2024 - 2025 年度报告 ANNUAL REPORT

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本册所列所有信息为2024年8月1日至2025年7月31日学术年期间

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.

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 2025, CSRC has 27 faculty members, 2 engineers, 27 postdoctoral fellows and 95 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 192 papers, organized 2 academic conferences and workshops, 1 colloquium on scientific frontiers, and 49 CSRC seminars. CSRC has also forged partnerships with many prestigious universities and research institutes around the world.

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.

CSRC

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；

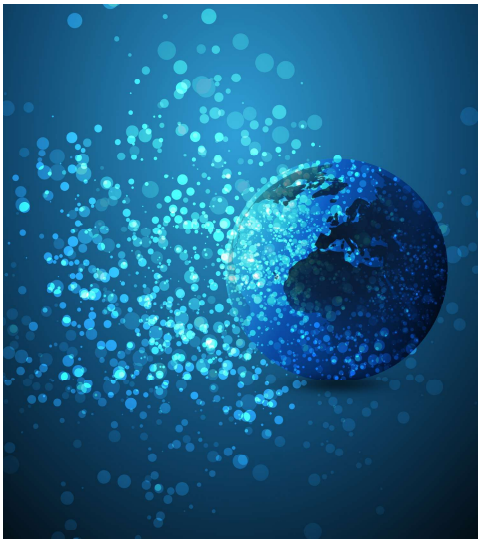
◇ 探索适于科研创新的管理体系，落实机制改革创新，提升我国科技自主创新能力，增强我国科技综合实力。

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。



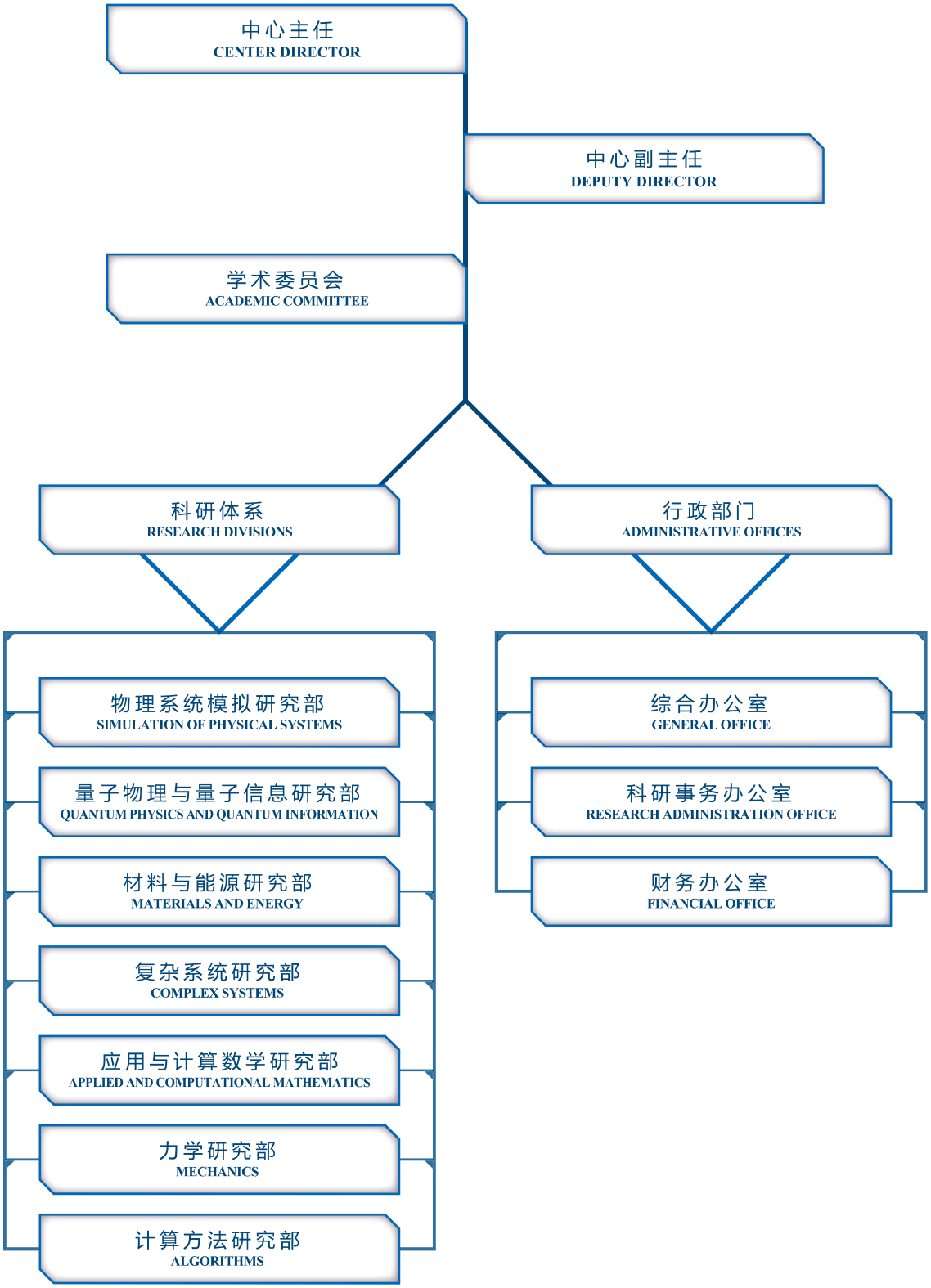
北京计算科学研究中心（以下简称中心）是隶属于中国工程物理研究院的独立法人单位，是以计算科学为牵引的多学科基础研究机构。中心成立于2009年8月。中心的定位是开展计算科学研究，促进科技发展，打造一个国际一流的开展计算科学及相关学科交叉研究的综合平台。

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2025年8月，中心的科研人才队伍包括10位讲座教授，3位教授，4位副教授，6位特聘研究员，1位研究副教授，3位特聘副研究员， 2位工程师和27位博士后。另外，中心还有博士/硕士研究生95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。

2024–2025学术年期间，中心公开发表国际学术论文192篇，主办合办国内外学术会议2场，举办科技前沿讲座1期，邀请学术报告49期，接待访问学者超过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。

ORGANIZATION 中心组织构架




CSRC
计算科学研究中心

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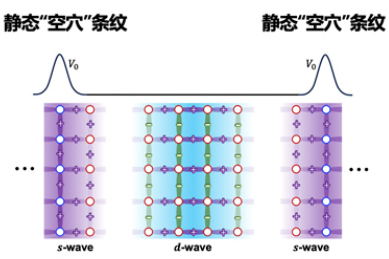
INVESTIGATION OF PAIRING SYMMETRY TRANSITION AND MICROSCOPIC PAIRING MECHANSIM IN HIGH-TEMPERATURE SUPERCONDUCTORS

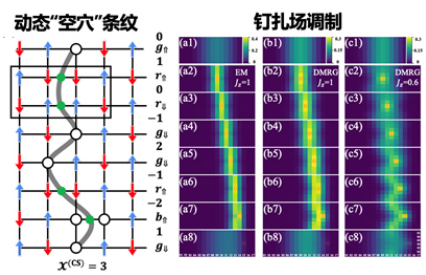
By Chao Chen, Peigeng Zhong, Xuelei Sui, Jialong Wang, Haiqing Lin, Shijie Hu, and Bing Huang

Charge stripes have been widely observed in various unconventional superconductors, exhibiting diverse periods and intensities. They are believed to play a crucial role in elucidating the mechanism of superconductivity, especially in cuprates. However, a comprehensive understanding of the interplay between charge stripes and superconducting properties remains exclusive. According to the early scenario proposed by Jan Zaanen, the charge-filled stripe phase (with one hole per unit cell of the charge order) can be regarded as interactive elastic quantum strings of holes, stabilized by π-phase shifts between neighboring magnetic domains. However, this scenario faces challenges in explaining electron pairing, as electron pairing requires the participation of hole pairs.

In the first work [1], we conducted large-scale unbiased numerical simulations on a general inhomogeneous Hubbard model and revealed that the period of static charge stripes—which varies across different real materials—can determine the pairing symmetry. By tuning the hole doping concentration and the amplitude of the charge stripes, we can trigger a transition from d-wave to s-wave pairing as well as a shift in magnetic correlations. In this process, the d-wave state transforms into a pairing-density wave state, which competes with the s-wave. These intriguing phenomena arise from the unusual behavior of stripe-induced selection rules for pairing symmetries within the stripe regions and between the stripes.

In the second work [2], we proposed a new effective model to describe the stripe phase in the hole-doped t-Jz model. Relative to the antiferromagnetic background, the model includes three types of color-labeled point defects coupled to an effective spin field, hence the name “colored string” model. Compared with the results from large-scale density matrix renormalization group simulations, we found semi-quantitative agreement in local hole density, magnetic moment, and the newly proposed spectral features of the effective spin field. By systematically analyzing the hole-density distribution and the scaling of the ground-state energy at different system sizes, we determined the effective core radius and the effective hopping amplitude of the quantum strings. We further demonstrated that the partially filled stripe phase (with fewer than one hole per unit cell of the charge order) can also be well described by the effective theory.





高温超导中配对对称性转变和配对微观机制的研究

陈超, 钟佩耕, 隋雪蕾, 汪嘉龙, 林海青, 胡时杰, 黄兵

电荷条纹在多种非常规超导体中已被广泛观察到，它们的周期和强度各异，被认为在阐明超导机制、尤其是在铜氧化物超导体中起着关键作用。然而，对于电荷条纹与超导性质之间相互作用的全面理解仍然不完整。根据 Jan Zaanen 早期的设想，充满电荷的条纹相(每个电荷序单元格有一个空穴)可以被视为空穴的相互作用弹性量子弦，这些量子弦通过相邻磁畴之间的 π 相位移动来稳定。然而，这一设想在解释电子配对方面存在挑战，因为电子配对需要空穴对参与。

在第一个工作中[1]，我们通过对一般非均匀 Hubbard 模型进行大规模无偏数值模拟，揭示了静态电荷条纹的周期（在不同实际材料系统中是可变的）能够决定配对对称性。通过调节空穴掺杂浓度和电荷条纹振幅，可以触发 d-s 波转变以及磁相关性的偏移，其中 d 波态转变为配对密度波态，并与 s 波竞争。这些有趣的现象源自条纹诱导的配对对称性选择规则在条纹区域和条纹间区域的异常行为。

在第二个工作中[2]，我们提出了一个新的有效模型，用于描述在空穴掺杂的 $t\text{-}J_z$ 模型中的条纹相。相对于反铁磁背景，该模型包含三种颜色标记的点缺陷与有效自旋场耦合，因此被称为“彩色弦”模型。与大规模密度矩阵重整化群数值模拟结果相比，我们在局部空穴密度、磁矩以及新提出的有效自旋场的谱特征方面发现了有效模型半定量的一致性。通过对不同系统尺寸下基态能量的标度分析以及空穴密度分布的系统分析，我们确定了量子弦的有效核心半径和有效跃迁振幅。我们进一步证明了部分填充的条纹相（每个电荷序单元格的空穴数少于一个）也可以通过有效理论很好地描述。

REFERENCES:

[1] Chao Chen, Peigeng Zhong, Xuelei Sui, Runyu Ma, Ying Liang, Shijie Hu,* Tianxing Ma,* Hai-Qing Lin, and Bing Huang,* Charge stripe manipulation of superconducting pairing symmetry transition, Nature Comm. 15, 9502 (2024).

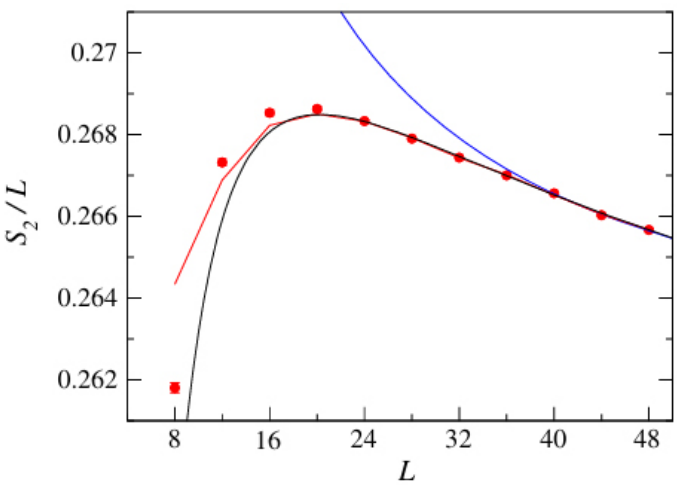
[2] Jialong Wang, Shijie Hu,* and Xuefeng Zhang, "Quantum colored strings in the hole-doped t-Jz model", Phys. Rev. B 111, 205121 (2025).

DIAGNOSING QUANTUM PHASE TRANSITION ORDER AND DECONFINED CRITICALITY VIA ENTANGLEMENT ENTROPY

By Zehui Deng, Lu Liu, Wenan Guo, and Hai-Qing Lin

Deconfined quantum criticality (DQC), describing continuous phase transition between two unrelated ordered states, is beyond the paradigm of Landau Ginzburg-Wilson. Sandvik invents the $J-Q_2$ model, realizing the valence-bond solid (VBS) to Néel transition in two-dimensional (2D) quantum spin systems. The model has no sign problem and, therefore, is amenable to quantum Monte Carlo (QMC) simulations. The $J-Q_3$ model, a variant of the $J-Q_2$ model, exhibits a similar VBS-Néel transition, with the VBS order enhanced in the VBS phase. Numerous QMC studies on these models have observed signatures of the DQC, with transitions appearing continuous. However, the conformal bootstrap calculation sets bounds on critical exponents. The exponents of the "continuous" VBS-Néel transitions do not satisfy the bounds, and thus alternative scenarios are suggested: the transition is described by a nonunitary conformal field theory (CFT) with complex fixed points, a multicriticality is involved, or it serves as a precursor to a weak first-order transition.

We study the scaling behavior of the Rényi entanglement entropy with smooth boundaries at the putative deconfined critical point separating the Néel antiferromagnetic and valence-bond-solid states of the two- dimensional $J-Q_3$ model. We observe a subleading logarithmic term with a coefficient indicating the presence of four Goldstone modes, signifying the presence of an $SO(5)$ symmetry at the transition point, which spontaneously breaks into an $O(4)$ symmetry in the thermodynamic limit. This result supports the conjecture that an $SO(5)$ symmetry emerges at the transition point, but reveals the transition to be weakly first-order. We demonstrate, through this Letter, a novel approach to detect emergent continuous symmetry and, more importantly, identify weakly first-order phase transitions efficiently, which have been notoriously challenging for conventional methods.



利用纠缠熵诊断量子相变的级和退禁闭临界性

邓泽辉, 刘录, 郭文安, 林海青

退禁闭量子临界性 (DQC) 一描述两种互不相关有序态之间的连续相变一超出了传统的Landau–Ginzburg–Wilson范式。Sandvik 提出了 $J-Q_2$ 模型，该模型在二维量子自旋系统中实现了从价键固体 (VBS) 相到 Néel 相的转变。该模型不存在符号问题，因此非常适合量子蒙特卡洛 (QMC) 模拟。其变体 $J-Q_3$ 模型表现出类似的 VBS–Néel 转变，但在 VBS 相中具有更强的 VBS 序。大量针对这些模型的 QMC 研究报告了与 DQC 相一致的特征，并且相变表现为连续的。然而，共形自举计算对临界指数给出了严格的界限，而这些“连续” VBS–Néel 转变的临界指数并不满足这些界限。这一差异促使研究者提出了几种可能的情景：相变可能由具有复定点的非幺正共形场论 (CFT) 描述，或者涉及多重临界性，抑或是弱一级相变的前兆。

在本工作中，我们研究了在二维 $J-Q_3$ 模型中 Néel 反铁磁态到 VBS 态的相变点处，具有光滑边界的 Rényi 纠缠熵的标度行为。我们观测到一个次级修正对数项，其系数对应于四个 Goldstone 模，表明在相变点出现了 $SO(5)$ 对称性，并在热力学极限下自发破缺为 $O(4)$ 对称性。该结果支持了在相变点涌现 $SO(5)$ 对称性的猜想，同时揭示了该相变是弱一级相变。我们的研究展示了一种探测涌现连续对称性的新方法，更重要的是，能够高效鉴别弱一级相变——这是传统方法长期面临的难题。

REFERENCES:

[1] Zehui Deng, Lu Liu, Wenan Guo*, and Hai-Qing Lin*, "Diagnosing Quantum Phase Transition Order and Deconfined Criticality via Entanglement Entropy, Physical Review Letters, 133. 100402.(2024).

SPIN FLUCTUATIONS IN THE DISSIPATIVE PHASE TRANSITIONS OF THE RABI MODEL

By Jiahui Li, Rosario Fazio, Yingdan Wang, and Stefano Chesi

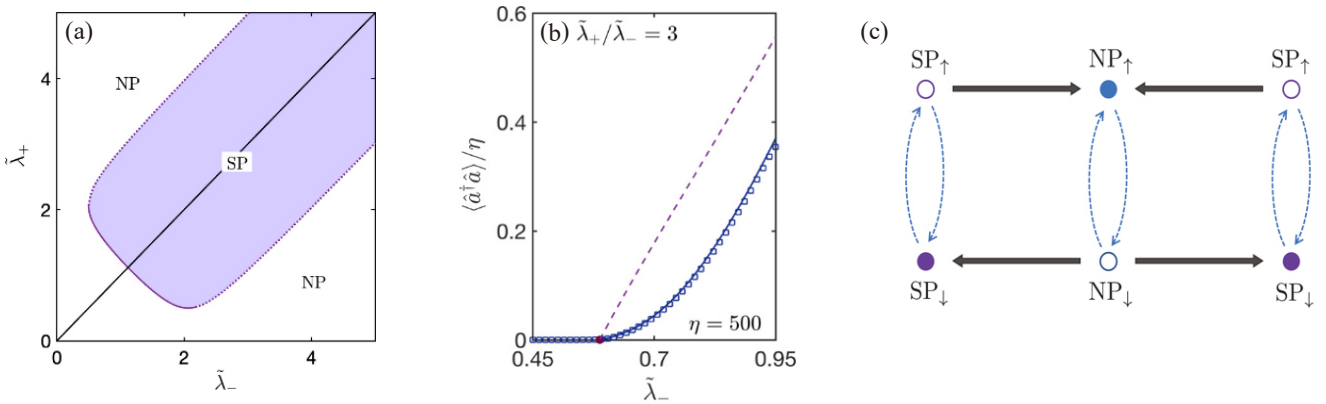


Fig. (a) Phase diagram of the system. (b) The numbers of photons (solid curve) is strongly reduced with respect to the case without fluctuations (dashed curve). (c) Transition processes between normal (NP) and superradiant (SP) states, giving a significant population in the excited NP state.

The quantum phase transition of the Rabi model occurs, remarkably, for a single qubit (or spin-1/2 system) interacting with a cavity mode. It has been widely studied, as it represents a minimal setting to explore few-body critical phenomena. The critical point between normal and superradiant phases is also very valuable for quantum metrology.

In a recent work [1], Prof. Stefano Chesi of CSRC and his former postdoc Prof. Jiahui Li (Henan University), together with Prof. Yingdan Wang (Institute of Theoretical Physics, CAS) and Prof. Rosario Fazio (ICTP, Italy), have analyzed in detail the effect of photon leakage on the critical behavior. This mechanism is naturally present in realistic setups and, as it turns out, has dramatic effects on the properties of the system. It induces large fluctuations of the two-level system, which can lead to an infinite- or even negative-temperature state. These spin fluctuations suppress the photon number in the superradiant phase and prevent the formation of a tri-stable phase predicted by mean-field theory.

The techniques developed in this work, as well as the tendency of forming extreme nonequilibrium states in the single-spin system, are expected to have general relevance in the study of dissipative phase transitions of few-body systems.

拉比模型耗散超辐射相变中的自旋涨落效应

李佳慧, Rosario Fazio, 王颖丹, **Stefano Chesi**

拉比模型的量子相变具有一个显著特点：仅需单个量子比特（或自旋-1/2系统）与一个腔模相互作用即可发生。该体系作为探索少体临界现象的最小化平台已被广泛研究。特别值得关注的是，其正常相与超辐射相之间的临界点在量子精密测量领域具有重要价值。

◀ 图 (a)系统的相图; (b)相比于无耗散的系统(虚线), 有耗散的系统中的光子数(实线)明显减少; (c)系统的状态在普通态和超辐射态之间的跃迁过程, 系统有很大的几率处在自旋向上的普通态。

在近期工作[1]中，北京计算科学研究中心的 Stefano Chesi 教授及其前博士后李佳慧博士（现任职于河南大学），以及王颖丹教授（中国科学院理论物理研究所）、Rosario Fazio 教授（国际理论物理研究中心，意大利），详细分析了腔中光子泄露对系统临界行为的影响。这种耗散机制普遍存在于实际实验装置中，并会对系统性质产生深远影响：它诱发了两能级系统的剧烈量子涨落，可能导致系统达到无限温度态甚至负温度态。这些自旋涨落显著抑制了超辐射相中的光子数，并阻止了平均场理论所预言的三稳态的形成。

本工作中使用的研究方法，以及单自旋系统中形成极端非平衡态的倾向，对少体系统的耗散相变研究具有普遍意义。

REFERENCES:

[1] J. Li, R. Fazio, Y. Wang, and **S. Chesi**, Phys. Rev. Res. 6, 043250 (2024) .

EXPERIMENTAL REVIVAL OF AN UNKNOWN STATE FROM THE PAST IN QUANTUM WALKS

By Bingzi Huo, Dengke Qu, Quan Lin, Gaoyan Zhu, Lei Xiao, Xiang Zhan, and Peng Xue

The physical process in the macroscopic world unfolds along a single time direction, while the evolution of a quantum system is reversible in principle. How to recover a quantum system to its past state is a complex issue of both fundamental and practical interests. In this article, we experimentally demonstrate a novel method for recovering the state in quantum walks (QWs), also known as full-state revival. Moreover, we observe two other important phenomena in QWs, recurrence and periodicity, via simplifying and repeatedly implementing the scheme, respectively. Our experiments show that obtaining these phenomena requires neither any information of the initial state nor full information of the coin operations. Our work sheds new light on quantum state engineering and recovery, and the initialization of quantum devices based on QWs.

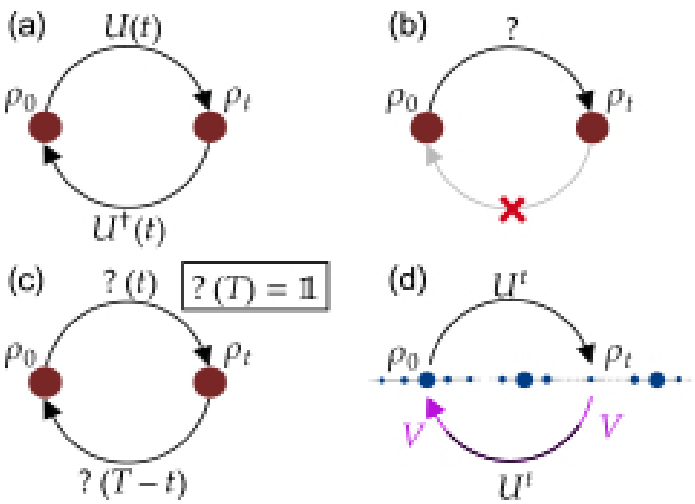


Fig. 1 Illustration of recovery of the initial state ρ0 of a QW after the t-step evolution.

量子行走中未知历史态的实验性复苏

霍丙子，曲登科，林泉，朱高岩石，肖磊，詹翔，薛鹏

宏观世界中的物理过程沿单一时间方向展开，而量子系统的演化在原理上是可逆的。如何使量子系统恢复至过去状态，是一个兼具基础研究价值与实际意义的前沿课题。本文通过实验展示了一种在量子行走中实现状态恢复（即全态复苏）的新方法。此外，我们分别通过方案简化和重复实施，观测到量子行走中另外两个重要现象——状态递归与周期演化。实验表明，实现这些现象既不需要初始状态的任何先验信息，也无需完全掌握硬币操作的全部信息。本研究为基于量子行走的量子态工程、状态恢复及量子设备初始化提供了新思路。

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FREQUENCY SHIFT CAUSED BY NONUNIFORM FIELD AND BOUNDARY RELAXATION IN MAGNETIC RESONANCE AND COMAGNETOMETERS

By Xiangdong Zhang, Jinbo Hu, Da-Wu Xiao & Nan Zhao

In magnetic resonance experiments, it is widely recognized that a nonuniform magnetic field can lead to an increase in the resonance line width, as well as a reduction in sensitivity and spectral resolution. However, a nonuniform magnetic field can also cause shifts in resonance frequency, which has received far less attention. The group led by Prof. Nan Zhao investigated the frequency shift caused by boundary relaxation and nonuniform magnetic field with arbitrary spatial distribution. They find that this frequency shift is spin-species dependent, implying a systematic error in NMR gyroscopes and comagnetometers. The first order correction to this systematic error is proportional to the difference of boundary relaxation rate, and dominates for small cells. In contrast, the third and higher order corrections arise from the difference of gyromagnetic ratios of spin species, and dominates for large cells. This insight helps understanding the unexplained isotope shifts in recent NMR gyroscopes and new physics searching experiments that utilize comagnetometers. Finally, They propose a tool for wall interaction research based on the frequency shift's dependency on boundary relaxation.

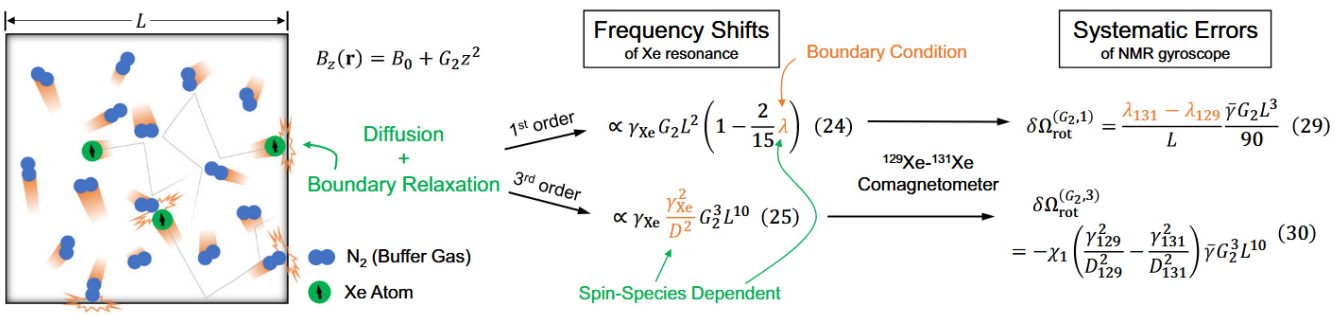

Fig. 1 Cartoon of the frequency shift mechanism.

非均匀场和边界弛豫在磁共振与共磁力计中引起的频移

张祥栋，胡锦波，肖大武，赵楠

在磁共振实验中，非均匀磁场会导致共振线宽增加、灵敏度与谱分辨率下降已是共识，但其引发的共振频移却长期被忽视。赵楠教授团队系统研究了任意空间分布的非均匀场与边界弛豫共同导致的频移效应，发现该频移具有自旋种类依赖性，会为核磁陀螺仪和共磁力计引入系统误差。研究揭示：对于小尺寸气室，系统误差的一阶修正项与边界弛豫率差值成正比；对较大尺寸而言，三阶及以上修正项（源于不同自旋种类的旋磁比差异）则起主导作用。这一发现不仅解释了近期核磁陀螺仪中未解的同位素频移现象，也对基于共磁力计的新物理搜索实验具有启示意义。最后，团队基于频移对边界弛豫的依赖特性，提出了一种新型器壁相互作用研究工具。

◀ 图 1 频移机制示意图。

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DRESSED MAJORANA FERMION IN A HYBRID NANOWIRE

By Guo-Jian Qiao, Xin. Yue, and C. P. Sun

Realizing Majorana fermions in condensed matter systems is the foundation of topological quantum computing. In recent years, experimental evidence supporting the existence of Majorana fermions has been reported successively. However, the key data in these studies have sparked widespread controversy, even leading to the retraction of many experimental papers. Since 2013, Chang-Pu Sun's team has been dedicated to research in this field and conducted a systematic analysis of the physical issues related to the "retraction incidents" [1, 2, 3]. Recently, they proposed a holistic theoretical approach that treats electrons in the nanowire and quasi-excitations in the superconductor on an equal footing to define Majorana fermions [4]. By the original definition of Majorana fermion—its antiparticle is own itself, this theory defines the "Dressed Majorana Fermion", that is the quasi-excitations of the entire hybrid system satisfy $\eta = \eta^{\dagger}$. From this, it directly determines the analytical conditions for the existence of Majorana fermions (topological phase). This topological phase diagram (the purple region in Fig. 1) depends not only on the chemical potential and magnetic field in the nanowire, but also on those in the superconductor. Since this approach is non-perturbative, the obtained results are valid for any strength of proximity tunneling and magnetic field. The work not only reveals why Majorana fermions—the "angel particles"—cannot be observed in nanowire-superconductor hybrid systems at present, but also points out the precise conditions for realizing Majorana fermion in the future.

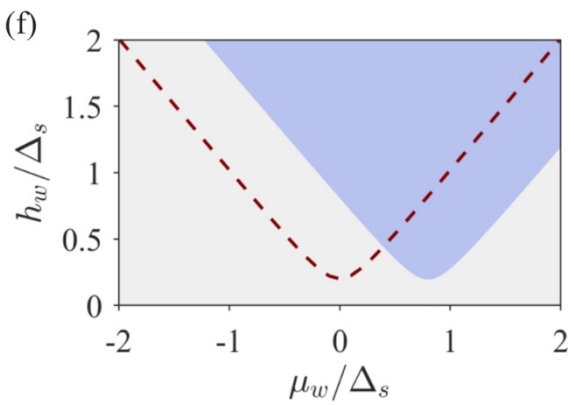

Fig. 1 In the space of the chemical potential and Zeeman energy, the more general topological phase (the light purple region) deviates from the phase diagram predicted by the low-energy theory (the red dashed line). For InSb-Al and InAs-Al hybrid systems, the shift of the chemical potential in the nanowire reaches the order of 1eV.

纳米线异质系统中“盛装”马约拉纳费米子

乔国健，岳鑫，孙昌璞

在凝聚态系统中，实现 Majorana 费米子是拓扑量子计算的基础。近年来，支持 Majorana 费米子存在的实验信号相继被报道。然而，这些研究中的关键数据引发了广泛争议，甚至导致许多发表在顶级期刊上的实验研究文章被撤稿。自 2013 年起，孙昌璞院士团队一直致力于该领域的研究, 并对“撤稿事件”相关物理问题进行了系统的分析[1,2,3]。最近，他们提出了一种整体理论方法—即平等地处理纳米线中的电子和超导体激发来定义马约拉纳费米子[4]。该理论基于马约拉纳粒子原始的定义—粒子与其反粒子相同，定义了“盛装马约拉纳费米子”（Dressed Majorana Fermion），即整个异质系统的准激发满足 $\eta = \eta^{\dagger}$。由此直接确定了 Majorana 费米子存在的精确解析条件（拓扑相）。其拓扑相图（图1中紫色区域）不仅取决于纳米线中的化学势和磁场，还与超导化学势和磁场有关。这个方法是非微扰的，因此得到的结果适用于任何近邻隧穿强度和任何磁场强度。该文不仅揭示了目前在纳米线-超导复合系统中观察不到 Majorana 费米子—“天使粒子”的原因，还指出了未来实现 Majorana 费米子的精确条件，从而在理论上回答了“天使粒子”何以存在的关键问题。

◀ 图 1 在 $\mu_w - h_w$ 空间中，更一般的拓扑相（浅紫色区域）的化学势偏离了低能理论所预测的相图（红色虚线）。对于实际的 InSb-Al 和 InAs-Al 异质系统，纳米线中化学势的偏移达 1eV 的量级。

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RECENT PROGRESS ON PHOTOINDUCED PHASE TRANSITIONS IN MATERIALS FROM FIRST-PRINCIPLES CALCULATIONS

By Yirui Lu, Yang Li*, and Bing Huang*

The interplay between light and matter is a crucial field in condensed matter physics, which not only gives rise to numerous fascinating physical phenomena, but also provides the physical foundations for the development of many modern technologies. When light interacts with a material, it can excite the electrons within a few femtoseconds. These excited electrons drive the system into non-equilibrium states through various mechanisms, including electron-electron interactions, electron-phonon coupling, phonon-phonon scattering and spin-orbit coupling effects. In the evolutionary process from the non-equilibrium state to the equilibrium state, the properties of the material undergo dramatic changes, leading to phase transitions in its electronic, crystal and magnetic structures. Because the manipulations of material properties using optical techniques are of great significance for developing advanced technologies, extensively efforts have been paid for exploring the physical mechanisms of photoinduced phase transitions.

In this review, we summarize the recent progress in the study of photoinduced phase transitions using real-time time-dependent density functional theory calculations. We first review the photoinduced phase transitions of electronic structure after photoexcitation, such as the insulator-to-metal transition and the melting of charge order in charge density wave systems. Subsequently, the redistribution of charge density induced by electron excitation generates forces on the atoms, potentially leading to ultrafast laser melting or structural transition of crystal. The amplitude and distribution of forces determine the features of atomic motions. In addition, we discuss the phonon excitation during structural phase transitions, such as the sequential phonon excitation at different steps of the transitions and the specific phonon excitation contributing to particular phase transitions. Furthermore, we introduce the self-amplification effect caused by the synergy between carrier relaxation and lattice deformation during structural phase transitions. Moreover, we also address the responses of the magnetic properties in materials stimulated by an external optical field, such as photoinduced magnetization, photoinduced demagnetization and ferromagnetic magnetic states induced by spin transfer. Finally, we offer some perspective on the future development of this active field.

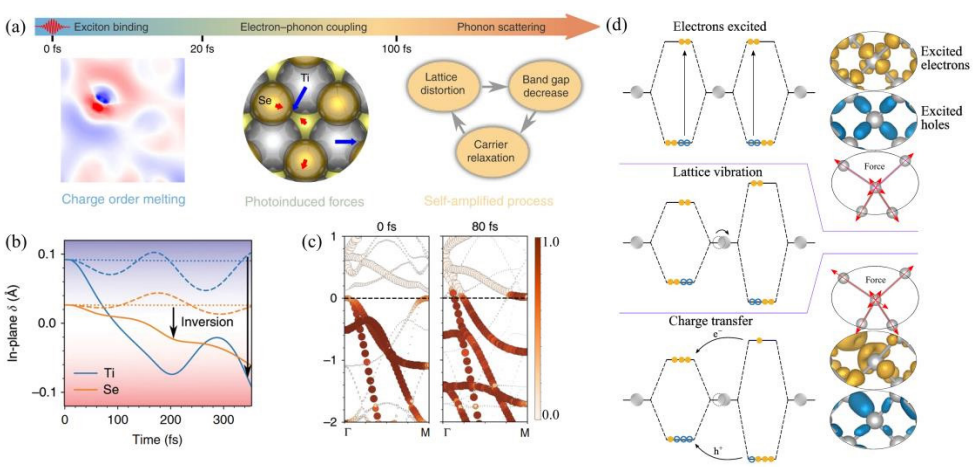

Fig. 1 Schematic diagram of the photoinduced phase transitions in 1T-TiSe2 and in crystalline silicon.

基于第一性原理计算的材料光诱导相变研究进展

芦一瑞，李阳*，黄兵*

光与物质的相互作用是凝聚态物理的重要研究领域，它不仅孕育了诸多的物理现象，也为许多现代技术的发展奠定了物理基础。当光与材料相互作用时，可以在飞秒时间尺度内激发电子。这些被激发的电子通过多种机制（包括电子–电子相互作用、电子–声子耦合、声子–声子散射以及自旋–轨道耦合效应）驱动体系进入非平衡态。在体系从非平衡态演化回平衡态的过程中，材料性质会发生显著变化，从而引发其电子结构、晶体结构和磁结构的相变。由于利用光学技术调控材料性质对于先进技术的发展具有重要意义，因此研究光诱导相变的物理机制已成为一个备受关注的课题。

本综述总结了利用实时含时密度泛函理论（RT-TDDFT）研究光诱导相变的最新进展。我们首先回顾了光激发后电子结构的相变过程，例如绝缘体–金属转变以及电荷密度波体系中的电荷有序融化。随后，我们讨论了电子激发引起的电荷密度重新分布如何在原子上产生作用力，并可能导致超快激光熔化或晶体结构转变。其中，作用力的幅值与分布决定了原子运动的特征。此外，我们探讨了结构相变过程中的声子激发，包括相变不同阶段的连续声子激发以及特定声子模式在特定相变中的作用。进一步地，我们介绍了在结构相变中，由载流子弛豫与晶格畸变协同作用引发的自放大效应。此外，我们还讨论了外部光场激发下材料磁性性质的响应，例如光诱导磁化、光诱导退磁化以及由自旋转移引起的铁磁态。最后，我们对这一快速发展的领域未来的研究方向提出了展望。

◀ 图 1 1T-TiSe 和晶体硅中光诱导相变的示意图。

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CORRELATED DIRAC FERMIONS IN TWISTED BILAYERS OF MOS_2

By Jun Kang*

Artificial honeycomb lattices are essential for understanding exotic quantum phenomena arising from the interplay between Dirac physics and electron correlation. This work shows that the top two moiré valence bands in rhombohedral-stacked twisted MoS_2 bilayers (tb-MoS_2) form a honeycomb lattice with massless Dirac fermions. The hopping and Coulomb interaction parameters are explicitly determined based on large-scale ab initio calculations. The system exhibits significant nonlocal Coulomb repulsion and can be described by the extended Hubbard model. At half-filling, strong Coulomb repulsion in freestanding tb-MoS_2 drives the system away from the semimetal phase, resulting in strongly correlated Dirac fermions. By varying the twist angle and dielectric environment, the Hamiltonian parameters can be tuned in a wide range, enabling transitions between distinct quantum phases. The high tunability makes tb-MoS_2 a promising simulator for exploring many-body effects of Dirac fermions.

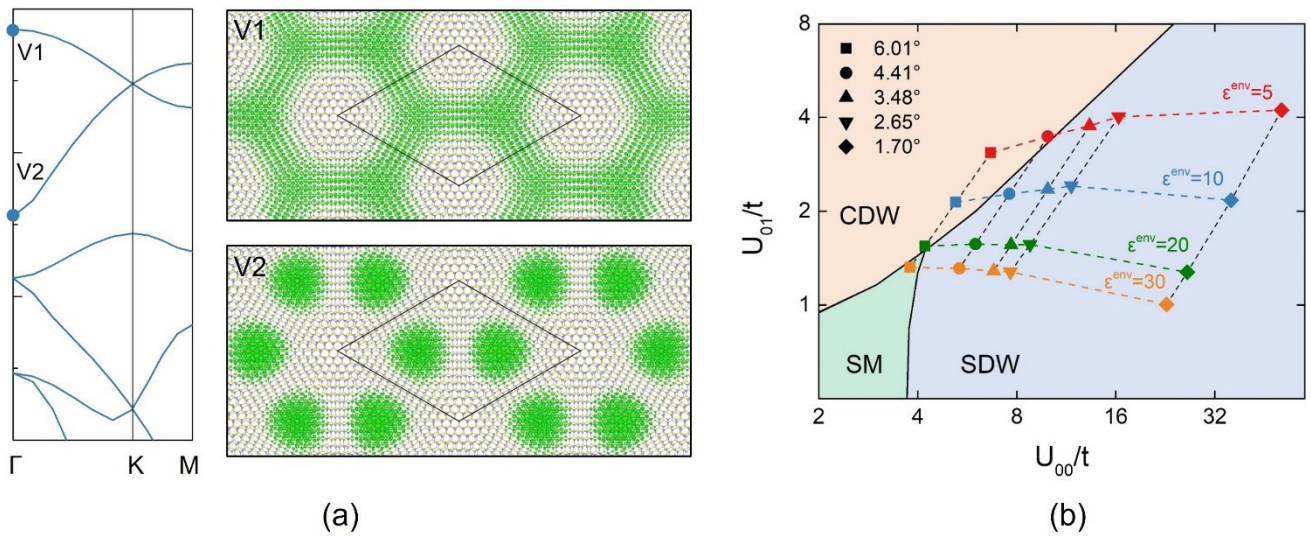

Fig. 1 (a) The moiré valence bands in twisted bilayer MoS_2. The top two bands exhibit Dirac cone dispersion. (b) Tuning correlation strength in twisted bilayer MoS_2 through twist angles and dielectric environments.

转角双层 MoS_2 中的强关联狄拉克费米子

康俊*

基于六角晶格上的哈伯德模型，人们预测许多强关联效应导致的狄拉克费米子体系中的新奇物相。石墨烯中存在狄拉克费米子，但其中的电子关联效应强度有限，难以呈现强关联物相。因此，如何在真实体系中实现具有强关联效应的狄拉克费米子，长期以来吸引着极大关注。我们通过大规模第一性原理计算发现，通过堆积方式的设计，在转角双层 MoS_2 莫尔超晶格中针对空穴可实现六角蜂窝排布的超晶格势阱，进而导致线性能量色散关系和狄拉克费米子的产生。通过对格点内和格点间库伦排斥作用的分析，发现库伦作用将远大于格点间的跃迁强度，因此体系中的狄拉克费米子具有强关联效应，在真空中体系将处于莫特绝缘态，而非半金属态。通过改变层间转角以及介电环境可实现对库伦能和跃迁强度的调控，进而引发体系在各类强关联物相间的转变，如从电荷密度波转变至自旋密度波。这些结果表明 MoS_2 莫尔超晶格将会是一个研究狄拉克费米子强关联效应的理想平台。

◀ 图 1 （a）转角双层 MoS_2 中的莫尔价带。最高的两条价带呈现狄拉克色散。（b）通过调节转角和介电环境改变转角双层 MoS_2 中的关联强度。

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QUANTUM EMISSION FROM COUPLED SPIN PAIRS IN HEXAGONAL BORON NITRIDE

By Song Li*, Anton Pershin & Adam Gali*

Optically addressable defect qubits in wide band gap materials are favorable candidates for room-temperature quantum information processing. Two-dimensional hexagonal boron nitride (hBN) is an attractive solid-state platform with great potential for hosting bright quantum emitters and quantum memories, leveraging the advantages of two-dimensional materials for scalable preparation of defect qubits. Although room-temperature bright defect qubits have been recently reported in hBN, their microscopic origin, the nature of the optical transition, and the optically detected magnetic resonance (ODMR) have remained elusive.

One major challenge is the identification of the exact defect structures responsible for SPEs and single-spin ODMR centers, which is a prerequisite for realizing deterministic formation and control. The observed photoluminescence (PL) spectra exhibit varying ZPL energies and phonon sidebands (PSBs), and many show similar optical lineshapes. These emissions may originate from various defects, but the similarities in optical lineshape imply the presence of common defect types in diverse crystalline environments.

An S = 1/2 paramagnetic defect with strong hyperfine interaction involving two equivalent nitrogen nuclei has been observed by electron paramagnetic resonance (EPR), and we assigned this signal to the negatively charged ONVB defect—i.e., oxygen substituting nitrogen adjacent to a boron vacancy—based on excellent agreement between experimental and simulated EPR spectra [1]. Notably, the existence of the ONVB defect was confirmed by subsequent annular dark-field scanning transmission electron microscopy (ADF-STEM) measurements. In addition, carbon and oxygen substitutions were simultaneously observed nearby using the same technique. This provides strong evidence that the extra charge on the ONVB defect giving rise to the EPR signal could originate from donor-like substitutions of boron by carbon (CB) or nitrogen by oxygen (ON). In other words, CB or ON may form donor-acceptor pairs (DAPs) with ONVB, where the S = 1/2 spin state arises from spin density localized around the ONVB component of the DAP. In this sense, the common defect type is the ONVB acceptor, while the variation in optical properties is governed by the type and position of the donor partner.

We perform comprehensive theoretical calculations on the optical properties of DAPs with varying separation distances. We find that the donor (CB and ON) indeed donates an electron to the ONVB defect, rendering it negatively charged. The donor-acceptor distance significantly influences the electronic structure, offering a possible explanation for the ZPL variation observed in experiments. We show that the ON–ONVB DAP is photostable, with quantum yields comparable to those of the isolated negatively charged ONVB. In contrast, the CB–ONVB pair exhibits metastable dim states at certain separations, which act as non-radiative decay pathways. Spin-flipping within these dim states can mix doublet and quartet multiplets, leading to spin polarization in the S = 1/2 ground state of the negatively charged ONVB when external magnetic fields lift the Kramers degeneracy. As a consequence, ODMR spectrum24 may arise from the CB–ONVB defect pair in the S = 1/2 ground state when subjected to a constant magnetic field [2].

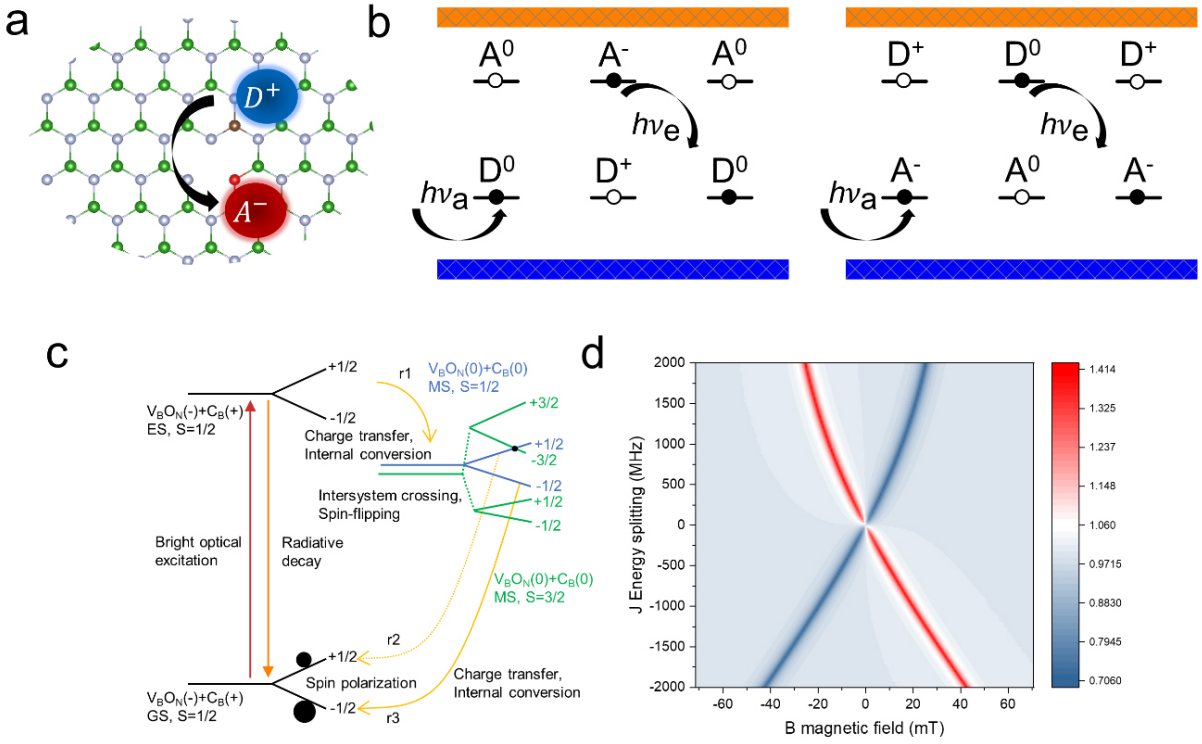

Fig. 1 **a)** The donor-acceptor model with oxygen and carbon impurities in hBN. **b)** Two mechanisms of optical transitions for DAPs in semiconductors. The two types differ whether charge transfer or direct recombination occurs: the excited electron can be trapped by A0 or D+, altering the charge state before relaxing back to the ground state. **c)** Bright excitation (red arrow) from the ground state (GS) to the excited state (ES) is localized on ONVB–. Through internal conversion, the ES can relax to the doublet metastable state of CB0–ONVB0, denoted as Ds. The Ds level is separated by an energy J > 0 from the quartet metastable state Qs of the same CB0–ONVB0 configuration. The ± 1/2 and ± 3/2 spin sublevels within Qs are split by zero-field splitting. The black dot indicates spin mixing between Ds and Qs, while the black circle indicates the population magnitude in the ground state. **d)** Spin sublevels in Ds and Qs under magnetic fields, shown for three values of J: − 3000, 0, and + 3000 MHz.

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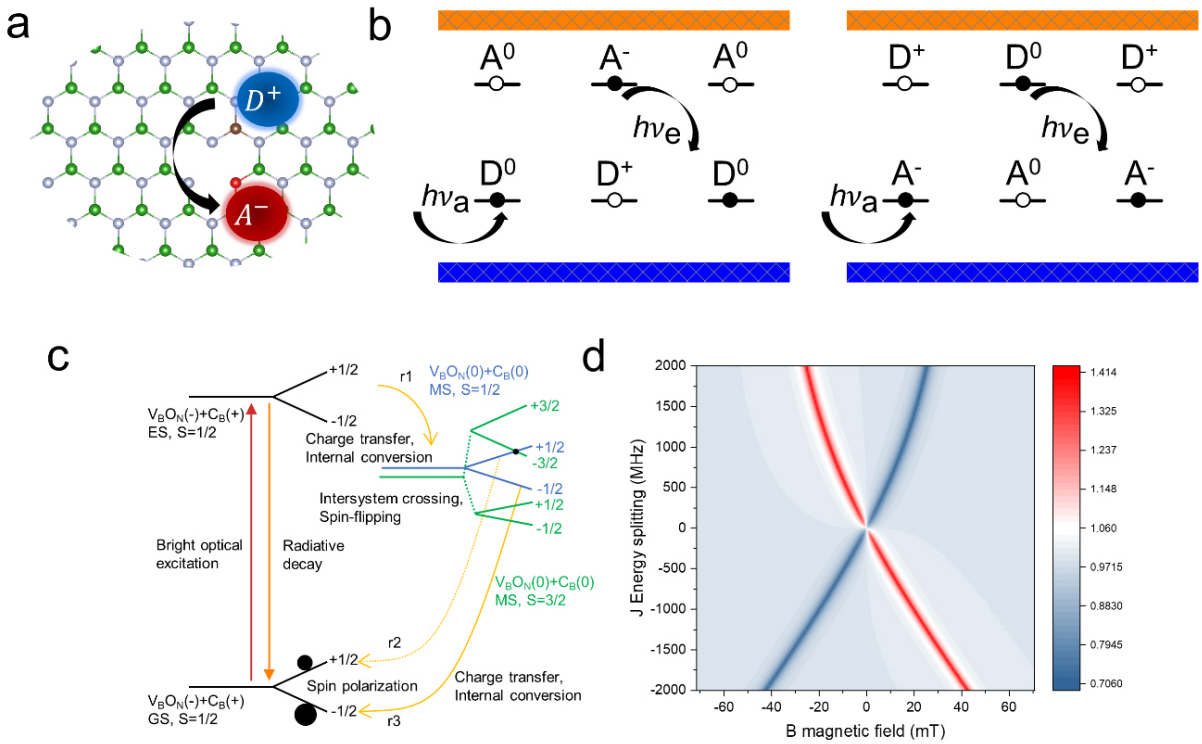

图 1 a）六方氮化硼（hBN）中含氧、碳杂质的施主-受主模型。b）半导体中施主-受主对（DAPs）的两种光学跃迁机制。两种类型的区别在于电荷转移与复合的方向：受激电子可被A0或D+捕获，在弛豫回基态前改变电荷状态。c）ONVB–基态（GS）到激发态（ES）的亮激发（红色箭头）。通过内转换，激发态可弛豫至CB0–ONVB0的二重亚稳态（记为 Ds）。Ds 能级与相同 CB0–ONVB0 构型的四重亚稳态（Qs）之间的能量差 $J>0$。Qs 内的 $\pm 1/2$ 和 $\pm 3/2$ 自旋子能级因零场分裂而分离。黑点表示 Ds 与 Qs 之间的自旋混合，黑圈表示基态中布居数大小。d）磁场下 Ds 和 Qs 的自旋子能级，图中展示了 J 的三个值：-3000、0 和 +3000 MHz。

六方氮化硼中耦合自旋对的单光子发射

李颂*, Anton Pershin & Adam Gali*

宽带隙半导体中可光寻址的色心是室温量子信息处理的潜在架构。六方氮化硼（hBN）凭借内部缺陷的规模化制备优势，成为极具吸引力的固态结构平台，在构筑高亮度量子光源和量子存储器方面展现巨大潜力。尽管近年来已在 hBN 中报道了室温下高亮度的色心量子比特，但其微观起源、光学跃迁特性以及光探测磁共振（ODMR）谱线的来源仍不明确。

实现色心的确定性制备和操控的前提是明确观测到的单光子源（SPEs）和单自旋 ODMR 的缺陷结构。实验中观测到的光致发光（PL）谱线呈现出多种零声子线（ZPL）能量和声子边带（PSBs），且许多光谱具有相似的谱线形状。这些单光子现象可能源于多种缺陷，但谱线形状的相似性表明，这颗坑是由于同种缺陷受到晶体环境影响引起的。

通过电子顺磁共振（EPR）观测到 S=1/2 的顺磁缺陷。基于实验与模拟 EPR 光谱的对比，我们将这一信号归于带负电的 ONVB 缺陷[1]。值得注意的是，后续的环形暗场扫描透射电子显微镜（ADF-STEM）测量证实了 ONVB 缺陷的存在。此外，实验观测到了其附近的碳、氧替位缺陷结构。这有力地证明，导致 EPR 信号的 ONVB 缺陷上的负电荷可能来源于施主杂质，如碳替位（CB）或氧替位（ON）。换句话说，CB 或 ON 可以与 ONVB 形成施主-受主对（DAPs），其中 S=1/2 自旋态来自局域在 ONVB 周围的自旋密度。我们猜测，实验观测到的光学特性变化是由施主杂质的类型和位置引起。

我们对不同间距的施主-受主对的光学特性进行了全面的理论计算。研究发现，施主（CB或ON）的确会向ONVB缺陷提供一个电子，使其带负电。施主-受主距离显著影响电子结构，这为实验中观测到的 ZPL 变化提供了解释。我们发现，ON-ONVB 施主-受主对具有光稳定性；相比之下，CB-ONVB 对在特定距离下会产生亚稳态暗态，这会为电子额外提供非辐射跃迁路径。在这些暗态中，自旋翻转会使二重态和四重态混合，当外部磁场消除 Kramers 简并时，导致带负电 ONVB 的 S=1/2 基态产生自旋极化。因此，当受到恒定磁场作用时，CB-ONVB 缺陷对在 S=1/2 基态下产生 ODMR 光谱,为实验观测到的 ODMR 光谱提供理论支持[2]。

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A GENERAL COLLOCATION ANALYSIS FOR WEAKLY SINGULAR VOLTERRA INTEGRAL EQUATIONS WITH VARIABLE EXPONENT

By Hui Liang, Martin Stynes*

Weakly singular Volterra integral equations (VIEs) of the second kind have the form $y(t) = g(t) + \int_{s=0}^{t} (t-s)^{-\alpha} K(t,s)\, y(s)\, ds$ for $0 \le t \le T$, where the given exponent $\alpha \in (0,1)$ is a constant and $y(t)$ is the unknown solution which must be determined. The numerical solution of such problems has been extensively studied in the research literature and in particular the use of collocation with piecewise polynomials is a commonly-used method. Our paper discusses the solution of this class of problems when the exponent is no longer constant but a given function:

$y(t) = g(t) + \int_{s=0}^{t} (t-s)^{-\alpha(t)} K(t,s)\, y(s)\, ds$ for $0 \le t \le T$. (Such problems are equivalent to certain variable-order fractional-derivative differential equations.) The numerical solution of this problem using collocation has been studied for the simplest case of piecewise linear polynomials (X.Zheng & H.Wang, SIAM J. Numer. Anal., 2020), but it is unclear whether this analysis can be extended to polynomials of higher degree and consequent greater accuracy.

Our paper uses novel techniques to discuss the general theory (existence, uniqueness, regularity of solutions) of variable-exponent weakly singular VIEs. These results then underpin an error analysis of collocation methods where piecewise polynomials of *any* degree can be used. This error analysis is also novel --- it makes no use of the usual resolvent representation, which is a key technique in the error analysis of collocation methods for VIEs in the current research literature. Furthermore, all the above analysis for a scalar VIE can be extended to certain nonlinear VIEs and to systems of VIEs. The sharpness of the theoretical error bounds obtained for the collocation methods is demonstrated by numerical examples.

带有变指数的弱奇异 VOLTERRA 积分方程的配置方法分析

梁慧, Martin Stynes*

第二类弱奇异 Volterra 积分方程（VIEs）具有形式 $y(t)=g(t)+\int_{s=0}^{t}(t-s)^{-\alpha}K(t,s)\,y(s)\,ds$ for $0\le t\le T$，其中给定的指标 $\alpha\in(0,1)$ 为常数，$y(t)$ 是需确定的未知解。在现有文献中，关于此问题的数值解已经被广泛研究，并且使用分片多项式的配置方法是一个常用方法。我们讨论这一类问题中的弱奇异指数不再是常数，而是一个给定函数的情况：$y(t)=g(t)+\int_{s=0}^{t}(t-s)^{-\alpha(t)}K(t,s)\,y(s)\,ds$ for $0\le t\le T$。（这类问题等价于某些变阶分数阶导数微分方程。）在（X.Zheng & H.Wang, SIAM J. Numer. Anal., 2020）中，对于最简单的分片线性多项式的情况，该问题的配置方法已经被研究，但是目前尚不清楚这种分析是否能适用于更高次的多项式以及从而达到更高的精度。

我们使用一个创新性的技巧讨论了变指数弱奇异 VIEs 的一般性理论（解的存在唯一性，正则性）。这些结果为使用任意阶的分片多项式配置方法的误差分析提供了依据。这个误差分析也是创新性的，其中不使用一般的预解表示，而这在现有文献中是 VIEs 的配置方法误差分析中的一个关键技巧。并且，这里所有针对标量方程的分析都可以拓展到某些非线性 VIEs 和 VIEs 系统。数值实验验证了该配置方法的理论误差界的准确性。

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PARAMETER INFERENCE AND NONEQUILIBRIUM IDENTIFICATION FOR MARKOV NETWORKS BASED ON COARSE-GRAINED OBSERVATIONS

By Bingjie Wu#, Chen Jia*

Most experiments can only detect a set of coarse-grained clusters of a molecular system, while the internal microstates are often inaccessible. Here, based on an infinitely long coarse-grained trajectory, we obtain a set of sufficient statistics which extracts all statistic information of coarse-grained observations. Based on these sufficient statistics, we set up a theoretical framework of parameter inference and nonequilibrium identification for a general Markov network with an arbitrary number of microstates and arbitrary coarse-grained partitioning (Fig. 1) [1]. Our framework can be used to identify whether the sufficient statistics are enough for empirical estimation of all unknown parameters and we can also provide a quantitative criterion that reveals nonequilibrium. Our nonequilibrium criterion generalizes the one obtained in Ref. [2] for a three-state system with two coarse-grained clusters, and is capable of detecting a larger nonequilibrium region compared to the classical criterion based on autocorrelation functions.

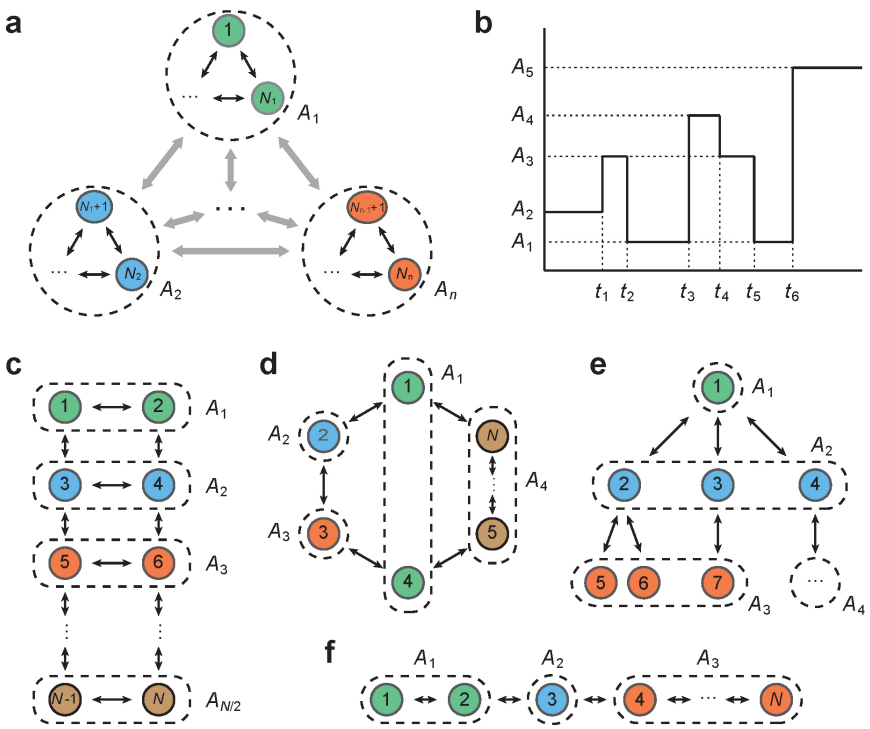

Fig. 1 Consider an N-state Markov network with n coarse-grained states A_1, ..., A_n, each composed of multiple microstates. Assume that an infinitely long trajectory of coarse-grained states can be observed. We obtain a set of sufficient statistics which extracts all statistic information of coarse-grained observations. Based on these sufficient statistics, we set up a theoretical framework of parameter inference and nonequilibrium identification for a general Markov network with an arbitrary number of microstates and arbitrary coarse-grained partitioning. Our framework can be used to identify whether the sufficient statistics are enough for empirical estimation of all unknown parameters and we can also provide a quantitative criterion that reveals nonequilibrium.

基于粗粒化观测的马尔可夫网络参数推断与非平衡判别

Bingjie Wu#, Chen Jia*

大多数实验只能探测到分子系统的一组粗粒化簇，而其内部的微观状态通常是无法直接观测到的。在本文中，我们基于一条无限长的粗粒化轨道，获得了一组充分统计量，它能够提取粗粒化观测所包含的全部统计信息。基于这些充分统计量，我们建立了一个适用于一般马尔可夫网络的理论框架，用于参数推断和非平衡判别，该框架适用于任意数量的微观状态和任意的粗粒化划分方式（见图1）[1]。我们的框架不仅可以判断这些充分统计量是否足以用于所有未知参数的经验估计，还能提供一个定量判据用于识别系统是否处于非平衡态。我们提出的非平衡判据是对文献[2]中针对具有两个粗粒化簇的三态系统所给判据的推广，并且相比于经典的自相关函数判据，它能够检测出更广泛的非平衡区域。

◀ 图 1 考虑一个具有 N 个微观状态的马尔可夫网络，这些状态被划分为 n 个粗粒化状态 $A_1, \ldots, A_n$，每个粗粒化状态由多个微观状态组成。我们假设可以观测到一条无限长的粗粒化状态轨道。在此基础上，我们构造出一组充分统计量，能够提取粗粒化观测中包含的全部统计信息。基于这些充分统计量，我们建立了一个适用于一般马尔可夫网络的理论框架，用于进行参数推断和非平衡判别，该框架适用于任意数量的微观状态和任意方式的粗粒化划分。我们的框架不仅可以判断这些充分统计量是否足以对所有未知参数进行经验估计，还能提供一个定量判据，用于识别系统是否处于非平衡状态。

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A HIGHLY EFFICIENT ASYMPTOTIC PRESERVING IMEX METHOD FOR THE QUANTUM BGK EQUATION

By Ruo Li, Yixiao Lu, Yanli Wang*

The quantum Boltzmann equation models the evolution of a dilute quantum gas flow, which was initially derived by Uehling and Uhlenbeck. It incorporates quantum effects that cannot be neglected for light molecules at low temperatures. This equation is now applied not only to low-temperature gases but also to model both bosons and fermions, potentially trapped by a confining potential.

The quantum Boltzmann equation is formulated in six-dimensional physical and phase space. The collision operator in this equation involves a five-dimensional integral, where the integrand is combined with complicated cubic terms. These complexities pose significant challenges in studying the quantum Boltzmann equation, both theoretically and numerically. Notably, the Bose-Einstein condensation is a phenomenon wherein the distribution function can exhibit finite blow-up or weak convergence towards Dirac deltas, even when the kinetic energy is conserved.

In this work, we propose an asymptotic preserving (AP) scheme for solving the quantum BGK equation using the Hermite spectral method. A specially chosen expansion center is adopted in the Gauss weight function to generate the related Hermite polynomials, enhancing the approximation accuracy of the basis functions. This method has been proven successful in solving the classical Boltzmann equation, and has been extended to address the collisional plasma scenarios. For the quantum BGK equation, a primary challenge of the Hermite spectral method lies in approximating the quantum equilibrium. We present a highly efficient algorithm to obtain the expansion coefficients of the equilibrium within the framework of the Hermite spectral method. The complex computations are eventually reduced to evaluating the value of the polylogarithm function, which can be further simplified into an one-dimensional integral.

In the numerical experiments, the simulations with periodic initial values are first tested, and the order of convergence validates the AP property of this numerical scheme. Subsequently, the Sod problem is implemented and the numerical results are compared with the solutions of the full quantum Boltzmann equation. The excellent agreement implies that the quantum BGK model serves as a good approximation of the original collision operator. Finally, the mixing regime problem and a spatially 2-dimensional lid-driven cavity flow are conducted to further demonstrate the superiority of this Hermite spectral method.

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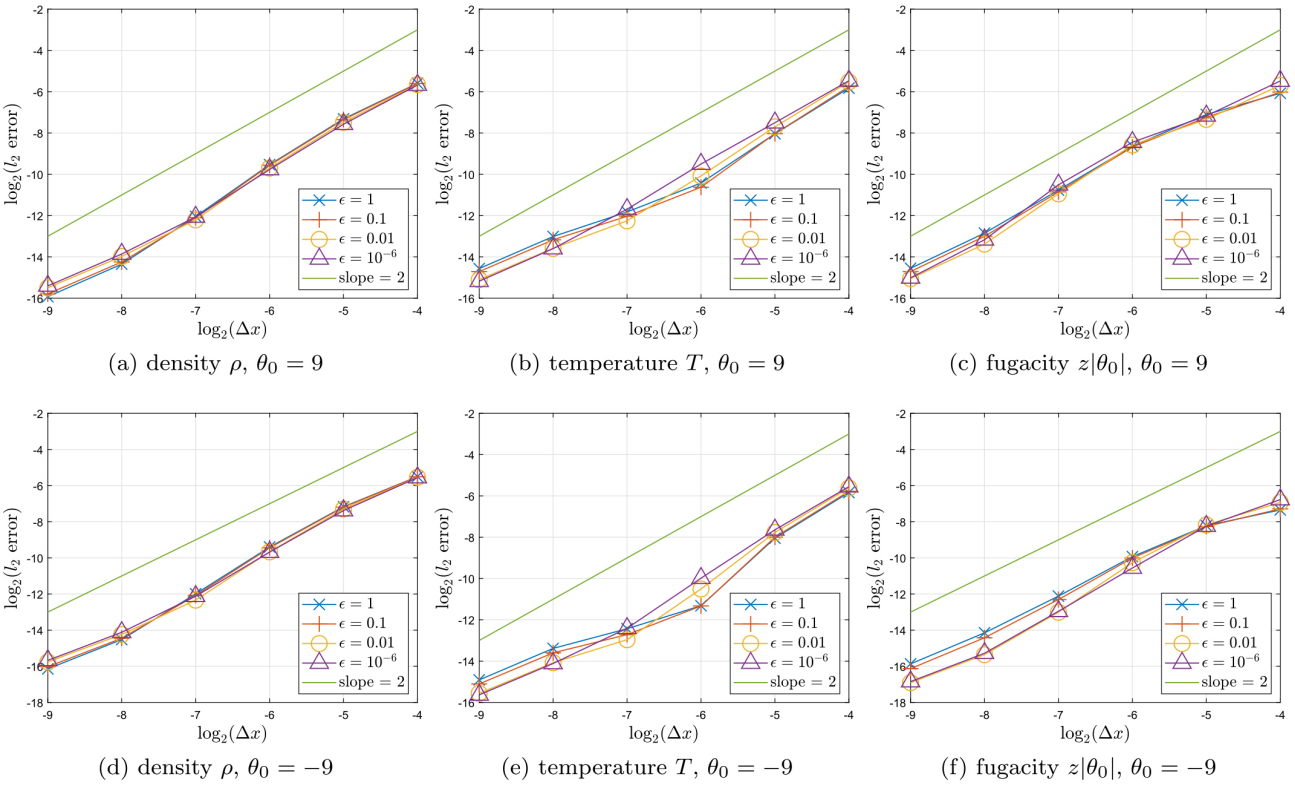
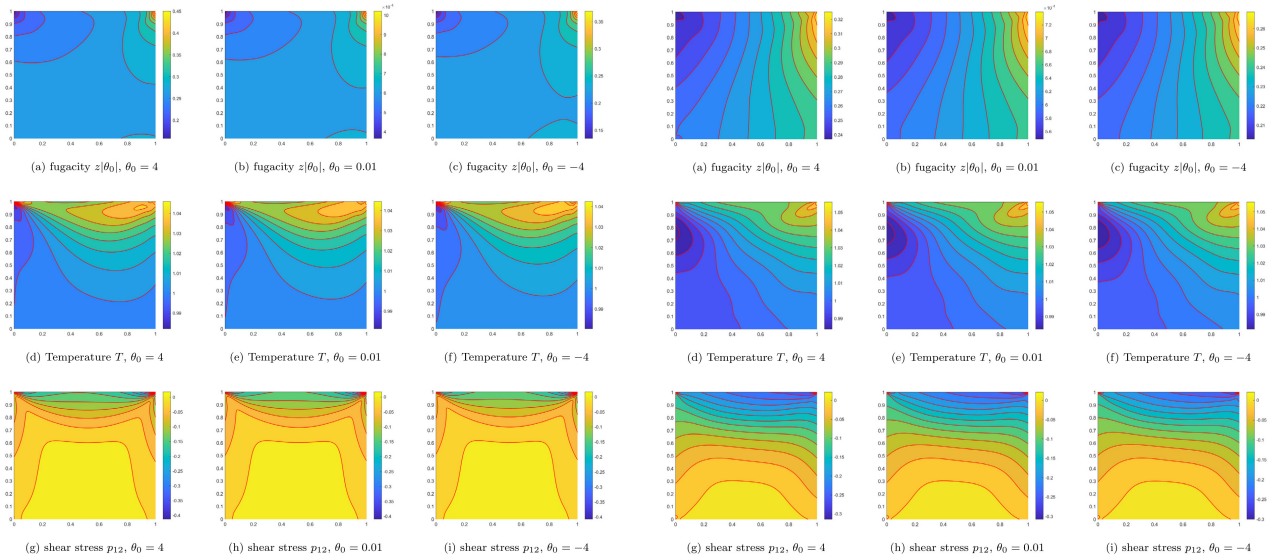


(a) density ρ, $\theta_0 = 9$ (b) temperature T, $\theta_0 = 9$ (c) fugacity $z|\theta_0|$, $\theta_0 = 9$

(d) density ρ, $\theta_0 = -9$ (e) temperature T, $\theta_0 = -9$ (f) fugacity $z|\theta_0|$, $\theta_0 = -9$

Fig. 1 AP test

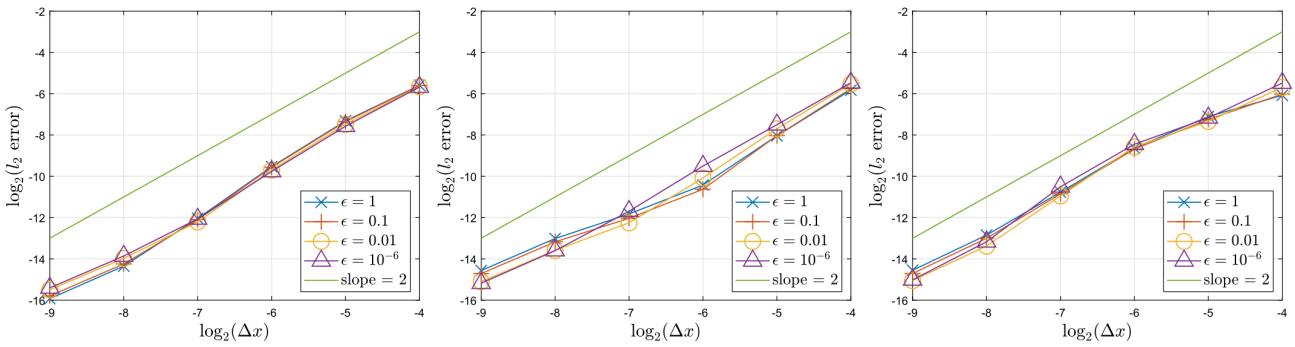


(a) fugacity $z|\theta_0|$, $\theta_0 = 4$ (b) fugacity $z|\theta_0|$, $\theta_0 = 0.01$ (c) fugacity $z|\theta_0|$, $\theta_0 = -4$ (a) fugacity $z|\theta_0|$, $\theta_0 = 4$ (b) fugacity $z|\theta_0|$, $\theta_0 = 0.01$ (c) fugacity $z|\theta_0|$, $\theta_0 = -4$

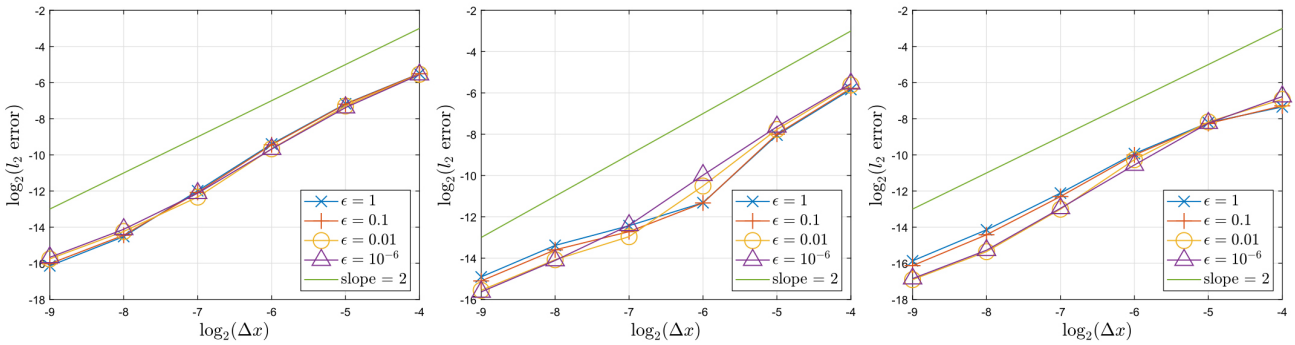
(d) Temperature T, $\theta_0 = 4$ (e) Temperature T, $\theta_0 = 0.01$ (f) Temperature T, $\theta_0 = -4$ (d) Temperature T, $\theta_0 = 4$ (e) Temperature T, $\theta_0 = 0.01$ (f) Temperature T, $\theta_0 = -4$

(g) shear stress p_{12}, $\theta_0 = 4$ (h) shear stress p_{12}, $\theta_0 = 0.01$ (i) shear stress p_{12}, $\theta_0 = -4$ (g) shear stress p_{12}, $\theta_0 = 4$ (h) shear stress p_{12}, $\theta_0 = 0.01$ (i) shear stress p_{12}, $\theta_0 = -4$

Fig. 2 The numerical solution of the 2D lid-driven cavity flow. Left: epsilon = 0.1. Right: epsilon = 1

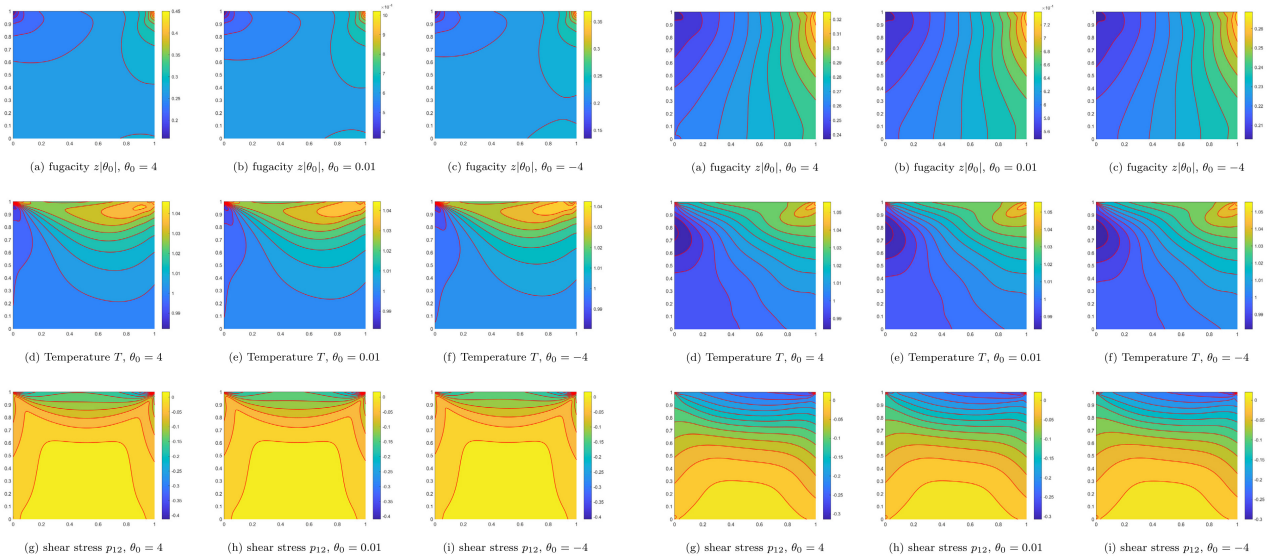


(a) density ρ, $\theta_0 = 9$ (b) temperature T, $\theta_0 = 9$ (c) fugacity $z|\theta_0|$, $\theta_0 = 9$



(d) density ρ, $\theta_0 = -9$ (e) temperature T, $\theta_0 = -9$ (f) fugacity $z|\theta_0|$, $\theta_0 = -9$

▲ 图 1 渐近保持性质测试



▲ 图 2 二维盖驱动方腔流问题。左: epsilon = 0.1. 右: epsilon = 1

一种求解量子 BGK 方程的高效渐近保持 IMEX 方法

李若，鲁一逍, 王艳莉*

量子玻尔兹曼方程刻画稀薄量子气体流动的演化过程，该模型最早由Uehling与Uhlenbeck推导提出，能够包含轻分子在低温条件下不可忽视的量子效应。该方程的应用范围已从低温气体拓展到同时可刻画受限域势约束的玻色子与费米子体系。

量子玻尔兹曼方程定义在六维的相空间中。其碰撞算子包含一个五维积分，且被积函数中伴随复杂的三次项。这些复杂性在量子玻尔兹曼方程的理论研究与数值求解中都带来了显著挑战。值得注意的是，玻色–爱因斯坦凝聚是一种现象，即使在动能守恒的情况下，分布函数仍可能出现有限时间爆破解或向狄拉克函数的弱收敛。

在本文中，我们提出了一种用于求解量子BGK方程的渐近保持（AP）格式，并采用Hermite谱方法实现。我们在Gauss权函数中选取了特定的展开中心来生成相关的Hermite多项式，从而提高基函数的逼近精度。该方法已在求解经典玻尔兹曼方程中取得成功，并被推广用于处理碰撞等离子体情形。对于量子BGK方程，Hermite谱方法的主要难点在于对量子平衡态的逼近。我们提出了一种高效算法，在Hermite谱方法框架下获得平衡态的展开系数。最终，复杂的计算可转化为多对数函数（polylogarithm function）数值的求取，并进一步简化为一维积分形式。

在数值实验中，我们首先对具有周期性初值的情形进行测试，其收敛阶验证了该数值格式的渐近保持（AP）性质。随后，我们实现了Sod问题，并将数值结果与完整量子玻尔兹曼方程的解进行比较。二者的高度一致性表明，量子BGK模型是原始碰撞算子的良好近似。最后，我们还进行了混合区间问题以及二维空间的盖驱动腔流动（lid-driven cavity flow）模拟，以进一步展示该Hermite谱方法的优越性。

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[3] L. Wu, A fast spectral method for the Uehling-Uhlenbeck equation for quantum gas mixtures: homogeneous relaxation and transport coefficients, J. Comput. Phys. 399 (2019) 108924.

During the 2024-2025 academic year, CSRC is undertakeing 39 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. 12 projects were concluded during the academic year.

2024-2025学术年期间，中心承担国家基金委、科学技术部、博士后科学基金，以及中物院等在研项目共39项，其中年内结题12项。

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	PROJECT TITLE 项目名称
1	罗民兴	国家自然科学基金委员会	联合基金项目	多体系物理模拟与功能设计研究	2023-01 - 2024-12
2	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
3	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
4	薛　鹏	国家自然科学基金委员会	重大研究计划	非厄米量子体系的构筑和操控及其在量子信息中的应用	2023-01 - 2026-12
5	康　俊	国家自然科学基金委员会	重大项目	量子级联结构的激发态理论及高效率器件设计	2024-01 - 2028-12
6	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
7	管鹏飞	国家自然科学基金委员会	国家杰出青年科学基金	无序合金结构与性能	2024-01 - 2028-12
8	Rubem Mondaini	国家自然科学基金委员会	优秀青年科学基金项目	平衡与非平衡量子多体系统的研究	2023-01 - 2025-12
9	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
10	张智民	国家自然科学基金委员会	国际(地区)合作与交流项目	有限元方法基本理论的再探讨	2023-04 - 2025-12

No.	PI 项目负责人	SOURCE 经费来源	CATEGORY 项目类别	PROJECT TITLE 项目名称	PROJECT TITLE 项目名称
11	Thomas Frauenheim	国家自然科学基金委员会	外国学者研究基金项目	Towards temperature dependent exciton properties in titania using properly screened density functional approximations	2023-01 - 2024-12
12	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
13	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
14	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
15	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
16	杨　文	国家自然科学基金委员会	面上项目	基于量子参数估计的最优化量子传感理论	2023-01 - 2026-12
17	贾　晨	国家自然科学基金委员会	面上项目	基因表达与细胞体积的耦合随机动力学	2023-01 - 2026-12
18	莫崇杰	国家自然科学基金委员会	面上项目	温/热稠密烧蚀层材料X射线汤姆逊散射的第一性原理建模与模拟研究	2024-01 - 2027-12
19	郭震林	国家自然科学基金委员会	面上项目	粘性流体中多组分囊泡相分离和形变动力学的数学建模和数值模拟	2024-01 - 2027-12
20	王　乾	国家自然科学基金委员会	面上项目	多几何构件复杂流动降阶模型研究	2024-01 - 2027-12
21	黄　兵	军委科技委	国防科技创新特区项目	基于色心晶体的THz高灵敏探测理论研究	2022-10 - 2024-10
22	王艳莉	中国工程物理研究院	院长基金自强项目	面向惯性约束聚变的辐射输运高精度、高效数值方法研究及其在靶丸辐射驱动不对称性研究中的应用	2023-01 - 2025-12
23	朱国怀	中物院研究生院	横向项目	高能量密度物理特征面处等离子体效应及其影响研究	2024-06 - 2025-05
24	曲登科	国家自然科学基金委员会	青年科学基金项目	基于量子行走的量子近似优化算法的实验研究	2024-01 - 2026-12

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	PROJECT TITLE 项目名称
25	陈祥友	国家自然科学基金委员会	青年科学基金项目	光与物质相互作用模型中A平方问题及其量子相变研究	2024-01 - 2026-12
26	陈泽华	国家自然科学基金委员会	青年科学基金项目	卤素钙钛矿多元合金相稳定性的热力学和动力学研究	2025-01 - 2027-12
27	李　阳	国家自然科学基金委员会	青年科学基金项目	二维磁性材料非线性光学性质的理论研究	2025-01 - 2027-12
28	陈家麒	中国博士后科学基金会	面上资助	费曼积分的约化方法与应用	2022-11 - 2024-10
29	陈祥友	中国博士后科学基金会	面上资助	光与物质相互作用系统中的临界动力学普适类研究	2022-11 - 2024-10
30	陈泽华	中国博士后科学基金会	面上资助	金属卤化物钙钛矿材料带隙随压强非单调变化的物理机制探索	2023-07 - 2025-06
31	曲登科	中国博士后科学基金会	面上资助	应用量子近似优化算法求解组合优化问题的实验研究	2023-07 - 2025-06
32	马　征	中国博士后科学基金会	面上资助	几类弱奇异Volterra型方程的高阶数值方法及其误差分析	2023-07 - 2025-06
33	王　敏	中国博士后科学基金会	面上资助	弱奇异积分微分方程的快速非多项式谱方法及其迭代超收敛算法	2024-07 - 2026-07
34	李　琪	中国博士后科学基金会	面上资助	三温辐射输运方程的隐式渐近保持格式研究	2025-07 - 2027-07
35	陈泽华	中国博士后科学基金会	特别资助	应变调控卤素钙钛矿稳定性及光电性质的机理探索	2024-07 - 2026-07
36	曲登科	中国博士后科学基金会	博士后创新人才支持计划		2023-11 - 2025-10
37	陈泽华	中国博士后科学基金会	国家资助博士后研究人员计划	三元混合卤素钙钛矿热力学稳定性研究	2024-01 - 2025-12
38	曾　维	中国博士后科学基金会	国家资助博士后研究人员计划	次扩散方程的映射方法及应用	2024-01 - 2025-12
39	王　敏	中国博士后科学基金会	国家资助博士后研究人员计划	Gierer-Meinhardt系统的保结构谱方法及其在图灵斑图动力学中的应用	2024-01 - 2025-12

2024-2025学术年期间，中心发表论文共计192篇。

During the 2024-2025 academic year, CSRC has published a total of about 192 papers.

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

1	Quantum metrology with optimal control under an arbitrary non-Markovian bosonic environment; **Zhou**, **LK**; **Yang**, **W**, COMMUNICATIONS IN THEORETICAL PHYSICS, 77, 2, 25108 (2025).
2	GHZ state, spin squeezed state, and spin coherent state for frequency estimation under general Gaussian noises; **Chai**, **Q**; **Yang**, **W**, COMMUNICATIONS IN THEORETICAL PHYSICS, 77, 6, 65106 (2025).
3	Polarization Modulation and Detection Based on Nonuniform Phase Gradient Metasurfaces; Pang, KW; **Zhang**, **W**, PLASMONICS (2025).
4	Modulated spiral order in the 1D Kondo lattice model; **Han, XH**; Ribeiro, P; **Chesi**, **S**, COMMUNICATIONS IN THEORETICAL PHYSICS, 77, 11, 115702 (2025).
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SIMULATION OF PHYSICAL SYSTEMS DIVISION 物理系统模拟研究部

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QUANTUM PHYSICS AND QUANTUM INFORMATION DIVISION 量子物理与量子信息实验室

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3	Planar Coil Design for Nuclear Magnetic Resonance Gyroscope Using Genetic Algorithm; **Shao**, **YM**; **Tang**, **F**; **Zhao**, **N**, IEEE SENSORS JOURNAL, 25, 5 (2025).
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MATERIALS AND ENERGY DIVISION 材料与能源研究部

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12	An improved DIIS method using a versatile residual matrix to accelerate SCF starting from a crude guess; Hu, LP; Sarwono, YP; **Ding**, **YL**; He, F; **Zhang**, **RQ**, JOURNAL OF COMPUTATIONAL CHEMISTRY, 45, 30 (2024).
13	Ferroelectric antiferromagnetic quantum anomalous Hall insulator in two-dimensional van der Waals materials; Liang, Y; Zhao, P; Zheng, FL; **Frauenheim**, **T**, PHYSICAL REVIEW B, 110, 20, 205421 (2024).
14	Oxygen Defect Site Filling Strategy Induced Moderate Enrichment of Reactants for Efficient Electrocatalytic Biomass Upgrading; Cheng, BX; Zhan, HY; Lu, YK; Xing, DN; Lv, XS; **Frauenheim**, **T**; Zhou, P; Wang, SY; Zou, YQ, ADVANCED SCIENCE (2024).
15	Synergy of rutile SnO2 and TiO2 in optoelectronic applications: Electronic structure and doping properties of TixSn1-xO2 alloys; Han, MM; Cai, XF; Wei, SH; Frauenheim, T; **Deák**, **P**, PHYSICAL REVIEW B, 110, 19, 195203 (2024).
16	All-Epitaxial Self-Assembly of Silicon Color Centers Confined Within Sub-Nanometer Thin Layers Using Ultra-Low Temperature Epitaxy; Aberl, J; Navarrete, EP; Karaman, M; Enriquez, DH; Wilflingseder, C; Salomon, A; Primetzhofer, D; Schubert, MA; Capellini, G; Fromherz, T; **Deak**, **P**; **Udvarhelyi**, **P**; **Song**, **L**; **Gali**, **A**; Brehm, M, ADVANCED MATERIALS (2024).
17	Platinum modification of metallic cobalt defect sites for efficient electrocatalytic oxidation of 5-hydroxymethylfurfural; Zhan, HY; Cheng, BX; Lu, YK; Xing, DN; Lv, XS; Huang, HN; **Frauenheim**, **T**; Wang, T; Zhou, P, JOURNAL OF ENERGY CHEMISTRY, 101(2025).

WORKSHOPS & CONFERENCES (2024-2025)

中心主办、合办的学术会议

时间 Date	会议名称 Title
2025.5.9-12	计算数学方法前沿论坛
2025.4.21-23	国产工业软件-高效数值方法与工业应用研讨会

计算数学方法前沿论坛

国产工业软件-高效数值方法与工业应用研讨会

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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。2024-2025学术年期间中心共举办专题讲座49期（总1344期）。

CSRC invites national and overseas leading researchers to give academic seminars. During academic year 2024-2025, CSRC has already held 49 seminars.

DATE\日期	SPEAKER\报告人	INSTITUTE\单位	TITLE/报告题目
2024.8.1	王轶凡 Yi-Fan Wang	北京大学 Peking University	张量神经网络及其应用
2024.8.1	胡　伟 Wei Hu	中国科学技术大学 University of Science and Technology of China	算法与算力驱动的第一性原理材料模拟
2024.8.6	李宏超 Hong-Chao Li	日本东京大学 University of Tokyo（Japan）	Yang-Lee Zeros, Semicircle Theorem, and Nonunitary Criticality in Bardeen-Cooper-Schrieffer Superconductivity
2024.8.8	胡　丹 Dan Hu	上海交通大学 Shanghai Jiao Tong University	DNN for PDEs: Residual-informed neural networks and non-uniform random walk for adaptive sampling
2024.8.22	方　洲 Zhou Fang	苏黎世联邦理工学院 ETH Zurich	A divide-and-conquer approach for biological filtering problems
2024.8.26	张　亿 Yi Zhang	北京大学 Peking University	Residue Imaginary Velocity May Induce Many-Body Delocalization
2024.8.30	衣学喜 Xue-Xi Yi	东北师范大学 Northeast Normal University	非厄米性可以提高参数估计精度?
2024.10.10	高文龙 Wen-Long Gao/ Malte Röntgen	宁波东方理工大学 Eastern Institute of Technology, Ningbo	Latent Symmetries Revealed by Graph Theoretical Tools for Hermitian and non-Hermitian Models
2024.10.10	刘　锋 Feng Liu	美国犹他大学 University of Utah（USA）	Excitonic Bose Einstein Condensation in a Quantum Semiconductor with Flat Band Edges

DATE\日期	SPEAKER\报告人	INSTITUTE\单位	TITLE/报告题目
2024.10.22	李向东 Xiang-Dong Li	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	熵、热力学第二定律及中心极限定理
2024.10.23	李逢苗 Feng-Miao Li	合肥国家实验室 Hefei National Laboratory (NFNL)	Bridging MBE and DFT for Studying Superconducting Films and Interfaces
2024.10.23	肖运龙 Yun-Long Xiao	新加坡科技研究局高性能计算研究院 A*STAR Institute of High Performance Computing (IHPC)，Singapore	Quantum Uncertainty Principles for Measurements with Interventions
2024.10.25	张　科 Ke Zhang	德国联邦物理技术研究院 Physikalisch-Technische Bundesanstalt （Germany)	Direct laser excitation of the Th-229 nucleus towards a nuclear clcok
2024.10.31	Peter Deák	德国不莱梅大学 University of Bremen(Germany)	Methodical Problems in Calculating Surfaces, Layers and Charged Defects in Semiconductors
2024.11.7	滕　飞 Fei Teng	复旦大学 Fudan University	From Scattering Amplitudes to Gravitational Wave Physics
2024.11.15	王亚娴 Ya-Xian Wang	中国科学院物理研究所 Institute of Physics, CAS	Nonequilibrium Electron-Phonon Dynamics: Dynamical Control of Quantum Matter
2024.11.22	陈　基 Ji Chen	北京大学 Peking University	机器学习量子蒙特卡洛计算
2024.11.28	赵宏健 Hong-Jian Zhao	吉林大学 Jilin University	反铁磁奈尔矢量探测
2024.12.6	宋　飞 Fei Song	中国科学院大学卡弗里理论科学研究中心 The Kavli Institute for Theoretical Sciences (UCAS)	From Non-Bloch Bands to Open Quantum Many-Body Systems: Insights Brought by Hermitization
2024.12.6	杨　康 Kang Yang	德国柏林自由大学 Freie Universität Berlin（Germany）	Non-Abelian Nodal Structures and Dissipation-Protected Chern Bands in Photonic Systems

CSRC SEMINAR 专题报告

DATE\日期	SPEAKER\报告人	INSTITUTE\单位	TITLE/报告题目
2024.12.8	胡振芃 Zhen-Peng Hu	南开大学 Nankai University	基于电子关联的电极材料催化性能调控
2024.12.11	徐小文 Xiao-Wen Xu	北京应用物理与计算数学研究所 Institute of Applied Physics and Computational Mathematics	特征修正预条件算法框架与智能解法器探讨
2024.12.12	张　扬 Yang Zhang	中国科学技术大学 University of Science and Technology of China	Multi-loop and Multi-leg: Analytic Computation of 2loop 6point and 3loop 5point Feynman Integrals
2024.12.13	孙兆茹 Zhao-Ru Sun	上海科技大学 ShanghaiTech University	Ab Initio Deep Neural Network Simulations of Carbonic Acid Dissociation and Proton Transfer Dynamics
2024.12.16	司新辉 Xin-Hui Si	北京科技大学 University of Science and Technology Beijing	有限方腔内FENE-P粘弹性流体电热对流的流动状态及热传递
2024.12.19	王　成 Cheng Wang	美国麻省大学达特茅斯分校 University of Massachusetts-Dartmouth (USA)	Unique Solvability and Convergence Analysis of the Lagrange Multiplier Approach for Gradient Flows
2024.12.19	杨海棠 Hai-Tang Yang	四川大学 Sichuan University	Obtain Einstein Equation from CFT_2 and Realize ER=EPR
2025.1.21	许传炬 Chuan-Ju Xu	厦门大学 Xiamen University	Gradient Flows: Modelling and Numerical Methods
2025.2.26	金翰文 Han-Wen Jin	英国帝国理工学院 Imperial College London（UK）	Excited States and Hot Carrier Dynamics in Plasmonic Materials
2025.2.27	斯　杭 Hang Si	大连理工大学 Dalian University of Technology	Introduction to Finite Eelement Mesh Generation and Adaptation
2025.3.27	秦伯韡 Bo-Wei Qin	复旦大学 Fudan University	复杂生物系统的数学模型和方法

DATE\日期	SPEAKER\报告人	INSTITUTE\单位	TITLE/报告题目
2025.4.2	Joachim Heinze	德国奥伯沃尔法赫数学研究所 Oberwolfach Stiftungsrat, MFO（Germany）	Redefining Research: The evolution of Scientific Publishing and Communication in the era of Artificial Intelligence
2025.4.11	费　飞 Fei Fei	华中科技大学 Huazhong University of Science and Technology	NS渐进保持性质的多尺度随机粒子方法
2025.4.11	刘红涛 Hong-Tao Liu	比利时鲁汶大学 KU Leugen（Belgium)	等离子体流动的离散统一气体动理学格式研究及应用
2025.4.18	Sebastian Eggert	德国凯泽斯劳滕理工大学 RPTU University of Kaiserslautern-Landau (Germany)	Transport in Quantum Wires: Fractional Charges and Non-Linear Luttinger Liquids
2025.4.21	Sebastian Eggert	德国凯泽斯劳滕理工大学 RPTU University of Kaiserslautern-Landau (Germany)	Floquet Theory of Resonances
2025.5.19	李思冶 Si-Ye Li	军事科学院军事智能研究院 AMII	Research on Intelligent Prediction Method with Graph Neural Networks for Compressible Flows and Its Application
2025.5.22	葛一凡 Yi-Fan Ge	中科院上海有机化学研究所生物与化学交叉中心 Interdisciplinary Research Center on Biology and Chemistry, CAS	Membrane Curvature as a Regulatory Mechanism of Tfam Prewetting
2025.5.23	刘　锋 Feng Liu	美国犹他大学 University of Utah（USA）	The Beauty and Richness of Yin-Yang Flat Bands: quantum geometry and anomalous Landau levels
2025.5.27	陈　扬 Yang Chen	北京大学医学部 Peking University Health Science Center	介导细胞间通讯的新型亚细胞结构“迁移体”
2025.6.11	马欢飞 Huan-Fei Ma	苏州大学 Soochow University	储备池计算：数据应用与机理融合
2025.6.13	尹璋琦 Zhang-Qi Yin	北京理工大学 Beijing Institute of Technology	从量子时间晶体到量子机器学习

CSRC SEMINAR 专题报告

DATE\日期	SPEAKER\报告人	INSTITUTE\单位	TITLE/报告题目
2025.6.16	宋卓洋 Zhuo-Yang Song	北京大学 Peking University	IdeaSearch：人工智能能够被用于科学探索吗？
2025.6.16	薛　玲 Ling Xue	哈尔滨工程大学 Harbin Engineering University	Mathematical Modeling and Optimization of Combination Immunotherapy for Breast Cancer: Integrating mRNA Vaccines and Anti-CTLA-4 Antibodies
2025.6.18	Aleksander Bach Lorentzen	西班牙多诺斯蒂亚国际物理中心 Donostia International Physics Center(Spain)	Simulating nanoelectronic devices driven by strong and transient fields
2025.6.25	韩锦森 Jin-Sen Han	国防科技大学&中国科学院半导体研究所 National University of Defense Technology&Institute of Semiconductor, CAS	半导体电子结构的第一性原理计算方法发展
2025.6.28	张　弘 Hong Zhang	国防科技大学 National University of Defense Technology	Time step rescaling resolves the lagging effect in stabilization single-step schemes for a class of L2 gradient flows
2025.7.2	王立联 Li-Lian Wang	新加坡南洋理工大学 Nanyang Technological University (Singapore)	Explicit Construction of Approximate Kolmogorov-Arnold Superpositions with C^2-Smoothness
2025.7.16	朱博南 Bo-Nan Zhu	北京理工大学 Beijing Institute of Technology	随机结构搜索在材料科学方面的应用与展望

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。自开展至今已举办十期。

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Since its establishment, more than 5000 visiting scholars from over 20 countries and regions have visited CSRC. CSRC faculty members went out for academic eschange for more than 2000 times. During the academic year 2024-2025, 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。2024-2025学术年期间，中心接待来访学者超过200人次。

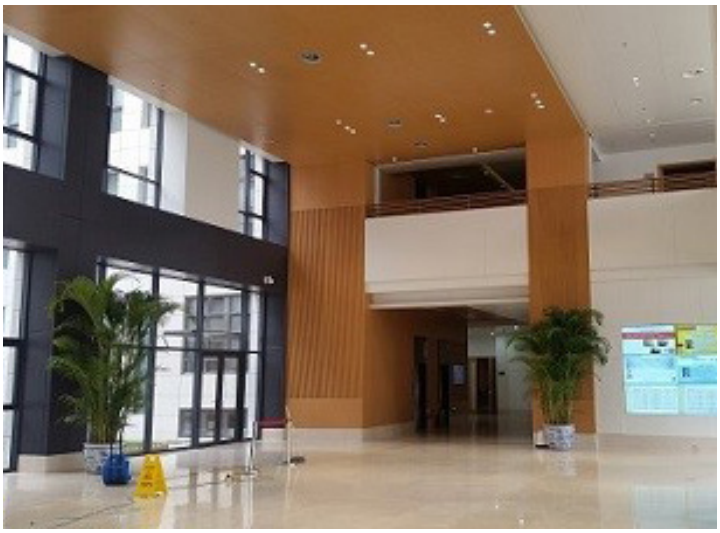
中心欢迎国内外各机构相关专业的科研人员和教师，以访问学者和客座研究人员的形式来访，进行短期或长期合作研究。中心也与同行们一起举办学术活动如会议、讲习班等。在中心访问期间，中心将提供一定的生活和住房补贴。

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.

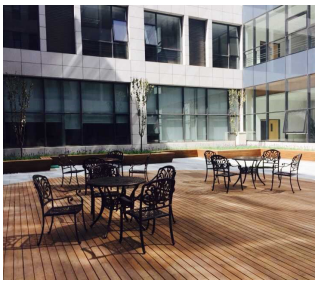
北京计算科学研究中心非常重视与科研机构及高校的合作，在积极组织承办国内外学术会议之时，也鼓励科研人员与国内外其他科研机构之间的互访交流，扩展学术视野和扩大学术影响。目前已与国际数所科研机构签署了合作协议，为打造中心作为国际一流的开展计算科学及相关学科交叉研究的综合平台而不断努力。

〖 中心办公楼效果图 〗 CSRC building

〖 大厅 〗 Lobby

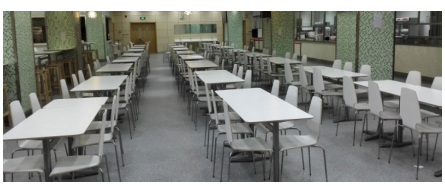


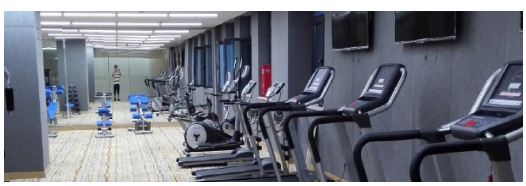
〖 中庭院 〗 Courtyard



〖 学术报告厅 〗 Auditorium

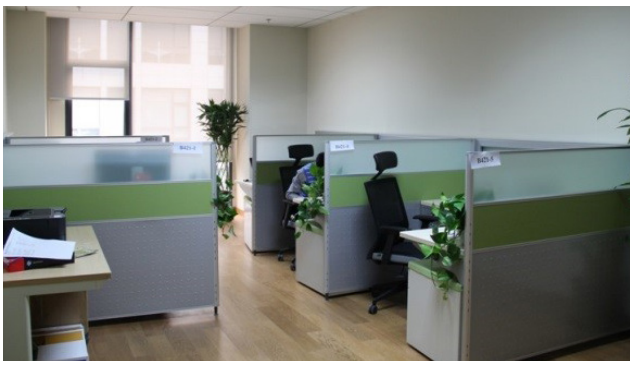
Seminar Rom 〖 学术会议室 〗 Common 〖 学术讨论区 〗



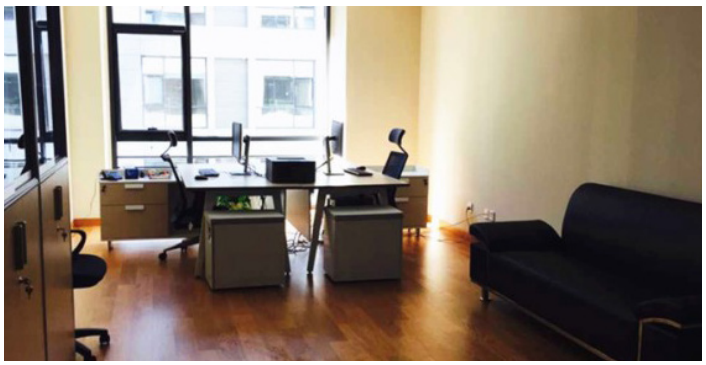


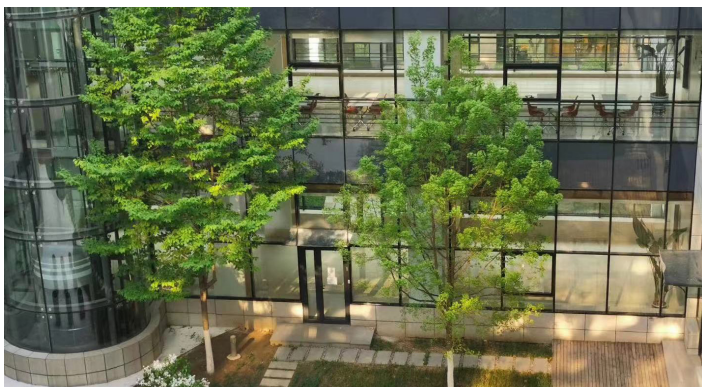
ZPark 〖 中关村软件园一二期鸟瞰图 〗

〖 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

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CLUSTER TIANHE2-JK

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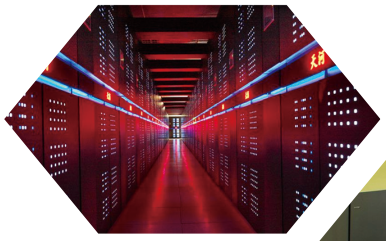
14112cores



131.1TB Memory

1440TB disks
2304TB back-up disks

80Gb/s QDR