2021 - 2022 年度报告 ANNUAL REPORT

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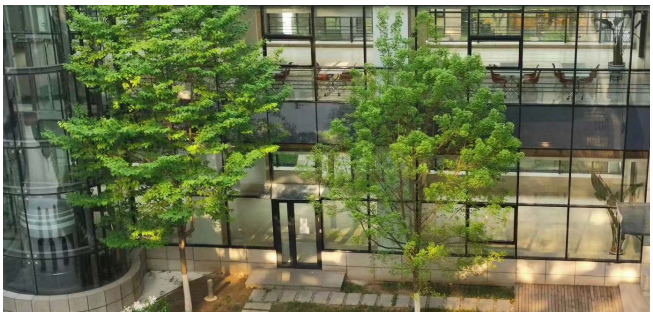
本册所列所有信息为2021年8月1日至2022年7月31日学术年期间

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2022年8月，中心的科研人才队伍包括13位讲座教授、3位教授、5位研究员、9位特聘研究员、5位特聘副研究员和3位工程师。另外，中心还有签约客座教授38位、博士后63位、博士/硕士研究生112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。

2021–2022学术年期间，中心公开发表国际学术论文423篇，主办合办国内外学术会议9场，开设培训班2场，举办科技前沿讲座2期，邀请学术报告147期，接待访问学者约200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;

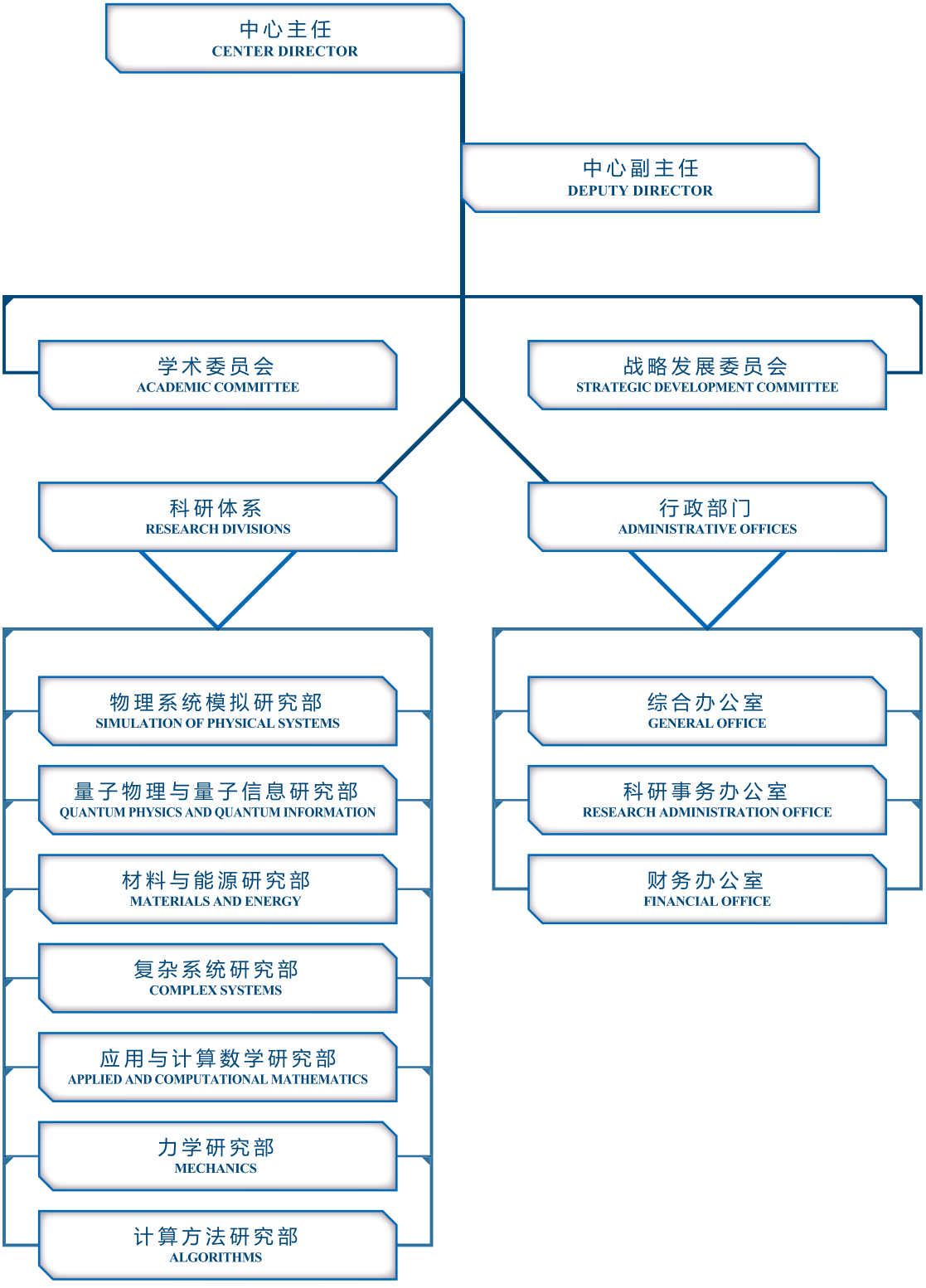
◎ Develop and maintain collaboration with research institutes elsewhere by building a comprehensive and internationalized research platform, to support academic and technological exchange and advancement;

◎ 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 2022, CSRC has 35 faculty members, 3 engineers, 38 associate members, 63 postdoctoral fellows and 112 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 423 papers, organized 9 academic conferences and workshops, 2 tutorials, 2 colloquium on scientific frontiers, and 147 CSRC seminars. CSRC has also forged partnerships with many prestigious universities and research institutes around the world.

ORGANIZATION 中心组织构架



QUANTUM CRITICAL POINTS AND THE SIGN PROBLEM

(By **Rubem Mondaini, Sabyasachi Tarat** and Richard T. Scalettar)

Extracting unbiased properties of quantum many-body systems exposes the challenge that numerical simulations in classical computers face in exploring quantum matter. Roughly put, one is trapped in a tale of two exponentials. On one side, a constraint arises due to the "exponential wall" associated with the growing dimension of the Hilbert space with the system size. On the other side, in avoiding retrieving exact quantum many-body wavefunctions and settling instead for a statistical estimation of physical quantities, one ends up facing the sign problem [1], which also leads to an exponential scaling of simulation times. The sign problem constitutes as the main hurdle that prevents systematic extraction of solutions of quantum many-body systems. It permeates a variety of fields, ultimately having a central impact on materials science, quantum chemistry and quantum field theory, as well as ultracold atoms and quantum computation. Thus, greater insight into the sign problem has important implications across these many disciplines.

Apart from some special (albeit important) limits such as the half-filled fermion Hubbard model [2], the latter 'wall' appears to be a generic (unavoidable) characteristic of quantum Monte Carlo (QMC) methods for fermionic and frustrated bosonic systems, and is conjectured to be NP-hard [3]. In practice, the common lore that permeates the application of QMC methods to quantum many-body systems dictates that once a sign problem occurs, that is, negative weights are obtained in the course of importance sampling, there is not much one can do, and moving to other techniques are deemed a better use of resources. Yet, recent progress in quantum many- body problems is the investigation of situations in which the sign problem can be alleviated [4] , eased [5] or mitigated [6] . Since the problem is known to be NP-hard, these approaches, although very interesting, just systematically delay the main bottleneck. If one lowers the temperature, increases the lattice size or enters a (typically more realistic) regime of parameters that is more prone to display large quantum fluctuations, the sign problem will reappear.

Faced by these difficulties, Prof. Rubem Mondaini (CSRC), together with his postdoc Sabyasachi Tarat (CSRC), collaborated with Prof. Richard Scalettar (University of California, Davis) to try a different approach that challenges the current paradigm: Instead of facing it as a hurdle, one can use the sign problem in determinant quantum Monte Carlo (DQMC) simulations as a tracker of quantum critical behavior. This demonstration (published in Science [7]) was done via the study of a number of fundamental models of condensed matter physics, all of whose critical properties are relatively well understood.

In particular, one of the models they studied was the SU(2) honeycomb Hubbard model (see Fig. 1A),

$$\hat{H} = -\sum_{ij\sigma} t_{ij}\left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}\right) - \sum_{i\sigma}\mu_i\hat{n}_{i\sigma} + U\sum_i\left(\hat{n}_{i\uparrow}-\tfrac{1}{2}\right)\left(\hat{n}_{i\downarrow}-\tfrac{1}{2}\right)$$

which exhibits a quantum critical point separating the Dirac semi-metal to a antiferromagneitc Mott insulator at the ratio of the interactions to the hopping energy $U_c/t \cong 3.8$, for simulations at half-filling ($\mu_i = 0$) . As there is no sign problem at this electronic occupation, a sign problem can be revealed by inserting a small perturbation ($\mu_i \neq 0$) . In this case, in approaching the thermodynamic limit $L \to \infty$, and the ground state regime ($T/t \to 0$) for an infinitely small sign-inducing perturbation ($\mu_i = 0^{+}$) , one can reveal the quantum critical point by the interaction strength at which the sign problem emerges [see Fig. 1B and 1C].

Generalizing such rationale for other Hamiltonians, as the U(1) honeycomb Hubbard model, and the SU(2) Ionic Hubbard model, Prof. Rubem Mondaini and his co-authors argue this phenomenon to be generic: if not protected by some symmetry of the problem, the sign problem appears in the regime of large quantum fluctuations, signaling quantum critical behavior. Ongoing research states that this is not a qualitative aspect of the sign problem but rather that the sign problem may quantitatively reveal aspects about the criticality of the transitions and the associated universality classes.

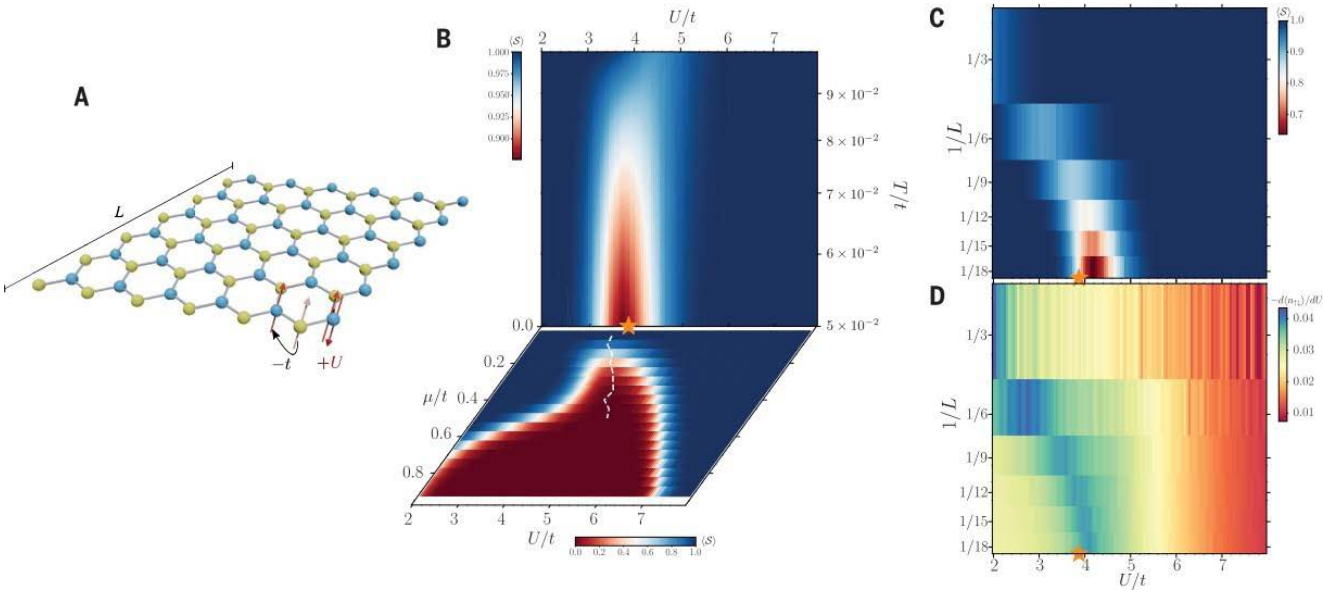


Fig. 1. The SU(2) Hubbard model on the honeycomb lattice. In the limit that the temperature $T \to 0$ the thermodynamic limit is achieved ($L \to \infty$) and the chemical potential is introduced as a perturbation $\mu \to 0^+$, the sign problem is worse at the critical point $U_c/t \cong 3.8$, separating the Dirac semi-metal from the antiferromagnetic Mott insulator. Adapted from Science 375, 418 (2022).

References:

[1] E. Loh, J. Gubernatis, R. Scalettar, S. White, D. Scalapino, and R. Sugar, *"Sign problem in the numerical simulation of many-electron systems"*, Phys. Rev. B **41**, 9301 (1990).

[2] J. E. Hirsch, *"Two-dimensional Hubbard model: Numerical simulation study"*, Phys. Rev. B **31**, 4403 (1985).

[3] M. Troyer and U.-J. Wiese, *"Computational complexity and fundamental limitations to fermionic quantum Monte Carlo simulations"*, Phys. Rev. Lett. **94**, 170201 (2005).

[4] Jan-Lukas Wynen, Evan Berkowitz, Stefan Krieg, Thomas Luu, and Johann Ostmeyer, *"Machine learning to alleviate Hubbard-model sign problems"*, Phys. Rev. B **103**, 125153 (2021)

[5] Dominik Hangleiter, Ingo Roth, Daniel Nagaj, and Jens Eisert, *"Easing the Monte Carlo sign problem"* Science Advances Vol. **6**, no. 33, eabb8341 (2020)

[6] Ryan Levy and Bryan K. Clark, *"Mitigating the Sign Problem through Basis Rotations"*, Phys. Rev. Lett. **126**, 216401(2021)

[7] R. Mondaini, S. Tarat, R. Scalettar, *"Quantum critical points and the sign problem"* Science **375** (6579), 418-424 (2022)

量子临界点与符号问题

(**Rubem Mondaini, Sabyasachi Tarat** and Richard T. Scalettar)

提取量子多体系统的无偏差属性暴露了通过经典计算机进行数值模拟探究量子性质时面临的挑战。粗略地说, 陷入了指数发散的约束之中。一方面, 希尔伯特空间的维度随系统的尺寸呈指数式增长; 另一方面, 为避免精确检索量子多体系统的波函数而改为对物理量进行统计估计时又面临着符号问题, 导致计算所需时间呈指数增长。符号问题作为系统性研究量子多体体系的主要瓶颈遍布于各个领域, 并对材料科学、量子化学和量子场论, 以及超冷原子和量子计算领域产生深远的影响。因此, 深入地探究符号问题对众多学科具有重要的意义。

图 1　蜂窝晶格中具有SU(2) 对称性的哈伯德模型。在温度趋于零 $T \to 0$ 以及系统尺寸趋于热力学极限的情况下 $L \to \infty$ 化学势作为一个正向的微扰被引入 $\mu \to 0^{+}$, 符号问题在临界点 $U_c/t \cong 3.8$ 处最严重, 刚好可以将狄拉克半金属相和反铁磁绝缘相区分开。 ▶

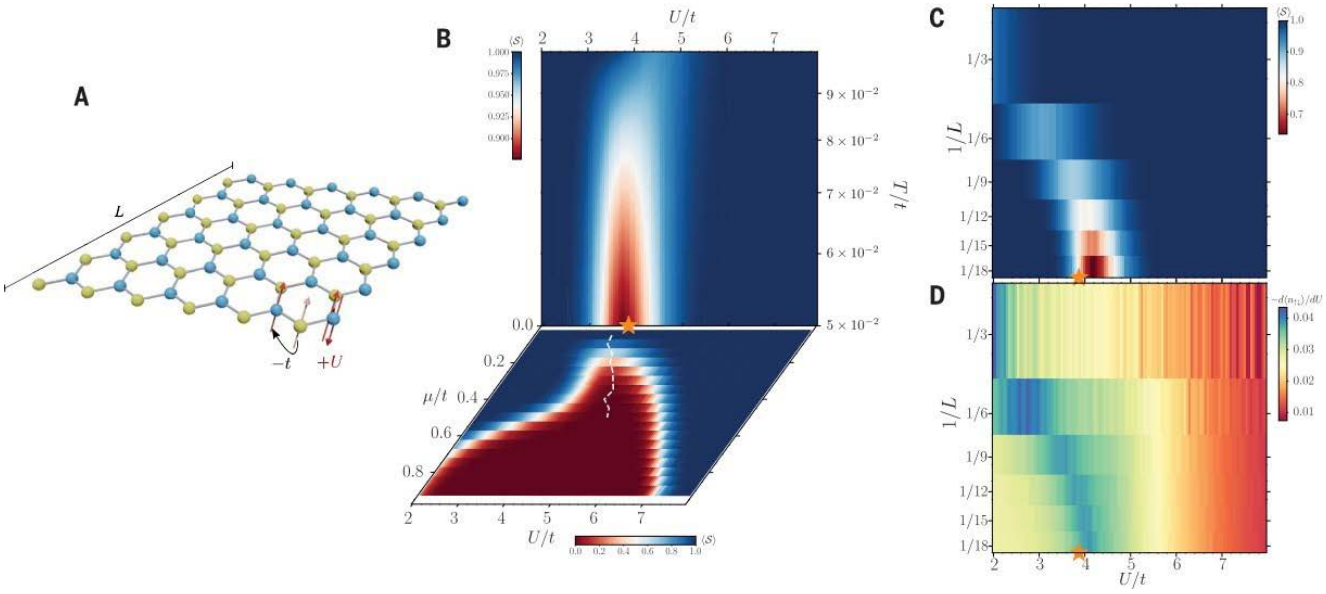
除了一些特殊模型(比如半满的费米子-哈伯德模型[2]), 符号问题似乎是量子蒙特卡罗方法(QMC)处理费米子系统和受阻挫的玻色子系统的普遍特征。事实上, 将量子蒙特卡罗方法应用于量子多体系统的过程中, 符号问题指在重要性抽样过程中出现负机率, 对于这种情况通常只能寄希望于其他手段。然而, 量子多体问题的最新研究进展集中于如何避免或者缓解符号问题 [4, 5, 6]。纵然这些方法非常有趣, 但其并没有从根本上解决符号问题。如果降低温度, 增大系统尺寸或者研究更实际的具有强量子涨落的参数区间, 符号问题将再次显现。

基于这些困难, 北京计算科学研究中心的Rubem Mondaini研究员及博士后Sabyasachi Tarat 与 美国加州大学戴维斯分校Richard Scalettar 教授合作尝试了一种挑战当前范式的不同方法: 将行列式量子模特卡罗模拟中的符号视为量子临界行为的追踪器, 而不是作为一个障碍。该项工作（发表在《科学》杂志 [7]）研究了凝聚态物理中的几个基本模型, 对这些模型的关键特性给予了很好的理解。

特别地, 他们研究了蜂窝晶格中具有SU(2) 对称性的哈伯德模型, 如图1A。其哈密顿量为

$$\hat{H} = -\sum_{ij\sigma} t_{ij}\left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}\right) - \sum_{i\sigma}\mu_i\hat{n}_{i\sigma} + U\sum_i\left(\hat{n}_{i\uparrow} - \tfrac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \tfrac{1}{2}\right)$$

在半满时存在一个由相互作用导致的从狄拉克半金属到反铁磁模特绝缘体的量子临界点 $U_c/t \cong 3.8$ 。虽然在此电子占据数下没有符号问题, 可通过引入微下的扰动来揭示符号问题 $(\mu_i \neq 0)$ 。当接近热力学极限情况 $L \to \infty$, 和无限小符号导致的扰动的基态时, 可通过符号问题表现的强度来揭示量子临界点, 如图1(B, C)。



Rubem Mondaini 研究员和他的合作者将这种现象推广到其他模型, 如蜂窝晶格中具有U(1) 对称性的哈伯德模型和正方晶格中具有SU(2) 对称性的ionic-Hubbard模型：如果没有受到某些对称性的保护, 符号问题出现在量子涨落很强的区域内, 这一现象预示着量子临界行为。正在进行的研究表明, 这不仅是符号问题的定性方面, 并且符号问题可以定量地揭示有关相变的临界行为和普适类的性质。

References:

[1] E. Loh, J. Gubernatis, R. Scalettar, S. White, D. Scalapino, and R. Sugar, *"Sign problem in the numerical simulation of many-electron systems"*, Phys. Rev. B **41**, 9301 (1990).

[2] J. E. Hirsch, *"Two-dimensional Hubbard model: Numerical simulation study"*, Phys. Rev. B **31**, 4403 (1985).

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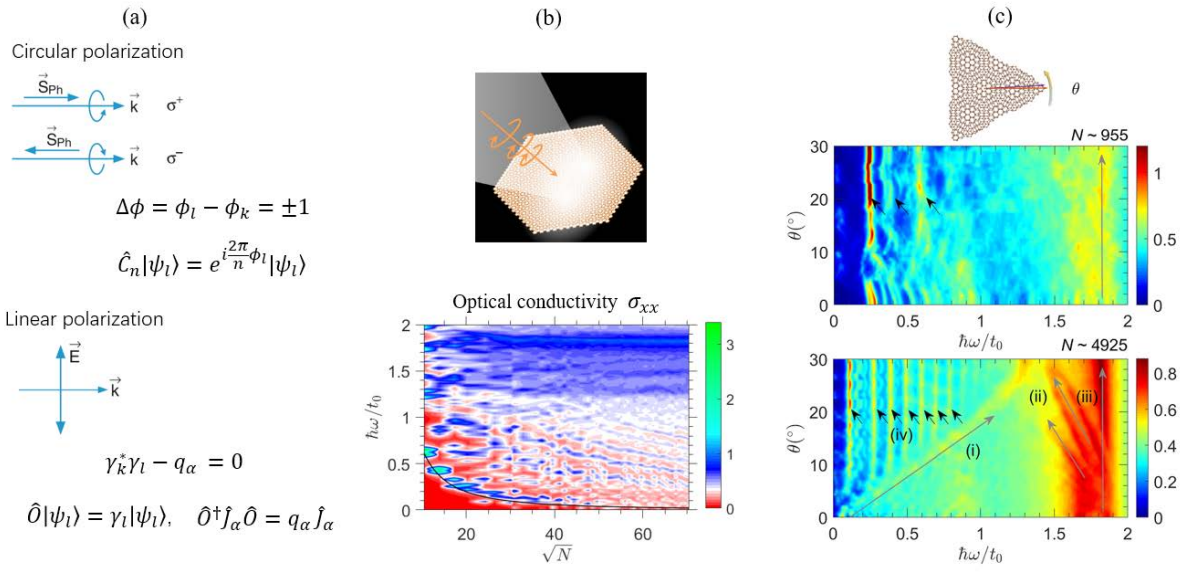
[7] R. Mondaini, S. Tarat, R. Scalettar, *"Quantum critical points and the sign problem"* Science **375** (6579), 418-424 (2022)

POLARIZATION-DEPENDENT SELECTION RULES AND OPTICAL SPECTRUM ATLAS OF TWISTED BILAYER GRAPHENE QUANTUM DOTS

(By **Yunhua Wang**, Guodong Yu, Malte Rösner, Mikhail I. Katsnelson, **Hai-Qing Lin**, and Shengjun Yuan)

Optical polarization has widespread applications in spectroscopic analysis, photodetectors, display technologies and quantum computation. Optical selection rules are essentially strict constraints resulting from both system symmetries and conservation laws. Therefore, it is of importance to reveal how symmetries encode the polarization of light into the selection rule in molecules and materials. It is known that the selection rules of both circularly and linearly polarized light for atoms in electric dipole approximation are described by the magnetic quantum number changes $\Delta m = \pm 1$ and $\Delta m = 0$, respectively. Here we generalize and augment the optical selection rules for both linear and circular polarizations in molecules and solids by a point group description. Our theory shows that (i) the selection rules of circularly polarized light are characterized by the changes in the rotational quantum number, and (ii) the selection rules of linearly polarized light in D_n, D_{nh}, D_{nd} and C_{nv} systems can be characterized by a two-fold rotational operator or reflection operator of systems.

Owing to shape- and size-controllable optical absorption as well as photoluminescence characteristics, graphene quantum dots hold high promises for applications in nanoscale carbon-based photodetectors, bioimaging and light-emitting diodes. Here, we present an extensive study of various twisted bilayer graphene quantum dots (TBGQDs) with ten different point groups. Applying the orthogonality theorem, we derive the optical selection rules for all these structures. Using these constructed selection rules, we further study how their optical properties rely on size, shape, twist angle, edge structure and correlation effects. We calculated the size-dependent scaling indexes of the band gap of energy spectrum and the optical band gap, and predicted a new type of optical conductivity features with multiple discrete absorption frequencies ranging from infrared to ultraviolet energy a result of quantum confinement effects.



偏振相关的选择定则和转角石墨烯量子点的光特性

(**王云华**, 于国栋, Malte Rösner, Mikhail I. Katsnelson, **林海青**, 袁声军)

光的偏振效应在光谱分析、光电器件、显示技术和量子计算等领域有着广泛应用, 光的选择定则本质上是守恒律和对称性约束的结果, 因此建立偏振光的选择定则具有基础和应用的双重重要性。在量子力学中我们熟知，对于原子而言，除了受角动量守恒约束外, 圆偏振光和线偏振光的选择定则分别由磁量子数的变化量即 $\Delta m = \pm 1$ 和 $\Delta m = 0$ 来描述。然而，对于分子和固体，人们并没有给出偏振光选择定则的一般描述。本研究建立了由常见点群描述的分子或固态系统的偏振光选择定则, 研究结果表明: (i) 圆偏振光的选择定则可由旋转量子数的变化量即 $\Delta\phi = \phi_l - \phi_k = \pm 1$ 来描述, 其中 ϕ_l 是系统旋转操作的本征量子数；(ii) 在 D_n、D_{nh}、D_{nd} 和 C_{nv} 系统，线偏振光的选择定则可由二重旋转操作或镜面反映操作的本征量子数的约束方程来描述。

实验研究表明, 石墨烯量子点的光吸收和光发射特征可由其尺寸和形状产生的量子限域效应来调控, 而且石墨烯量子点在微纳米碳基光电二极管、生物荧光标记、光电探测器和显示器件等领域有潜在应用前景。本研究基于正交性定理系统地建立了十种转角石墨烯量子点的选择定则数据库, 结合偏振光选择定则研究了这些量子点的电子结构和光诱导激发对体系尺寸、空间构型、对称性、扭转角度和关联效应的依赖性。我们计算出了转角石墨烯量子点的能谱带隙和光吸收带隙的尺寸依赖幂指数, 还预报了一种由有限尺寸的量子限域效应产生的从红外到紫外的多重离散吸收的新特征。

◀ 图 1　(a)偏振光选择定则，(b) D_{6d} 转角石墨烯量子点光电导率的尺寸依赖性，(c)三角量子点光电导率的转角依赖性。

Fig. 1. (a) Optical selection rules for circular and linear polarizations, (b) Optical conductivity σ_{xx} for D_{6d} TBGQDs as a function of $\sqrt{N}$ with N as the number of atoms, (c) Twist angle dependence of optical spectrum for triangular quantum dots.

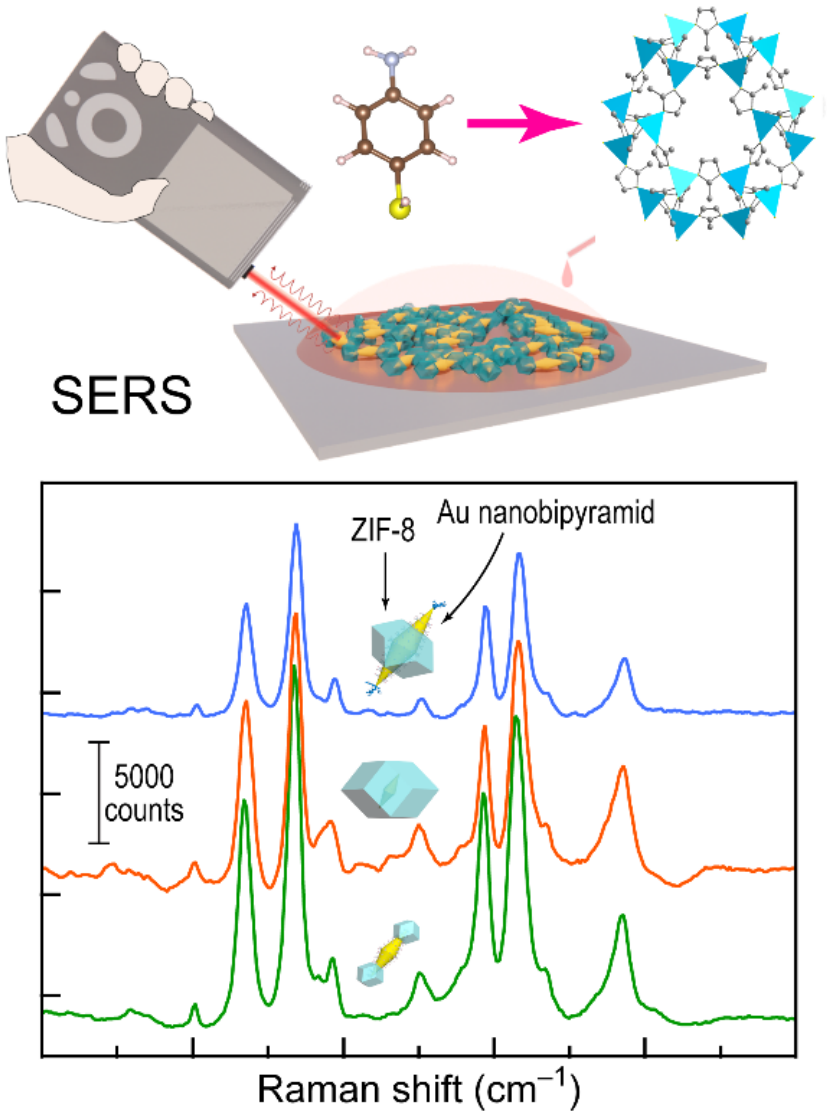
References:

Yunhua Wang, Guodong Yu, Malte Rösner, Mikhail I. Katsnelson, Hai-Qing Lin, and Shengjun Yuan, Polarization-Dependent Selection Rules and Optical Spectrum Atlas of Twisted Bilayer Graphene Quantum Dots, Physical Review X, 12, 021055 (2022).

SITE-SELECTIVE DEPOSITION OF METAL-ORGANIC FRAMEWORKS ON GOLD NANOBIPYRAMIDS FOR SURFACE-ENHANCED RAMAN SCATTERING

(By **Xueqing Yang**, Yi Liu, Shiu Hei Lam, **Jing Wang**, **Shizheng Wen**, **ChiYung Yam**, **Lei Shao**, Jianfang Wang)

Plasmonic hotspots, where electromagnetic field is highly concentrated, are crucial for achieving high detection performance for surface-enhanced Raman scattering (SERS). Controlled deposition of metal-organic frameworks (MOFs) on the specific sites of plasmonic nanocrystals is a highly effective approach for improving the SERS detection performance of plasmonic nanocrystals because the deposited MOFs can effectively capture and concentrate target analyte molecules at the hotspots. In this work, we report on a new approach for site-selective deposition of a MOF (ZIF-8) at the ends, waist, and around the entire surface of elongated gold nanocrystals, including gold nanobipyramids (NBPs) and nanorods. Deposition of ZIF-8 at the ends of Au NBPs leads to the best SERS performance. ZIF-8 can effectively capture and concentrate small molecules at the hotspots through the molecular sieving effect. Moreover, vapor-phase analytes can also be captured by the ZIF-8 component at the ends of Au NBPs and detected by SERS. Our synthetic protocol provides a new route for the design of hybrid nanostructures out of plasmonic nanocrystals and MOFs, where the MOF can capture and concentrate analyte molecules at the plasmonic hotspots for SERS detection. The route also opens up many possibilities for applications in plasmonic sensing, optical switching, and plasmonic catalysis.



有分子选择性的等离激元表面增强拉曼基底设计与构筑

(杨雪清, 刘怡, 林劭僖, 王晶, 温世正, 任志勇, 邵磊, 王建方)

分子的振动转动能级信息相当于分子的“指纹”, 不同物质具有其独特的“指纹”信息, 这一信息可以被拉曼光谱分析技术所取得。表面增强拉曼散射(SERS) 是一种通过将分子的微弱拉曼信号放大, 进而可达到单分子精度识别的强大检测技术, 它在生物医学、材料和环境监测、以及国家安全等领域有着广泛的应用。贵金属纳米晶由于其等离激元共振特性可以产生极强的局域电磁场, 所以被广泛应用于SERS检测中。然而, 相关的技术推广仍然受制于贵金属纳米结构对目标分子有限的富集和筛选性能, 发展出可以浓缩和筛选分子的等离激元SERS基底就成为这项技术实用的关键。

我们报道了一种金属有机骨架(MOFs)材料在金纳米双锥上的择位沉积技术, 并将这种技术制备的纳米结构应用于富集和筛选目标分子, 从而提高分子SERS检测性能。具体而言, 我们在金纳米双锥表面择位沉积ZIF-8金属有机框架多孔材料。通过对结构的电磁学模拟以及对待测分子性质的第一性原理计算分析表明, 多孔ZIF-8晶体起了分子筛的效果, 可将具有活性官能团和合适尺寸的小分子吸附并富集在等离激元热点区域(即局域电磁场增强比较大的区域), 从而实现信号增强。在进一步的工作中, 我们研究团队发现无论是液相还是气相待测物质, 择位沉积复合结构在SERS测试中均表现出了对合适尺寸的小分子良好的富集和选择性拉曼增强。本研究为利用等离激元纳米晶–MOF材料复合结构的制备提供了一条很有前景的方法, 所制备的复合结构在分子传感、光开关和等离激元催化等领域具有巨大的应用潜力。

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STARK MANY-BODY LOCALIZATION ON A SUPERCONDUCTING QUANTUM PROCESSOR

(By Qiujiang Guo, Chen Cheng, Hekang Li, Shibo Xu, Pengfei Zhang, Zhen Wang, Chao Song, Wuxin Liu, Wenhui Ren, Hang Dong, **Rubem Mondaini**, Haohua Wang)

The eigenstate thermalization hypothesis [1,2] provides a basic framework for studying the long-time evolution of isolated general quantum systems, that is, the macroscopic properties of non-equilibrium steady state after equilibration can be predicted by the thermodynamic average of the system. However, some quantum systems are known to not satisfy it. In particular, the phenomenon of many-body localization (MBL) caused by disorder [3,4] is a famous counterexample. Additionally, recent studies have shown that even in the absence of disorder, the phenomenon of many-body localization can also be observed by applying a linear chemical potential to a one-dimensional interacting quantum system [5]. This brings to the many-body realm the concept of Stark localization, being thus dubbed Stark MBL.

As the focus of the study of thermalization and many-body localization involves the non-equilibrium regime at high-energies of the system, a complement of both theoretical and numerical research is necessary. In recent years, the rapid development of quantum computing platforms provides a new way to solve this type of many-body problems. Continuing the previous cooperation [6], Prof. Rubem Mondaini of the Beijing Computational Science Research Center and the quantum experimental group led by Professor Wang Haohua from Zhejiang University systematically studied the Stark many-body localization phenomenon using superconducting quantum chips. The scientific research collaborators used the most advanced 32-bit chip to simulate the hard-core boson model on an engineered triangular ladder, and adjusted the detuning of the qubits to realize the linear chemical potential. In the unitary evolution starting from a large number of random product states, the collaborators fully characterized the transition of thermal many-body localization by measuring the Hamming distance, correlation function and quantum Fisher information of the system, and clearly demonstrated the Bloch oscillation behavior unique to Stark many-body localization.

This work is a typical example of theoretical, numerical and experimental cooperation. The experimental measurement and chip preparation are mainly undertaken by Dr. Guo Qiujiang and Dr. Li Hekang of Zhejiang University, and the numerical calculation is completed by young researcher Chen Cheng from Lanzhou University. It is worth mentioning that the joint effort of theoretical and numerical experiments accompanied by the research of quantum many-body problems using the quantum simulation platforms are the forefront of current international frontier research trends. Interestingly, simultaneously to this work, two other well-known research teams also used to rival platforms of either cold atoms [7] or ion traps [8] to similarly study the Stark many-body localization phenomenon. The results of the collaboration in China stand out for the clear characterization of entanglement capping, a hallmark of the many-body localization phenomenon.

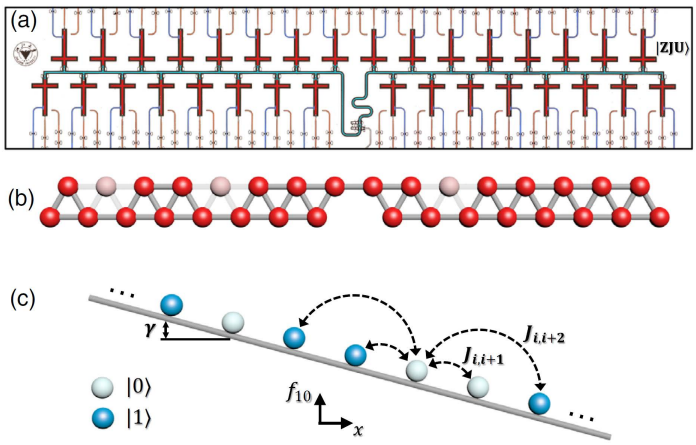

Fig. 1. (a) the schematic diagram of the 32-bit chip used in this work is obtained by coloring the optical micrograph photos. (b) Triangular ladder lattice simulated by quantum chip. (c) Schematics of the Hamiltonian used to simulate the Stark many-body localization phenomenon. The linear chemical potential can be realized by adjusting the detuning of the qubits.

利用超导量子芯片研究STARK-多体局域化

(郭秋江, 程晨, 李贺康, 徐世波, 张鹏飞, 王震, 宋超, 刘武新, 任文慧, 董航, **Rubem Mondaini**, 王浩华)

本征态热化假说[1,2]为研究孤立一般量子体系的长时演化行为提供了基本的框架, 即经过长时间演化的非平衡稳态的宏观性质可以由体系的热力学平均预测。然而, 并非所有的量子系统都满足本征态热化假说, 由无序导致的多体局域化[3,4]现象就是著名的反例。最近的研究表明, 在没有无序存在的情况下, 向一维相互作用量子系统施加以线性化学势也能观测到多体局域化现象, 即Stark-多体局域化[5]。

在研究本征态热化假说及多体局域化的相关问题时, 所涉及的研究对象是相互作用的多体量子系统, 且人们更多关注体系的非平衡态和高能本征态。面对这类问题, 理论和数值两方面的研究均存在各自的困难, 近年来高速发展的量子计算为解决这类多体问题的提供了新的思路。延续之前的合作[6], 北京计算科学研究中心的Rubem Mondaini研究员和来自浙江大学王浩华教授领导的量子实验组利用超导量子芯片系统地研究了Stark-多体局域化现象。科研合作者们采用最先进的32-比特芯片模拟了三角梯子模型上的硬核玻色子模型, 并调节量子比特的失谐以实现了线性化学势。在由大量随机直积态出发的幺正演化中, 合作者们通过测量体系的Hamming距离、关联函数及量子Fisher信息等, 证据充分地表征了热化-多体局域化的转变、并清晰展示了Stark-多体局域化特有的Bloch震荡行为。

◀ 图 1　(a) 该工作采用的32比特芯片示意图, 由光学显微镜照片后期上色得到; (b) 由量子芯片模拟的三角梯子格点; (c) 用于模拟Stark-多体局域化现象的哈密顿量示意图, 线性的化学势可通过调节量子比特的失谐实现。

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FIRST-PRINCIPLES CALCULATION IN DARK MATTER DIRECT DETECTION

(By Zheng-Liang Liang, **Chongjie Mo**, Fawei Zheng, Ping Zhang)

Migdal effect refers to a phenomenon that the suddenly recoiled atom struck by dark matter particles is easier to excite its electrons. Based on this effect, it is promising to use semiconductor targets to realize the direct detection on the sub-GeV dark matter particles, belonging to the weakly interacting massive particles (WIMPs). In order to meet the requirement of such experiments, combining the bremsstrahlung-like description of the recoiled ion with the electronic many-body effect in solids, we provide a first-principles method for the estimation of event rates for dark matter particles in a semiconductor. We also investigate the in-medium effect on the detection of the solar-reflected DM flux in silicon-based detectors. Recently, we further introduce the multi-phonon process triggered by an incident DM particle into our first-principles method through electronic excitation induced by the exchange of a virtual phonon. Surprisingly, this approach can effectively push the sensitivities of the semiconductor targets further down to the MeV DM mass region. This work is selected as an editors' suggestion in Physical Review D.

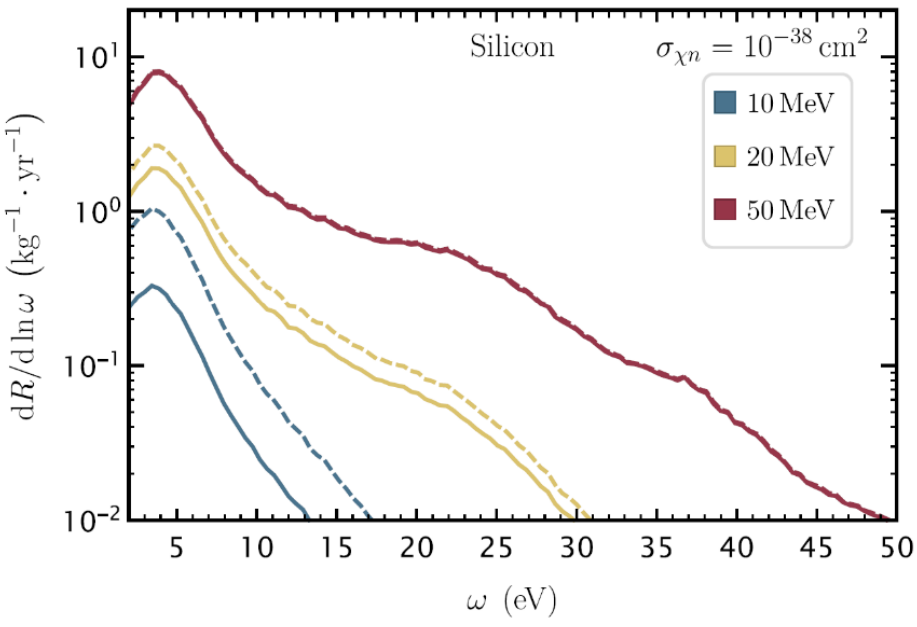

Fig. 1. The differential Migdal electronic excitation event rates in bulk silicon for a reference cross section of 10−38 cm2 and DM masses of 10 (emerald), 20 (orange) and 50 MeV (maroon), respectively; the solid lines and the dashed lines are calculated using the phonon-mediated approach and the bremsstrahlung-like approach, respectively.

暗物质直接探测中的第一性原理计算

(梁振良, **莫崇杰**, 郑法伟, 张平)

Migdal效应指的是暗物质粒子碰撞原子核使其反冲引起核外电子电离的现象。基于该效应, 科学家有望通过半导体靶实现亚GeV暗物质候选粒子, 即WIMP的直接探测。为了更好地服务于暗物质探测实验, 我们将固体电子系统的多体效应和反冲离子的类韧致描述相结合, 从理论上提供了一套估计半导体中暗物质事例率的第一性原理模拟方法。通过该方法, 我们还研究了在对太阳反射到地表的暗物质粒子流探测实验中, 硅靶的介质效应。近期, 基于虚声子交换引起电子激发的图像, 我们创新性地将暗物质引发的多声子过程引入了第一性原理方法中。预测结果表明, 该方法有望将半导体靶对暗物质粒子的敏感度降低到MeV的量级。该工作被选为《物理评论D》的编辑推荐。

◀ 图 1　参考散射截面为 10^{-38} cm^2 且暗物质粒子质量分别为10(红), 20(黄)和50 MeV(蓝) 的情况下, 体硅中Migdal电子激发事例率的微分截面; 实线和虚线分别为声子参与方法和类韧致方法的计算结果。

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GIANT ATOMS IN A SYNTHETIC FREQUENCY DIMENSION

(By **Lei Du**, Yan Zhang, Jin-Hui Wu, Anton Frisk Kockum, and **Yong Li***)

Giant atoms, which interact with the surrounding environment (waveguides) at multiple points, have attracted rapidly growing interest in the past few years due to various intriguing phenomena arising from them [1]. In general, giant atoms can be achieved by coupling (artificial) atoms to propagating fields whose wavelengths are much smaller than the atomic sizes (e.g., surface acoustic waves), or by coupling atoms to meandering waveguides at separated points. For such structures, one should naturally consider phase accumulations of the field between different atom-waveguide coupling points, which lead to a series of striking phenomena that are absent for small atoms [2-3].

On the other hand, the concept of synthetic dimensions has been recently proposed and extensively explored in a variety of physical system. With synthetic dimensions, it is possible to explore richer physical effects with fewer geometric dimensions. The construction of synthetic dimensions not only enables significant reduction of physical resources, but also provides possibilities for manipulating the relevant degrees of freedom.

Here we demonstrate how to implement giant atoms in a synthetic frequency dimension [4], where the one-dimensional frequency lattice acting as a discrete waveguide is achieved with a dynamically modulated superconducting resonator. As shown in Fig. 1(a), we consider a Δ-type artificial atom, where two of the transitions are coupled to different sites of the frequency lattice and the third one is driven by an external field. If the atom supports both a single-photon resonant transition and a two-photon one with large detuning, it can be effectively described as a two-level giant atom with two coupling points in the frequency dimension, as shown in Fig. 1(b). We reveal that the effective model can not only simulate some typical effects of real-space giant atoms such as long-lived populations, but can also be used to manipulate light frequency and achieve chiral quantum optical effects in the frequency dimension. Moreover, the effective giant atom in the frequency dimension can also be implemented with a ladder-type three-level atom, which is coupled to different sites of the frequency lattice via multiple two-photon resonant transitions, as shown in Fig. 1(c).

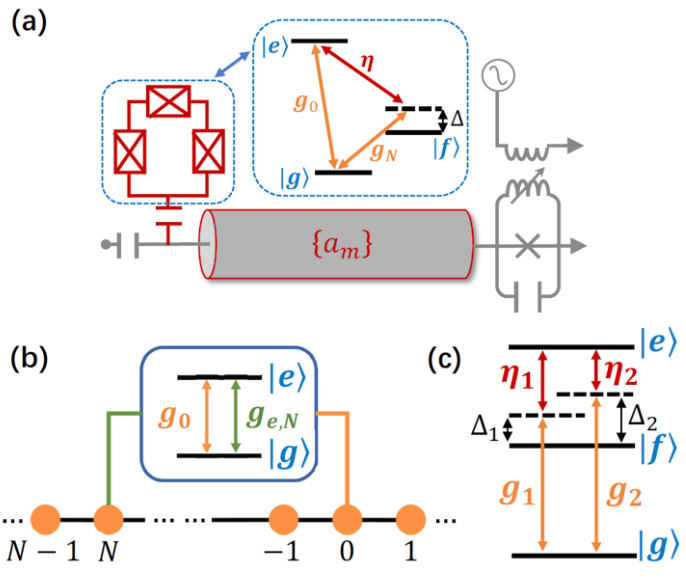

Fig. 1. (a) Schematic illustration of the model under consideration. The SQUID coupled to the superconducting resonator is modulated in time. A Δ-type artificial atom interacts with two resonant modes of the resonator and is driven by an external field. (b) Effective two-level giant atom after adiabatic elimination. (c) Ladder-type implementation scheme of the effective giant atom.

双层银纳米棒超表面晶格共振诱导手性选择透明

(**杜磊**, 张岩, 吴金辉, Anton Frisk Kockum, **李勇**)

作为近年来波导量子电动力学的研究热点之一，“巨型原子”通常是指在空间上与波导存在非局域多点耦合的量子发射器[1]。巨型原子系统由于其自干涉效应，可以呈现出许多常规波导量子电动力学系统所无法实现的奇特量子光学现象[2-3]。然而这一结构特征使得巨型原子系统通常有着较大的空间尺寸，不利于进一步的片上集成，并且在某些情况下（如考虑波导为耦合腔阵列时）会消耗较多的物理资源。为解决这类问题，本文考虑在一维合成频率维度中[4]构造有效的巨型原子结构。其中，一维频率晶格可以通过动态调制多模谐振腔的边界来产生，而非局域的原子--晶格相互作用则可以考虑将三能级人造原子通过不同类型的原子跃迁（如单光子和双光子共振跃迁）或多个不同的双光子共振跃迁过程与不同的频率晶格格点（对应不同的腔模）耦合来实现（见图1）。这种合成维度中的模型不仅为研究巨型原子效应提供了更加小型化和资源节约的平台，并且为构造更高维度中的巨型原子结构提供了可行的方案。此外，该论文还展示了在合成维度中实现手性量子光学现象和级联相互作用的可能性，这为相关自由度的操控提供了新的思路。

◀ 图 1　模型示意图。(a) Δ型人工原子与多模超导谐振腔的两个不同模式耦合，且被外部激光场驱动。此外，本文考虑对谐振腔的边界进行适当的含时调制。(b) 合成频率维度中的有效二能级巨型原子。(c) 可用于实现频率维度中巨型原子的梯型能级人工原子。

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OBSERVATION OF NON-HERMITIAN TOPOLOGICAL ANDERSON INSULATOR IN QUANTUM DYNAMICS

(By **Quan Lin**, Tianyu Li, **Lei Xiao** , **Kunkun Wang** , Wei Yi , & **Peng Xue**)

Disorder and non-Hermiticity dramatically impact the topological and localization properties of a quantum system, giving rise to intriguing quantum states of matter. The rich interplay of disorder, non-Hermiticity, and topology is epitomized by the recently proposed non-Hermitian topological Anderson insulator that hosts a plethora of exotic phenomena. Here we experimentally simulate the non-Hermitian topological Anderson insulator using disordered photonic quantum walks, and characterize its localization and topological properties. In particular, we focus on the competition between Anderson localization induced by random disorder, and the non-Hermitian skin effect under which all eigenstates are squeezed toward the boundary. The two distinct localization mechanisms prompt a non-monotonous change in profile of the Lyapunov exponent, which we experimentally reveal through dynamic observables. We then probe the disorder-induced topological phase transitions, and demonstrate their biorthogonal criticality. Our experiment further advances the frontier of synthetic topology in open systems.

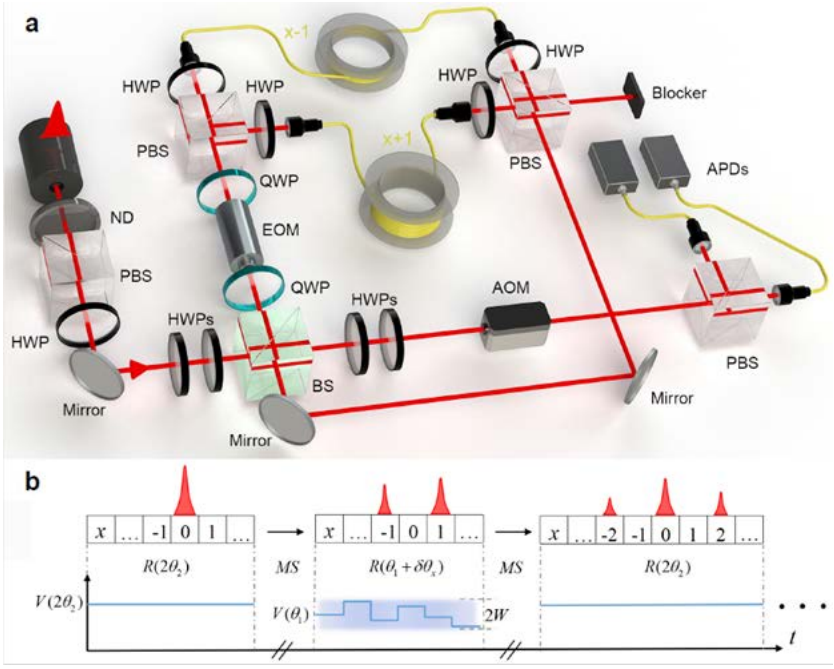

Fig. 1. Experimental setup for observing non-Hermitian topological Anderson insulator.

A Photons are coupled in and out of an interferometric network through a low-reflectivity beam splitter (BS, reflectivity 5%). The coin operation is carried out with wave plates and a dynamic electro-optic modulator (EOM). The shift operator is realized by splitting the light, using a polarizing beam splitter (PBS), into two single-mode fibers of length of 160,000 and 167,034 m, respectively. As such, the spatial modes are encoded into the polarization-dependent temporal shift within a time step. The out-coupled photons are detected using the avalanche photodiodes (APDs), in a time- and polarization-resolved fashion. An optical switch acousto-optic modulator (AOM) is used to protect the APDs such that photons are only allowed to reach the APDs at the time of measurement. b Illustration of the operation sequence of the time-multiplexed quantum walk. Here V is the control voltage applied to the EOM for generating rotations with the coin parameter.

薛鹏团队在实验观测非厄米拓扑安德森绝缘体方面取得重要进展

（林泉，李天宇，肖磊，王坤坤，易为，薛鹏）

日前，北京计算科学研究中心薛鹏教授团队及合作者在非厄米拓扑量子系统的研究中取得重要进展，首次在量子行走体系中观测到了非厄米拓扑安德森绝缘体。 研究成果以“Observation of non-Hermitian topological Anderson insulator in quantum dynamics”为题，于2022年6月9日在线发表于Nature Communications。

在传统的拓扑材料中，拓扑边缘态由拓扑不变量所刻画，其稳定性源于体系本征态在希尔伯特空间的全局几何特性。然而，这一传统范式在无序或非厄米体系中受到挑战：一方面，体系中的无序在导致局域化的同时，也可能诱导出具有全局拓扑性质的拓扑安德森绝缘体；另一方面，许多非厄米拓扑模型的本征态在非厄米趋肤效应的影响下，会失去布洛赫波的空间延展性而趋向体系边界，这些非厄米体系的拓扑边缘态因而需要用非布洛赫拓扑不变量描述。薛鹏团队将上述两个对体系拓扑产生重要影响的因素融合在一起，在实验上观测到由无序导致的局域化和非厄米趋肤效应在量子行走系统中的相互竞争，以及由无序诱导的拓扑相变，从而实现了对非厄米拓扑安德森绝缘体的动力学量子模拟。

◀ 图 1　实验装置图

薛鹏团队及合作者通过时间域光量子实验平台，观测到了非厄米趋肤效应以及安德森局域化现象。通过对动力学过程的量子模拟，验证了趋肤效应与局域化之间的竞争关系。且在此基础上，首次在实验上观测到了非厄米拓扑量子体系中由无序造成的拓扑相变。

这一实验工作奠定了在具有趋肤效应的非厄米多体系统中研究局域化问题的基础，开辟了对可集成量子态传输，可控光量子设备的应用道路。

这项研究是该团队继观测新型非厄米拓扑体边对应关系[Nat. Phys. 16，761–766 (2020)]，非布洛赫宇称时间对称相变的观测[Phys. Rev. Lett. 126，230402 (2021)]，非布洛赫拓扑不变量的直接测量[Phys. Rev. Lett. 127，270602 (2021)]之后，在非厄米系统新奇物性研究方面取得的又一重要成果。

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[1] Q. Lin, T. Y. Li, K. K. Wang, W. Yi, and P. Xue, Observation of non-Hermitian topological Anderson insulator in quantum dynamics, Nat. Commun. 13, 3229 (2022).

DETERMINISTIC SEARCH ON STAR GRAPHS VIA QUANTUM WALKS

(By **Dengke Qu**, Samuel Marsh, **Kunkun Wang**, **Lei Xiao**, Jingbo Wang and **Peng Xue**)

We propose a novel algorithm for quantum spatial search on a star graph using interleaved continuous-time quantum walks and marking oracle queries. Initializing the system in the star's central vertex, we determine the optimal quantum walk times to reach full overlap, matching the well-known lower bound of Grover's search. We implement the deterministic search in a database of size seven on photonic quantum hardware, and demonstrate the effective scaling of the approach up to size 115. This is the first experimental demonstration of quantum walk-based search on the highly noise-resistant star graph, which provides new evidence for the applications of quantum walk in quantum algorithms and quantum information processing.

Our work is the first experimental demonstration of this new and more flexible database search framework, as well as the first experimental demonstration of deterministic spatial search. In doing so we show the advantages of selecting a graph to suit the quantum hardware. This work thus demonstrates the alternating phase-walk framework's advantages on near-term quantum hardware in reducing the impacts of noise, on the widely applicable problem of searching a database.

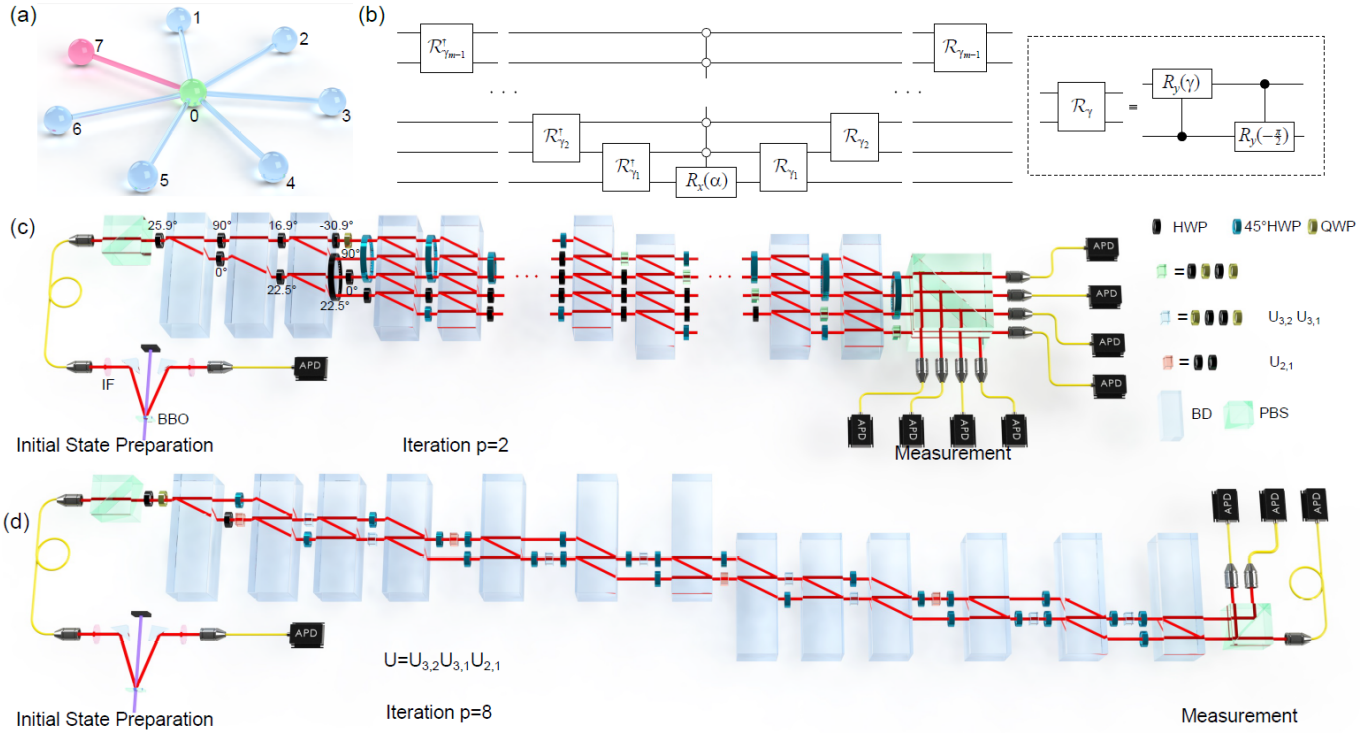


Fig. 1. (a) star graph S7, consisting of seven outer vertices connected to a central vertex. (b) Efficient quantum circuit to simulate a CTQW over the star graph. (c),(d) Experimental setup. A pair of photons is generated via the spontaneous parametric down-conversion, with one serving as a trigger and the other as a single photon.

薛鹏团队实现星图中的确定性搜索

(**曲登科**，Samuel Marsh，**王坤坤**，肖磊，王静波，**薛鹏**)

近日，北京计算科学研究中心薛鹏教授团队及合作者在连续时间量子行走的研究中取得重要进展。他们通过交替使用连续时间量子行走与oracle查询，提出并实验实现了一种新奇的星图中的确定性量子空间搜寻算法。研究成果以“Deterministic Search on Star Graph via Quantum Walks”为题，于2022年1月10日发表于 Physical Review Letters.

Grover搜索算法是量子计算的一个标志性应用，在对未排序的数据库进行搜寻时，与经典搜索算法相比具有平方根加速的优势。Grover搜寻算法证明在包含N个元素的数据库中去找到一个标记的元素，需要oracle查询的次数最优为大约$\pi/4\sqrt{N}$。 然而Grover算法存在1/N的数量级的失败率。

另一方面，量子行走作为经典随机行走在量子世界的对应，其平方式增长的扩散速度体现出量子资源的重要优势，可以实现普适的量子计算。而其中连续时间的量子行走，更被广泛应用于搜寻算法。

北京计算科学研究中心薛鹏教授团队及合作者在基于前期对量子行走研究的积累下，通过交替使用连续时间量子行走与oracle查询，提出并实验实现了一种新奇的确定性的量子空间搜寻算法。他们将Grover搜寻算法中的Grover算子替换为连续时间的量子行走，此种新型的量子确定性搜寻算法与Grover算法相比有着相同的效率，即需要oracle查询的次数为$\pi/4\sqrt{N}$的量级。他们将新型的量子搜寻算法应用到星图的数据库搜寻中，该类图具有抗噪声的能力，因此星图的数据库存在着额外的优势。

该团队利用单光子和线性光学系统实验实现了任意的幺正演化的方案，在数据库大小为7的星图中演示了该确定性的搜寻算法，并且利用三维子空间模拟了更大数据库的搜寻算法，证明了该算法的可扩展性。这一工作首次在实验中实现了这种新的且更灵活的数据搜寻框架，也是确定性的空间搜寻算法的首次实验说明。该工作选择了适合量子硬件的星图来完成，证明了在数据库搜寻问题中，交替使用相位-行走框架在降低噪声影响方面的优势。该工作为量子行走在量子算法和量子信息处理中的应用提供了新的证据。

◀ 图 1　(a). 星图S_7，由7个外部顶点连接到一个中心点。(b). 有效量子线路用于模拟星图上的连续时间量子行走。(c). 星图S_7的确定性量子搜寻算法的实验装置。(d). 在子空间中实现搜寻算法的实验装置。

References:

[1] D. K. Qu, S. Marsh, K. K. Wang, J. B. Wang, and P. Xue, Deterministic search on star graphs via quantum walks, Phys. Rev. Lett. 128, 050501 (2022).

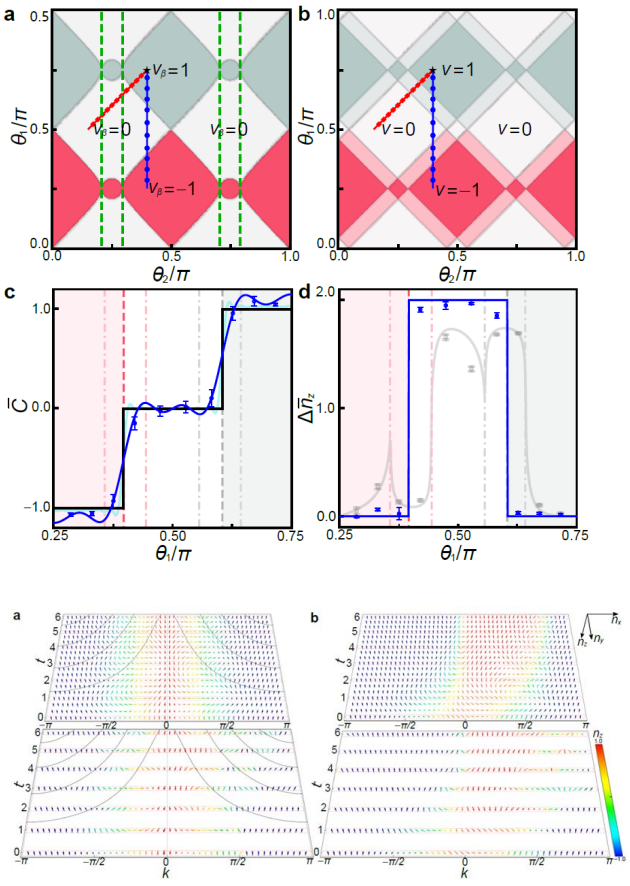
DETECTING NON-BLOCH TOPOLOGICAL INVARIANTS IN QUANTUM DYNAMICS

(By **Kunkun Wang**, Tianyu Li, **Lei Xiao**, Yiwen Han, Wei Yi and **Peng Xue**)

Non-Bloch topological invariants preserve the bulk-boundary correspondence in non-Hermitian topological systems, and are a key concept in the contemporary study of non-Hermitian topology. Here we report the dynamic detection of non-Bloch topological invariants in single-photon quantum walks, revealed through the biorthogonal chiral displacement, and crosschecked with the dynamic spin textures in the generalized quasimomentum-time domain following a quantum quench. Both detection schemes are robust against symmetry-preserving disorders, and yield consistent results with theoretical predictions. Our experiments are performed far away from any boundaries, and therefore underline non-Bloch topological invariants as intrinsic properties of the system that persist in the thermodynamic limit. Our work sheds new light on the experimental investigation of non-Hermitian topology.

Consistent with the theoretical characterization of non-Bloch topological invariants, our experiment is hinged upon the concept of non-Bloch band theory, where the application of the GBZ is essential. The experiment thus serves to further underline the importance of the non-Bloch band theory in providing a coherent understanding regarding lattice models with non-Hermitian skin effects. As both of our detection schemes are sensitive to the non-Bloch PT symmetry, they also provide dynamic probes to the non-Bloch exceptional points. For future studies, it would be desirable to devise detection schemes for non-Bloch topological invariants in models of higher dimensions.

Fig. 2. Experimental (lower layer) and numerical results (upper layer) of dynamic spin textures.



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[1] K. K. Wang, T. Y. Li, Y. W. Han, W. Yi, and P. Xue, Detecting non-Bloch topological invariants in quantum dynamics, Phys. Rev. Lett. 127, 270602 (2021).

薛鹏团队在量子动力学演化中实现非布洛赫拓扑不变量的直接测量

（王坤坤，李天宇，肖磊，韩奕文，易为，薛鹏）

日前，北京计算科学研究中心薛鹏教授团队及合作者在对非厄米量子系统拓扑性质的研究中取得重要进展。实验在单光子非厄米量子行走的动力学演化中，通过观测演化过程中光子的平均手性位移，以及量子行走动力学淬火过程中动量—时间域的斯格明子结构两种不同的方式，首次实现了对非布洛赫(non-Bloch)拓扑不变量的直接测量。研究成果以“Detecting Non-Bloch Topological Invariants in Quantum Dynamics”为题，于2021年12月30日发表于Physical Review Letters。

近年来，随着对量子开放体系中拓扑物相研究的逐步深入，开放体系呈现出诸多区别于封闭系统的拓扑特性。其中一个典型的案例是非厄米趋肤效应引起的非厄米拓扑体系体边对应关系的失效。在非厄米趋肤效应下，非厄米系统中的体态与拓扑边缘态均局域在体系边界附近，定义在传统布里渊区上的布洛赫拓扑不变量与开边界下的拓扑边缘态不再一一对应。为重新建立非厄米系统中的体边对应关系，理论研究者引入了非布洛赫能带理论，在修正的广义布里渊区上重新定义出非布洛赫拓扑不变量。在前期的研究中，封闭系统布洛赫拓扑不变量已经被实验证明可以通过统计矩、平均手性位移和量子淬火中的衍生拓扑结构等方式进行探测，而开放系统中的非厄米趋肤效应及非布洛赫体边对应关系也都得到了实验验证。但能否对非布洛赫拓扑不变量进行实验探测，仍是悬而未决的重要课题。

该团队利用线性光学系统，搭建了非厄米量子行走实验装置，不仅精确地测量了动力学演化过程中的平均手性位移，还通过模拟淬火动力学演化，观测到了非布洛赫能带理论下动量—时间空间中的斯格明子结构。两种测量方式相互印证，实现了对非厄米拓扑不变量的直接观测。实验表明，基于非布洛赫能带理论的拓扑不变量可以通过体态的动力学演化在热力学极限下得到，充分说明了非布洛赫能带论的普适性。 同时，实验通过引入静态及动态两种不同的微扰，证明了两种测量方案的鲁棒性。

◀ 图 2　淬火过程中非布洛赫能带理论下定义的动量—时间空间中衍生斯格明子结构及布洛赫理论下自旋结构的演化。

这是该团队继实验实现开放系统的非厄米量子行走[Nature Physics 13， 1117 (2017)]，直接测量其拓扑不变量[Physical Review Letters 119, 130501 (2017)]，模拟多体拓扑系统的非厄米动力学量子相变[Physical Review Letters 122, 020501 (2019)]并观测其斯格明子结构[Nature Communications 10, 2293 (2019)]，模拟并观测非厄米临界现象[Physical Review Letters 123, 230401 (2019)]和非厄米金属拓扑能带结构[Physical Review Letters 127, 026404 (2021)]，观测非厄米趋肤效应并验证非布洛赫体边对应关系[Nature Physics 16, 761 (2020)]，观测非布洛赫奇异点(Physical Review Letters 126, 230402(2021))之后，对开放系统中新型非厄米拓扑物态的实验研究中取得的又一重要进展。这一工作首次在实验上实现了开放系统中非布洛赫拓扑不变量的直接观测，不仅为非布洛赫能带理论提供重要实验支持，进一步加深人们对开放系统拓扑物相的了解，更为开放系统拓扑物相的研究提供了新的手段。

STATE-INDEPENDENT TEST OF QUANTUM CONTEXTUALITY WITH EITHER SINGLE PHOTONS OR COHERENT LIGHT

(By **Dengke Qu**, **Kunkun Wang**, **Lei Xiao**, Xiang Zhan and **Peng Xue**)

Contextuality is a phenomenon at the heart of quantum mechanics different from classical behavior and has been recently identified as a resource in quantum information processing. Experimental demonstration of contextuality is thus an important goal. We experimentally demonstrate a test of state-independent contextuality in a four-dimensional Hilbert space with single photons and violate the inequality by at least 387 standard deviations. Despite imperfections and possible measurement disturbance, our results cannot be explained in non-contextual models. We also provide a theoretical analysis of a test of contextuality with a coherent light field and show how the definitions affect the emergence of non-classical correlations. Our result sheds new light on the conflict between quantum and classical physics.

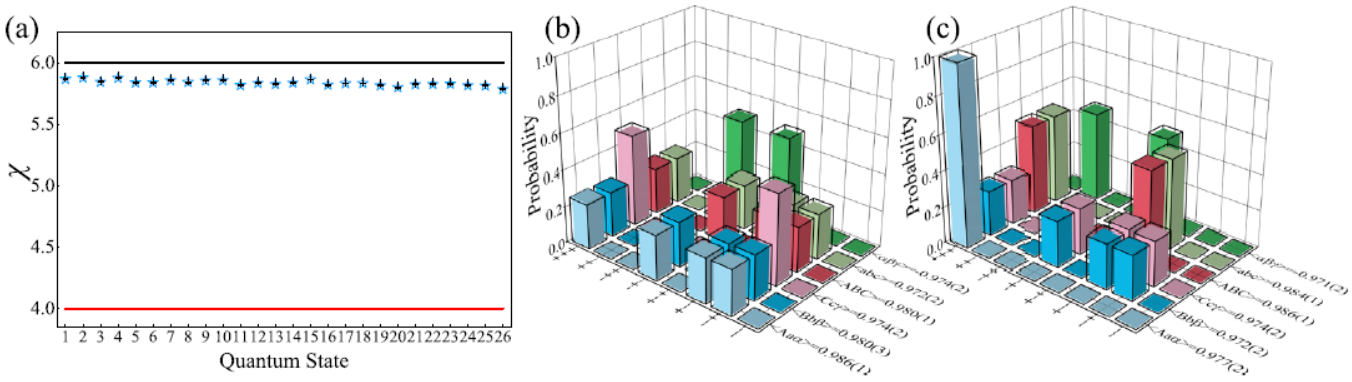
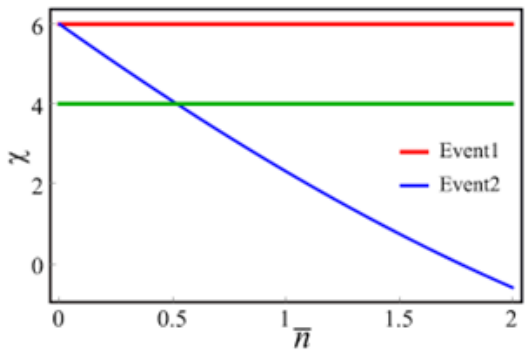


Fig. 1. State-independent violation of the inequality.

The Kochen–Specker theorem states that no non-contextual hidden-variable theory can reproduce the predictions of quantum mechanics for correlations between measurement outcomes of some sets of observables. In this work, we experimentally demonstrate a test of state-independent contextuality in a four-dimensional Hilbert space with single photons. We show that 26 different single-photon states violate an inequality that involves correlations between results of sequential compatible measurements by at least 387 standard deviations. Despite imperfections and possible measurement disturbance, under the assumption of fair sampling, our results cannot be explained in non-contextual models. We also provide a theoretical analysis of test of contextuality with a coherent light field and show how the definitions affect the emergence of non-classical correlations.

Fig. 2. Theoretical predictions of left-hand side (green line) and right-hand side (red and blue lines) of the inequality χ for a coherent light under different measurement events E1 and E2.



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[1] D. K. Qu, K. K. Wang, X. Zhan, and P. Xue, State-independent test of quantum contextuality with either single photons or coherent light, npj Quantum Information 7, 154 (2021).

使用单光子或相干光对量子上下文进行状态无关测试

（曲登科，王坤坤，肖磊，詹翔，薛鹏）

互文性在量子信息和计算的发展中变得非常重要。互文性是量子力学的这一关键特征，其代表了最有价值的量子资源之一。著名的 Bell-Kochen-Specker 定理指出，没有任何非上下文隐变量理论能够重现量子力学的预测。

之后，由Peres和 Mermin提出了一个更简单的证明，在文献中被称为Peres-Mermin正方形。目前为止，已经对各种物理系统进行了量子上下文测试。然而，这些测试需要产生特殊的量子态。 在2008年Cabello推导出了一组不等式，这些不等式由非上下文隐变量理论满足，但对于任何量子态都被量子力学违反。这提供了一个通过有限精度实验来测试非上下文性的机会，而不需要特殊的量子态。

在本研究中，展示了 Kochen-Specker 定理在四维希尔伯特空间中的实验证明。用单光子进行实验，证明与非上下文的状态无关冲突。尽管存在缺陷和可能的测量干扰，但结果无法在非上下文模型中解释。本研究还提供了对具有相干光场的上下文测试的理论分析，并展示了定义如何影响非经典相关性的出现。

◀ 图 1　不等式的态不依赖的违背。

考虑九个可以在单体系统中测量的双值可观测量。基于兼容性关系，这些测量可以在以下三元组中进行 $\{A,a,\alpha\},\{B,b,\beta\},\{C,c,\gamma\},\{A,B,C\},\{a,b,c\},\{\alpha,\beta,\gamma\}$。任何理论，其中九个可观测量具有预定义的非上下文结果 -1 或 1 必须满足以下不等式：

$$\langle A\cdot a\cdot\alpha\rangle+\langle B\cdot b\cdot\beta\rangle+\langle C\cdot c\cdot\gamma\rangle+\langle A\cdot B\cdot C\rangle+\langle a\cdot b\cdot c\rangle-\langle\alpha\cdot\beta\cdot\gamma\rangle\leq 4$$

对于一个四维系统，这里有一组可观测量可以使不等式在任何量子态下的量子预测达到6。本本研究选取了 $A=X\otimes I, a=I\otimes X, \alpha=X\otimes X, B=I\otimes Y, b=Y\otimes I, \beta=Y\otimes Y, C=X\otimes Y, c=Y\otimes X, \gamma=Z\otimes Z$

尽管语境性被认为是非经典行为的内在特征，但一直有人提出是否可以使用经典光来测试语境性的问题。通过用经典光替换预示的单光子来显示不同的结果。与提供明确定义的测量事件的单个光子相比，对于每组测量，光子都由与 D0 处的触发光子相关联的 D1 检测到，对于作为光子源的相干光场，多光子的概率不可忽略，如图所示。因此，需要将测量事件重新定义为 E1 仅用于一个检测器点击，E2 用于多个检测器点击（由于相干光的真空分量，也有可能没有检测器点击。

研究表明，26 种不同的单光子状态违反了一个不等式，该不等式涉及至少 387 个标准偏差的连续兼容测量结果之间的相关性。尽管存在缺陷和可能的测量干扰，但在公平抽样的假设下，实验结果无法在非上下文模型中解释。本研究还提供了对具有相干光场的上下文测试的理论分析，并展示了定义如何影响非经典相关性的出现。与表现出上下文的单光子相比，经典相干光的上下文强烈依赖于测量事件的具体定义。

◀ 图 2　淬不同测量事件 E1 和 E2 下相干光的不等式 χ 左侧（绿线）和右侧（红线和蓝线）的理论预测。

HIGH-PRECISION MEASUREMENT OF SPIN-EXCHANGE PARAMETERS IN NUCLEAR SPIN MAGNETIC RESONANCE GYROSCOPE

(By **Bowen Song**, Yanhua Wang and **Nan Zhao***)

Spin-exchange between alkali-metal atoms and noble gas atoms is essential to the various applications including nuclear magnetic resonance gyroscope. The team lead by Nan Zhao experimentally studied the Rb-Xe spin-exchange optical pumping process. The dependence of the spin-exchange rate on the intensity of the pumping light was measured at different temperatures under low magnetic fields. They demonstrated that the spin-exchange rate will decrease as the Rb spin polarization increases, which agreed well with the theoretical prediction. In the measurement, three spin exchange and spin relaxation mechanisms, namely, the spin exchange rates between Rb and Xe atoms caused by van der Waals molecule and binary collision processes, and the spin relaxation rate due to the wall collision of Xe atoms, had comparable magnitudes. These rates were extracted separately from the measured data with different Rb spin polarization at various temperatures. This work provided a comprehensive confirmation of the physical picture of the spin-exchange optical pumping process. [Song, B., Wang, Y., & Zhao, N.. Spin-polarization dependence of the Rb-Xe spin-exchange optical pumping process. *Physical Review A, 104*(2), 023105 (2021)]

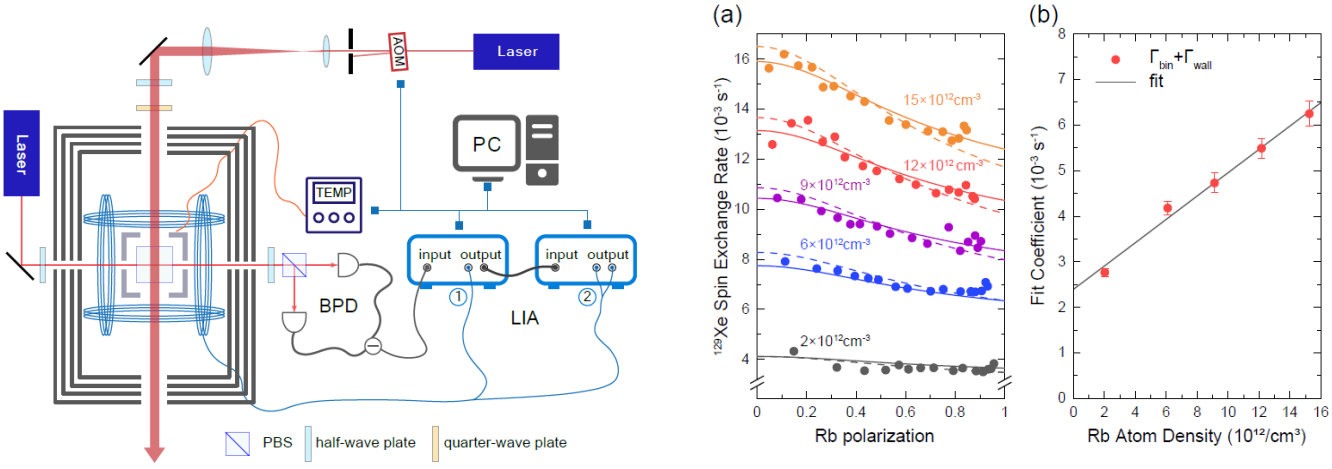

Fig. Left: Experimental setup.
Right: Experimental data showing the Rb-polarization dependence of the Rb-Xe spin exchange rate, from which different spin-exchange processes can be distinguished.

核磁共振陀螺系统中自旋交换碰撞过程的精确测量

（宋博文，王彦华，赵楠）

自旋交换碰撞过程是核磁共振陀螺系统中的关键物理过程。这一过程决定了陀螺的信噪比和核自旋的相干时间等关键物理参数，并将直接影响核磁共振陀螺精度等重要性能指标。人们通过前期研究已经了解到，核磁共振陀螺系统中Rb原子-Xe原子自旋交换过程可以分为两个类型：Rb-Xe两体碰撞过程和在缓冲气体N2氮气辅助参与下的Rb-Xe-N2三体范德瓦尔斯过程。在适当的气体分压条件下，后者对自旋交换碰撞的贡献占主导地位。然而，虽然几十年来人们对Rb-Xe-N2三体范德瓦尔斯过程有了较深入的理论认识，整个实验验证和实验参数的精确测量仍然不完备。例如，理论预言Rb-Xe-N2三体范德瓦尔斯过程对Rb自旋极化度的依赖关系始终没有的到实验的直接观测。北京计算科学研究中心赵楠研究团队搭建了核磁共振陀螺实验系统，并通过一系列完整的实验设计，首次实验观测到了Rb-Xe-N2三体范德瓦尔斯过程对Rb自旋极化度的依赖关系，并精确测定了Rb-Xe-N2三体范德瓦尔斯过程的关键碰撞参数，填补了这一问题的实验空白。通过这一工作，赵楠研究团队对核磁共振陀螺中的微观物理机制有了深入、定量的理解，为进一步优化核磁共振陀螺性能，推进陀螺研究依托深层次的物理原理全面开展奠定了坚实的基础。【Song, B., Wang, Y., & Zhao, N.. Spin-polarization dependence of the Rb-Xe spin-exchange optical pumping process. Physical Review A, 104(2), 023105 (2021)】

◀ 左图：实验装置示意图。右图：实验数据显示了Rb-Xe自旋交换速率对温度和Rb原子自旋极化度的依赖关系，从中提取出Rb-Xe自旋交换过程的关键参数。

GENERAL MODEL FOR DEFECT DYNAMICS IN IONIZING-IRRADIATED SIO_2/SI STRUCTURES

(By Yu Song, Guanghui Zhang, Xuefen Cai, Baoying Dou, Zhihao Wang, Yang Liu, Hang Zhou, Le Zhong, Gang Dai, Xu Zuo, and **S.-H. Wei**)

Irradiation damage is a key issue for the reliability of semiconductor devices under extreme environments. For decades, the ionizing-irradiation-induced damage in transistors with silica-silicon (SiO_2/Si) structures at room temperature has been modeled by a uniform generation of $E'\gamma$ centers in the bulk silica region through the capture of irradiation-induced holes, and an irreversible conversion from $E'\gamma$ to P_b centers at the SiO_2/Si interface through reactions with hydrogen molecules (H_2). However, the traditional model fails to explain experimentally-observed dose dependence of the defect concentrations, especially at low dose rate. We proposed that the generation of E'_g centers is decelerated because the protons migrate dispersively in disordered silica and the diffusion coefficient decays as the irradiation goes on. We also proposed that the conversion between E'_g and P_b centers is reversible because the huge activation energy of the reverse reaction can be effectively reduced by a "phononkick" effect of the vibrational energy of H_2 and P_b centers obtained from nearby nonradiative recombination centers. We demonstrate that the derived analytic model based on these two new concepts can consistently explain the experimentally observed fundamental but puzzling dose dependence of the defect concentrations for an extremely wide dose rate range.

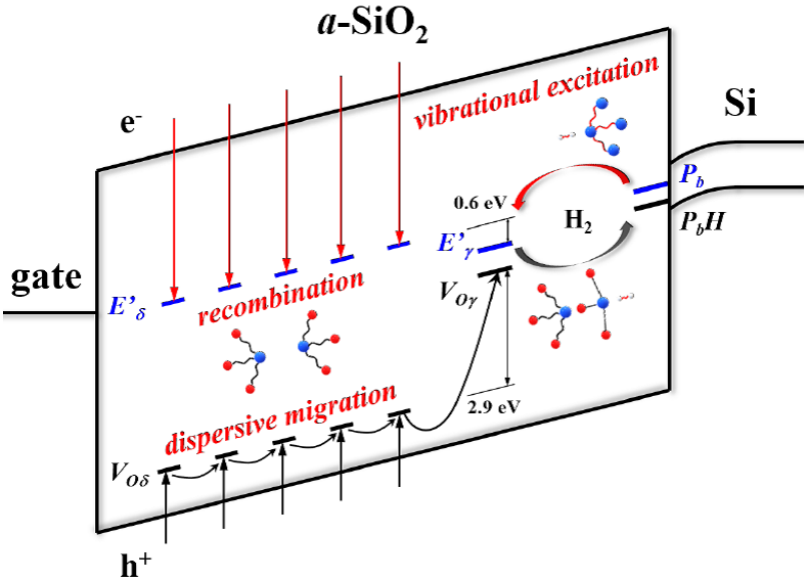

Fig. 1. Summarized new understanding of the defect dynamics. While it is still a generation-conversion framework, the recombination, dispersive migration, and vibrational excitation processes are essentially different from the traditional understanding.

电离辐照 SiO_2/Si 结构中缺陷动力学的普适模型

（宋宇，张光辉，**蔡雪芬**，**窦保英**，**王智灏**，刘杨，周航，钟乐，代刚，左旭，**魏苏淮**）

硅基器件的总剂量效应起源于a-SiO_2/Si结构中氧化物陷阱电荷（$E'\gamma$）和界面陷阱电荷（P_b）的产生和转化。长期以来，人们一直认为 $E'\gamma$ 的产生是匀速的，且 $E'\gamma$ 向 P_b 的转化是不可逆的。但我们发现这种传统模型无法解释电荷密度对总剂量的基本实验规律，特别是低剂量率下 $E'\gamma$ 的非单调行为。本文中，我们基于热氧化a-SiO_2的材料特性提出总剂量效应的两个全新概念。

第一，由于a-SiO_2的无序结构，辐照诱导的空穴和质子在材料中分散式地迁移。这使得迁移随辐照的进行越来越慢，$E'\gamma$ 的产生是减速的。第二，由于a-SiO_2的超宽带隙，体系中的缺陷和杂质被激发到高能振动态。这使得反应势能曲线被强烈调制，有效反应势垒大大降低，高剂量率下 $E'\gamma$ 和 P_b 之间的转化是可逆的。基于这两个全新概念，我们推导获得 $E'\gamma$ 和 P_b 随辐照总剂量变化的解析模型。与实验数据的比对表明，该模型可以自洽且定量地描述很宽剂量率范围和温度范围内的实验数据，这些数据具有非常显著且不同的非线性特征。这些普适的结果表明，我们的模型可用于预测低剂量率、高温辐照下硅基器件的总剂量效应，支持其抗辐射加固设计。

◀ 图 1　总结了对缺陷动力学状态的新认识。虽然它仍然是一个产生-转换模型，但载流子重组、色散迁移和振动能吸收和激发过程与传统的理解有本质的不同。

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[1] Yu Song*, Guanghui Zhang, **Xuefen Cai, Baoying Dou**, **Zhihao Wang**, Yang Liu, Hang Zhou, Le Zhong, Gang Dai, Xu Zuo, **Su-Huai Wei**, and S.-H. Wei*, Small **18**, 2107516 (2022).

ORIGIN OF LIGHT-INDUCED EFFICIENCY ENHANCEMENT IN HYBRID PEROVSKITE SOLAR CELLS

(By **Xie Zhang** and **Su-Huai Wei**)

Pronounced light-induced lattice expansion and accordingly an enhancement in the solar conversion efficiency have been experimentally observed in hybrid perovskites, but the origin remains elusive. By performing rigorous first-principles calculations for a prototypical hybrid perovskite FAPbI3 (FA: formamidinium), we show that 1% lattice expansion could already reduce the nonradiative capture coefficient by one order of magnitude. Unexpectedly, the suppressed nonradiatve capture is not caused by changes in the band gap or defect transition level due to lattice expansion, but originates from enhanced defect relaxations associated with charge-state transitions in the expanded lattice. These insights not only provide a rationale for the light-induced efficiency enhancement in hybrid perovskites, but also offer a general approach to manipulating nonradiative capture via light-lattice coupling in a wide spectrum of optoelectronic materials.

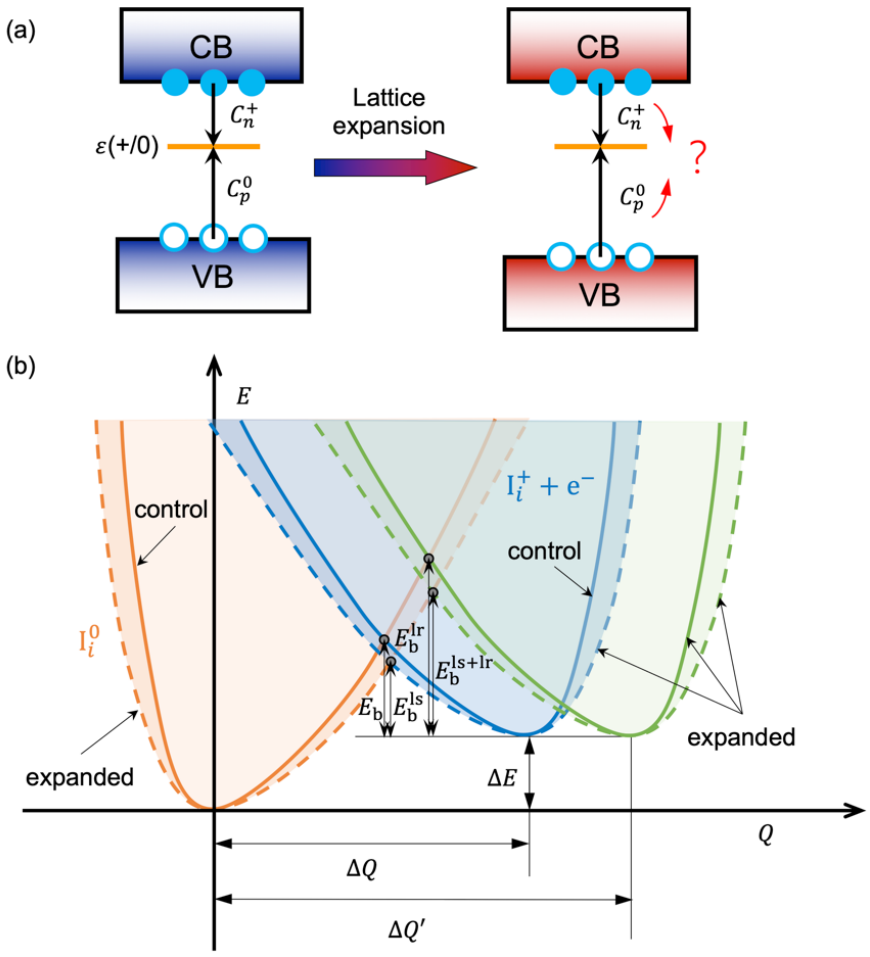

Fig. 1. (a) Schematic illustration of the impact of lattice expansion on the charge-state transition level and nonradiative capture coefficients. (b) Schematic showing the impact of lattice expansion on the electron capture barrier of I_i^+.

光致杂化钙钛矿太阳能电池效率提升的根源

（张燮，魏苏淮）

实验上观测到杂化钙钛矿在光照下会发生显著的晶格膨胀和效率提升，但其根源并不明了[H. Tsai *et al*., Science 360, 67 (2018)]。通过对典型的杂化钙钛矿$FAPbI_3$进行精确的第一性原理计算发现，仅仅1%的晶格膨胀就可以使得载流子非辐射捕捉系数降低一个数量级。尤其意想不到的是，非辐射复合的抑制与晶格膨胀引起的带隙或缺陷能级的变化基本无关，而是由于晶格膨胀之后缺陷在进行价态转变时结构驰豫增强。这些重要的认知不仅很好地解释了光照导致杂化钙钛矿太阳能电池效率提升的实验现象，更提供一种通过光和晶格相互作用来调控光电材料中载流子非辐射复合的新方法。

◀ 图 1 （a）晶格膨胀对缺陷转变能级和非辐射捕获系数影响规律的示意图。（b）晶格膨胀对 I_i^+ 电子捕获势垒影响规律的示意图。

References:

[1] X. Zhang, S.-H. Wei, Phys. Rev. Lett. **128**, 136401 (2022).

STRONGLY-CORRELATED STATES IN MOIRÉ SUPERLATTICE

(By **J. An** and **J. Kang**)

Recently, the electronic properties in moiré superlattices, which consist of two-dimensional van der Waals materials, have become a topic of great interest. The induced moiré potential with long periodicity results in the formation of flat bands and strongly correlated states, making moiré superlattice a good platform to study strong-correlation physics. A key issue in the research of moiré superlattice is how to modulate the correlation strength to realize different quantum phases. We use large-scale electronic structure calculation methods to investigate this problem.

Using twisted bilayer γ-graphyne (TBGY) as an example, we show that it is possible to create multiple flat bands in carbon allotropes without the requirement of a specified magic angle. The origin of the flat bands can be understood by a simple two-level coupling model. The narrow bandwidth and strong localization of the flat band states might lead to strong correlation effects, which make TBGY a good platform for studying correlation physics. On the basis of the two-level coupling model, we further propose that the width and extent of localization of flat bands can be tuned by an energy mismatch ΔE between the two layers of TBGY, which can be realized by either applying a perpendicular electric field or introducing a heterostrain. This allows continuous modulation of TBGY from the strongcorrelation regime to the medium- or weak-correlation regime, which could be utilized to study the quantum phase transition. [1]

A two-dimensional nanosheet has top and bottom open surfaces, allowing the specific case of doubly aligned super-moiré lattice to serve as a toy model for studying the tunable lattice symmetry and the complexity of related electronic structures. We discovered that in doubly aligned BN/graphene/BN heterostructure, due to the modulation of moiré potential, there is a band renormalization around the Fermi level, resulting the formation of flat minibands with narrow band width. The corresponding electronic states in the flat bands are strongly-correlated. Together with the collaboration from experiment groups, it is shown that at partial occupation of these bands, correlation-driven metal-insulator transition occurs. [2]

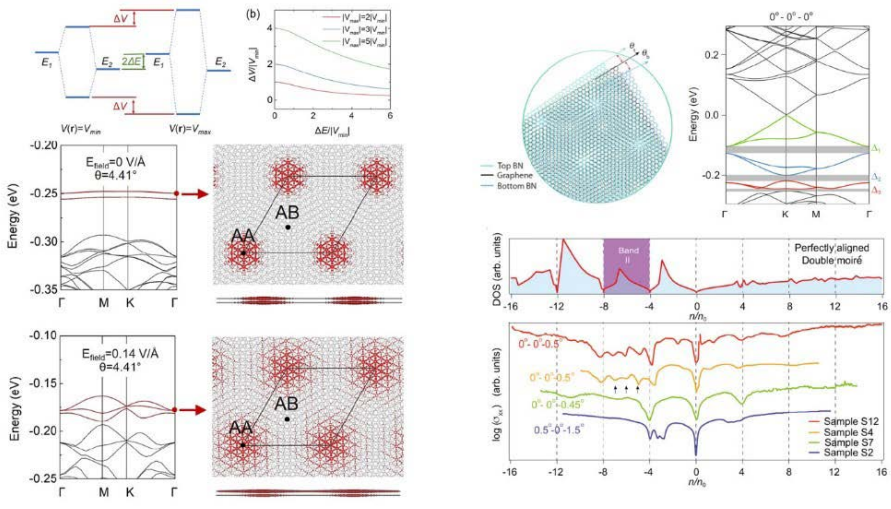

Fig. 1. Flat bands and strongly-correlated states in twisted bilayer γ-graphyne (left panel) and BN/graphene/BN moiré superlattice (right panel).

摩尔超晶格中的强关联电子态

（安娇，康俊）

近年来，由二维范德瓦尔斯材料堆叠而成的摩尔超晶格的电子结构引起广泛关注。超晶格中长周期的摩尔势将诱导产生强关联的平带电子态，使其成为研究强关联物理效应的理想平台。相关研究的关键问题之一是如何有效地调控电子态的关联强度从而实现不同的强关联物相。课题组利用大规模电子结构计算针对这一问题开展研究。

以二维转角石墨炔体系为例，提出通过调控层间能级匹配改变摩尔超晶格中的关联强度。当层间转角足够小时，石墨炔摩尔超晶格中产生平带，体系处于强关联作用区域。通过改变层间能级的相对位置，可以改变摩尔超晶格势的强度，从而改变平带电子态局域程度及带宽并调控关联作用强度，使得石墨炔摩尔超晶格发生强关联至弱关联作用的转变。该工作为调控摩尔超晶格中的关联强度提供了思路。

与实验合作，研究了BN/graphene/BN三层摩尔超晶格中的电子结构。计算发现，在BN/graphene/BN摩尔超晶格中，费米能级附近的价带发生重组，形成多组平带。平带电子态表现出很强的关联效应。当平带部分占据时，体系不再是金属态，而将打开能隙，转变为强关联绝缘态。相应的实验结果证实了理论的预测。该工作表明了在使役条件下，摩尔超晶格中的强关联效应对电子结构的显著影响。

◀ 图 1　转角双层 γ-graphyne （左） 和 BN/graphene/BN （右）摩尔超晶格中的强关联电子态。

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[1] J. An and **J. Kang***, *J. Phys. Chem. Lett*. 12, 12283, (2021).

[2] X. Sun, S. Zhang, Z. Liu, H. Zhu, J. Huang, K. Yuan, Z. Wang*, K. Watanabe, T. Taniguchi, X. Li, M. Zhu, J. Mao, T. Yang, **J. Kang***, J. Liu*, Y. Ye*, Z. V. Han*, and Z. Zhang, *Nat. Commun*. 12, 7196 (2021).

CYCLE DEFORMATION ENABLED CONTROLLABLE MECHANICAL POLARITY OF BULK METALLIC GLASSES

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

Tuning anisotropy in bulk metallic glasses, ideally isotropic, is of practical interest in optimizing properties and of fundamental interest in understanding the amorphous structure and its instability. Here we propose a quasi-elastic AMC training method and used it to achieve mechanical anisotropy of MGs without destroying samples or inducing mechanical annealing or rejuvenation effects. The degree of polarity and the anelastic limit can be well controlled by regulating the amplitude of mechanical cycling. We find that only plastic STZs corresponding to the training direction can be consumed by asymmetric cycling and the anelastic rearrangements are still however observable in trained glasses. The achieved anisotropic behavior originates from the exhaustion of plastic STZs in the training direction. While usual structural indicators are not sensitive probes for induced anisotropy, the asymmetric local yield stresses distribution works well to capture the polarization. Moreover, the increase in quasi-elastic limit is always accompanied by the decrease of potential energy, when the MG sample is processed by thermal or mechanical annealing. However, the AMC protocol significantly improves the quasi-elastic (anelastic) limit in the target direction, while rejuvenating other physical properties that may be sensitive to the energy state, which pro- vides a potential way to achieve the multi-performance regulation of MGs. In fact, many experimental testing or preparation methods are quasi-elastic asymmetrical mechanical cyclic loadings, such as the dynamic mechanical spectroscopy method, and the ultrasonic vibration synthesis of BMGs. It should be very interesting to verify our prediction in further experimental investigations. Our finding is of fundamental importance, which furthers our understanding of the mechanical deformation of metallic glasses and sheds some light on the prospects for improved properties through induced anisotropy.

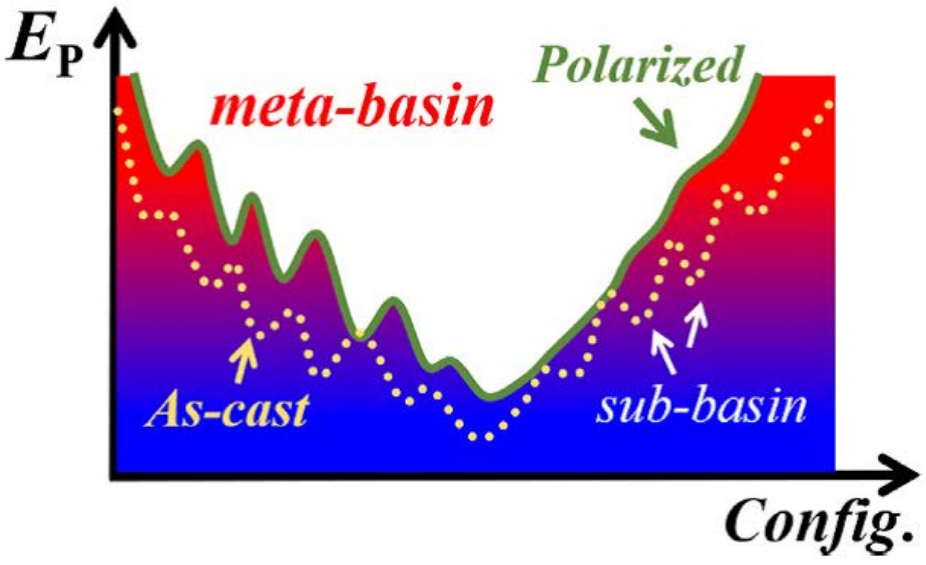

Fig. 1. Schematic illustration of tl
inherent features of potential energy surfa
(PES) for the as-cast (the dashed line) a
polarized (the solid line) samples.

非对称加载诱导非晶合金性能各向异性及其微观机理

（管鹏飞课题组）

块体非晶材料一般认为具有理想的各向同性，如何实现其性能的各向异性调控对优化性能和理解非晶结构及其失稳特性具有重要的意义。管鹏飞课题组提出了一种非对称、准弹性、循环加载的训练方法，利用该方法在不破坏样品、不引起机械退火或回春效应的情况下实现了非晶合金材料的力学各向异性调控。通过调节机械循环的振幅，可以很好地控制材料物性力学性能的极化程度和准弹性极限。基于原子尺度的分析，我们发现：只有与训练方向对应的“塑性重排单元”可以被非对称循环加载消耗，而“准弹性重排”在训练后的样品中仍然可见，表明通过训练所获得的各向异性行为源于训练方向上 “塑性重排单元”的耗尽。事实上，许多实验测试或制备方法都是准弹性非对称机械循环加载，如动态机械能谱法、非晶合金的超声振动合成等，而这种加载方式所引入的不可忽略的各项异性并没有在实验中得到重视。因而，如何设计合理的实验验证我们的预测，并基于此综合调控非晶材料的性能是非常有意义的研究方向。我们的发现进一步加深了我们对非晶合金力学变形的理解，并为通过诱导各向异性改善材料的性能提供了新思路。

◀ 图 1　非对称加载诱导极化非晶合金体系势能曲面形貌示意图。

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[1] **Baoshuang Shang**, Weihua Wang, **Pengfei Guan***, Cycle deformation enabled controllable mechanical polarity of bulk metallic glasses, *Acta Mater*. 225, 2117557(2022).

[2] Bing Wang, **BaoShuang Shang**, XuanQiao Ga, YiTao Su, JiChao Qia, WeiHua Wang, MingXiang Pan, **PengFei Guan***, Local structural signs for distinct crystallization behaviors of monatomic metals, *Journal of Non-Crystalline Solids*. 576, 121247(2022).

INTERPLAY BETWEEN QUANTUM ANOMALOUS HALL EFFECT AND MAGNETIC SKYRMIONS

(By **Y. Li**, S. Xu, J. Wang, C. Wang, B. Yang, **H. Lin**, W. Duan, and **B. Huang**)

Quantum anomalous Hall effect (QAHE) and magnetic skyrmion (SK) represent two typical topological states in momentum (*K*) and real (*R*) spaces, respectively. However, little is known about the interplay between these two states. Here, we propose that the coexistence of QAHE and SK may generate a previously unknown SK state, named the RK joint topological skyrmion (*RK*-SK), which is characterized by the SK surrounded by nontrivial chiral boundary states (CBSs). Interestingly, beyond the traditional SK state that can solely be used via creation or annihilation, the number and chirality of CBS in RK-SK can be tunable under external fields as demonstrated in Janus monolayer (ML) $MnBi_2X_2Te_2$ (X = S, Se), creating additional degrees of freedom for SK-state manipulations. Moreover, it is also found that external fields can induce a continuous topology phase transition from K-space QAHE to *R*-space SK in ML $MnBi_2X_2Te_2$, providing an ideal platform to understand the cross-over phenomena of multiple-space topologies.

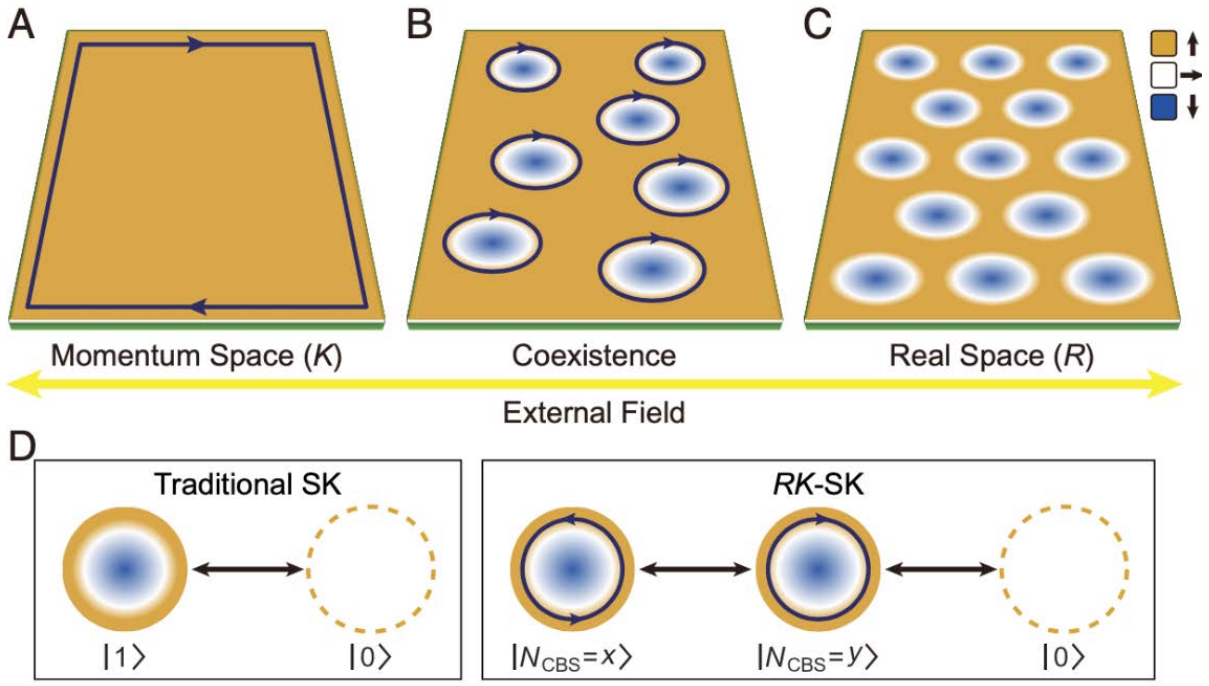

Fig. 1. Schematic diagram of the external field–tunable topological phase transition from K space to *R* space. (A) QAHE with chiral edge states. (B) *RK*-SK states with external field-tunable NCBS may appear under certain conditions in the region where QAHE and SK can coexist. (C) An SkX state. (D) Comparison between traditional SK and *RK*-SK. D, Left shows that traditional SK can mainly be used via creation and annihilation. D, Right shows that there is an additional degree of freedom NCBS in *RK*-SK (i.e., the number and chirality of N_{CBS}) for SK manipulation. Herein, x and y represent different values of N_{CBS}, in which the anticlockwise or clockwise arrows demonstrate the different chirality.

反常量子霍尔效应和磁斯格明子之间的相互作用

（**李阳**，徐胜男，王建峰，王冲，**杨百顺**，**林海青**，段文晖，**黄兵**）

反常量子自旋霍尔效应(QAHE)和磁斯格明子(SK)分布是倒空间和实空间拓扑态的典型代表。尽管这两种效应已经有了比较充分的研究，它们之间的相互作用依然非常不清楚。我们提出当QAHE和SK共存时候，可能会在一定的条件下诱导出一种全新的SK态，我们命名为RK-SK态。不同于传统的SK态，RK-SK态附近会出现环绕在SK附近的非平庸边界态，这个边界态会根据体系费米能级位置表现出不同的宏观输运行为，可被实验观测。特别是，我们可以通过调控边界态的陈数和手性，实现多种不同的RK-SK态的存储和读写。这和传统的SK态不同，传统的SK态只能通过产生和湮灭实现两种状态的存储。我们提出的这个概念可能被用来设计新一代的基于SK态的自旋存储，并解释了多空间拓扑态耦合可以延伸出全新的量子态。

◀ 图 1　从倒空间反常量子霍尔效应 (A) 到实空间磁斯格明子 (C) 可能会经过一个特殊的多空间纠缠量子态 (B), 我们定义为多空间斯格明子态。 (D) 不同于传统的斯格明子态，我们新发现的多空间斯格明子态可以通过调控其边缘态的手性和陈数来实现更高维度的量子存储和读写。

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[1] Y. Li, S. Xu, J. Wang, C. Wang, B. Yang, H. Lin, W. Duan, and **B. Huang***, PNAS **119**, 2122952119 (2022).

BACTERIAL MOTION IN COMPLEX FLUID

(By S. Kamdar, S. Shin, **P. Leishangthem**, L. Francis, **X. L. Xu***, and X. Cheng*)

Teaser: "Persistence, in spite of obstacles", something we might all learn from the bacterial swimming behaviors in complex fluids.

For years, science fictions authors have written about the idea of using microswimmers that could perform surgeries or deliver medicines to humans. However, swimming through complex fluids and environments such as the human body proves to be very different in comparison to swimming in water, as demonstrated by the intensive research works by scientists since the 1960s. Previous studies have consistently found that bacteria swim faster in thick polymer solutions, which is surprising given the mounting hydrodynamic resistance in thick polymer solutions in comparison to water. After six decades of active research, the nature and origin of such motility enhancement are still under heated debate.

In a recent collaboration between the theoretical group led by Prof. Xinliang Xu at Beijing Computational Science Research Center and the experimental groups led by Prof. Xiang Cheng and Prof. Lorraine Francis at the University of Minnesota, bacterial swimming behavior in complex fluids is quantitatively described. In this study, a simple physical model is proposed to describe the mechanical properties of the hook connection between bacterial body and flagellar bundle. Based on this model, these researchers are able to study how hydrodynamic interaction in complex fluids influences the structural configuration of the hook connection, and how such structural configuration behavior is related to bacterial wobbling dynamics and thus bacterial motility in complex fluids. With no free parameters, this model quantitatively explains bacterial wobbling dynamics and motility enhancement in both colloidal and polymeric fluids. In specific, the "obstacles in the suspension" (colloids or polymer chains) exert an effective torque on bacteria that on average lowers the amplitude of bacterial wobbling, leading to higher velocity moving forward. This study provides a unified understanding of bacterial swimming through complex fluids relevant to a wide range of microbiological processes, and is published in Nature [1].

Fig. 1. Keep Moving Forward: Provided by Chinese artist Yi Su, based on the scientific findings in research article

勇往直前：细菌在复杂流体中的运动

(S. Kamdar, S. Shin, **P. Leishangthem**, L. Francis, 徐辛亮*, and 程翔*)

“Persistence, in spite of obstacles”，或许细菌在复杂流体中勇往直前的运动行为对我们所有人都可以有一点启示。

多年以来，通过让微型机器人进入人体循环系统，进而完成微手术、药物投递等功能一直是热门的科幻题材。然后不同于纯净水，人体循环系统中充斥着如血红蛋白等各种有机物，是很典型的复杂流体环境。关于细菌在这种环境中的运动行为，人们从上个世纪60年代开始进行了长期的持续而深入的研究，并发现了细菌在充斥着有机聚合物的溶液中反而运动的更快这一普遍存在然而却有悖于我们常理的现象。

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美国明尼苏达大学Xiang Cheng教授实验组以及Lorraine Francis教授实验组通力合作，实现了对细菌在复杂流体环境中的运动行为的定量描述。通过对细菌身体和鞭毛连接部分的力学性质建立简单的物理模型，研究人员对流体相互作用与该连接部分的结构形态的关系、该连接部分结构形态与细菌运动的摇摆幅度的关系，以及细菌摇摆幅度与细菌向前运动速度的关系进行了研究。该模型在无可调参数的情况下完美的解释了实验在不同复杂流体溶液中所观察到的所有细菌运动结果，揭示了流体相互作用在影响细菌运动方面的核心作用。该研究特别指出，溶液中充斥的障碍物通过流体相互作用给予细菌一个有效力矩，反而减小了细菌的摇摆幅度，使得其在前进方向运动的速度更快，更加持续的向前运动。研究成果于最近在《自然》杂志成文发表【1】。

◀ 《Keep Moving Forward》：作品由中国美术艺术工作者苏艺，根据本文内容所创作。

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[1] S. Kamdar, S. Shin, P. Leishangthem, L. Francis, X. L. Xu*, and X. Cheng*, “The colloidal nature of complex fluids enhances bacterial motility”, Nature **603**, 819-823 (2022).

HOW AN ENZYME MAY UTILIZE THE FLEXIBILITY OF SINGLE STRAND DNA TO CONTROL ACTIVITIES

(By Jinghua Li, Jianbing Ma, Vikash Kumar, Chunhua Xu, Shuang Wang, Qi Jia, Qinkai Fan, Xuguang Xi, Ming Li, Haiguang Liu, and Ying Lu)

Flexible regions in biomolecular complexes, although crucial to understanding structure–function relationships, are often unclear in high-resolution crystal structures. In this study, we showed that single-molecule techniques, in combination with computational modeling, can characterize dynamic conformations not resolved by high-resolution structure determination methods.

In partner with a group led by Prof. Ming Li and Dr. Ying Lu, from the Institute of Physics, we investigated this issue by taking two Pif1 helicases (ScPif1 and BsPif1) as model systems. We found that, besides a few tightly bound nucleotides, adjacent solvent-exposed nucleotides interact dynamically with the helicase surfaces. This cannot be directly observed from high-resolution structure determination method, because only 6 nucleotides can be seen from crystal structures. We applied computational approach to extend the DNA and carried out extensive simulations. The whole nucleotide segment possessed curved conformations and covered the two RecA-like domains of the helicases, which are essential for the inch-worm mechanism. The synergetic approach reveals that the interactions between the exposed nucleotides and the helicases could be reduced by large stretching forces or electrostatically shielded with high-concentration salt, subsequently resulting in reduced translocation rates of the helicases. The dynamic interactions between the exposed nucleotides and the helicases were observed in all-atom molecular dynamics simulations. Such interactions underlay the force- and salt- dependences of their enzymatic activities. The present single-molecule based approach complements high-resolution structural methods in deciphering the molecular mechanisms of the helicases.

The simulation work is done at CSRC, mainly by Dr. Vikash Kumar, who was a postdoc researcher in Prof. Haiguang Liu's group. The work was carried out with a close collaboration with groups led by Prof. Ming Li and Dr. Ying Lu from Institute of Physics (IoP, CAS). The wetlab experiments using single molecule techniques were detailed executed by the IoP group members.

References:

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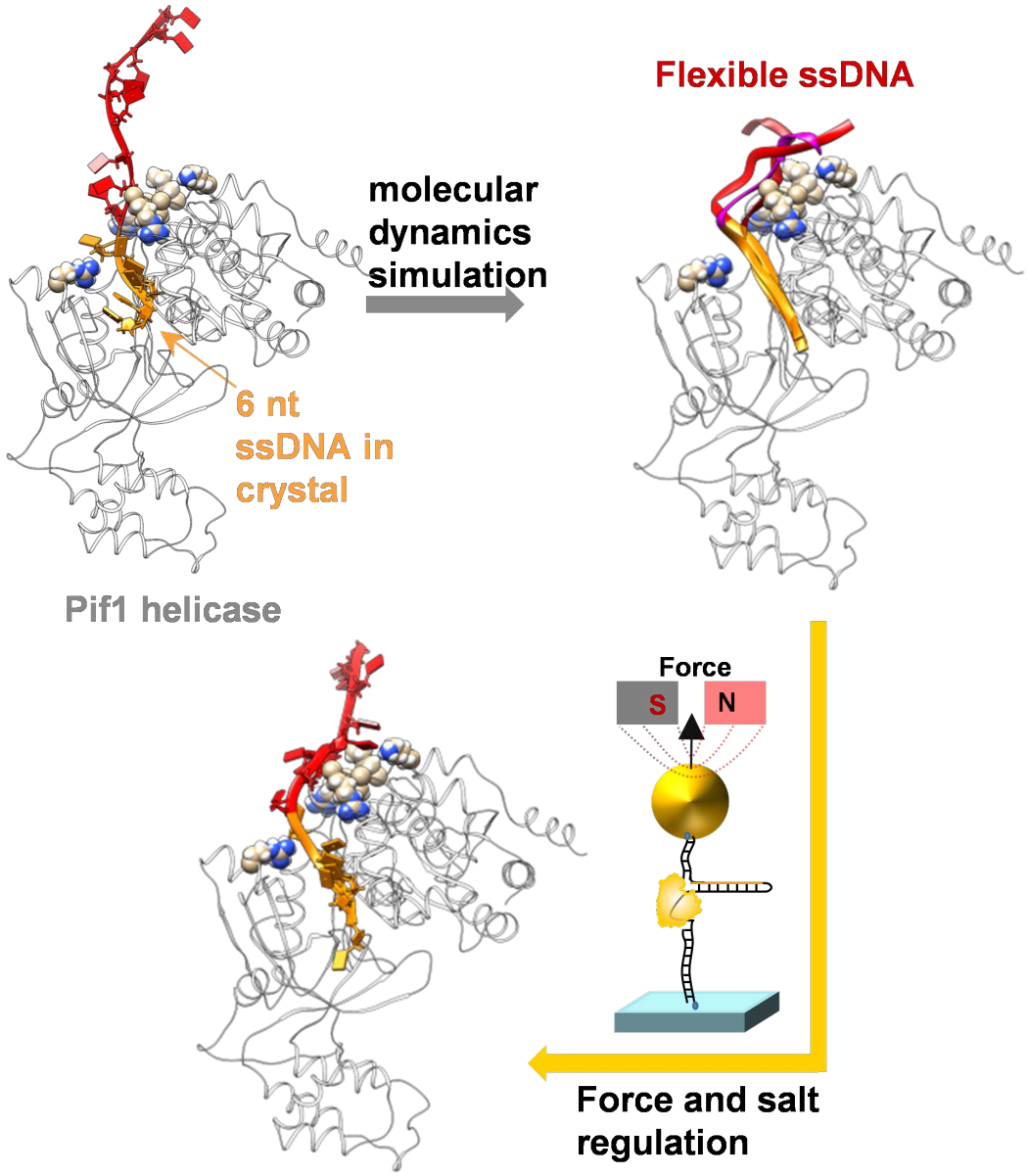

Fig. Computational simulations reveal curved DNA conformations when bound to helicase protein. Key interactions between DNA and helicase are also identified. The single molecular experiments found the activity of helicase depends on the pulling force and salt concentration of the buffer, both are well-explained by the curved conformation of DNA and its interactions with helicase positively charged surface.

CONVERGENCE OF RENORMALIZED FINITE ELEMENT METHODS FOR HEAT FLOW OF HARMONIC MAPS

(By Xinping Gui, Buyang Li, **Jilu Wang**)

The heat flow of harmonic maps can be viewed as the L^2 gradient flow of the energy functional. And it appears in many applications, including the Landau--Lifshitz equation of magnetization dynamics (as the limiting case when the damping parameter tends to ∞), the nematic liquid crystals model (coupled with the Navier--Stokes equations to describe the local molecular direction), and color image denoising. The solution of the heat flow of harmonic maps automatically stays on the unit sphere when the initial function satisfies the unit length constraint. Many efforts have been devoted to developing efficient numerical methods and analyzing stability and convergence of numerical solutions for the heat flow of harmonic maps and its related PDEs, including the Landau--Lifshitz equation and the nematic liquid crystals equations, e.g., linearly unconstrained FEMs and nonlinearly implicit constrained FEMs. The former kind of methods can not preserve the unit length of solutions, and the latter is computationally expensive and no convergence rates have been given for this kind of methods. The simplest method to restore the unit length is to artificially renormalize the numerical solutions by a post-processing technique, i.e., changing the numerical solution m_h^n to $m_h^n/|m_h^n|$ artificially after solving the equation at every time level, before proceeding to the next time level. However, the error analysis of such a simple renormalization method with commonly used FEMs and time-stepping schemes is still challenging.

Recently, Xinping Gui (CSRC), Buyang Li (The Hong Kong Polytechnic University), and Jilu Wang (CSRC) consider a renormalized lumped mass finite element method for the heat flow of harmonic maps:

(1) For given m_h^{n-1} in a finite element space S_h^r, compute an auxiliary numerical solution $\widetilde{m}_h^n$ by

$$\left(\frac{\widetilde{m}_h^n - m_h^{n-1}}{\tau}, v_h\right)_h + (\nabla \widetilde{m}_h^n, \nabla v_h) = (|\nabla m_h^{n-1}|^2 \widetilde{m}_h^n, v_h) \; \forall v_h \in S_h^r$$

where $(\cdot,\cdot)_h$ denotes the discrete inner product in the lumped mass FEM.

(2) Renormalize the auxiliary numerical solution to

$$m_h^n = I_h(\widetilde{m}_h^n/|\widetilde{m}_h^n|)$$

where I_h denotes the Lagrange interpolation onto the finite element space S_h^r.

$\tau\backslash h$	1/16	1/32	1/64	1/128	Convergence rate
1/80	1.874e-7	1.827e-8	2.082e-9	2.535e-10	≈ 3.04
1/160	1.377e-7	1.497e-8	1.792e-9	2.214e-10	≈ 3.02
1/320	1.178e-7	1.357e-8	1.658e-9	2.060e-10	≈ 3.01

$h\backslash\tau$	1/20	1/40	1/80	1/160	Convergence rate
1/32	2.247e-3	8.443e-4	3.691e-4	1.784e-4	≈ 1.05
1/64	2.247e-3	8.444e-4	3.691e-4	1.784e-4	≈ 1.05
1/128	2.247e-3	8.444e-4	3.691e-4	1.784e-4	≈ 1.05

Table. 1. Spatial discretization error $\|m_{h,\tau}^N - m_{h/2,\tau}^N\|_2$ (left) and temporal discretization error $\|m_{h,\tau}^N - m_{h,\tau/2}^N\|_2$ (right) with Q_2 element

The paper [1] presents an optimal-order error estimate of $O(\tau + h^{r+1})$ for a linearly implicit renormalized lumped mass FEM on rectangular mesh under the grid-ratio condition $\tau \geq \kappa h^{r+1}$ for $r \geq 1$, where κ is any positive constant. This condition is very mild compared with restrictions like $c_1 h \leq \tau \leq c_2 h$ and $h^2 \leq \tau \leq h^{1+\varepsilon}$ given in [2,3]. And the discretization errors are displayed in Table 1 by using Q_2 element, which shows the desired convergence rates in time and space. On a triangular mesh, paper [1] yields $O(\tau + h^r)$ under the condition $\tau \geq \kappa h^r$ for $r \geq 1$. The proof of the error estimates is based on a geometric relation between the auxiliary and renormalized numerical solutions. And the techniques in this paper would also work for related PDEs, including the Landau--Lifshitz equation and nematic liquid crystals equations, as the common difficulty for all these equations is the analysis of stability for the renormalization technique in approximating the time derivative.

针对调和映射热流的重整化有限元方法的收敛性分析

（桂新平，李步扬，**王冀鲁**）

调和映射热流的解也可以看作是 L^2 梯度流能量泛函在单位球上的极值点。另外，调和映射热流出现在许多应用中，包括磁化动力学的Landau—Lifshitz方程(阻尼参数趋于无穷大时即可转化为调和映射热流)，向列相液晶模型(结合Navier- Stokes方程描述局部分子方向)和彩色图像去噪等。调和映射热流的解具有特殊的结构，即当初始函数 m^0 模长为 1 时，之后任意时刻均自动满足约束 $|m|=1$ 。大量文献分析了许多工作致力于发展高效的数值方法，并且分析调和映射热流及相关偏微分方程数值解的稳定性和收敛性，包括Landau—Lifshitz方程和向列相液晶方程等。比如线性无约束的有限元方法和非线性隐式的有限元方法。前一类方法不能保证解的单位长度，后一类方法计算量大而且还未证明出收敛阶。实际上，恢复单位长度最简单的方法是通过后处理技术对数值解进行重整化(单位化)，即在每个时间层解完方程后，人为地将数值解 m_h^n 改为 $m_h^n/|m_h^n|$，然后再进入下一个时间层。然而，将这种简单的重整化方法与常用的有限元方法和时间步进格式结合起来进行误差分析仍是一个挑战。

最近，桂新平 (北京计算科学研究中心)、李步扬 (香港理工大学) 和王冀鲁 (北京计算科学研究中心) 研究了针对调和映射热流的重整化集中质量有限元方法:

（1）给定第 $n-1$ 时间层的重整化后的数值解 m_h^{n-1}，先计算第 n 层的辅助数值解 $\tilde{m}_h^n$：

$$\left(\frac{\tilde{m}_h^n-m_h^{n-1}}{\tau},v_h\right)_h+\left(\nabla\tilde{m}_h^n,\nabla v_h\right)=\left(|\nabla m_h^{n-1}|^2\,\tilde{m}_h^n,v_h\right)\forall v_h\in S_h^r$$

这里 $(f,g)_h$ 为插值型数值积分，插值节点选为每个单元上的Guass- Lobatto节点，即在每个单元上都是用Guass-Lobatto数值积分逼近。

（2）再对所求得的第 n 层辅助数值解进行重整化 $m_h^n=I_h(\tilde{m}_h^n/|\tilde{m}_h^n|)$，这里 I_h 为拉格朗日插值算子。

当网格比条件为 $\tau\geq\kappa h^{r+1}$ 时，其中 κ 为任意正常数且 $r\geq 1$，文章 [1] 给出了在矩形网格上针对线性隐式带重整化步骤的集中质量有限元方法 （1）-（2） 的最优阶误差估计 $O(\tau+h^{r+1})$。与 [2,3] 中所需的 $c_1h\leq\tau\leq c_2h$ 和 $h^2\leq\tau\leq h^{1+\varepsilon}$ 等限制条件相比，这个网格比条件非常温和。表 1 给出了利用该格式使用张量型 Q_2 元时所得的误差结果，从表中可以看出收敛阶和理论分析相同。在三角形网格上，当 $\tau\geq\kappa h^r$ 且 $r\geq 2$ 时，相似地可以得到收敛阶 $O(\tau+h^r)$。文章 [1] 中误差分析结果的证明是基于辅助解和重整化数值解之间的几何关系，该技术也适用于相关的偏微分方程，包括 Landau—Lifshitz 方程和向列液晶方程等。

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CHARACTERIZING NON-EXPONENTIAL GROWTH AND BIMODAL CELL SIZE DISTRIBUTIONS IN FISSION YEAST: AN ANALYTICAL APPROACH

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

Advances in microscopy enable us to follow single cells over long timescales from which we can understand how their size varies with time and the nature of innate strategies developed to control cell size. These data show that in many cell types, growth is exponential and the distribution of cell size has one peak, namely there is a single characteristic cell size [1]. However data for fission yeast show remarkable differences: growth is non-exponential (see Fig. 1a) and the distribution of cell sizes has two peaks, corresponding to different growth phases [2]. Here we construct a novel stochastic model of cell size dynamics in fission yeast (see Fig. 1b); by solving the cell size distribution analytically, we show that it is able to predict the two peaked distributions of cell size seen in experiments (see Fig. 1c). In particular, our theory shows that the left peak in the bimodal distribution is associated with cells in the elongation phase, while the right peak is due to cells in the septation and reshaping phases. Furthermore, by fitting the model to the data, we infer values for the rates of all microscopic processes in our model. This method is shown to provide a much more reliable inference than conventional methods and shed light on how the strategy used by fission yeast cells to control their size varies with external conditions. We also show that the variability in added size and the strength of size control in fission yeast depend weakly on the temperature but strongly on the culture medium. More importantly, we find that stronger size homeostasis and larger added size variability are required for fission yeast to adapt to unfavorable environmental conditions.

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[1] Tanouchi, Y. et al. A noisy linear map underlies oscillations in cell size and gene expression in bacteria. Nature 523, 357–360 (2015).

[2] Nakaoka, H. & Wakamoto, Y. Aging, mortality, and the fast growth trade-off of Schizosaccharomyces pombe. PLoS Biol. 15, e2001109 (2017).

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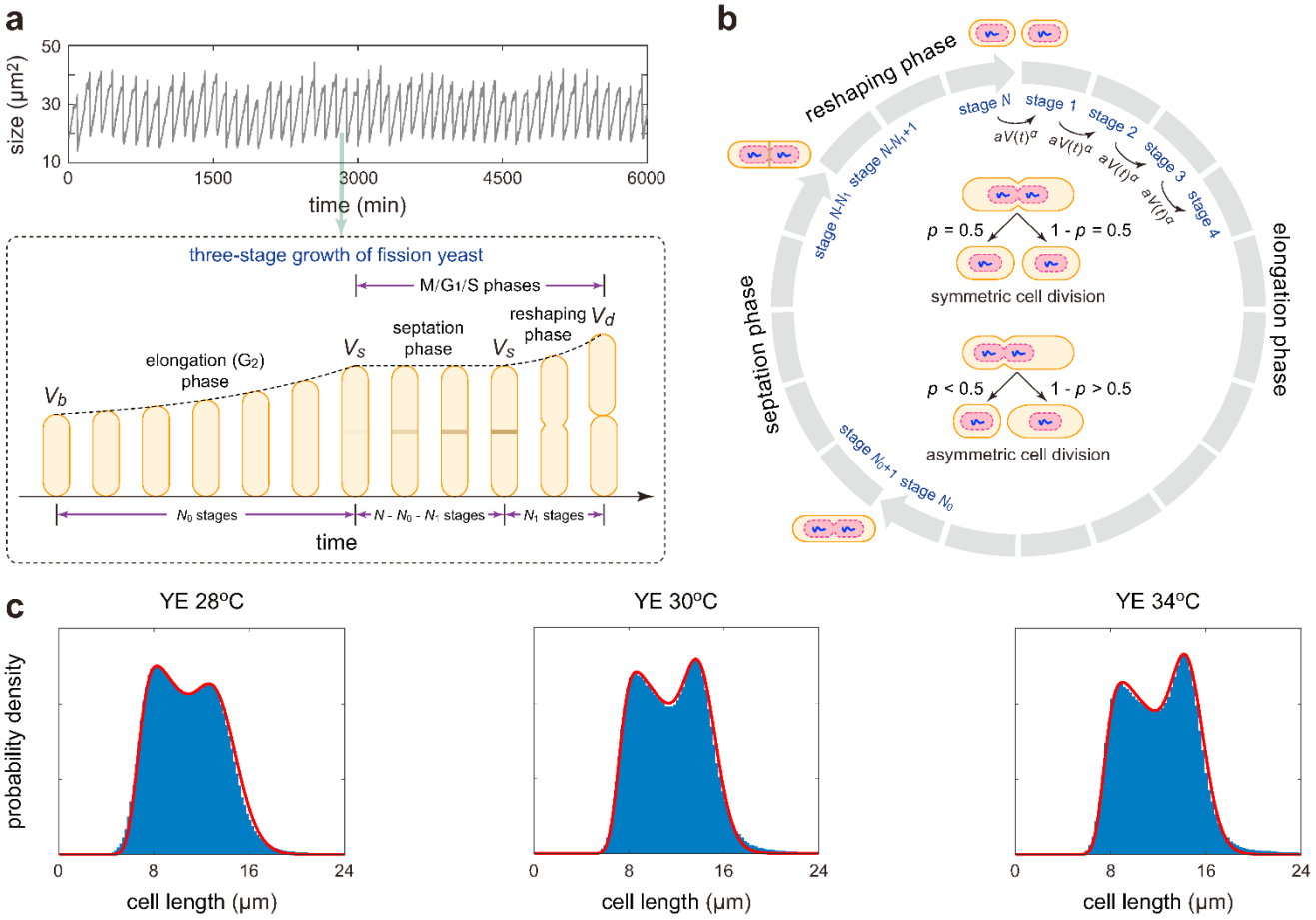

Fig. 1. A detailed model of cell size dynamics in fission yeast.

a. Three-stage growth pattern of fission yeast: an elongation phase where cell size grows exponentially with rate g_0 , followed by a septation phase during which the septum is formed and cell size remains constant, and then followed by a reshaping phase during which the new cell end forms a hemisphere and cell length increases with a higher exponential growth rate $g_1 > g_0$. Here V_b is the size at birth, V_s is the size at septation, and V_d is the size at division.

b. Schematic illustrating a detailed model of cell size dynamics describing three cell growth phases, size homeostasis, and symmetric or asymmetric partitioning at cell division (see inset graph). Each cell can exist in N effective cell cycle stages. Cell elongation occurs during the first N_0 stages, septation occurs during the intermediate $N - N_0 - N_1$ stages, and reshaping occurs during the last N_1 stages. The transition rate from one stage to the next at time t is proportional to the ath power of the cell size $V(t)$ with $a > 0$ being the strength of size control and $a > 0$ being the proportionality constant. This guarantees that larger cells at birth divide faster than smaller ones to achieve size homeostasis. At stage N, a mother cell divides into two daughters that are typically different in size via asymmetric cell division. Symmetric division is the special case where daughters are equisized.

c. Fitting the experimental cell size distributions (blue bars) to the three-stage model (red curve) for fission yeast cells cultured in the yeast extract medium at 28°C, 30°C, and 34°C.

裂殖酵母的非指数生长与双峰细胞体积分布的解析理论

(贾晨#, Abhyudai Singh. Ramon Grima*)

近年来，显微镜学的进展允许我们在很长的时间尺度内追踪单细胞的演化行为。这些实验可以帮助我们理解细胞体积随时间的动力学变化，揭示细胞体积之所以能维持恒定态所需的体积调控策略。实验数据表明，在很多细胞类型中细胞体积的生长是指数的，且细胞体积分布是单峰的，即只存在唯一的典型细胞体积[1]。然而，裂殖酵母数据却呈现出完全不同的动力学行为：细胞体积的生长是非指数的（见图1a），且细胞体积分布是双峰的，这两个峰分别对应于两个不同的生长阶段[2]。在本文中，我们构建了裂殖酵母细胞体积动力学的全新数学模型（见图1b）。通过对细胞体积分布进行解析求解，我们发现该模型可以精确地描述实验中观测到的双峰细胞体积分布（见图1c）。特别地，我们的理论表明分布的左峰对应于处于延伸阶段（elongation phase）的细胞，而分布的右峰对应于处于分隔阶段（septation phase）与重塑阶段（reshaping phase）的细胞。进一步，通过与数据进行拟合，我们推断了模型微观过程所涉及的所有速率参数。与传统的方法相比，我们的参数推断方法更加可信，且能够揭示裂殖酵母细胞体积的调控策略如何随外部环境进行变化。我们的结果表明，裂殖酵母细胞体积增量的变异性以及细胞体积调控的强度对温度有较弱的依赖，但对培养基有很强的依赖。更重要地，我们发现裂殖酵母需要更强的体积调控策略以及更大的体积增量变异性以适应不利的环境条件。

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[1] Tanouchi, Y. et al. A noisy linear map underlies oscillations in cell size and gene expression in bacteria. Nature 523, 357–360 (2015).

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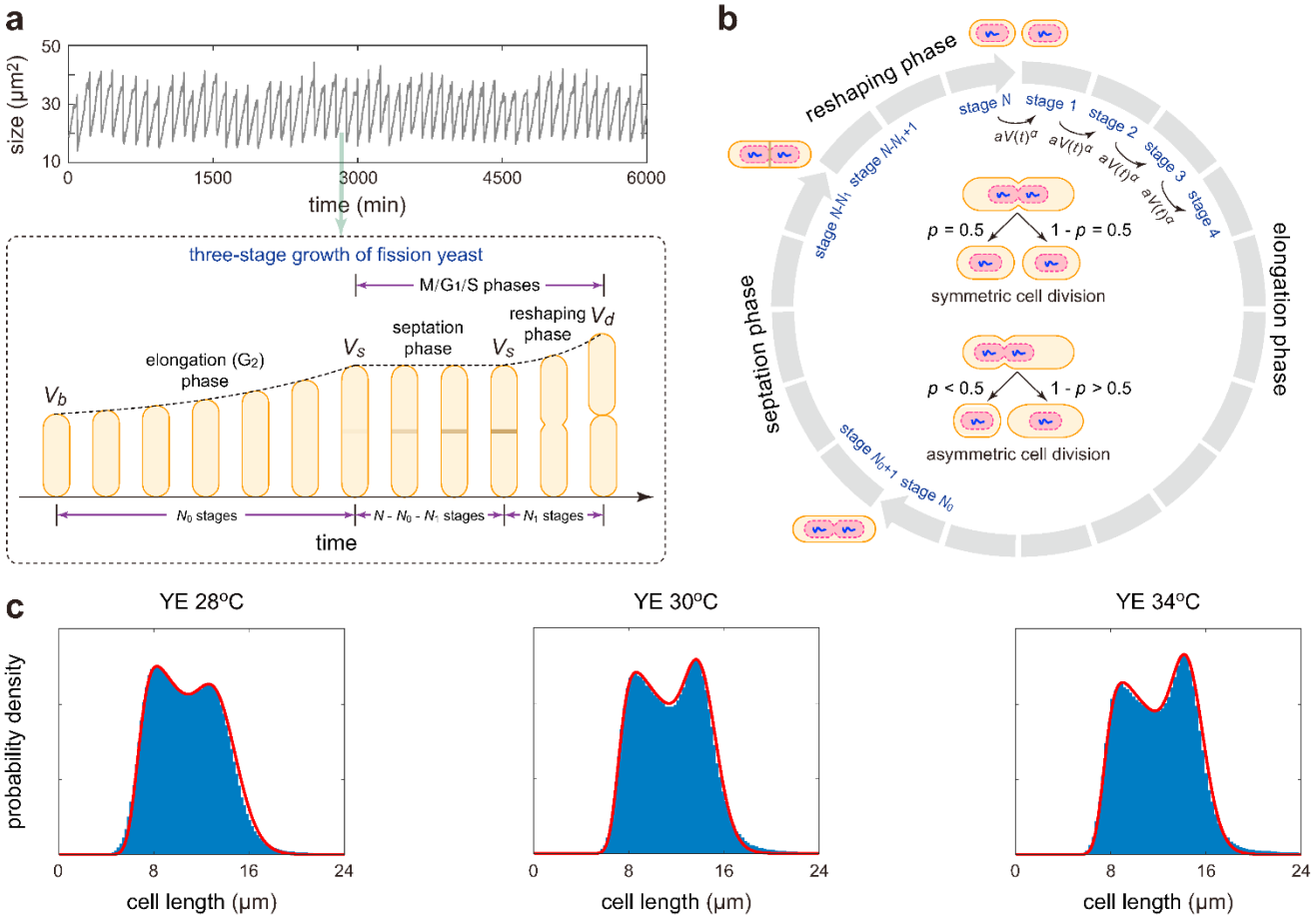


图 1　裂殖酵母细胞体积动力学的精细模型。a. 裂殖酵母的三阶段生长模式: 在延伸阶段细胞体积以 g_0 的速率进行指数生长，随后在分隔阶段细胞的隔膜开始形成且细胞体积保持不变，最后在重塑阶段新细胞的端点形成半球形且细胞长度以更大的速率 $g_1 > g_0$ 进行指数生长。其中 V_b 为细胞出生时的体积, V_s 为细胞在分隔阶段的体积，V_d 为细胞分裂时的体积。b. 细胞体积动力学精细模型的示意图。该模型描述了裂殖酵母的三个细胞生长阶段，体积调控策略，以及对称或非对称细胞分裂（见内插图）。每个细胞周期被分为 N 个等效阶段，细胞延伸发生在前 N_0 个阶段，细胞分隔发生在中间的 $N - N_0 - N_1$ 个阶段，而细胞重塑发生在最后的 N_1 个阶段。在 t 时刻从某个阶段转移到下一阶段的转移速率正比于细胞体积 $V(t)$ 的 a 次幂，其中 $a > 0$ 为体积调控强度且 $a > 0$ 为比例系数。这确保出生时体积较大的细胞比出生时体积较小的细胞分裂地更快，通过该机制细胞可以实现体积恒定态。在第 N 个阶段, 母细胞分裂为两个子细胞。在对称分裂情形，两个细胞拥有相同的体积；而在非对称分裂情形，两个细胞拥有不同的体积。c. 细胞体积分布的实验测量（蓝色柱子）与三阶段模型拟合（红色曲线）。三张子图分别对应于在28°C, 30°C与34°C这三个温度、在酵母提取物培养基下培养的裂殖酵母。

A C^1 CONFORMING PETROV-GALERKIN METHOD FOR CONVECTION-DIFFUSION EQUATIONS AND SUPERCONVERGENCE ANALYSIS OVER RECTANGULAR MESHES

(By Waixiang Cao, **Lueling Jia**, and **Zhimin Zhang***)

In Scientific and engineering computing, there are situations where we are as interested in the derivatives (gradient) as the solution itself, examples are stress/strain versus displacement in solid mechanics, pressure versus velocity in fluid dynamics, etc. Since the C^1-conforming method provides a better approximation for derivatives without increasing the computational cost, we present a new C^1-L^2 Petrov-Galerkin method (i.e., the tensor product C^1 polynomial space Q_k for trial space and the L^2 piecewise Q_{k-2} polynomial for test space) for 2D convection-diffusion equation. In this work, we provide a unified mathematical approach to establish convergence theory for the C^1-L^2 Petrov-Galerkin method. Optimal error estimates in the L^2-, H^1-, H^2-norms are established and interesting superconvergence results are discovered, including: 1) h^{2k-2} superconvergence rate for approximations of both the function value and the first-order derivatives ($e_{u,n}$ and $e_{\nabla u,n}$) at mesh nodes; 2) h^{k+2} for the function value approximation ($e_{u,J}$) at the roots of a special Jacobi polynomial; 3) h^{k+1} for the first-order and h^k for the second-order derivative approximations ($e_{\nabla u,l}$ and $e_{\Delta u,g}$) at Lobatto lines and Gauss lines, respectively; 4) the Petrov-Galerkin solution u_h is superconvergent to a particular Jacobi projection u_I of the exact solution u in the L^2-, H^1-, H^2-norms. With relatively fewer requirements on the global smooth of u , we further established interior estimates and proved that a superconvergence phenomenon may still exist for the numerical solution over a compact subdomain Ω_0 even the solution is singular or has low regularity. To recover the global optimal convergence for singular solution, the graded mesh is used to treat the singularity. Table 1 indicates numerical results in $\Omega=[0,1]^2$ when u is singular near the origin and $u\in H^{2.5-\delta}(\delta>0)$. Under uniform mesh, convergence orders are limited by finite regularity in Ω but higher in sub-domain Ω_0 excluding the singular point. By adopting graded mesh, all superconvergence results are recovered.

uniform mesh	$\|u-u_h\|_{0,\Omega}$		$\|u-u_h\|_{1,\Omega}$		$\|u-u_h\|_{2,\Omega}$		$\|u-u_h\|_{2,\Omega_0}$		$\|u_h-u_I\|_{2,\Omega_0}$	
M	error	order	error	order	error	order	error	order	error	order
32	3.4e-7	-	1.0e-4	-	5.1e-2	-	1.1e-7	-	7.5e-10	-
64	6.1e-8	2.5	3.7e-5	1.5	3.6e-2	0.5	1.4e-8	3.0	6.5e-11	3.5
128	1.1e-8	2.5	1.3e-5	1.5	2.5e-2	0.5	1.8e-9	3.0	5.8e-12	3.5
256	1.9e-9	2.5	4.6e-6	1.5	1.8e-2	0.5	2.2e-10	3.0	-	-
graded mesh	$e_{u,n}$		$e_{\nabla u,n}$		$e_{u,J}$		$e_{\nabla u,l}$		$e_{\Delta u,g}$	
M	error	order	error	order	error	order	error	order	error	order
4	2.4e-4	-	2.6e-3	-	2.5e-4	-	3.9e-3	-	6.6e-2	-
8	7.6e-6	5.0	9.3e-5	4.8	1.1e-5	4.6	2.3e-4	4.1	7.2e-3	3.2
16	1.3e-7	5.9	2.2e-6	5.4	1.9e-7	5.8	9.9e-6	4.5	6.1e-4	3.6
32	1.9e-9	6.1	3.9e-8	5.8	3.1e-9	5.9	3.4e-7	4.9	4.3e-5	3.8

Table. 1. M: the partition size in each direction; $k=4$.

求解对流扩散方程C^1协调的Petrov-Galerkin方法及其矩形网格下的超收敛分析

（曹外香，贾略羚，张智民*）

在科学和工程计算领域，许多情况下人们对解的导数（梯度）逼近和解函数本身逼近同样感兴趣，例如固体力学中的应力/应变和位移，流体动力学中的压力和速度等等。由于 C^1 协调元能够在不增加计算量的前提下更好的逼近导数，我们以二维对流扩散方程为例，系统地研究了 C^1-L^2 Petrov-Galerkin方法（其中试探空间和检验空间分别取作 C^1 多项式空间 Q_k 和分片 L^2 多项式空间 Q_{k-2}，Q_k 是 k 次张量型多项式空间）的收敛性理论。这项工作建立了该方法在 L^2-, H^1-, H^2-范数意义下的最优误差估计以及如下的超收敛结论：

1) 网格节点处函数值逼近($e_{u,\,n}$)和一阶导数值逼近($e_{\nabla u,\,n}$)的超收敛阶均为 h^{2k-2}；

2) 特殊Jacobi多项式的零点处函数值逼近($e_{u,\,J}$)的超收敛阶为 h^{k+2}；

3) 沿Lobatto线一阶导数值逼近($e_{\nabla u,\,l}$)、沿Gauss线二阶导数值逼近($e_{\Delta u,\,g}$)的超收敛阶分别为h^{k+1} 和 h^k；

4) 数值解 u_h 在 L^2-, H^1-, H^2-范数意义下超逼近于与真解 u 的特定Jacobi投影 u_I。

当 u 具有较低的全局光滑性时，我们进一步对该方法建立了内估计，证明了在解有奇性时，远离奇性的区域仍然存在超收敛现象。为了恢复更高的收敛阶，我们提出了使用几何网格处理局部奇异性的策略。设区域 $\Omega=[0,1]^2$，真解 u 仅在原点处有奇异性，满足 $u\in H^{2.5-\delta}(\delta>0)$，表1给出了相应的数值计算结果。在均匀网格下，区域 Ω 上最优误差的收敛阶受限于 u 的正则性，但在一个不包含奇异点的子区域上 Ω_0 上，误差有较高的收敛阶。应用几何网格后，所有的最优超收敛都得到了恢复。

References:

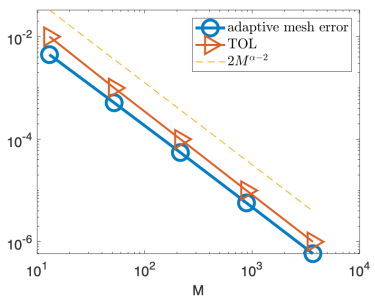
[1] W.X. Cao, L.L. Jia, and Z.M. Zhang*, A C^1 conforming Petrov-Galerkin method for convection-diffusion equations and superconvergence analysis over rectangular meshes, SINUM, 60-1, (2022) pp.274-311.

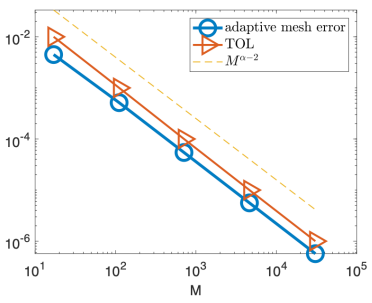
A POSTERIORI ERROR ANALYSIS FOR VARIABLE-COEFFICIENT MULTITERM TIME-FRACTIONAL SUBDIFFUSION EQUATIONS

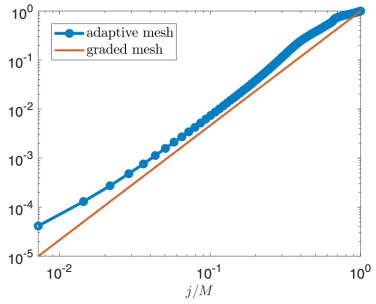
(By Natalia Kopteva and **Martin Stynes***)

Consider the multiterm time-fractional subdiffusion problem $\sum_{i=1}^{\ell}[q_i(t)D_t^{\alpha_i}u(x,t)] + \mathcal{L}u(x,t) = f(x,t) for (x,t) \in \Omega \times (0,T]$ satisfying the initial and boundary conditions $u(x,0) = u_0(x)$ for $x \in \Omega$, $u(x,t) = 0$ for $x \in \partial\Omega$ and $0 < t \le T$. Here ℓ is a positive integer, the constants α_i satisfy $0 < \alpha_\ell < \cdots < \alpha_2 < \alpha_1 \le 1$, while each $q_i \in C[0,T]$ with $q_i(t) \ge 0$ and $\sum_{i=1}^{\ell} q_i(t) > 0$ for $t \in [0,T]$. Each $D_t^{\alpha_i}$ is a Caputo derivative of order α_i, defined in the usual way. The problem is posed in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ with $d \in \{1,2,3\}$; $\mathcal{L}$ is a linear second-order elliptic spatial operator satisfying $\int_\Omega (\mathcal{L}r)\, r \ge \lambda \| r \|^2$ for some $\lambda > 0$ where $\|\cdot\|$ is the $L^2(\Omega)$ norm.

Let u_h be an approximate numerical solution to this problem that is computed by any numerical method such that the residual $R_h(x,t) := \left(\sum_{i=1}^{\ell} q_i(t)D_t^{\alpha_i} + \mathcal{L}\right)u_h(x,t) - f(x,t)$ is defined for almost all $(x,t) \in \Omega \times (0,T]$. Then under some reasonable regularity hypotheses on u and u_h (see [1]), if $\| R_h(\cdot,t) \| \le \left(\sum_{i=1}^{\ell} q_i(t)D_t^{\alpha_i} + \lambda\right)\mathcal{E}(t)$ for all $t > 0$, where $\mathcal{E} \ge 0$ is a suitable user-chosen barrier function, one has $\| (u_h - u)(\cdot,t) \| \le \mathcal{E}(t)$ for all $t \ge 0$. Suggestions for choosing $\mathcal{E}$ are given in [1]. Hence, for example, one gets *the a posteriori bound* $\| (u_h - u)(\cdot,t) \| \le \sup_{0<s\le t}\left\{\frac{\| R_h(\cdot,s) \|}{\mathcal{R}_0(s)}\right\}$ for $t \in [0,T]$, where $\mathcal{R}_0(t) := \lambda + \sum_{i=j}^{\ell} q_i(t)t^{-\alpha_i}/\Gamma(1-\alpha_i)$. Using this $\mathcal{R}_0$, we show some typical numerical results that are generated by an adaptive algorithm based on the above a posteriori bound combined with the standard L1 discretisation in time. This algorithm does not use any analytical information about the true solution and the user does not guide the choice of temporal mesh that is generated; the computation of this mesh is one-dimensional in nature and is independent of the number of spatial dimensions, since it is based on the scalar quantity $\| R_h(\cdot,t) \|$ The left and centre graphs display the maximum of $\| (u_h - u)(\cdot,t) \|$ over $[0,T]$ for $\alpha = 0.4$ and $\alpha = 0.8$ respectively, for various values of the parameter TOL specified by the user, while the right graph compares the adaptively generated mesh with the theoretically optimal graded mesh. Our computed solution attains the optimal order of convergence $O(M^{\alpha_1 - 2})$, where the temporal mesh has M mesh points.







变系数多项时间分数次扩散方程的后验误差分析

(Natalia Kopteva and Martin Stynes*)

考虑如下多项时间分数阶次扩散问题 $\sum_{i=1}^{\ell}[q_i(t)D_t^{\alpha_i}u(x,t)]+\mathcal{L}u(x,t)=f(x,t) for (x,t)\in\Omega\times(0,T]$ 满足初边值条件 $u(x,0)=u_0(x)$ 其中 $x\in\Omega$，$u(x,t)=0$ 其中 $x\in\partial\Omega$，$0<t\leq T$。这里 ℓ 是一个正整数，常数 α_i 满足 $0<\alpha_\ell<\cdots<\alpha_2<\alpha_1\leq 1$，每个 $q_i\in C[0,T]$ 满足 $q_i(t)\geq 0$，$\sum_{i=1}^{\ell}q_i(t)>0$ 其中 $t\in[0,T]$。每个 $D_t^{\alpha_i}$ 表示 α_i 阶Caputo导数。该问题定义在有界Lipschitz 区域 $\Omega\subset\mathbb{R}^d$，$d\in\{1,2,3\}$；$\mathcal{L}$ 表示线性二阶椭圆空间运算满足 $\int_\Omega(\mathcal{L}r)\,r\geq\lambda\|r\|^2$ 其中 $\lambda>0$，这里 $\|\cdot\|$ 表示 $L^2(\Omega)$ 范数。

令 u_h 为用任何数值方法求解该问题的近似数值解，它的残差定义式为

$$R_h(x,t):=\left(\sum_{i=1}^{\ell}q_i(t)D_t^{\alpha_i}+\mathcal{L}\right)u_h(x,t)-f(x,t)$$

然后在一些合理的对 u 和 u_h 正则性假设下(参见 [1]), 如果 $\|R_h(\cdot,t)\|\leq\left(\sum_{i=1}^{\ell}q_i(t)D_t^{\alpha_i}+\lambda\right)\mathcal{E}(t)$，$t>0$，其中 $\mathcal{E}\geq 0$ 是一个合适的障碍函数, 假设选择[1]中给出的 $\mathcal{E}$，我们可得 $\|(u_h-u)(\cdot,t)\|\leq\mathcal{E}(t)$，$t\geq 0$。例如我们可得后验误差估计 $\|(u_h-u)(\cdot,t)\|\leq\sup_{0<s\leq t}\left\{\frac{\|R_h(\cdot,s)\|}{\mathcal{R}_0(s)}\right\}$，$t\in[0,T]$，其中 $\mathcal{R}_0(t):=\lambda+\sum_{i=j}^{\ell}q_i(t)t^{-\alpha_i}/\Gamma(1-\alpha_i)$ 用这个 $\mathcal{R}_0$，我们给出了一些典型的数值结果，这些结果是由基于上述后验界结合标准的L1时间离散得到的的自适应算法。该算法不使用任何关于真解的信息，也不用指定选择时间网格；因为它基于标量 $\|R_h(\cdot,t)\|$，所以该计算本质上是一维的，与空间维度的数量无关。左边和中间的图形分别展示了 $\alpha=0.4$ 和 $\alpha=0.8$ 在 $[0,T]$ 上的最大误差 $\|(u_h-u)(\cdot,t)\|$，其中 TOL 为指定的数，右边的图比较了自适应生成的网格和理论上最优的梯度网格. 我们的计算结果可得到最优收敛阶 $O(M^{\alpha_1-2})$，其中 M 为时间网格点数。

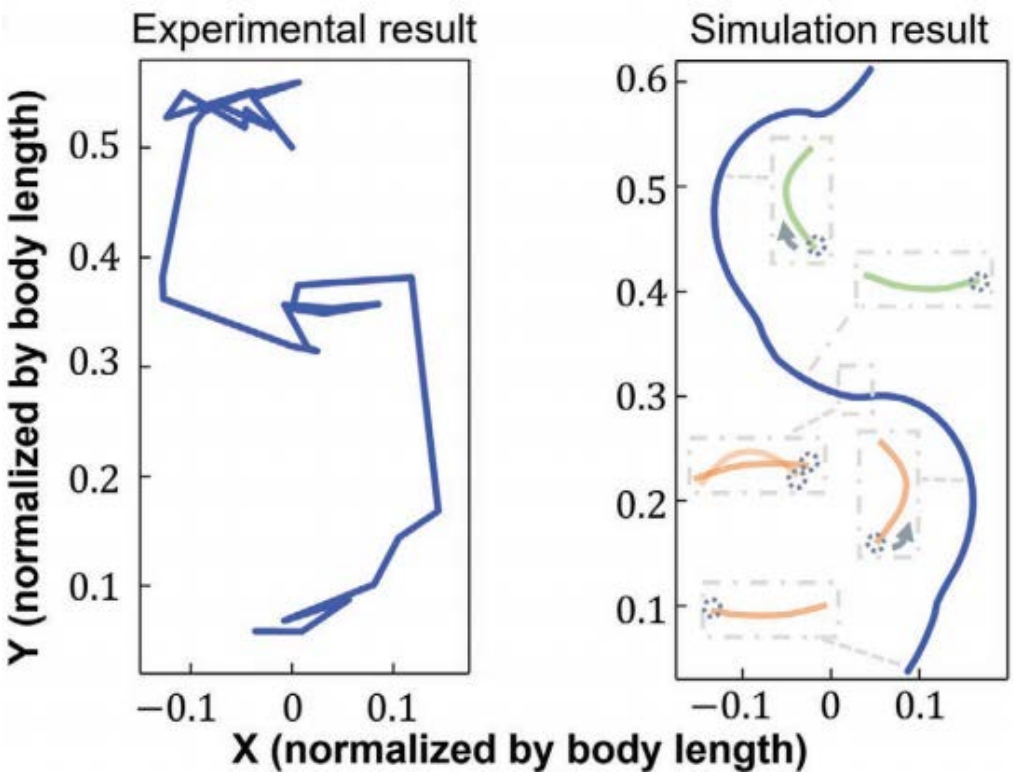
References:

[1] Natalia Kopteva & Martin Stynes, A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations, J. Sci. Comput. 92 (2022), paper no.73. doi:10.1007/s10915-022-01936-2

DECOUPLING AND REPROGRAMMING WIGGLING MOTION OF MIDGE LARVAE USING A SOFT ROBOTIC PLATFORM

(By Neng Xia, **Bowen Jin**, Dongdong Jin, Zhengxin Yang, Chengfeng Pan, Qianqian Wang, Fengtong Ji, Veronica Iacovacci, Carmel Majidi, **Yang Ding**, Li Zhang)

The efficient motility of invertebrates helps them survive under evolutionary pressures. Reconstructing the locomotion of invertebrates and decoupling the influence of individual basic motion are crucial for understanding their underlying mechanisms, which, however, generally remain a challenge due to the complexity of locomotion gaits. A team led by Prof. Yang Ding from CSRC and Prof. Li Zhang from CUHK developed a magnetic soft robot to reproduce midge larva's key natural swimming gaits, and investigated the coupling effect between body curling and rotation on motility [1]. Through the team's systematically decoupling studies using programmed magnetic field inputs, the soft robot (named LarvaBot) experiences various coupled gaits, including biomimetic side-to-side flexures, and unveils that the optimal rotation amplitude and the synchronization of curling and rotation greatly enhance its motility. The LarvaBot achieves fast locomotion and upstream capability at the moderate Reynolds number regime. The soft robotics-based platform provides new insight to decouple complex biological locomotion, and design programmed swimming gaits for the fast locomotion of soft-bodied swimmers.



使用软机器人平台解耦和重编程子孓的游动

（夏能，**靳博文**，金东东，杨正馨，潘程枫，王乾乾，纪凤同，Veronica Iacovacci，Carmel Majidi，**丁阳**，张立）

动物的有效运动有助于它们在进化压力下生存。重建动物在各种环境下的运动和解耦基本运动模式对其整体运动性能的影响对于理解它们的运动机理至关重要，然而，由于运动步态的复杂性，这通常仍然是一个挑战。由北京计算科学研究中心的丁阳教授和香港中文大学的张立教授领导的团队开发了一种磁软机器人来重现子孓的关键自然游泳步态，并研究了身体卷曲和旋转对运动的耦合效应[1]。通过该团队使用程序化磁场输入的系统解耦研究，软机器人（名为 LarvaBot）体验了各种耦合步态，包括仿生侧向弯曲，并揭示了最佳旋转幅度以及卷曲和旋转的同步极大地增强了它的动力。 LarvaBot 在中等雷诺数范围内实现了快速运动和上游能力。基于软体机器人的平台为解耦复杂的生物运动提供了新的见解，并为软体游泳者的快速运动设计了可以编程的游泳步态。

◀ 实验（左）和模拟（右）得到的仿子孓机器人的轨迹。长度单位为身长。

References:

[1] Neng Xia, Bowen Jin, Dongdong Jin, Zhengxin Yang, Chengfeng Pan, Qianqian Wang, Fengtong Ji, Veronica Iacovacci, Carmel Majidi, Yang Ding, Li Zhang, Decoupling and Reprogramming the Wiggling Motion of Midge Larvae Using a Soft Robotic Platform, *Advanced Materials* 34(17),2109126 (2022)

NUMERICAL SOLVER FOR THE BOLTZMANN EQUATION WITH SELF-ADAPTIVE COLLISION OPERATORS

(By Zhenning Cai, Yanli Wang*)

In the kinetic theory, Boltzmann equation is always adopted as the governing equation in the gas dynamics. One of the numerical difficulties in the discretization of the Boltzmann equation lies in the high-dimensional integral form of the quadratic collision term. To compute the collision term efficiently, the velocity variable in the distribution function is usually discretized by high-order schemes such as the spectral methods, discontinuous Galerkin methods, etc. Here, we are focusing on the Hermte/Burnett spectral method, which can be linked to the moment method since the coefficients in the spectral expansion are actually the moments of the distribution function.

In the previous work, by taking the idea of the Shakhov operator, the authors divided all moments of the distribution function into two sets, with one set including low-order moments describing the sketch of the distribution function, and the other including high-order moments providing the details. For the set with low-order moments, the quadratic collision operator is applied, while for the set with high-order moments, a simple relaxation towards the equilibrium is used as an approximation. One parameter in this hybrid approach is the critical order M0 that defines the “low-order” and “high-order” moments. Since the parameter M0 defines the modeling accuracy, it is expected that the choice of M0 should depend on the “modeling error” given by some differences between the current collision model and the exact binary collision model when applied to the current distribution function. Once such an error indicator is obtained, we can change the value of M0 dynamically during our simulation. However, the construction of such an error indicator is far from trivial due to the following reasons:

1) Unlike the a posteriori error estimation in the finite element methods, we do not have an equation to define the “residual” as an

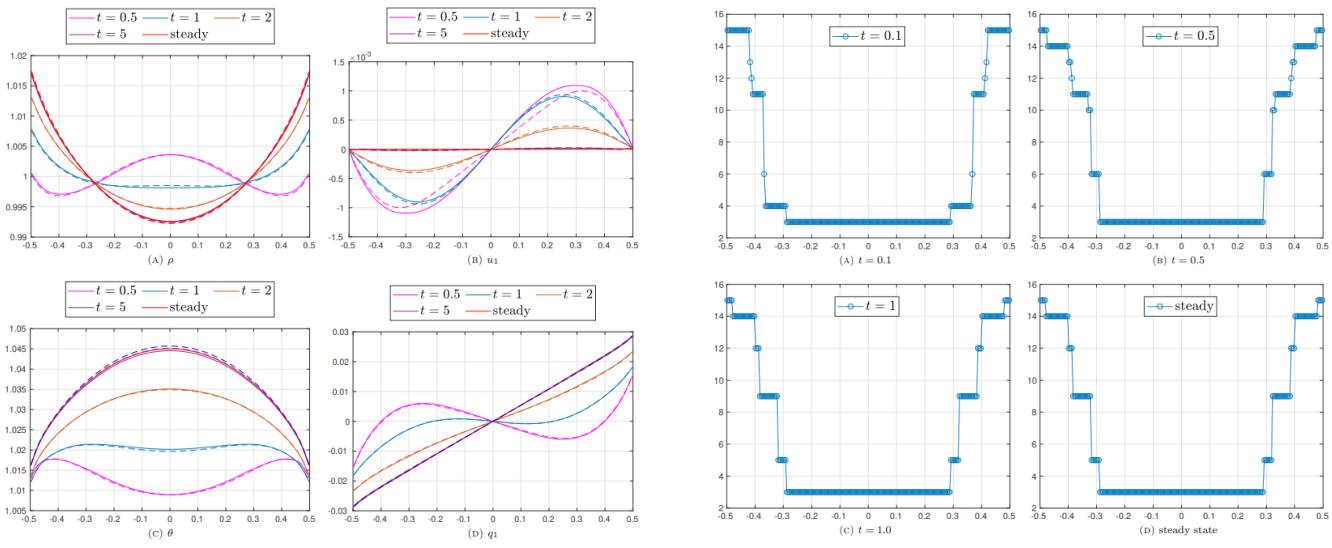
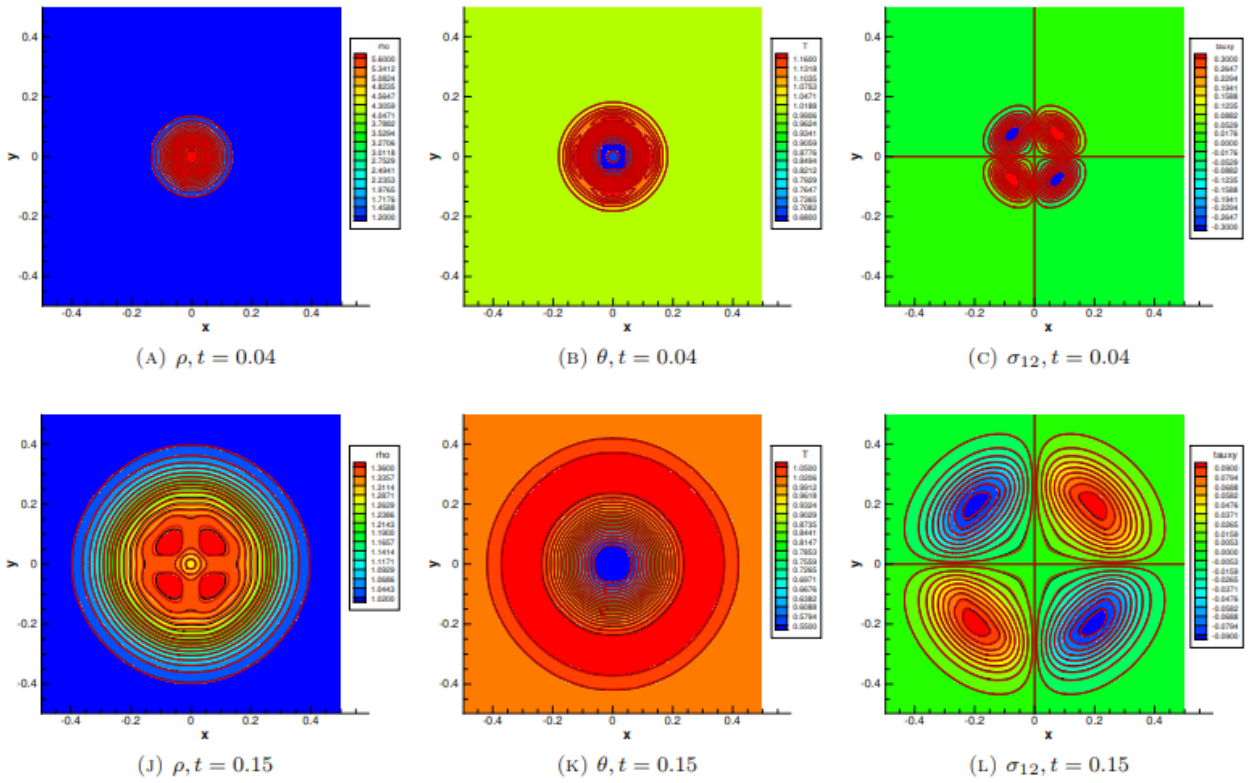


Fig. 1. Couette flow (left:Evolution of the numerical solution, right: change of M_0)



(A) $\rho, t = 0.04$ (B) $\theta, t = 0.04$ (C) $\sigma_{12}, t = 0.04$

(J) $\rho, t = 0.15$ (K) $\theta, t = 0.15$ (L) $\sigma_{12}, t = 0.15$

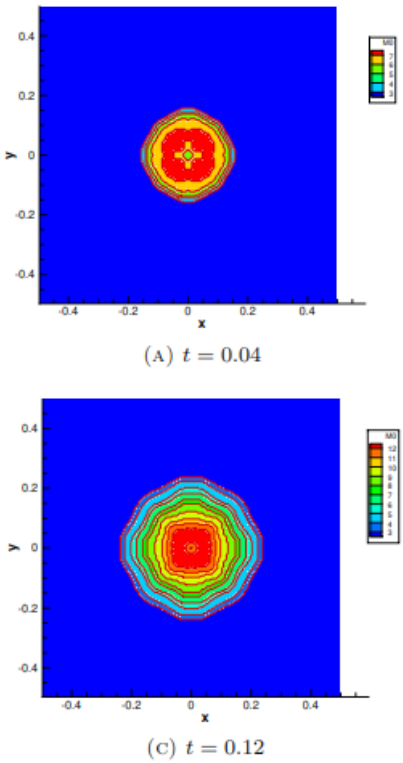
Fig. 2. Fluid diffusion (Numerical solution at different time)

error indicator.

2) The collision operator is generally unbounded, so that even an a priori error estimation is non-trivial.

3) Another common technique by comparing the current model and a more accurate model with larger M0 is not applicable here due to the rapid growth of the computational cost with respect to M0 (usually M08).

Because of these difficulties, we, in this work, look for non-standard techniques to quantify the error. The goal of this paper is to establish an error indicator with low computational cost compared to the collision term. With this error indicator, we are able to choose this modeling parameter M0 adaptively on each spatial grid cell at each time step with the purpose to reduce the computational time on the collision terms. Due to the high computational complexity with respect to M0, reducing M0 can effectively save the computational cost. This work contributes to the adaptive methods for the Boltzmann equation. Several numerical examples such as the 1D Couette flow and 2D fluid diffusion problem are studied to validate this new method. [This work is now published in SISC, 44(2), 2022].



(A) $t = 0.04$

(C) $t = 0.12$

Fig. 3. Fluid diffusion (M_0 at different time)

针对Boltzmann方程二元碰撞模型的自适应求解算法

（蔡振宁，王艳莉）

Boltzmann方程作为动理学中的基本方程而被广泛应用。但由于其二元碰撞模型包含高维非奇性积分，高效数值求解Boltzmann方程充满困难。因此，人们发展了一系列数值方法来模拟Boltzmann方程复杂的二元碰撞模型，例如谱方法，间断Galerkin方法等。在该项工作中，论文作者主要关注Hermite/Burnett谱方法。

目前，论文作者利用Shakhov碰撞模型的思路，在Hermite谱方法框架下构造了混合碰撞模型来近似二元碰撞模型。具体地，分布函数矩系数被分为高阶与低阶两个部分，其中低阶部分认为对刻画分布函数至关重要，因此使用原始二元碰撞模型演化，高阶部分对分布函数起到修饰作用，使用简单的BGK碰撞模型演化。在这个混合模型中，一个重要参数为M0，其定义了低阶与高阶矩的阶数。由于M0决定了混合模型近似二元碰撞模型的精度，因此，一般情况下M0的数值取决于混合模型与原始二元碰撞模型间的误差。如果可以寻找到一个合适的指示子来表示该误差，即可在数值模拟中动态修改M0，做到在保证计算精度的前提下，大幅减少计算量。然而，传统构造误差指示子的方法在这里并不适用，具体地

1) 不同于有限元中的后验误差估计，不存在一个可以定义残差的方程；

2) 二元碰撞算子一般是无界算子，因此不存先验误差估计；

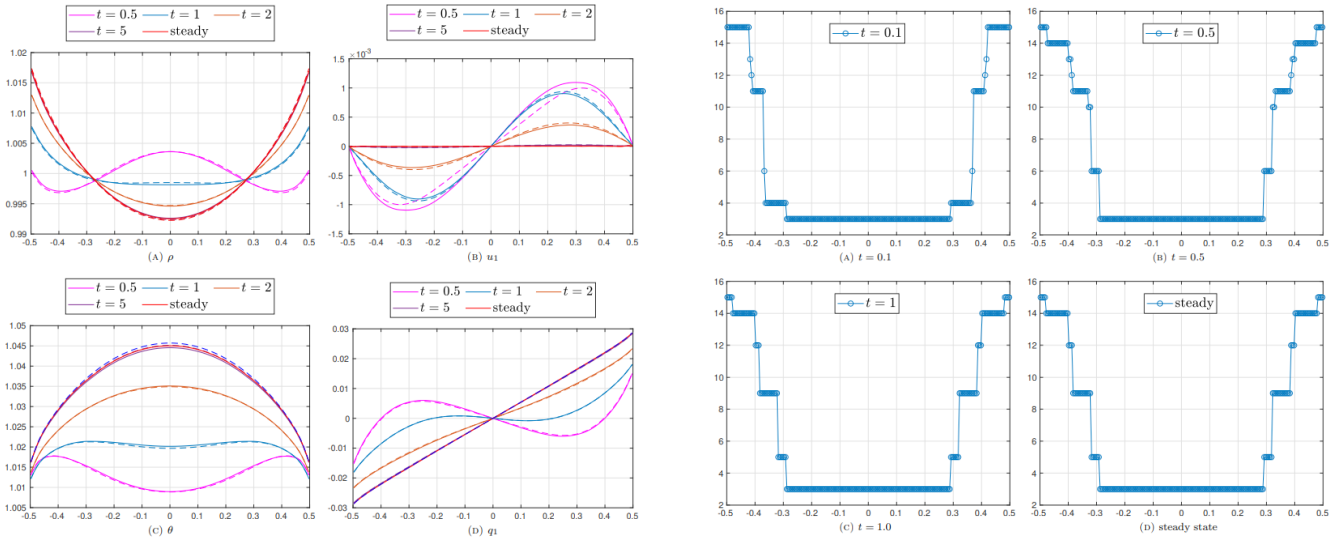
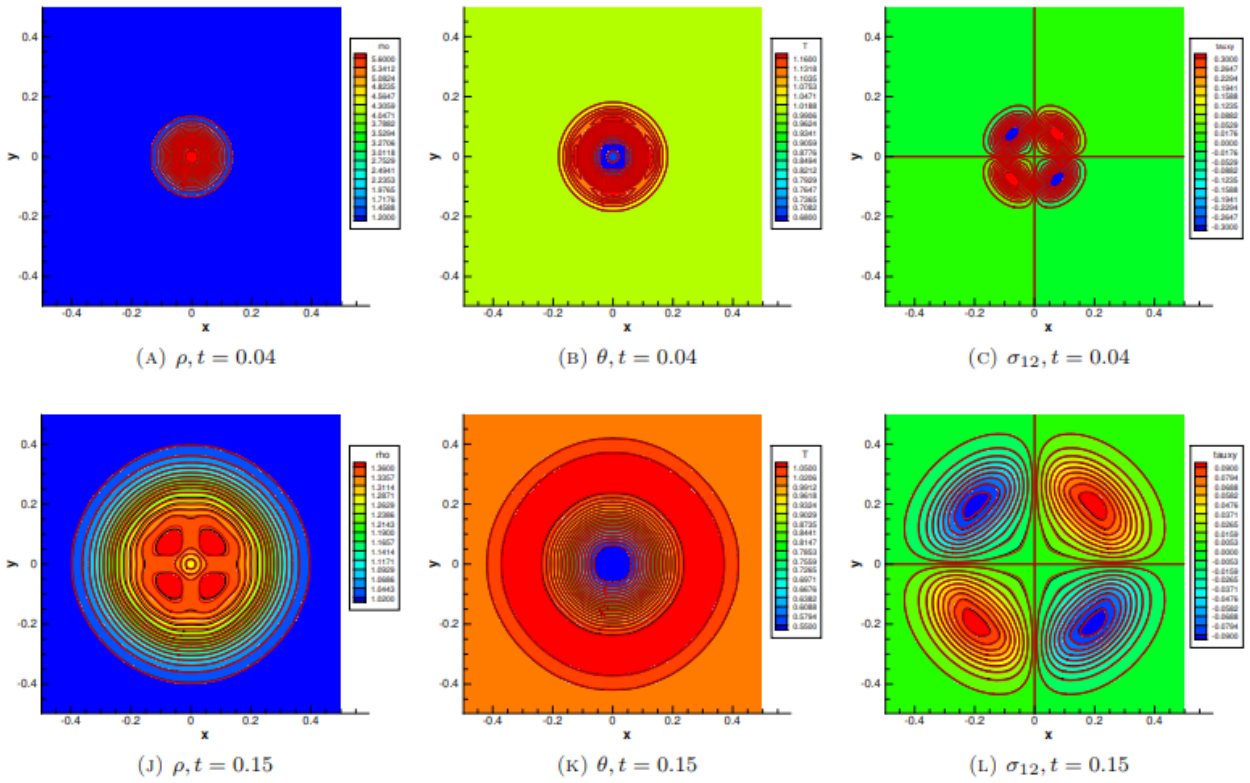


Fig. 1. Couette flow (left:Evolution of the numerical solution, right: change of M_0)



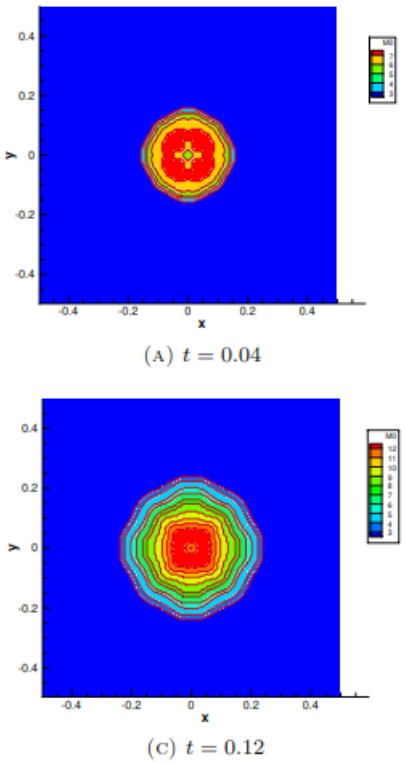
(A) $\rho, t = 0.04$ (B) $\theta, t = 0.04$ (C) $\sigma_{12}, t = 0.04$

(J) $\rho, t = 0.15$ (K) $\theta, t = 0.15$ (L) $\sigma_{12}, t = 0.15$

Fig. 2. Fluid diffusion (Numerical solution at different time)

3) 由于计算不同M0模型间误差的计算量为（M08），通过比较现有模型与更精确模型间误差来构造指示子方法也不适用。

由于这些困难，论文作者寻找非典型的估计方法来量化该误差。该工作的目标是通过比较小计算量来构建误差估计指示子，并在每个时间层的空间网格点上，自适应选择M0，达到平衡计算精度与减少计算量的效果。论文测试了1维Couette流与二维扩散问题等算例来检验该方法的有效性。(目前该文章发表于SISC, 44(2), 2022).



(A) $t = 0.04$

(C) $t = 0.12$

Fig. 3. Fluid diffusion (M_0 at different time)

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。

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.

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
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	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
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	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
12	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
13	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
14	管鹏飞	国家自然科学基金委员会	国际(地区)合作与交流项目	二维金属玻璃：从制备，物理力学性能到合金设计	2022-01 - 2025-12
15	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
16	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
17	Stefano Chesi	国家自然科学基金委员会	外国学者研究基金项目	Spin coherence and collective effects in solid-state quantum devices	2022-01 - 2023-12
18	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
19	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
20	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
21	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
22	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
23	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
24	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

续表

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	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
37	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

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
38	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
39	Martin Stynes	国家自然科学基金委员会	面上项目	分数阶导数问题α-鲁棒性数值方法构造与分析	2022-01 - 2025-12
40	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
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	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
49	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
50	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

续表

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
51	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
52	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
53	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
54	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
55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	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

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
64	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
65	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
66	邹　芬	国家自然科学基金委员会	理论物理专款	腔光力杂化系统中的动力学声子阻塞与N声子束辐射效应研究	2022-01 - 2022-12
67	景晓波	国家自然科学基金委员会	理论物理专款	介观尺度下细胞中液液相分离现象的非平衡态机理研究及数值模拟	2022-01 - 2022-12
68	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
69	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
70	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
71	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
72	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
73	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
74	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
75	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
76	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

续表

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
77	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
78	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
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	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
87	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
88	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

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	FROM AND TO 起始时间
89	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
90	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
91	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
92	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
93	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
94	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
95	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
96	赵志稳	中国博士后科学基金	面上二等资助	复合材料中的椭圆方程和方程组	2021-11 - 2023-11
97	蔡文涛	中国博士后科学基金	面上二等资助	变密度的不可压缩流体方程有限元解最大Lp正则性及其误差估计研究	2021-11 - 2023-11
98	陶　琪	中国博士后科学基金	面上二等资助	空间高阶导数方程局部间断有限元方法的后处理技术研究	2021-11 - 2023-11
99	邹　芬	中国博士后科学基金	面上二等资助	腔光力系统中的动力学声子阻塞与N声子束辐射效应研究	2021-11 - 2023-11
100	葛　磊	中国博士后科学基金	面上二等资助	光场自注入下太赫兹量子级联激光器光频梳动力学研究	2022-06 - 2024-06

2021-2022学术年期间，中心合计发表论文约423篇，其中归属中心（包括第一单位及通讯作者第一单位）论文208篇，其他合作论文215篇。

During the 2021-2022 academic year, CSRC has published a total of about 423 papers.

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4	DNA sequencing based on electronic tunneling in a gold nanogap: a first-principles study; Zou, Hao; Wen, Shizheng; Wu, Xiaoyan; Wong, Ka-Wai; Yam, ChiYung; PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 24, 9 (2022)
5	Numerical Approximations of Phase Field Models using a General Class of Linear Time-Integration Schemes; Chen, Lizhen; Zhang, Zengyan; Zhao, Jia; COMMUNICATIONS IN COMPUTATIONAL PHYSICS, 30, 5 (2021)
6	Solutions of Atomic and Molecular Schrodinger Equations with One-dimensional Function Approach; Sarwono, Yanoar Pribadi; Ur Rahman, Faiz; Zhao Rundong; Zhang Ruiqin; CHEMICAL JOURNAL OF CHINESE UNIVERSITIES-CHINESE, 42, 7 (2021)
7	Efficient SVV stabilized triangular spectral element methods for incompressible flows of high Reynolds numbers; Chen, Lizhen; Tang, Tao; Xu, Chuanju; ADVANCES IN AERODYNAMICS, 4, 1 (2022)

WORKSHOPS & CONFERENCES (2021-2022) 中心主办、合办的学术会议

时间 Date	会议名称 Title
2022.8.11-13	6th Conference on Numerical Methods for Fractional-derivative Problems 第六届分数导数问题数值方法会议
2022.8.4	Mini-Workshop on Applied and Computational Mathematics 应用与计算数学小型研讨会
2022.7.23-24	Computational and Applied Mathematics Workshop II 计算与应用数学研讨会II
2022.5.28-29	先生之风山高水长——纪念钱敏先生学术传承研讨会 Conference on academic inheritance in memory of Professor Min Qian
2022.5.28-29	Computational and Applied Mathematics Workshop I 计算与应用数学研讨会I
2022.4.27	多物理问题数值计算研讨会 Workshop on Numerical Computing for Multiple Physics Problems

TUTORIALS (2021-2022) 培训班

时间 Date	会议名称 Title
2021.11.15-18	扭转电子学(Twistronics)的实验进展及理论方法培训班
2021.10.17-20	“材料与能源前沿科学： 材料腐蚀热力学 与动材料腐蚀热力学”院内培训班

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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。2021-2022学术年期间中心共举办专题讲座147期（总1157期）

CSRC invites national and overseas leading researchers to give academic seminars. During academic year 2021-2022, CSRC has already held 147 seminars.

No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
1	2021-8-31	陈理想 Li-Xiang Chen	厦门大学 Xiamen University	Orbital Angular Momentum: Sorting, Sensing, Imaging, and Beyond
2	2021-9-16	芮洪兴 Hong-Xing Rui	山东大学 Shandong University	Stabilized Hybrid Mixed Element Method for Poroelasticity
3	2021-9-17	刘 峥 Zheng Liu	清华大学高等研究院 Institute for Advanced Study, Tsinghua University	Insights into frustrated magnets via first-principles hyperfine coupling calculation
4	2021-9-17	常 超 Chao CHANG	军科院国防创新院	太赫兹生物物理研究进展报告
5	2021-9-18	杨 宇 Yu Yang	北京应用物理与计算数学研究所 Institute of Applied Physics and Computational Mathematics	铀铌合金氢蚀的动力学蒙特卡罗模拟研究
6	2021-9-28	褚维斌 Weibin Chu	美国南加州大学 University of Southern California	能源材料中的激发态载流子动力学
7	2021-9-29	汪艳秋 Yan-Qiu Wang	南京师范大学 Nanjing Normal University	基于广义重心坐标的有限元离散
8	2021-10-12	李有泉 You-Quan Li	浙江大学 Zhejiang University	Nonabelian Ginzburg-Landau Theory for Ferroelectrics
9	2021-10-15	Georgios Akrivis	University of Ioannina	The energy technique for BDF methods
10	2021-10-15	陈 天 Tian Chen	北京理工大学 Beijing Institute of Technology	量子随机行走的拓扑现象及应用研究

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No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
11	2021-10-28	胡光辉 Guang-Hui Hu	澳门大学 University of Macau	Efficient computation in density functional theory
12	2021-11-3	张家军 Jia-Jun Zhang	中山大学 Sun Yat-sen University	三维基因组结构和基因表达的理论建模与机制
13	2021-11-4	焦　锋 Feng Jiao	广州大学 Guangzhou University	Approximating gene transcription dynamics using steady-state formulas
14	2021-11-9	刘铁钢 Tie-Gang Liu	北京航空航天大学 Beihang University	Characteristic-featured troubled-cell indicator for Conservation Laws based on Artificial Neural Network
15	2021-11-11	周　涛 Tao Zhou	中国科学院数学与系统科学研究院Academy of Mathematics and Systems Science, CAS	Normalizing field flow: solving forward and inverse stochastic differential equations using physics-informed flow model
16	2021-11-11	洪　柳 Liu Hong	中山大学 Sun Yat-sen University	随机动力学、大偏差理论和非平衡态热力学
17	2021-11-18	兰岳恒 Yue-Heng Lan	北京邮电大学 Beijing University of Posts and Tele communications	Reconstruction of nonlinear dynamics fro m noisy time series
18	2021-11-26	曾凡海 Fan-Hai Zeng	山东大学 Shandong University	Fast convolution quadrature for the fractional operators
19	2021-11-29	张　勇 Yong Zhang	天津大学 Tianjin University	A Spectrally Accurate Numerical Method For Computing The Bogoliubov-De Gennes Excitations Of Dipolar Bose-Einstein Condensates
20	2021-12-2	曲风龙 Feng-Long Qu	烟台大学 Yantai University	Mathematical theory and numerical methods for several kinds of scattering by complex obstacles
21	2021-12-2	张海 文Hai-Wen Zhang	中国科学院数学与系统科学研究院Academy of Mathematics and Systems Science, CAS	Direct and inverse elastic scattering by unbounded rough surfaces
22	2021-12-2	李建樑 Jian-Liang Li	长沙理工大学 Changsha University of Science and Technology	Inverse scattering for a random source/ potential

No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
23	2021-12-3	刘晓东 Xiao-Dong Liu	中国科学院数学与系统科学研究院Academy of Mathematics and Systems Science, CAS	Data completion algorithms and their applications in inverse acoustic scattering with limited-aperture backscattering data
24	2021-12-3	孟世旭	中国科学院数学与系统科学研究院Academy of Mathematics and Systems Science, CAS	Sampling methods in acoustic and electromagnetic waveguides
25	2021-12-6	沈　捷 Jie Shen	美国普渡大学 Purdue University	Positivity/bound preserving schemes for complex nonlinear systems
26	2021-12-7	雷锦志 Jin-Zhi Lei	天津工业大学 Tiangong University	异质性干细胞增殖的数学模型框架
27	2021-12-7	邹秀芬 Xiu-Fen Zou	武汉大学 Wuhan University	Data-driven Mathematical Modeling and Quantitative Analysis for Tumor Microenvironment
28	2021-12-8	刘可伋 Ke-Ji Liu	上海财经大学 Shanghai University of Finance and Economics	Inverse problems in a stratified ocean waveguide
29	2021-12-8	梁正良 Zheng-Liang Liang	北京化工大学 Beijing University of Chemical Technology	First-principles calculation in dark matter direct detection
30	2021-12-8	和建刚 Jian-Gang He	北京科技大学 University of Science and Technology Beijing	利用高通量密度泛函理论计算加速新型热电材料的发现
31	2021-12-9	李春贺 Chun-He Li	复旦大学 Fudan University	Landscape and flux in gene networks
32	2021-12-13	邱建贤 Jian-Xian Qiu	厦门大学 Xiamen University	A conservative semi-Lagrangian HWENO scheme for linear transport equations
33	2021-12-14	杨哲森 Zhesen Yang	中国科学院卡弗里理论科学研究所 The Institute of Theoretical Physics, CAS	非厄米趋肤效应和广义布里渊区理论
34	2021-12-15	沈　捷 Jie Shen	美国普渡大学 Purdue University	Some Recent Advances on the SAV Approach with Applications to Navier-Stokes and related equations

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35	2021-12-15	王坤坤 Kun-Kun Wang	安徽大学 Anhui University	利用单光子干涉仪模拟非厄米拓扑金属
36	2021-12-15	张　勇 Yong Zhang	北京邮电大学 Beijing University of Posts and Tele communications	基于金刚石NV色心的量子纠缠和量子计算
37	2021-12-16	满　怡 Yi Man	北京大学 Peking University	Synchronization in biological filaments
38	2021-12-17	李晓丽 Xiao-Li Li	山东大学 Shandong University	Error analysis and numerical simulations of high-precision algorithms for the Cahn-Hilliard-Navier-Stokes model
39	2021-12-17	Wei Yi	中国科学技术大学 University of Science and Technology of China	Cold Atoms and Quantum Simulation
40	2021-12-17	张　融 Rong Zhang	南京邮电大学 Nanjing University of Posts and Telecommunications	基于量子行走制备最大纠缠态
41	2021-12-23	孟　雄 Xiong Meng	哈尔滨工业大学 Harbin Institute of Technology	Superconvergence of the local discontinuous Galerkin method for 1D nonlinear convection-diffusion equations
42	2021-12-29	祁　宏 Hong Qi	山西大学 Shanxi University	钙信号调控细胞凋亡机制的动力学研究
43	2022-1-5	鲁汪涛 Wang-Tao Lu	浙江大学 Zhejiang University	PML and high-accuracy boundary integral equation solver for wave scattering by a locally defected periodic surface
44	2022-1-10	周　达 Da Zhou	厦门大学 Xiamen University	多细胞层次结构的一些数学模型
45	2022-1-11	陈景润 Jing-Run Chen	中国科学技术大学 University of Science and Technology of China	Second-order semi-implicit methods for Landau-Lifschitz equation
46	2022-1-13	吴怀志 Huai-Zhi Wu	福州大学 Fuzhou University	Cavity optomechanics with parametric amplification

No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
47	2022-1-17	楼　元 Yuan Lou	上海交通大学 Shanghai Jiao Tong University	On principal eigenvalues for time-periodic parabolic operators
48	2022-1-17	王　斌 Bin Wang	西安交通大学 Xi'an Jiaotong University	Structure-preserving methods for charged-particle dynamics in a strong magnetic field
49	2022-1-20	张　林 Lin Zhang	陕西师范大学 Shaanxi Normal University	Parametrically control of quantum state with spin
50	2022-1-20	孔　嘉 Jia Kong	杭州电子科技大学 Hangzhou Dianzi University	15万亿高温原子宏观纠缠态的制备与探测
51	2022-1-20	王　成 Cheng Wang	美国麻省大学达特茅斯分校 University of Massachusetts Dartmouth	A positivity preserving, energy stable finite difference scheme for the Flory-Huggins-Cahn-Hilliard-Navier-Stokes system
52	2022-1-24	杨志国 Zhi-Guo Yang	上海交通大学 Shanghai Jiao Tong University	The gPAV method and its error estimate for some dissipative systems
53	2022-2-7	张继伟 Ji-Wei Zhang	武汉大学 Wuhan University	Recent progress on variable-time-step schemes for subdiffusion and diffusion equations
54	2022-2-14	刘　洋 Yang Liu	内蒙古大学 Inner Mongolia University	On discrete energy dissipation of Maxwell's equations in a Cole-Cole dispersive medium
55	2022-2-16	何晓明 Xiaoming He	美国密苏里科学技术大学 Missouri University of Science and Technology	A decoupled, linear, and unconditionally energy stable finite element method for a two-phase ferrohydrodynamics model
56	2022-2-18	曹延昭 Yanzhao Cao	美国奥本大学 Auburn University	A Stochastic Neural Network for uncertainty quantification of deep neural networks
57	2022-2-21	刘海亮 Hailiang Liu	美国爱荷华州立大学 Iowa State University	Selection dynamics for deep neural networks
58	2022-2-25	鞠立力 Lili Ju	美国南卡罗莱纳大学 University of South Carolina	High-Order Multirate Explicit Time-Stepping Schemes for the Baroclinic-Barotropic Split Dynamics in Primitive Equations

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59	2022-3-1	汪　波 Bo Wang	湖南师范大学 Hunan Normal University	Fast multipole method in Layered media
60	2022-3-4	孙志忠 Zhi-Zhong Sun	东南大学 Southeast University	二维抛物方程交替方向隐格式解的无穷模估计
61	2022-3-4	王　东 Dong Wang	香港中文大学（深圳） The Chinese University of Hong Kong, Shenzhen	An efficient unconditionally stable method for Dirichlet partitions in arbitrary domains
62	2022-3-7	李继春 Jichun Li	美国内华达大学拉斯维加斯分校 University of Nevada Las Vegas (UNLV), USA	Finite element analysis and simulation for wave propagation in the Cole-Cole medium
63	2022-3-15	Ricardo H. Nochetto	美国马里兰大学帕克分校 University of Maryland, College Park, USA	Large Isometric Deformations and their L DG Approximation
64	2022-3-16	赵凯锋 Kai-Feng Zhao	复旦大学 Fudan University	Spin-noise spectrum of hot vapor atoms in an antirelaxation-coated cell
65	2022-3-18	王　宏 Hong Wang	美国南卡罗来纳大学 University of South Carolina	An optimal control of a variable-order fractional PDE
66	2022-3-21	张晓飞 Xiao-Fei Zhang	华中师范大学 Central China Normal University	Exploring Tumor Heterogeneity Based on Differential Graphical Models
67	2022-3-21	J. Markus Melenk	维也纳科技大学 Technische Universität Wien, Austria	Stability and convergence of Galerkin dis cretizations of the Helmholtz equation in piecewise smooth media
68	2022-3-22	宋永利 Yong-Li Song	杭州师范大学 Hangzhou Normal University	反应扩散方程的分支理论及斑图动力学
69	2022-3-23	孙启文 Qiwen Sun	广州大学 Guangzhou University	Stochastic gene transcription and its dynamical behavior
70	2022-3-24	张小鹏 Xiaopeng Zhang	南京大学 Nanjing University	Modeling on the mechanism of cellular re sponse to hypoxia

No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
71	2022-3-25	石东洋 ongyang Shi	郑州大学 Zhengzhou University	Quasi-uniform Error Estimates for the Fourth Order Singularly Perturbed Bi-wave Problem
72	2022-3-25	王　乾 Qian Wang	瑞士洛桑联邦理工学院 EPFL	Reduced-Order and High-Order Methods in Computational Fluid Dynamics
73	2022-3-28	蒋世东 Shidong Jiang	美国西蒙斯基金会Flatiron研究所 Flatiron Institute, Simons Foundation, USA	An overview of integral equation methods and fast algorithms
74	2022-3-28	王瑞琦 Ruiqi Wang	上海大学 Shanghai University	基于动力学摄动方法的生物网络分析
75	2022-3-28	盛长滔 Changtao Sheng	上海财经大学 Shanghai University of Finance and Economics	Efficient numerical methods for fractional PDEs and their applications to fractional Schrodinger eigenvalue problems
76	2022-3-29	楼　元 Yuan Lou	上海交通大学 Shanghai Jiao Tong University	Perthame-Souganidis model, Lei Model and beyond
77	2022-3-31	王海金 Haijin Wang	南京邮电大学 Nanjing University of Posts and Telecommunications	Some recent developments of IMEX-LDG methods
78	2022-4-1	龚新奇 Xin-Qi Gong	中国人民大学 Renmin University of China	设计新智能算法解决生物医学难题
79	2022-4-1	赵国焕 Guo-Huan Zhao	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	Stochastic flows for SDEs with singular drifts and their applications
80	2022-4-6	刘　锐 Rui Liu	华南理工大学 South China University Of Technology	基于高维数据的复杂生物系统临界状态预警方法
81	2022-4-6	李培森 Pei-Sen Li	北京理工大学 Beijing Institute of Technology	Exponential ergodicity of branching processes with immigration and competition
82	2022-4-6	李海刚 Haigang Li	北京师范大学 Beijing Normal University	Babuska Problem in Composite Materials and Suspension Problem in Stokes Flow

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83	2022-4-7	席福宝 Fu-Bao Xi	北京理工大学 Beijing Institute of Technology	Stabilization of state-dependent regime-switching processes by feedback control based on discrete time observations
84	2022-4-8	倪旭敏 Xu-Min Ni	北京交通大学 Beijing Jiaotong University	群体遗传学中的概率模型及其应用
85	2022-4-8	鲁兴业 Xing-Ye Lu	北京师范大学 Beijing Normal University	Spinon Fermi Surface Spin Liquid in a Triangular Lattice Antiferromagnet NaYbSe2
86	2022-4-8	仲杏慧 Xinghui Zhong	浙江大学 Zhejiang University	Compact WENO Limiters for Discontinuous Galerkin Methods
87	2022-4-10	庾建设 Jian-She Yu	广州大学 Guangzhou University	A General Periodic Discrete Model on Wolbachia Transmission Dynamics in Mosquito Populations
88	2022-4-11	李学志 Xue-Zhi Li	河南财政金融学院 Henan Finance University	Modeling and research on an immuno-epidemiological coupled system with coinfection
89	2022-4-12	朱　毅 Yi Zhu	清华大学 Tsinghua University	Three-fold Weyl points for the periodic Schrödinger operator
90	2022-4-14	刘桂荣 Gui-Rong Liu	山西大学 Shanxi University	Stochastic dynamics of an SIS epidemic on networks
91	2022-4-14	蒋建华 Jian-Hua Jiang	苏州大学 Soochow University	Seeing topological quantum effects in synthetic materials
92	2022-4-14	季　霞 Xia Ji	北京理工大学 Beijing Institute of Technology	Inverse acoustic scattering with phaseless far field data
93	2022-4-15	易　鸣 Ming Yi	中国地质大学（武汉） China University of Geosciences, Wuhan	蛋白质结构评估及微小RNA预测问题启发下的数据分析
94	2022-4-18	肖燕妮 Yanni Xiao	西安交通大学 Xi'an Jiaotong University	Modeling impacts of massive movements on COVID-19 epidemic
95	2022-4-19	黄启华 Qi-Hua Huang	西南大学 Southwest University	A hybrid parabolic and hyperbolic equation model for a population with separate dispersal and stationary stages: well-posedness and population persistence

No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
96	2022-4-20	帅建伟 Jian-Wei Shuai	厦门大学 Xiamen University	蛋白质质谱大数据深度学习分析
97	2022-4-20	刘胜强 Sheng-Qiang Liu	天津工业大学 Tiangong University	阶段结构资源-消费者动力模型研究
98	2022-4-20	王筱平 Xiaoping Wang	香港中文大学（深圳） Chinese University of Hong Kong, Shenzhen	Recent progress on topology optimization
99	2022-4-21	郎利君 Li-Jun Lang	华南师范大学 South China Normal University	Interplay of non-Hermiticity and topological states in quantum models
100	2022-4-21	刘茂省 Mao-Sheng Liu	中北大学 North University of China	网络传染病动力学建模分析及疾病最优控制
101	2022-4-25	郑小琪 Xiao-Qi Zheng	上海师范大学 Shanghai Normal University	围绕肿瘤纯度估计和肿瘤异质性分析的若干计算模型
102	2022-4-27	黄旻怡 Minyi Huang	浙江理工大学 Zhejiang Sci-Tech University	Some problems related to the dilation of PT-symmetric systems
103	2022-4-27	孙桂全 Gui-Quan Sun	中北大学 North University of China	干旱半干旱区域植被斑图动力学
104	2022-4-28	曹志兴 Zhi-Xing Cao	华东理工大学 East China University of Science and Technology	基于微分机器学习的基因表达建模与求解
105	2022-5-5	林聪萍 Cong-Ping Lin	华中科技大学 Huazhong University of Science and Technology	Domino-like transient dynamics at seizure onset in epilepsy
106	2022-5-5	曹外香 Waixiang Cao	北京师范大学 Beijing Normal University	A class of efficient Hamiltonian conservative spectral methods for Korteweg-de Vries equations
107	2022-5-5	付　培 Pei Fu	瑞典乌普萨拉大学 Uppsala University	High order cut discontinuous Galerkin methods for hyperbolic conservation laws
108	2022-5-6	陈华杰 Huajie Chen	北京师范大学 Beijing Normal University	Stability of the Minimal Energy Path

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109	2022-5-9	龚思宁 Sining Gong	美国布朗大学 Brown University	Convergence of Lagrange FEM for Maxwell Eigenvalue Problem in 3D
110	2022-5-9	徐礼虎 Li-Hu Xu	澳门大学 University of Macau	Approximation to stochastic variance reduced gradient Langevin algorithms by stochastic differential delay equations
111	2022-5-10	李国君 Guo-Jun Li	山东大学 Shandong University	重构基因组的新的组装算法
112	2022-5-10	徐　岩 Yan Xu	中国科学技术大学 University of Science and Technology of China	Structure-preserving finite volume arbitrary Lagrangian -Eulerian WENO schemes for the shallow water equations
113	2022-5-10	熊云丰 Yun-Feng Xiong	北京大学 Peking University	A characteristic-spectral-mixed scheme for six-dimensional Wigner-Coulomb dynamics
114	2022-5-11	夏银华 Yin-Hua Xia	中国科学技术大学 University of Science and Technology of China	A hybrid WENO scheme for steady-state simulations of Euler equations
115	2022-5-11	林支桂 Zhi-Gui Lin	扬州大学 YangzhouUniversity	早期四级应急响应和目前动态清零的模型分析
116	2022-5-12	郭瑞晗 Rui-Han Guo	郑州大学 Zhengzhou University	High order linearized spectral deferred correction methods based on low order time integration schemes for nonlinear PDEs
117	2022-5-12	崔景安 Jing-An Cui	北京建筑大学 Beijing University of Civil Engineering and Architecture	异质性传染病动力学模型与应用
118	2022-5-17	张本龚 Ben-Gong Zhang	武汉纺织大学 Wuhan Textile University	单细胞数据缺失值插补的若干问题研究
119	2022-5-17	潘　亮 Liang Pan	北京师范大学 Beijing Normal University	High-order gas-kinetic scheme for compressible flows
120	2022-5-18	李小舟 Xiaozhou Li	中国科学技术大学 University of Electronic Science and Technology of China	Filtering for Discontinuous Galerkin Method: Challenging the Assumption of Uniformity
121	2022-5-19	张　强 Qiang Zhang	南京大学 Nanjing University	Error estimate to smooth solutions of high order Runge–Kutta discontinuous Galerkin method for scalar nonlinear conservation laws with and without sonic points

No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
122	2022-5-20	卢键方 Jianfang Lu	华南理工大学 South China University of Technology	An inverse Lax-Wendroff procedure for finite difference schemes on the Cartesian mesh
123	2022-6-1	阮士贵 Shigui Ruan	美国迈阿密大学 University of Miami	The Influence of Human Behavior and Social Factors on the Spread of Infectious Diseases
124	2022-6-2	任景莉 Jing-Li Ren	郑州大学 Zhengzhou University	Short-to-medium range structure and glass-forming ability in metallic glasses
125	2022-6-6	陈　龙 Long Chen	美国加州大学欧文分校 University of California at Irvine	Immersed Virtual Element Methods for Interface Problems in Three Dimensions
126	2022-6-9	李茂枝 Mao-Zhi Li	中国人民大学 Renmin University of China	从拓扑的角度认识非晶无序结构中的序
127	2022-6-13	李　晓 Xiao Li	香港理工大学 Hong Kong Polytechnic University	Generalized SAV-exponential integrator schemes for Allen-Cahn type gradient flows
128	2022-6-13	张　倩 Qian Zhang	美国密歇根理工大学 Michigan Technological University	Nonconforming finite elements for the Brinkman problem and the quad-curl problem on cuboid meshes
129	2022-6-16	金瑜亮 Yu-Liang Jin	理论物理研究所 Institute of Theoretical Physics	无序中的对称性——从自旋玻璃相变到Gardner相变
130	2022-6-23	郭汝驰 Ruchi Guo	美国加利福尼亚大学 University of California	A Deep Direct Sampling Method for Geometric Inverse Problems
131	2022-6-23	鲁　振 Zhen Lu	中科院物理所 Institute of Physics, CAS	稳态非晶合金中局域类晶体序
132	2022-6-27	王士召 Shi-Zhao Wang	中国科学院力学研究所 Institute of Mechanics, CAS	流动噪声四极子声源的频域修正模型
133	2022-6-28	Yong-Liang Zhao	四川师范大学 Sichuan Normal University	A preconditioning technique for an all-at-once system from Volterra subdiffusion equations with graded time steps
134	2022-6-30	王　琦 Qi Wang	中国工程物理研究院材料研究所 China Academy of Engineering Physics	数据+机器学习：探索非晶结构性能关联的新范式

CSRC SEMINAR 专题报告

No.	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
135	2022-7-1	Yao Cheng	苏州科技大学 Suzhou University of Science and Technology	On the local discontinuous Galerkin method for singularly perturbed problems
136	2022-7-4	孙家昶 Jia-Chang Sun	中国科学院软件研究所 The Institute of Software, Chinese Academy of Sciences (ISCAS)	特征值计算中的几何网格因式分解算法
137	2022-7-7	马　恩 E. Ma	西安交通大学 Xi’an Jiaotong University	Local chemical order starting from chemical short-range order in high/medium entropy alloys
138	2022-7-11	周栋焯 Douglas Zhou	上海交通大学 Jiaotong University Shanghai	神经元网络连接结构的重构
139	2022-7-13	邱志鹏 Zhi-Peng Qiu	南京理工大学 Nanjing University of Science and Technology	Modeling the role of macrophages in HIV persistence during antiretroviral therapy
140	2022-7-14	张　勇 Yong Zhang	北京科技大学 University of Science &Technology Beijing	多元高熵非晶加工成形技术
141	2022-7-18	张　磊 Lei Zhang	北京大学 Peking University	Nucleation of Quasicrystals
142	2022-7-19	Rui-lian Du	常州大学 Changzhou University	A temporal second-order scheme for time fractional mixed diffusion and wave equation with an initial singularity
143	2022-7-21	姚永刚 Yong-Gang Yao	华中科技大学 Huazhong University of Science and Technology	多元高熵合金催化剂
144	2022-7-25	邓伟华 Weihua Deng	兰州大学 Lanzhou University	Generators and Feynmann-Kac operators for the time-changed strong Markov processes
145	2022-7-26	李方廷 Fangting Li	北京大学 Peking University	Nonlinear, stochastic effects and nonequilibrium in yeast cell-cycle process
146	2022-7-28	蒋虽合 Sui-He Jiang	北京科技大学 University of Science and Technology Beijing	Radiation tolerance of metallic materials strengthened by superlattice nanoprecipitates
147	2022-7-28	刘雪峰 Xuefeng Liu	日本新潟大学 Niigata University, Japan	特征值的形状最优化问题的计算机辅助数学证明方法

COLLOQUIUMS 百旺科学论坛

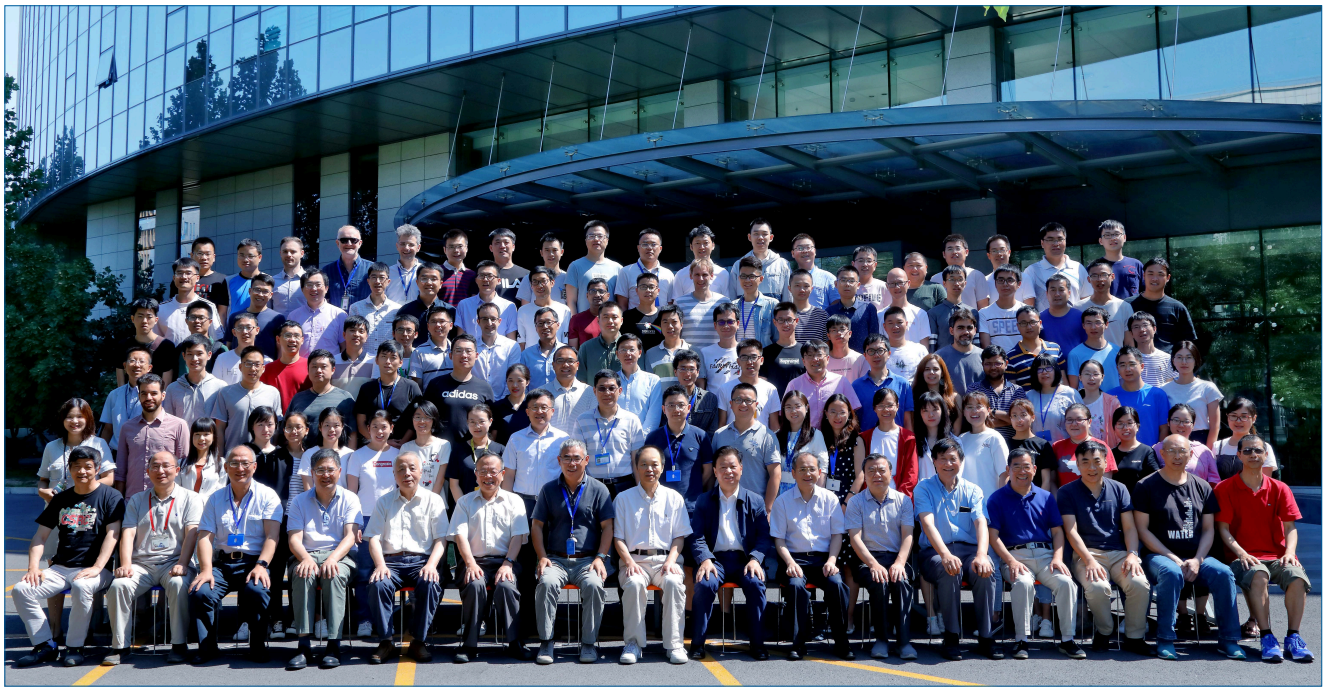
百旺科学论坛是由中物院研究生院、北京计算科学研究中心、北京高压科学研究中心联合举办的高端学术论坛。论坛组织邀请国内外优秀学者做前沿科学报告。论坛侧重于基础科学研究，致力于为广大科研工作者提供不同的视角，提供展示交流的平台，促进学科交叉相互启发，对重要的科学进展进行普及。自开展至今已举办六期。

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
- 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 1800 times. During the academic year 2021-2022, CSRC has hosted around 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。2021-2022学术年期间，中心接待来访学者约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。

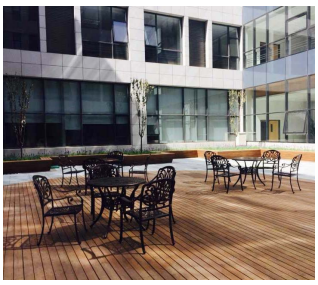
中心欢迎国内外各机构相关专业的科研人员和教师，以访问学者和客座研究人员的形式来访，进行短期或长期合作研究。中心也与同行们一起举办学术活动如会议、讲习班等。在中心访问期间，中心将提供一定的生活和住房补贴。

〖 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

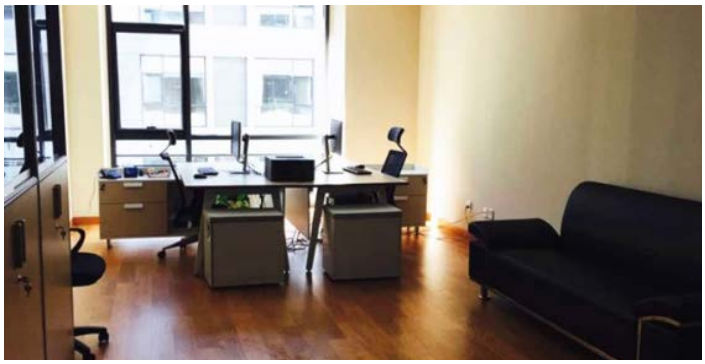


〖 学术报告厅 〗 Auditorium

Seminar Rom 〖 学术会议室 〗

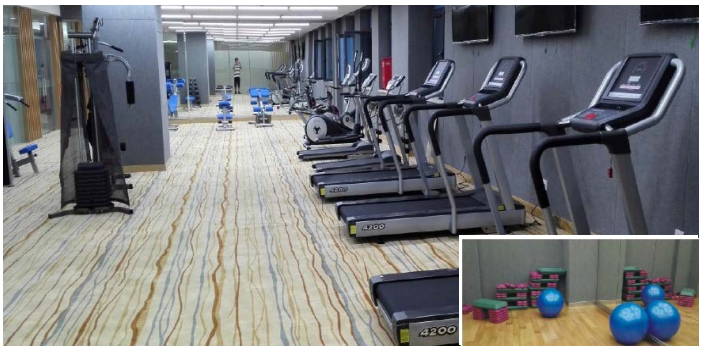
Common 〖 学术讨论区 〗

〖 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

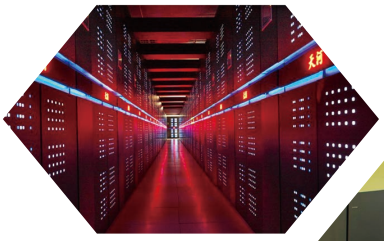
〖 餐厅 〗 Canteen

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