2022 - 2023 年度报告 ANNUAL REPORT

# CONTENTS 目录



本册所列所有信息为2022年8月1日至2023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2023年8月，中心的科研人才队伍包括13位讲座教授、4位教授、6位研究员、7位特聘研究员、3位特聘副研究员、3位工程师和32位博士后。另外，中心还有博士/硕士研究生108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。

2022-2023学术年期间，中心公开发表国际学术论文299篇，主办合办国内外学术会议6场，开设培训班2场，举办科技前沿讲座1期，邀请学术报告68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。

## 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.

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.

## Mission of CSRC

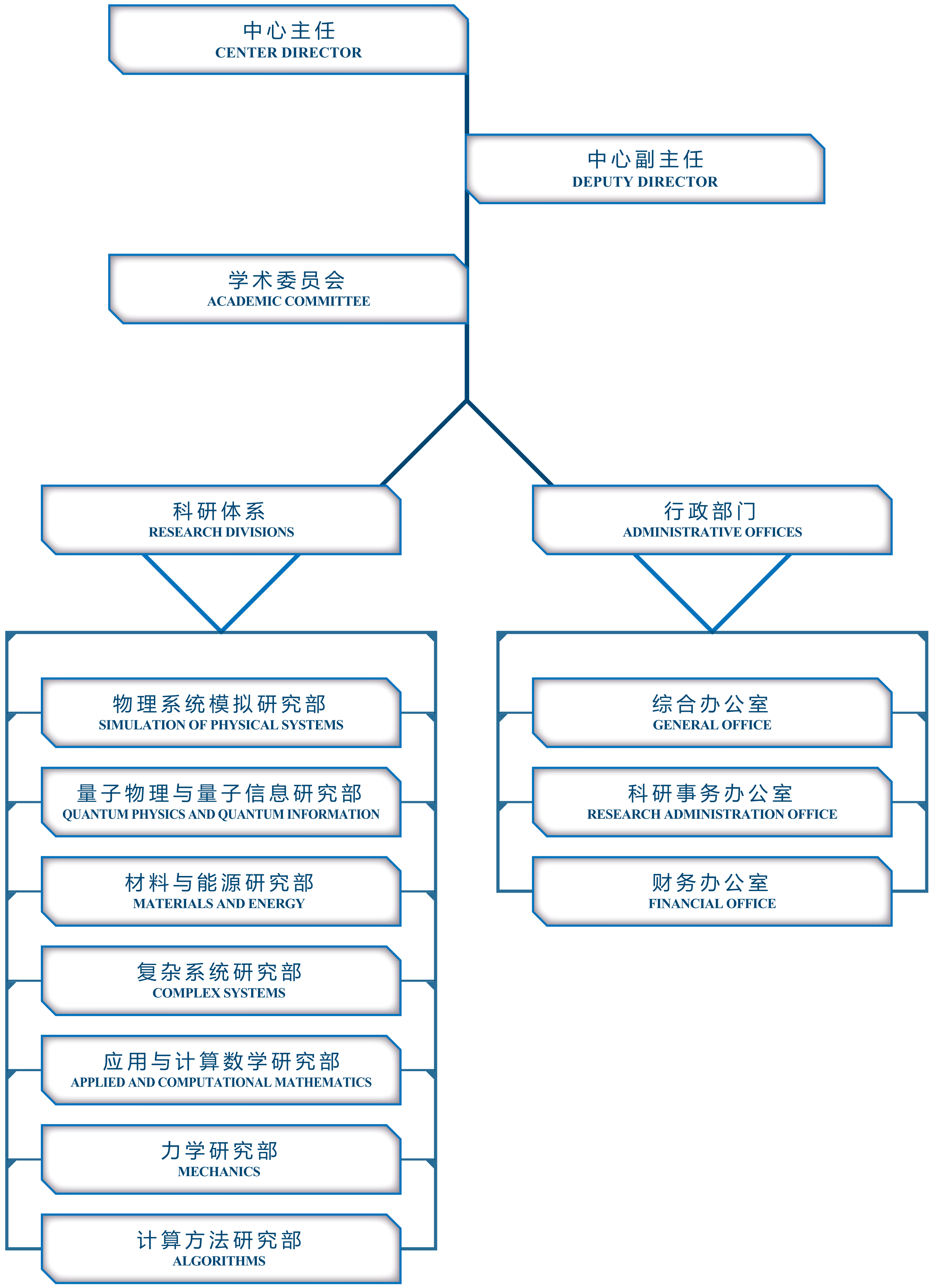
◎ Carry out fundamental, frontier, critical, and multidisciplinary research with advanced computational approaches, thereby attract talents worldwide and train highly qualified research personnel, to support grand scientific development and technology innovation in China;

◎ 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.

As of August 2023, CSRC has 33 faculty members, 3 engineers, 32 postdoctoral fellows and 108 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 299 papers, organized 6 academic conferences and workshops, 2 tutorials, 1 colloquium on scientific frontiers, and 68 CSRC seminars. CSRC has also forged partnerships with many prestigious universities and research institutes around the world.

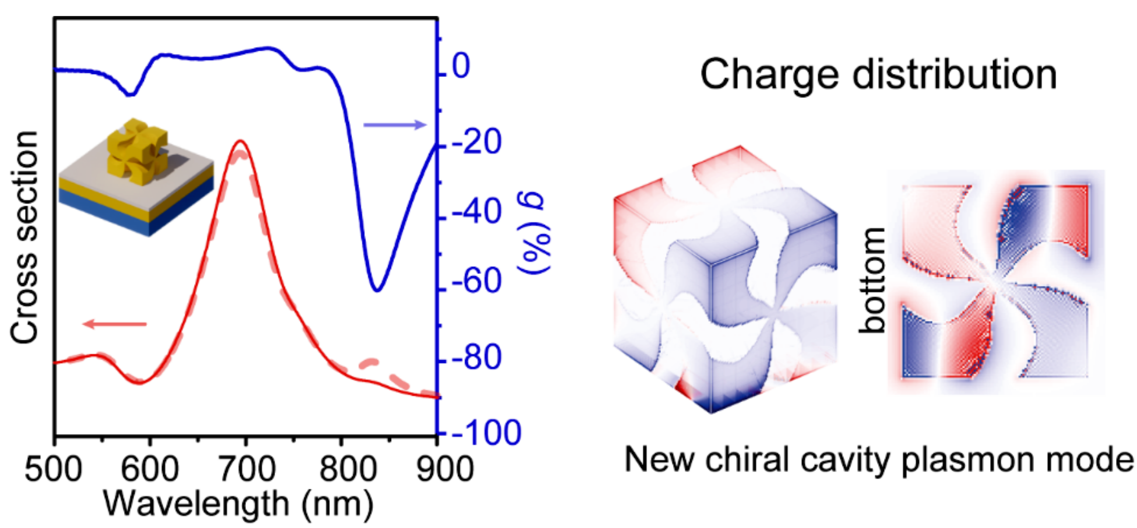
# ORGANIZATION 中心组织构架



# EXCITATION OF CHIRAL CAVITY PLASMON RESONANCES IN FILM-COUPLED CHIRAL AU NANOPARTICLES

By Jing Wang, Jiapeng Zheng, Kwai Hei Li, Jianfang Wang, Hai-Qing Lin, Lei Shao

Chiral plasmonic nanostructures have attracted increasing attention because of their superchiral near-fields as well as strong far-field chiral optical response. Recently, the development of chemical synthesis methods enabled the large-scale manufacturing of three-dimensional colloidal chiral plasmonic nanocrystals. Further improving the chiral optical response of such nanostructures will greatly facilitate their practical applications. In this work, it is found both in calculations and experiments that chiral cavity plasmon resonances can be excited in film-coupled chiral Au helicoid nanoparticles, enabling the significant enhancement of the nanostructure chiral optical response. In addition, it is demonstrated from simulation that the chiral cavity mode can modulate the emission polarization of a point electric dipole placed in the nanocavity formed by the nanoparticle and the Au film, allowing the emission of almost circularly polarized photons by the linear dipole with the emission circular polarization anisotropy factor reaching as high as 93%. The film-coupled chiral plasmonic nanoparticles therefore provide a promising platform for the construction of advanced chiral optical devices such as on-chip nonreciprocal nanoscale light sources, chiral plasmonic sensors, chiral metamaterials, plasmonically enabled valleytronic devices, and nanophotonic circuits for future on-chip communication applications.



# 等离激元纳腔增强纳米颗粒的手性光学响应

**王晶**, 郑嘉鹏, 李携曦, 王建方, **林海青**, 邵磊

手性等离激元纳米结构在包括负折射率人工材料构建、偏振调制与探测、手性分子传感、手性选择性光催化等领域具有广泛的应用前景。纳米结构的手性光学性质越强, 即结构对左旋偏振光与右旋偏振光的响应差异越大, 越有利于上述应用。近年来, 溶液生长手性胶体金属纳米颗粒的制备方法取得突破, 极大地降低了手性纳米结构的制备成本, 为人们将手性纳米结构应用于不同领域扫除了最大的障碍, 引起了研究人员极大的兴趣。然而, 与高成本的物理方法制备出的结构相比, 胶体手性纳米颗粒由于其结构与形状的限制, 手性光学响应还远不够高。如果可以高效地激发出结构中电子螺旋振荡对应的手性等离激元共振模式, 那么纳米颗粒的手性光学响应将被大幅提高, 十分有利于这些结构的应用。

研究团队发现, 通过构筑简单的手性颗粒—薄膜耦合体系, 在金属间隙处可以激发起新的等离激元纳腔模式, 该模式具有显著增强的手性光学响应。理论计算模拟和实验测量均表明, 手性等离激元纳腔模式的吸收/散射不对称因子可达0.6以上, 远大于单个手性纳米颗粒不对称因子的最大值(0.12)。这种模式可以将电场与磁场能量局域在纳米颗粒与金膜之间形成的纳米腔中, 并且敏感地依赖于手性纳米颗粒的大小以及间隔层的材料与厚度, 其共振波长可以通过结构参数设计从可见波段连续地调制到红外波段。模拟结果也证明了, 手性纳腔等离激元对应着电荷的螺旋振荡行为, 其可以近似看成是电等离激元和磁等离激元模式相互作用的结果。理论计算进一步表明, 上述手性等离激元纳腔模式的近场性质可以用于调制量子发光体的辐射偏振。这种优异的性质有望将胶体手性纳米颗粒的应用拓展至圆偏振纳米光源、能谷光电子器件等领域。

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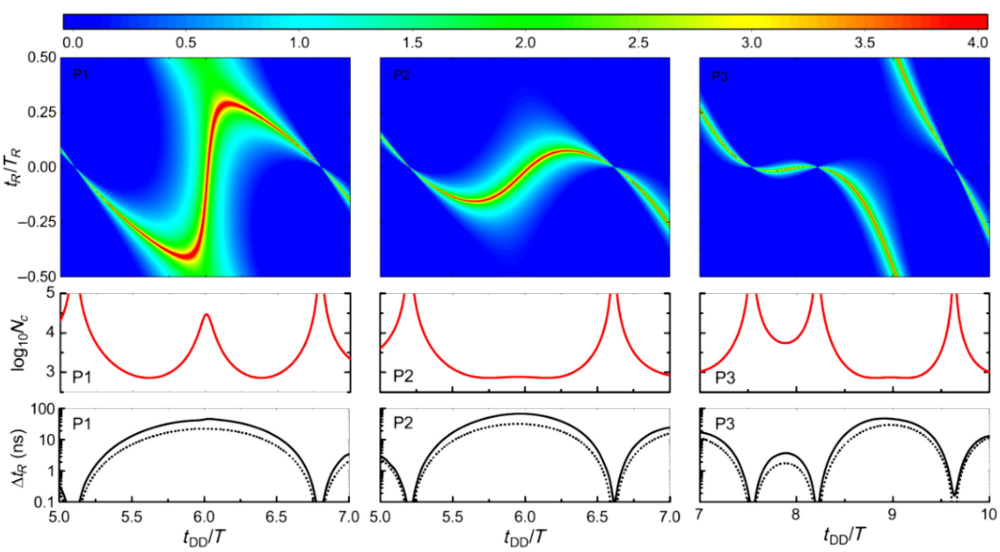
# USING WEAK MEASUREMENTS TO SYNTHESIZE PROJECTIVE MEASUREMENT OF NONCONSERVED OBSERVABLES

By Ping Wang, Wen Yang, Renbao Liu

Projective measurement on the nuclear spin is useful for quantum technologies based on hybrid electron-nuclear spin systems. The measurement of the nuclear spin is difficult and is often realized indirectly via measurement of a nearby electron spin. However, for remote nuclear spins weakly coupled to the electron, it is hard to establish perfect electron-nuclear entanglement, as required for projective measurement on the nuclear spin via measuring the electron spin.

Recently, Wen Yang group in Beijing Computational Science Research Center in collaboration with Renbao Liu group in the Chinese University of Hong Kong proposed a general method to synthesize projective measurements of a nuclear spin by a sequence of weak measurements via weakly coupled auxiliary electron spin. The procedure consists of two steps. First, dynamical decoupling is applied to the electron spin to establish weak electron-nuclear entanglement, followed by a projective measurement on the electron spin to mediate a single weak measurement on the nuclear spin. Second, we apply a sequence of such weak measurements to the nuclear spin and tune the evolution of the nuclear spin between neighboring measurements to meet the stroboscopic quantum nondemolition (QND) condition, so that this sequence of weak QND measurements form a single projective measurement on the nuclear spin. Compared with the traditional QND condition that requires the observable to be a conserved quantity commuting with the Hamiltonian, our method allows measurement of non-conserved nuclear spin observables. We further identify a set of tunable parameters for flexible, in situ control of the observable and find optimal parameters to stabilize the projective measurement against control errors. This work is relevant to state preparation, quantum sensing, and quantum error correction via projective measurements.




Upper panels: contour of $\log_{10}N$ (N is the QND lifetime) for three different magnetic fields and CPMG periods as a function of controlling parameters. Middle and lower panels: $\log_{10}N_c$ ($N_c$ is the number of weak measurements to construct a projective measurement) and error tolerance for the waiting time $t_R$.

# 用弱测量合成对不守恒观测量的投影测量

王评, **杨文**, 刘仁保

对原子核自旋做投影测量对基于电子-核自旋复合系统的各类量子技术非常重要。直接测量核自旋很困难,通常对核自旋的测量是通过测量近邻的电子自旋来间接实现的。但是, 当核自旋与电子自旋的耦合非常微弱时, 很难在电子自旋和被测核自旋间建立强纠缠, 从而无法通过测量电子自旋来实现对核自旋的投影测量。

最近, 北京计算科学研究中心杨文研究组与香港中文大学刘仁保研究组合作提出一种普遍的方法, 可以利用弱耦合的电子自旋来实现对核自旋的投影测量。该方法由两步组成: (1) 对电子自旋施加动力学去耦脉冲, 在电子自旋与核自旋间建立弱纠缠, 然后对电子自旋做投影测量, 它等效于对核自旋的弱测量; (2) 施加一系列上述弱测量, 通过调控相邻两次测量之间的核自旋演化, 使得这些弱测量满足量子非破坏测量的条件, 从而合成一个投影测量。传统的量子非破坏测量要求被测物理量跟自由演化哈密顿量对易, 而我们的方法可以测量不守恒的物理量, 还进一步提供了一系列可调参数来实时调控被测物理以及测量对实验误差的鲁棒性。我们的工作为基于投影测量的量子态制备、量子传感和量子纠错提供了理论指导。

◀ 第一行: 量子非破坏性的寿命(对数图$\log_{10}N$)随控制参数的变化
第二行: 合成一个投影测量所需弱测量的数量(对数图$\log_{10}N_c$ )随动力学去耦脉冲总时间的变化。
第三行: 控制参数$t_R$的容错性随动力学去耦脉冲总时间的变化。
每行的三副图分别对应三种不同的磁场和动力学去耦脉冲的组合

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# SUBGAP MODES IN TWO-DIMENSIONAL MAGNETIC JOSEPHSON JUNCTIONS

By Yinan Fang, Seungju Han, Stefano Chesi, and Mahn-Soo Choi

The interplay between ferromagnetism and superconductivity leads to remarkable phenomena, such as the formation of Yu-Shiba-Rusinov (YSR) bound states, the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) pairing mechanism, and the occurrence of 0-π phase transitions. A magnetic Josephson junction, formed by sandwiching a thin ferromagnetic (FM) layer between two superconductors (S), represents an ideal testbed for such fundamental effects, while also having important applications which range from weak signal sensing to quantum information processing.

So far, most studies considered 1D or quasi-1D models of such junctions, but a recent collaboration lead by Prof. Stefano Chesi of the Beijing Computational Research Center (CSRC) and Prof. Mahn-Soo Choi from Korea University, with a prominent role played by former CSRC researcher Dr. Yinan Fang (currently a faculty at Yunnan University), has discovered important features associated with the transverse motion of quasiparticles bounded to the ferromagnetic layer.

More specifically, the authors analyze a model which takes fully into account the two-dimensional geometry of the S/FM/S junction, thus allowing them to investigate in detail the subgap modes of the ferromagnetic junction. For clean superconductor-ferromagnet interfaces with strong interface coupling, the subgap modes develop flat quasiparticle bands, which turns out to be useful in engineering states which are highly localized by magnetic domain walls. Furthermore, the subgap modes undergo a 0-π transition that depends strongly on the momentum along the junction interface. The novel momentum-dependent transition would be seen in wave-vector-resolved measurements of the Josephson current. These findings might lead to other useful applications to spintronics, e.g., facilitate controlling the domain walls with high precision and speed.

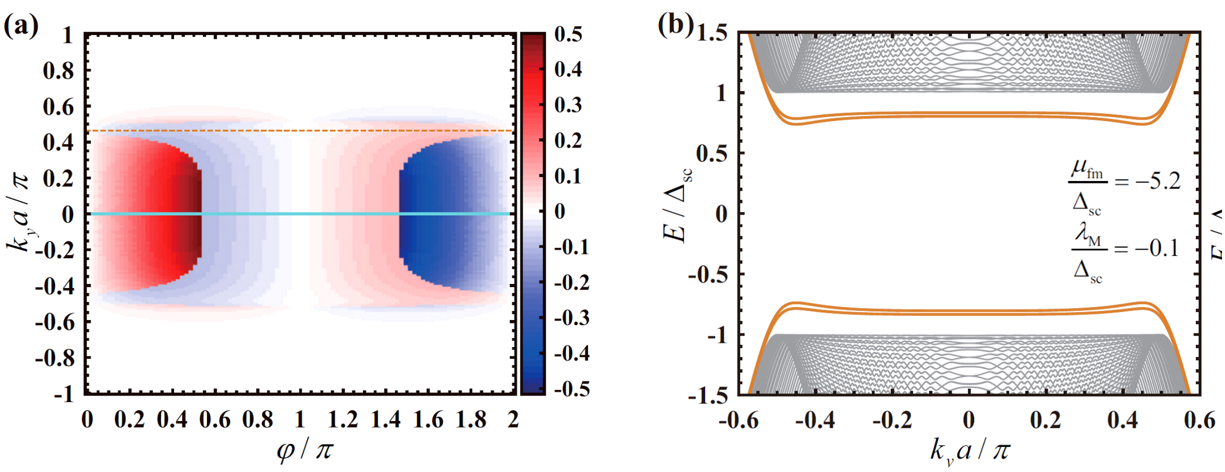


**Fig.** (a) Momentum-dependent Josephson current, (b): Subgap modes with a nearly flat dispersion

# 二维磁性约瑟夫森结中的亚能隙模式

房一楠, Seungju Han, Stefano Chesi, Mahn-Soo Choi

超导序与铁磁序的交互作用能够导致重要的物理现象, 如Yu-Shiba-Rusinov(YSR)束缚态的形成, Fulde–Ferrell–Larkin–Ovchinnikov(FFLO)配对机制, 以及0-π相变的发生。由两块超导体及夹在其之间的薄铁磁(FM)层构成的磁性约瑟夫森结是研究这些基本物理效应的理想系统, 并且无论是从微弱信号感知还是到量子信息处理, 它都具有重要的物理应用。

到目前为止, 绝大多数以往研究的关注点均是一维或者准一维的磁性约瑟夫森结, 然而最近一项由北京计算科学研究中心Stefano Chesi研究员以及其前博士后房一楠博士(现任职于云南大学)与高丽大学Mahn-Soo Choi教授领导的合作研究中指出, 束缚于铁磁层中准粒子的横向运动能够导致重要的物理效应。

具体而言, 该项工作的研究者们分析了具有二维几何特征的S/FM/S磁性约瑟夫森结, 通过理论模型他们仔细的研究了磁性约瑟夫森结的亚能隙模式。对于具有强界面耦合的干净超导-铁磁界面, 这些亚能隙模式能够导致具有平带特征的准粒子色散, 这有助于调控由于磁畴壁束缚引起的准粒子束缚态。此外, 这些亚能隙模式的0-π转变还强烈的依赖性于平行于磁性约瑟夫森结界面的动量。这一新奇的动量依赖效应可以通过波矢分辨的约瑟夫森电流测量加以观测。该项研究结果有助于自旋电子学中的相关应用，例如对铁磁纳米线中磁畴壁的高精度控制及其快速移动。

◀ 图 (a): 动量依赖的约瑟夫森电流； (b): 具有平带特征的亚能隙模式。

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# UNIVERSALITY AND CRITICALITY OF THE FERMI SIGN PROBLEM

By Rubem Mondaini, Sabyasachi Tarat and Richard T. Scalettar

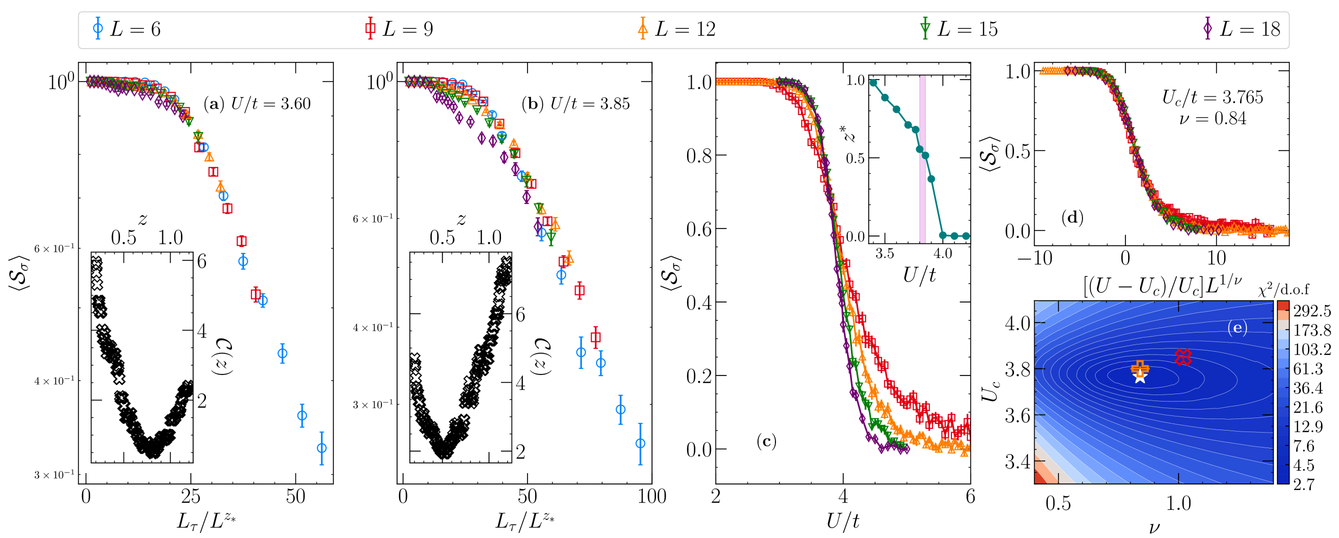
The sign problem (SP) is the main hurdle that prevents the systematic extraction of solutions to quantum many-body problems. It permeates various fields, ultimately having a central impact on materials science, quantum chemistry, and quantum field theory, as well as ultracold atoms and quantum computation. Thus, greater insight into the sign problem has important implications across these many disciplines.

Concretely, it manifests when instead of obtaining exact quantum many-body wave functions, one instead settles for statistical estimation of physical quantities via a Monte Carlo scheme, for example. In the absence of special symmetries, the corresponding weights of the quantum configurations that govern the construction of the Markov chain can be negative. This stands in contrast with classical models in which these weights (or corresponding probabilities) are positively defined. To overcome this hurdle and construct an importance sampling obeying detailed balance, one takes the absolute values of the weights, which results in the statistical estimation of the physical quantities being modified, incorporating the average value of the sign of the weights in it. It is often argued that the SP is not intrinsic to the physics of particular Hamiltonians, because its behavior can be influenced by the choice of algorithm.

Despite that, Prof. Rubem Mondaini (CSRC), together with his former postdoc Sabyasachi Tarat (CSRC), collaborated with Prof. Richard Scalettar (University of California, Davis) and took a 'step back' to understand how the sign problem was tied to critical behavior. The demonstration of this conjecture is simple: Given that phase transitions are inherently reflected in non-analytic behavior of the free energy (or compositions of it, as the partition function), this means that the average sign, being a ratio of partition functions of the original and the reference system [1, 2],

$$\langle s \rangle_{|W|} = \frac{\mathcal{Z}_W}{\mathcal{Z}_{|W|}}$$

can be used to reflect critical behavior at a



given point $x_c$ if the original physical model (and original partition function $\mathcal{Z}_W$ is non-analytic at this same point, provided that $\mathcal{Z}_{|W|}$ is sufficiently analytic in this domain.

To show the generality of this argument, they have studied a variety of physical models that host either quantum or thermal phase transitions (see Fig. 1 for an example of the former) and obtained the location of the corresponding critical point, matching the best estimates to date that take into account the scaling of physical l quantities. By further allowing the extraction of the related critical exponents associated with the divergence of the correlation lengths at the transition, they can use that to have a 'peek' at the corresponding universality classes of the corresponding phase transitions. This research, recently published in the Physical Review B [3], after a qualitatively studied recently published in Science [4] along the same lines, has spurred the systematic investigation of a variety of other cases within Prof. Mondaini's group in which this rationale is systematically applied. The hope is that by corroborating the results of known phase transitions, one can use the same ideas for phase transitions which are still under debate and for which no field-theory description exists thus far.

**Fig 1.** The scaling of the spin-resolved sign $\langle \mathcal{S}_\sigma \rangle$ in the SU(2) Hubbard model on the honeycomb lattice. $\langle \mathcal{S}_\sigma \rangle$ exhibits scaling behavior $\langle \mathcal{S}_\sigma \rangle(u, L, L_\tau) = f(uL^{1/\nu}, L_\tau/L^z)$ similar to that of physical quantities, which establish the way at which one approaches the non-analytic behavior at $U = U_c$ . By independently fitting the parameters associated with both arguments of the scaling function, we find the critical coupling $U_c$ and the critical exponent governing the divergence of the correlation lengths $\nu$ to be close to the best estimations to date of these parameters, obtained by using physical quantities instead. Adapted from Phys. Rev. B 107, 245144 (2023), Ref. [3].

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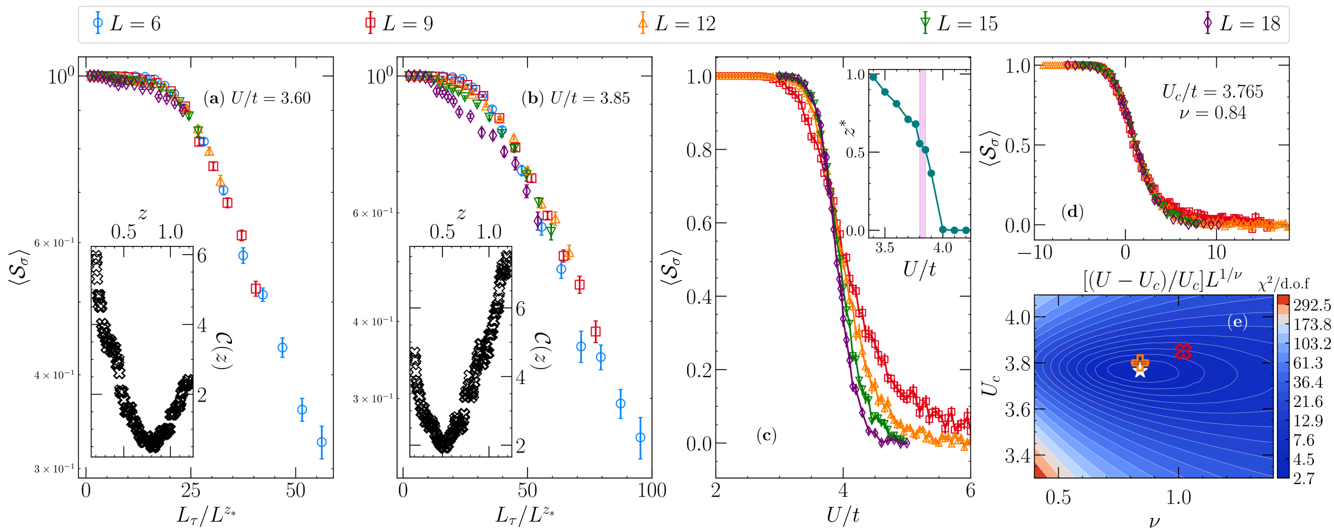


图 1: 蜂窝格子上的SU(2)哈伯德模型的自旋分解符号 $\langle \mathcal{S}_\sigma \rangle$ 的标度。$\langle \mathcal{S}_\sigma \rangle$ 存在与物理量类似的标度行为 $\langle \mathcal{S}_\sigma \rangle(u, L, L_\tau) = f(uL^{1/\nu}, L_\tau/L^z)$，这意味着它在 $U = U_c$ 处表现出非解析性。通过独立拟合与标度函数相关的两个参数，发现临界耦合参数 $U_c$ 与决定关联长度的散度的临界指数 $\nu$ 接近于迄今为止从物理量得到的此二参数的最佳估计值。*图引自 Phys. Rev. B 107, 245144 (2023), Ref. [3]*。


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# 费米符号问题的普适性和临界性

Rubem Mondaini, Sabyasachi Tarat and Richard T. Scalettar

符号问题是系统地求解量子多体问题的主要障碍。它涉及到多个领域, 最终对材料科学、量子化学、量子场论以及超冷原子和量子计算产生至关重要的影响。因此，更深入地符号问题对上述学科有着重大的意义。

具体地说, 它表现在通过蒙特卡洛方案求解物理量的统计估计值，而不是求解严格的量子多体波函数。在没有特殊对称性的情况下, 控制马尔可夫链构造的量子构型对应的权重可以是负的, 而这些权重(或相应的概念)在经典模型中总是被很好的定义。为了克服这一阻碍, 我们需要构造一个服从细致平衡条件的重要性采样, 取权重的绝对值, 从而修改物理量的统计估计值, 使其包含权重的符号的平均值。符号问题通常不被认为是特定哈密顿量的物理所固有的, 以为它的表现会受到所选择的算法的影响。

尽管如此, Rubem Mondaini教授(北京计算科学研究中心)及其前博士后Sabyasachi Tarat(北京计算科学研究中心)与Richard Scalettar教授(美国加州大学戴维斯分校)合作, “退一步”去理解符号问题如何与临界行为联系在一起。这个猜想的证明很简单: 考虑到相变本质上反映在自由能(或它作为配分函数的组成部分)的非解析行为中, 这意味着符号的平均值, 就是原始系统和参考系统的配分函数的比值[1, 2]

$$\langle s \rangle_{|W|} = \frac{\mathcal{Z}_W}{\mathcal{Z}_{|W|}}$$

它可以用来反应给定的原始物理系统(或原始配分函数 $\mathcal{Z}_W$ )非解析但在剩下的参数区域都解析的点的临界行为。

为了证明这一论点的普遍性, 他们研究了各种物理模型, 如量子相变和力学相变 (图1是前者的一个例子), 获得了与迄今为止通过物理量获得的标度的最佳估计值相匹配的临界点的位置。通过进一步提取关联长度临界指数, 他们可以使用它来“窥视”相变对应的普适性类。在近期发表在《科学》 [4]上的一项基于同样思路的定性研究之后, 发表在《物理评论B》[3]上的这项研究, 激发了Mondaini研究团队中对各种其他案例的系统性研究(这些案例基本都应用了这一理论基础)。希望通过验证已知相变的结果, 可以将同样的思想用于仍在争论中并且迄今为止还没有场论描述的相变。

# PHONON-MEDIATED MIGDAL EFFECT IN SEMICONDUCTOR DETECTOR

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). While there have been well-established methods treating the Migdal effect in isolated atoms, a coherent and complete description of the valence electrons in a semiconductor is still absent. The bremsstrahlung-like approach is a promising attempt, but it turns invalid for DM masses below a few tens of MeV. In this work, we lay out a framework where phonon is chosen as an effective degree of freedom to describe the Migdal effect in semiconductors. In this picture, a valence electron is excited to the conduction state via exchange of a virtual phonon, accompanied by a multi-phonon process triggered by an incident DM particle. Under the incoherent approximation, it turns out that this approach can effectively push the sensitivities of the semiconductor targets further down to the MeV DM mass region. This work was published in Physical Review D as an editor's suggestion.

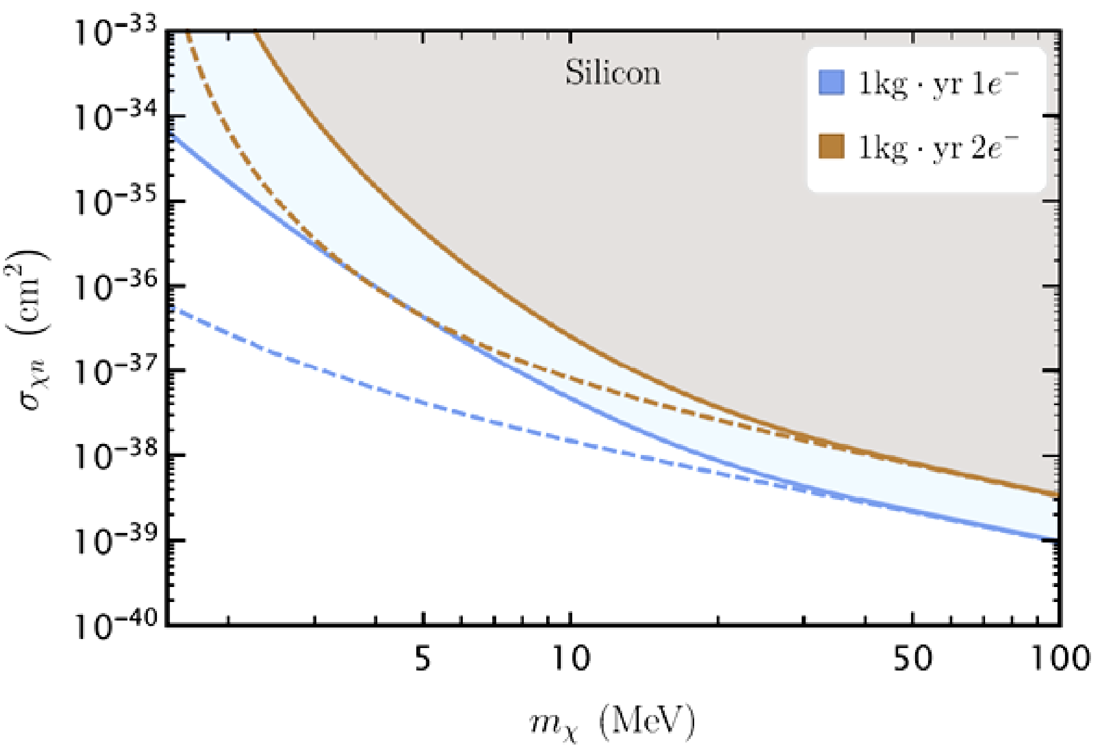


**Fig 1.** The sensitivities of single-electron (blue) and two-electron (orange) ionization signals caused by Migdal effect detected by silicon detectors. The solid and the dashed curves are calculated using the phonon-mediated approach and the bremsstrahlung-like approach.

# 半导体探测器中声子介导的 MIGDAL 效应

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 (WIMP) 的直接探测。尽管现有方法能够完善地处理孤立原子的 Migdal 效应, 但对半导体中的价电子仍然缺乏自洽完备的描述。科研人员尝试通过类韧致方法解决该问题, 结果表明该方法无法用于质量低于几十 MeV 暗物质的探测。为了克服上述问题, 北京计算科学研究中心莫崇杰副研究员、北京化工大学梁正良博士、北京理工大学郑法伟教授和北京应用物理与计算数学研究所张平研究员合作,将声子作为有效自由度建立了一套描述半导体中 Migdal 效应的理论框架。基于该图像, 价电子通过虚拟声子的交换激发到传导态, 同时伴随入射暗物质粒子触发的多声子过程。结果表明该方法可以有效地将半导体靶材的灵敏度推向 MeV 暗物质质量范围。

该工作作为编辑推荐在《物理评论D》上发表。

◀ 图 1: 硅探测器探测 Migdal 效应引起单电子(蓝色)和双电子(橙色)电离信号的灵敏度。实线和虚线分别表示声子介导和类韧致辐射的结果。

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# STABLE ATOMIC MAGNETOMETER IN PARITY-TIME SYMMETRY BROKEN PHASE

By Xiangdong Zhang#, Jinbo Hu, Nan Zhao*

Random motion of spins is usually detrimental in magnetic resonance experiments. The spin diffusion in nonuniform magnetic fields causes broadening of the resonance and limits the sensitivity and the spectral resolution in applications like magnetic resonance spectroscopy. Here, by observation of the parity-time (PT) phase transition of diffusive spins in gradient magnetic fields, we show that the spatial degrees of freedom of atoms could become a resource, rather than harmful, for high-precision measurement of weak signals. In the normal phase with zero or low gradient fields, the diffusion results in dissipation of spin precession. However, by increasing the field gradient, the spin system undergoes a PT transition, and enters the PT symmetry broken phase. In this novel phase, the spin precession frequency splits due to spatial localization of the eigenmodes. We demonstrate that, using these spatial-motion-induced split frequencies, the spin system can serve as a stable magnetometer, whose output is insensitive to the inevitable long-term drift of control parameters. This opens a door to detect extremely weak signals in imperfectly controlled environments.

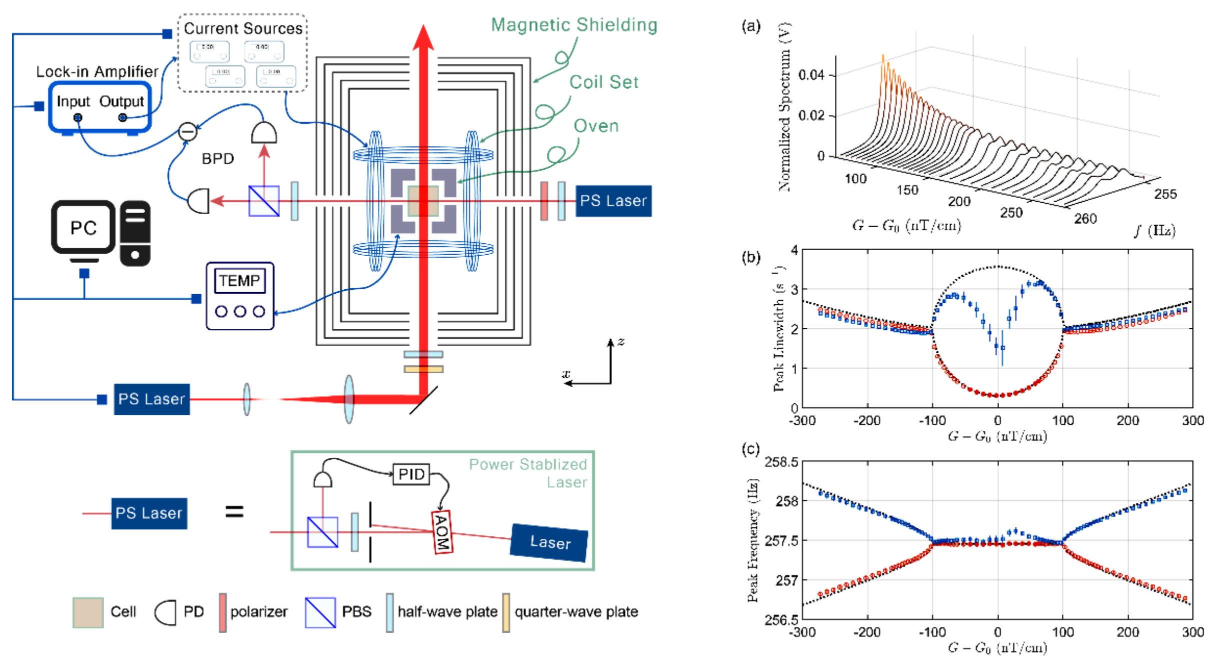


**Fig 1.** Left subplot, experimental setup. A cubic glass cell containing Xe gas and Rb metal is placed inside a magnetic shielding and heated. A parametric magnetometer is used to detect the nuclear spin signals. Right subplot, the eigenvalue spectrum of diffusive spins. (a) The Fourier spectrum of measured FID signals of $^{129}$Xe spins as a function of gradient field strength $\boldsymbol{G}$. (b), (c) The linewidth and precession frequency of $^{129}$Xe FID signal. An exceptional point can be found at $|G-G_0| \approx 100$ nT/cm, indicating a PT symmetry breaking at that position.

# 利用PT破缺相的稳定原子共磁力仪

张祥栋#，胡锦波，赵楠*

在气体核磁共振系统中，扩散效应通常起到负面的作用。在非均匀的磁场中，自旋扩散会导致磁共振谱线的展宽，从而限制谱线的分辨率和测量灵敏度。然而，通过求解 Torrey 方程可以发现，当磁场梯度大于某一个阈值时，扩散效应会使自旋系统的本征模式发生 PT 对称性破缺。在 PT 破缺相中，扩散效应使自旋磁共振谱线发生劈裂，引入了额外的实验可观测量。在这个工作中，我们在 $^{129}$Xe-$^{131}$Xe 核磁共振系统中对此PT对称性破缺过程进行了深入的研究，观测到了完整的对称性破缺过程，并利用 PT 破缺相提供的额外可观测量，实现了对环境变化不敏感的稳定原子共磁力仪，极大地提高了原子共磁力仪的长期稳定性。这一实验工作加深了我们对核自旋空间分布演化规律的理解，同时也改变了原子共磁力仪研究中一贯认为的“磁场梯度需要尽可能地消除”这一常识，为原子共磁力仪技术的发展提供了一种新的思路。

图　左图：实验装置示意图。右图：实验观测到的核自旋 FID 的本征值谱，PT 对称性破缺发生在(b)(c)图中的分叉点。(a)不同磁场梯度 $G$ 下观测到的 $^{129}$Xe 核自旋 FID 频谱。(b)(c) FID信号的线宽和共振频率，在 $|G-G_0|\approx 100$ nT/cm 处可以看到 EP 点，指示该处可能发生了 PT 对称性破缺。

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# PROBING THE SYMMETRY BREAKING OF A LIGHT–MATTER SYSTEM BY AN ANCILLARY QUBIT

By Shuai-Peng Wang, Alessandro Ridolfo, Tiefu Li*, Salvatore Savasta*, Franco Nori, Y. Nakamura & J. Q. You*

Hybrid quantum systems in the ultrastrong, and even more in the deep-strong, coupling regimes can exhibit exotic physical phenomena and promise new applications in quantum technologies. In these nonperturbative regimes, a qubit–resonator system has an entangled quantum vacuum with a nonzero average photon number in the resonator, where the photons are virtual and cannot be directly detected. The vacuum field, however, is able to induce the symmetry breaking of a dispersively coupled probe qubit. We experimentally observe the parity symmetry breaking of an ancillary Xmon artificial atom induced by the field of a lumped-element superconducting resonator deep-strongly coupled with a flux qubit. This result opens a way to experimentally explore the novel quantum-vacuum effects emerging in the deep-strong coupling regime.

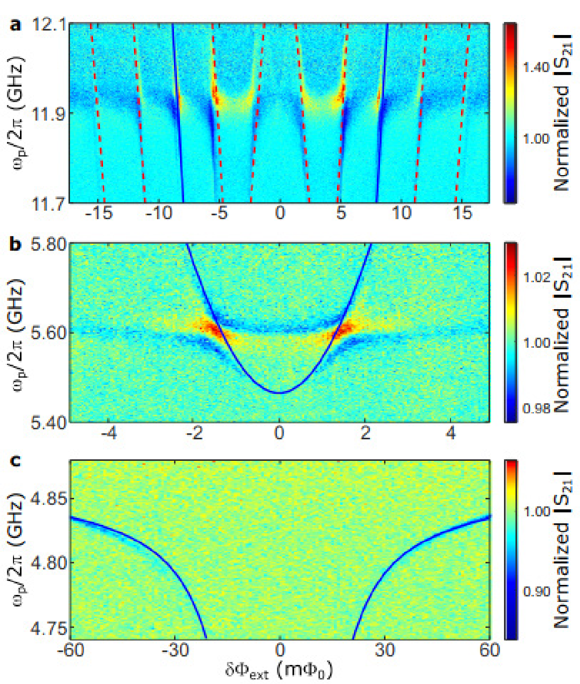


**Fig 1.** (left). Reflection spectra. Reflection spectra of the deep-strongly coupled qubit–resonator system versus the external flux bias $\delta\Phi_{ext}$ and the probe frequency $\omega_p$. The solid blue curves in a–c are the fitted transition frequencies between the ground state to the third-, second- and first-excited states of the qubit–resonator system, respectively (i.e., $\omega_{03}$, $\omega_{02}$, and $\omega_{01}$). In a, the additional transitions indicated by the dashed red curves correspond to sideband transitions (assisted by the Xmon levels) in the system.

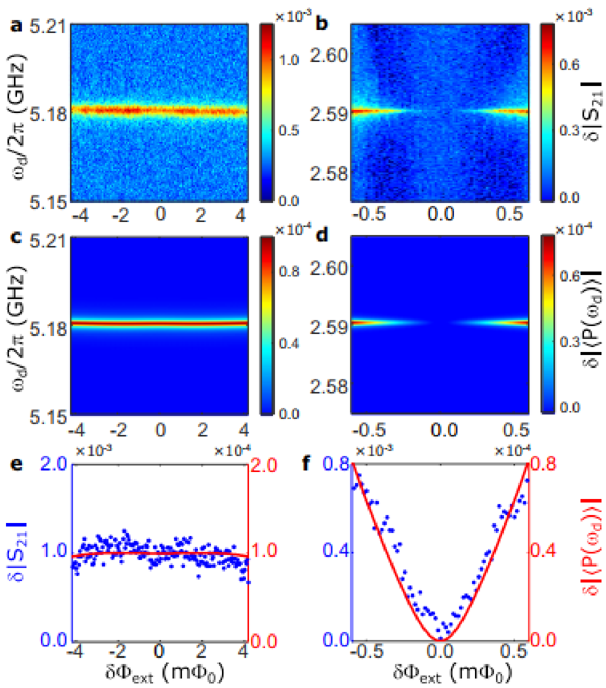


**Fig 2.** (right). Excitation spectra. Excitation spectra of the Xmon qubit versus the external flux bias $\delta\Phi_{ext}$ and the drive frequency $\omega_d$. a and b show the experimental results, corresponding to the single- and two-photon transitions of the Xmon qubit with frequencies $\omega_X$ and $\omega_X/2$ , respectively. c and d show the simulated results. The theoretical calculations display the changes in the amplitude of the Xmon polarization $|\langle P(\omega_d)\rangle|$. e, f Cross sections along the excitation spectra in a (b) and c (d) when $\omega_d/2\pi$ = 5.181 GHz (2.5905 GHz).

# 利用辅助量子比特探测光–物质耦合系统的对称性破缺

王帅鹏, Alessandro Ridolfo, 李铁夫*, Salvatore Savasta*, Franco Nori, Y. Nakamura, 游建强*

杂化量子系统在超强，或更进一步在深强耦合区域，将展现奇异的物理现象，对量子技术的新应用具有潜在价值。在这些非微扰区域，一个量子比特与谐振腔耦合的系统将具有纠缠的量子真空，其中谐振腔的平均光子数非零，但这些光子是虚光子，无法直接探测。然而，这一真空场却能够诱导一个与之色散耦合的探针量子比特发生对称性破缺。我们在实验上观测到了一个辅助 Xmon 人工原子的宇称对称破缺，这一破缺是由与一个集总元件谐振腔的真空场相互作用所诱导的。谐振腔真空场的特殊性来源于与一个超导磁通量子比特之间的深强耦合相互作用。这一实验结果为后续进一步研究光与物质深强耦合区域的量子真空效应打开了道路。

◀ 图 1 (左图)：深强耦合量子比特与谐振腔耦合系统的反射谱。图a到图c中的蓝色实线表示从系统基态到第三，第二和第一激发态的跃迁频率 (即 $\omega_{03}$， $\omega_{02}$和 $\omega_{01}$）。图a中红色虚线是系统中由 Xmon 辅助产生的边带跃迁。

图 2 (右图)：探针量子比特激发谱。图a和b是实验结果，分别表示 Xmon 量子比特的单光子和双光子跃迁。同时存在单光子和双光子跃迁表示探针比特发生宇称对称破缺。图c和d是数值模拟结果。图e和f是在频率 $\omega_d/2\pi$ = 5.181 GHz（2.5905 GHz）位置的截线。

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# TOPOLOGICAL PHASE TRANSITIONS AND MOBILITY EDGES IN NON-HERMITIAN QUASICRYSTALS

By Quan Lin, Tianyu Li, Lei Xiao, Kunkun Wang, Wei Yi*, and Peng Xue*

Non-Hermiticity significantly enriches the properties of topological models, leading to exotic features such as the non-Hermitian skin effects and non-Bloch bulk-boundary correspondence that have no counterparts in Hermitian settings. Its impact is particularly illustrating in non-Hermitian quasicrystals where the interplay between non-Hermiticity and quasi periodicity results in the concurrence of the delocalization-localization transition, the parity-time (PT)-symmetry breaking, and the onset of the non-Hermitian skin effects. Here we experimentally simulate non-Hermitian quasicrystals using photonic quantum walks. Using dynamic observables, we demonstrate that the system can transit from a delocalized, PT-symmetry broken phase that features non-Hermitian skin effects, to a localized, PT-symmetry unbroken phase with no non-Hermitian skin effects. The measured critical point is consistent with the theoretical prediction through a spectral winding number, confirming the topological origin of the phase transition. Our work opens the avenue of investigating the interplay of non-Hermiticity, quasi periodicity, and spectral topology in open quantum systems.

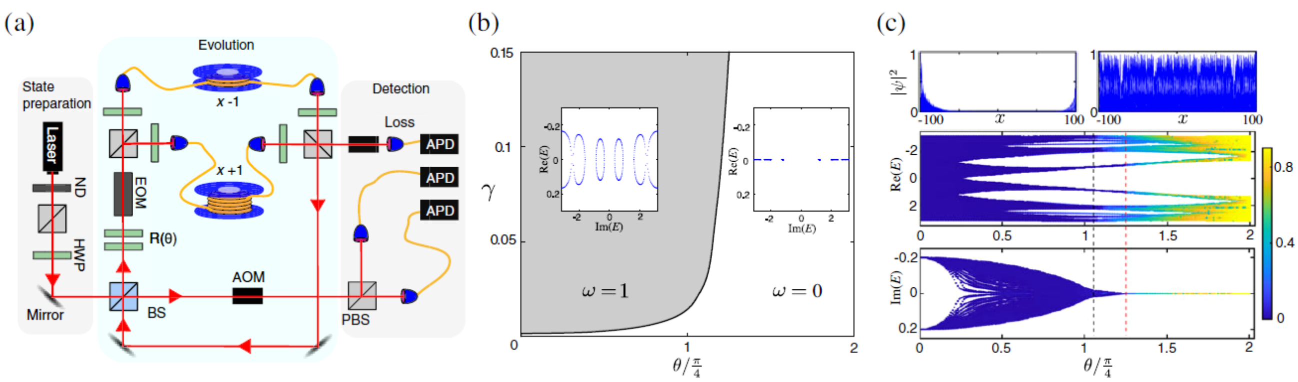


**Fig 1.** Simulation of non-Hermitian quasicrystals. (a) A cartoon illustration of \Tout{the} quantum-walk dynamics. Operators S and R are defined in the main text. Lattice sites are located at the crossing points of the laser beams (red). The dashed grey curves illustrate the quasiperiodic phase (or a quasiperiodic potential for the effective Hamiltonian) introduced by the phase operator $P_{1,2}$. (b) A time-multiplexed implementation of the photonic quantum walk illustrated in (a). ND: neutral density filter; HWP: half-wave plate; AOM: optical switch acousto-optic modulator; EOM: electro-optic modulator; BS: beam splitter; PBS: polarizing beam splitter; APD: avalanche photo-diode. (c) Phase diagram of the spectral winding number ω. Insets are the typical eigenspectra of the two phases on the complex plane with a fixed $\Upsilon=0.1$, and $\theta=\pi/8$ for $\omega=1$ and $\theta=3\pi/8$ for $\omega=0$. The phase boundary here not only marks the onset of the non-Hermitian skin effect, but also the PT-symmetry breaking point and the delocalization-localization transition. (d) Top panel: spatial distribution of all eigenstates of U under the OBC, for the phase with $\omega=1$ (left) and $\omega=0$ (right), respectively. Middle panel: The real components of the eigenenergies E of the effective Hamiltonian H (under PBC) with increasing θ, colored according to their respective inverse participation ratio IPR. Lower panel: The imaginary components of the eigenenergies with increasing θ (under PBC), colored according to the IPR. For the numerical simulations, we take the lattice size N=200 and $\Upsilon=0.1$.

# 非厄米准晶中的拓扑相变和迁移率边

林泉，李天宇，肖磊，王坤坤，易为*，薛鹏*

非厄米性显著丰富了拓扑模型的性质，导致了非厄米趋肤效应和非布洛赫体边对应等在厄米环境中没有对应物的奇异特性。它的影响尤其体现在非厄米准晶中，非厄米和准周期性之间的相互作用导致了退局域化-局域化转变，宇称-时间 (PT) 对称性破缺和非厄米趋肤效应的出现。我们利用光子量子行走实验模拟了非厄米准晶，且利用动力学可观测量，我们证明了系统可以从具有非厄米趋肤效应的PT对称破缺相转变为无非厄米趋肤效应的局域 PT 对称未破缺相。测量的临界点通过一个光谱缠绕数与理论预测一致，证实了相变的拓扑起源。更有趣的是，我们还提供了非厄米诱导的迁移率边的第一个实验证据。我们的工作为研究开放量子系统中非厄米性、准周期性和谱拓扑的相互作用开辟了新的途径。

◀ 图 1: 非厄米准晶的模拟。(a)光子量子行走的时分复用实现。ND：中性密度滤膜；HWP：半波片；AOM：光开关声光调制器；EOM：电光调制器；(P) BS：(偏振)分束器；APD：雪崩光电二极管。(b)频谱绕数的相图。嵌入的子图为特定参数下的复平面上两相的典型本征谱。这里的相边界不仅标志着非厄米趋肤效应的开始，也是PT对称破缺点和退局域化-局域化转变。(c)上面板：分别为相位为 $\omega=0$ (左)和 $\omega=1$ (右)的 U 在 OBC 下所有本征态的空间分布。中间面板：有效哈密顿量H (在PBC下) 的本征能量E的实分量随 $\theta$ 的增加的变化，根据它们各自的逆参与率 IPR 着色。下面板：本征能量随 $\theta$ 增加的虚部变化(PBC)，且按 IPR 着色。对于数值模拟，我们取晶格尺寸为200且 $\Upsilon=0.1$。黑色和红色垂直虚线分别表示迁移率边在特征谱分中出现和结束的位置。

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# SYNCHRONOUS OBSERVATION OF BELL NONLOCALITY AND STATE-DEPENDENT CONTEXTUALITY

By Peng Xue*, Lei Xiao, G. Ruffolo, A. Mazzari, T. Temistocles, M. Terra Cunha, and R. Rabelo*

Bell nonlocality and Kochen-Specker contextuality are two remarkable nonclassical features of quantum theory, related to strong correlations between outcomes of measurements performed on quantum systems. Both phenomena can be witnessed by the violation of certain inequalities, the simplest and most important of which are the Clauser-Horne-Shimony-Holt (CHSH) and the Klyachko-Can-Binicioğlu-Shumovski (KCBS), for Bell nonlocality and Kochen-Specker contextuality, respectively. It has been shown that, using the most common interpretation of Bell scenarios, quantum systems cannot violate both inequalities concomitantly, thus suggesting a monogamous relation between the two phenomena. In this Letter, we show that the joint consideration of the CHSH and KCBS inequalities naturally calls for the so-called generalized Bell scenarios, which, contrary to the previous results, allows for joint violation of them. In fact, this result is not a special feature of such inequalities: We provide very strong evidence that there is no monogamy between nonlocality and contextuality in any scenario where both phenomena can be observed. We also implement a photonic experiment to test the synchronous violation of both CHSH and KCBS inequalities. Our results agree with the theoretical predictions, thereby providing experimental proof of the coexistence of Bell nonlocality and contextuality in the simplest scenario, and lead to novel possibilities where both concepts could be jointly employed for quantum information processing protocols.

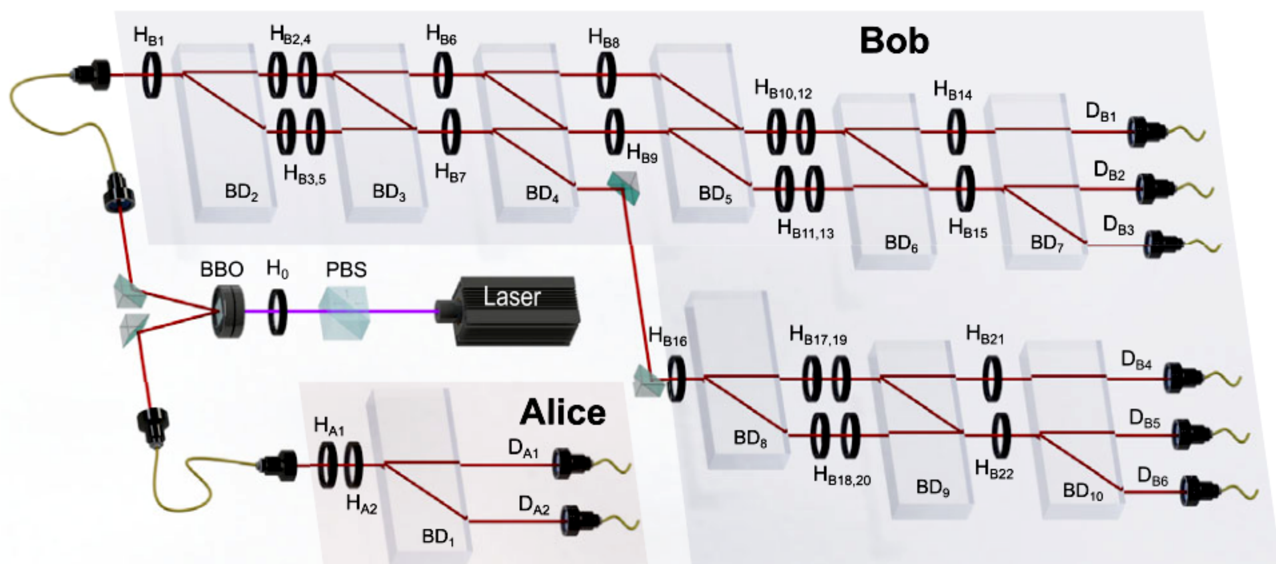


**Fig. 1.** Illustration of the experimental setup. Polarization entangled photon pairs are generated via type-I spontaneous parametric down-conversion where two joint β-BBO crystals are pumped by a continuous wave diode laser. Qubit is encoded in the horizontal and vertical polarizations of one photon of each pair, while qutrit is encoded in both polarizations and spatial modes of the other photons of the entangled pairs, which are split in different paths dependent on their polarizations via a beam displacer (BD). For Alice, observables Ai are measured via standard polarization measurements using a half-wave place (HWP) and a BD. For Bob, cascade Mach-Zehnder interferometers for sequentially measuring observables $B_j$ and $B_{j+1 \text{ mod} 5}$ are used to test the KCBS inequality.

# 贝尔非局域性和态依赖的互文性的同步观测

薛鹏*，肖磊, G. Ruffolo, A. Mazzari, T. Temistocles, M. Terra Cunha, and R. Rabelo*

Bell 非局域性和 Kochen-Specker 互文性是量子理论的两个显著的非经典特征，与对量子系统进行测量的结果之间的强相关性有关。这两种特性都可以通过违反某些不等式来证明，其中最简单且最重要的是 Clauser-Horne-Shimony-Holt（CHSH）和 Klyachko-Can-Binicio lu-Shumovsky（KCBS）不等式，他们分别用于Bell非局域性和 Kochen-Specker 互文性的验证。已经证明，使用 Bell 场景的最常见解释，量子系统不能同时违反这两个不等式，因此暗示了这两种现象之间的一种单婚性关系。在我们的研究工作表明，联合考虑 CHSH 和 KCBS 不等式自然引出的广义贝尔场景，这与以前的结果相反，允许它们的联合违反。实际上，这个结果并不是这些不等式的特殊特征：我们提供了非常强的证据，表明在任何可以观察到这两种现象的场景中，非局域性和情境性之间都不存在单婚性。我们还用单光子实验验证了同时违反 CHSH 和 KCBS 不等式。我们的结果与理论预测一致，从而为 Bell 非局域性和互文性在最简单的场景中的共存提供了实验证据，并引出了两个概念可以共同用于量子信息处理协议的新可能性。

◀ 图 1：实验设备的示意图。通过I-型自发参量下转换制备纠缠光子对，其中两个胶合的 β-BBO 晶体被连续波二极管激光器泵浦，生成偏振纠缠的光子对。量子比特被编码在每对光子的偏振中，其中一个光子的三能级量子体系则被编码在纠缠光子的偏振和空间模式中，这些光子通过光束位移器 (BD) 分开到不同的路径中。对于 Alice，通过使用半波片 (HWP) 和 BD 进行标准的偏振测量来测量观察量 $A_i$。对于 Bob，通过级联马赫-曾德尔干涉仪依次测量观察量 $B_j$ 和 $B_{j+1\ \mathrm{mod}5}$，用来测量 KCBS 不等式。

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# OBSERVATION OF DARK EDGE STATES IN PARITY-TIME-SYMMETRIC QUANTUM DYNAMICS

By Peng Xue*, Xingze Qiu, Kunkun Wang, Barry C. Sanders and Wei Yi

Topological edge states arise in non-Hermitian parity-time (PT)-symmetric systems, and manifest themselves as bright or dark edge states, depending on the imaginary components of their eigenenergies. As the spatial probabilities of dark edge states are suppressed during the non-unitary dynamics, it is a challenge to observe them experimentally. Here we report the experimental detection of dark edge states in photonic quantum walks with spontaneously broken PT symmetry, thus providing a complete description of the topological phenomena therein. We experimentally confirm that the global Berry phase in PT-symmetric quantum-walk dynamics unambiguously defines topological invariants of the system in both the PT-symmetry-unbroken and-broken regimes. Our results establish a unified frame work for characterizing topology in PT -symmetric quantum-walk dynamics, and provide a useful method to observe topological phenomena in PT -symmetric non-Hermitian systems in general.

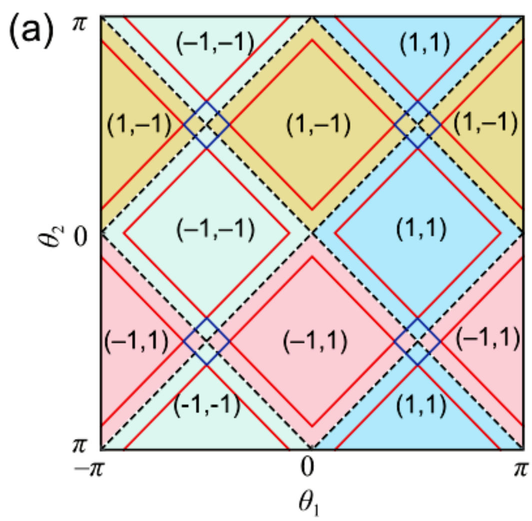


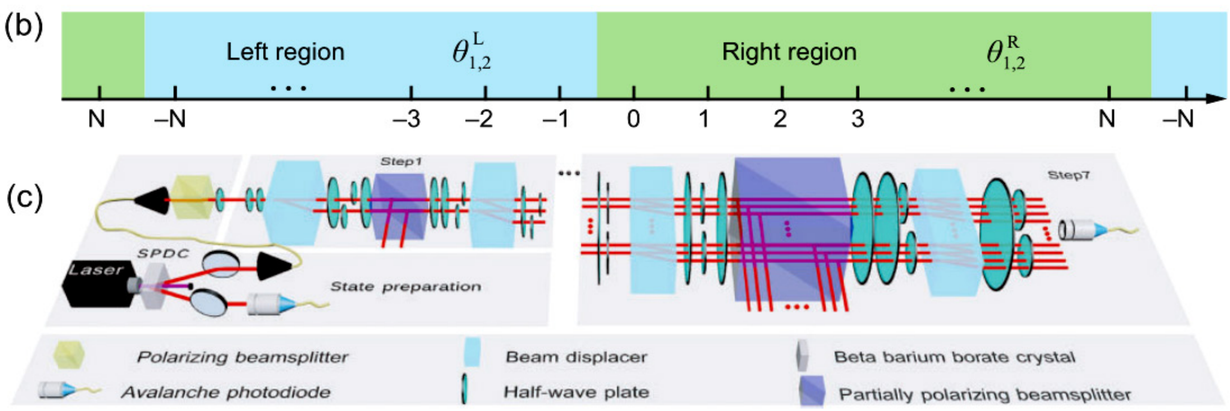

**Fig 1.** Phase diagram and experimental setup. (a) Phase diagram for PT -symmetric non-unitary QWs governed by **U**, with coin parameters ( $\theta_1$ , $\theta_2$ ) and corresponding topological numbers ( $\nu_0$ , $\nu_\pi$ ). Dashed black lines represent topological phase boundaries. Solid red lines represent boundaries between PT -symmetry-unbroken and -broken regimes, with PT -symmetry-broken regimes lying in between the red lines near topological phase boundaries. Solid blue squares represent regimes with completely broken PT symmetry, where the eigenspectra are purely imaginary. (b) Left $(x<0)$ and right $(x\geq 0)$ regions for the PT-symmetric QW. (c) Experimental setup for PT -symmetric QWs with alternating losses. The photon pair is created via spontaneous parametric down-conversion (SPDC). One photon serves as a trigger. The other photon is projected into the polarization state $|\pm\rangle$ (or $(|+\rangle + i|-\rangle)/\sqrt{2}$ and then proceeds through the quantum-walk interferometric network. Finally, the photon is detected by an avalanche photodiode (APD), in coincidence with the trigger one. Photon counts give measured probabilities after correcting for relative efficiencies of the different APDs.

# 在宇称–时间对称的动力学中观测到暗边界态

薛鹏*，邱型泽，王坤坤, Barry C. Sanders, 易为

非厄米的宇称-时间对称的系统中是存在边界态的，一般来说，根据边界态所对应的本征值虚部大小，边界态可以表现为亮边界态或者或暗的边界态。在非幺正动力学过程中，暗边界态的空间概率被抑制，这使得在实验中观测它们成为一项挑战。在这里，我们在具有PT自发破缺的光子量子行走中实验检测到了暗边缘态，从而完整描述了其中的拓扑现象。我们实验证实，PT 对称量子行走动力学中的全局Bell相可以无歧义地定义系统的拓扑不变量，无论 PT 对称未破缺还是破缺状态。我们的结果确立了一个统一的框架，用于表征 PT 对称量子行走动力学中的拓扑，并提供了一种观察 PT 对称非厄米系统中拓扑现象的有用方法。

▼ 图 1：相图和实验设备的示意图。(a)由 U 控制的 PT 对称非幺正量子行走的相图，其中包括硬币参数 ( $\theta_1$ , $\theta_2$ ) 和相应的拓扑数 ( $\nu_0$ ,$\nu_\pi$ )。虚线黑线表示拓扑相界限。实线红线表示 PT 对称未破缺和破缺状态之间的边界，而 PT 对称破缺状态则位于红线附近的拓扑相界限附近。实心蓝色方块表示完全破缺 PT 对称性的状态，其中本征谱是纯虚的。(b)PT 对称量子行走的左侧 (x＜0) 和右侧 (x ≥ 0) 区域。(c)带有交替损耗的 PT 对称量子行走的实验设置。光子对是通过自发参量下转换 (SPDC) 创建的。一个光子用作触发器，另一个光子被投射到极化态 $|\pm\rangle$(or $(|+\rangle + i|-\rangle)/\sqrt{2}$，然后通过量子行走干涉网络。最后，光子被雪崩光电二极管 (APD) 探测到，并与触发器光子实现符合测量。

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# ORIGIN OF STRUCTURE AND ZERO-PHONON-LINE ANOMALIES OF XV (X=Si, Ge, Sn, Pb) CENTERS IN DIAMOND

By Chen Qiu, Hui-Xiong Deng*, Songyuan Geng, Su-Huai Wei*

Color centers in diamonds have emerged as a promising candidate for quantum information and quantum computing applications. Compared to the well-known and widely studied nitrogen-vacancy NC-VC (NV) color center with $C_{3v}$ symmetry, the group-IV-vacancy color centers VC-X-VC (XV, X=Si, Ge, Sn, Pb), exhibit structures with the $D_{3d}$ symmetry, which give rise to more stable coherent optical transitions for the zero-phonon-line (ZPL) due to its inversion-symmetry. Moreover, it is experimentally found that the ZPL peak of XV centers increases from Si to Sn to Ge to Pb, i.e., it does not vary monotonically with the atomic numbers. So far, the physical origin of the unusual local structures and the abnormal trend of ZPL of the XV centers are not well understood. Researchers at CSRC, based on density functional theory calculations and symmetry analysis, demonstrate that the large size of the X atoms plays a dominant role in moving the X atoms away from the substitution site to the bond center site between the two carbon vacancies to form the $D_{3d}$ structure that can effectively reduce the local strain energy. Meanwhile, we find that the abnormal trends of ZPL of the XV centers derives from a competition of the $p-p$ coupling and $p-d$ coupling between X atoms and the divacancy based on the band coupling mechanism. Our study, therefore, provides insights into the origin of the abnormal trends of ZPL and the local structure of XV centers in diamonds.[1]

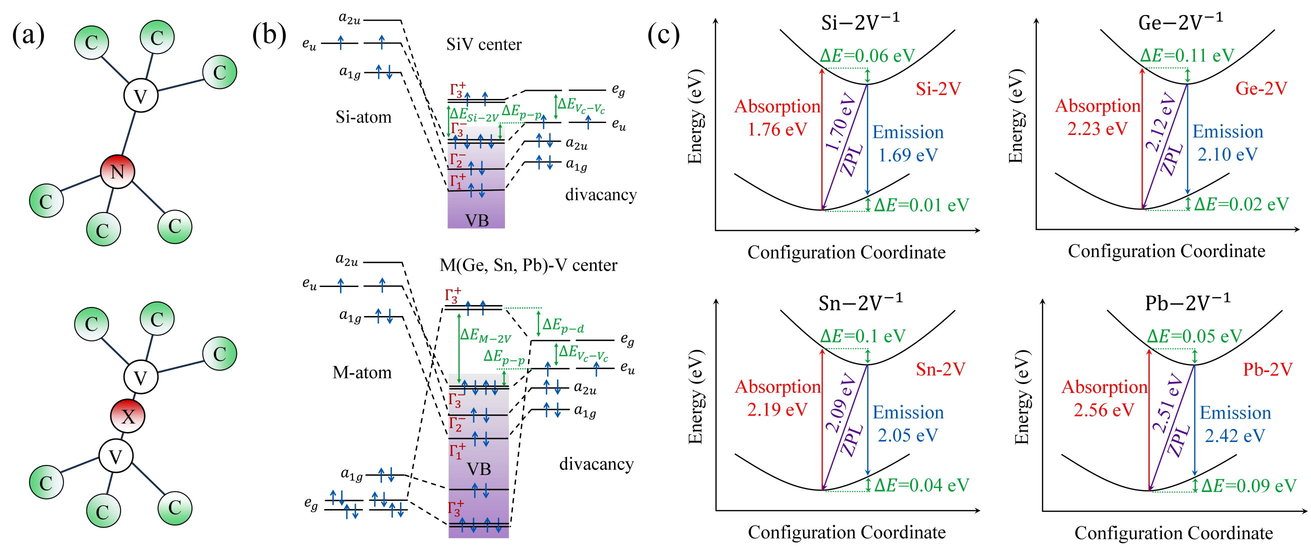


**Fig 1.** (a) Schematic plot of local structures of NV center and XV centers. The green balls are carbon atoms, white balls are lattice-vacancy and red balls are impurities. (b) The band coupling diagrams of the neutral SiV and MV (M=Ge, Sn, Pb) centers in diamond. The irreducible representations of the atomic orbitals and band states under $D_{3d}$ point group is shown. The orbitals of the Si and M atoms and the six-carbon dangling bond states of divacancy in diamond couples to form the valence band as schematically depicted. For simplicity, the level splitting caused by spin-orbital coupling is not considered in the diagrams. (c) Configuration coordinate diagrams for spin-conserving triplet excitation. Excitation cycles for $SiV^{1-}$ center, $GeV^{1-}$ center, $SnV^{1-}$ center and $PbV^{1-}$ center in diamond. Absorption, emission, structure-relaxation and ZPL transitions are indicated, along with their HSE06 calculated energies.

# 金刚石中四族色心结构与零声子线异常的起源

**邱晨**，邓惠雄*，耿松源，**魏苏淮***

金刚石中的色心已经在量子信息和量子计算应用中展现广泛的应用前景。与广为人知且深入研究的具有 $C_{3v}$ 对称性的氮-碳空位（氮替位-空位缺陷对）缺陷色心相比，四族空位色心（空位-四族元素间隙-空位缺陷对，四族元素分别为硅、锗、锡、铅）具有 $D_{3d}$ 对称性的结构。因为四族空位色心具有空间反演对称性，这使得其零声子线的相干光学跃迁更加稳定。此外，实验观察表明四族空位色心的零声子线峰值从硅逐步增加至锡、锗，再到铅，并未随着原子序数的增加而单调变化。迄今为止，四族空位色心具有空间反演对称性的局部结构及其零声子线异常趋势的物理本质仍未完全阐明。在本研究中，基于密度泛函理论计算和对称性分析，我们详细阐述了四族原子的较大尺寸对四族原子从替代位点转移至两个碳空位之间的键合中心位点以形成 $D_{3d}$ 结构的关键原因是这样的局部结构畸变能够极大的降低局部应力能。与此同时，我们发现四族空位色心中心的零声子线的异常趋势源于四族原子与双空位之间基于能带耦合机制的 $p-p$ 轨道耦合和 $p-d$ 轨道耦合间的竞争机制。由此，本研究深入揭示了四族空位色心异常零声子线趋势及其局部结构的物理起源。

◀ 图 1: a)氮-碳空位缺陷和四族空位缺陷局部结构的示意图。绿色球代表碳原子，白色球代表晶格空位，红色球代表杂质。b)金刚石中中性四族间隙-空位缺陷中心的能带耦合示意图。在 $D_{3d}$ 点群下，原子轨道和能带态的不可约表示如图所示。四族原子的轨道以及金刚石中双空位最近邻六个碳原子悬挂键按照示意图的方式耦合。为简单起见，示意图中未考虑自旋-轨道耦合引起的能级分裂。c)自旋守恒三重态激发的构型坐标图。

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# PLASMONIC PHOTOCATALYSIS WITH NONTHERMALIZED HOT CARRIERS

By Shengxiang Wu, Yu Chen, and Shiwu Gao*

Hot electron-hole pairs generated by plasmonic damping could provide an electronic channel for photocatalysis. However, its mechanism is unclear regarding how the nonthermalized hot carriers dynamically activate and promote the energy transfer processes. In addition, the competition with possible thermal effect is also under debate. Here, we develop a quantum-mechanical model to describe the molecular vibrational excitation and bond breaking based on the theory of vibrational heating induced by hot electrons. By treating the reaction rates with and without light illumination on equal footing, it is found that the nonthermal electrons in the high energy region can, albeit its much smaller populations, provide an efficient and dominant channel for photodissociation in the low-temperature and quantum plasmon regime. For $O_2$ dissociation on silver nanoparticles, this model well captures the wavelength dependence of photodissociation and qualitatively reproduces the enhancement factors observed in experiments. The results reveal the nonthermal hot-carrier mechanism and the underlying dynamics involved in plasmonic photocatalysis. It also provides a theoretical framework for quantitative analysis of the plasmonic energy harvesting and conversion utilizing surface plasmons.

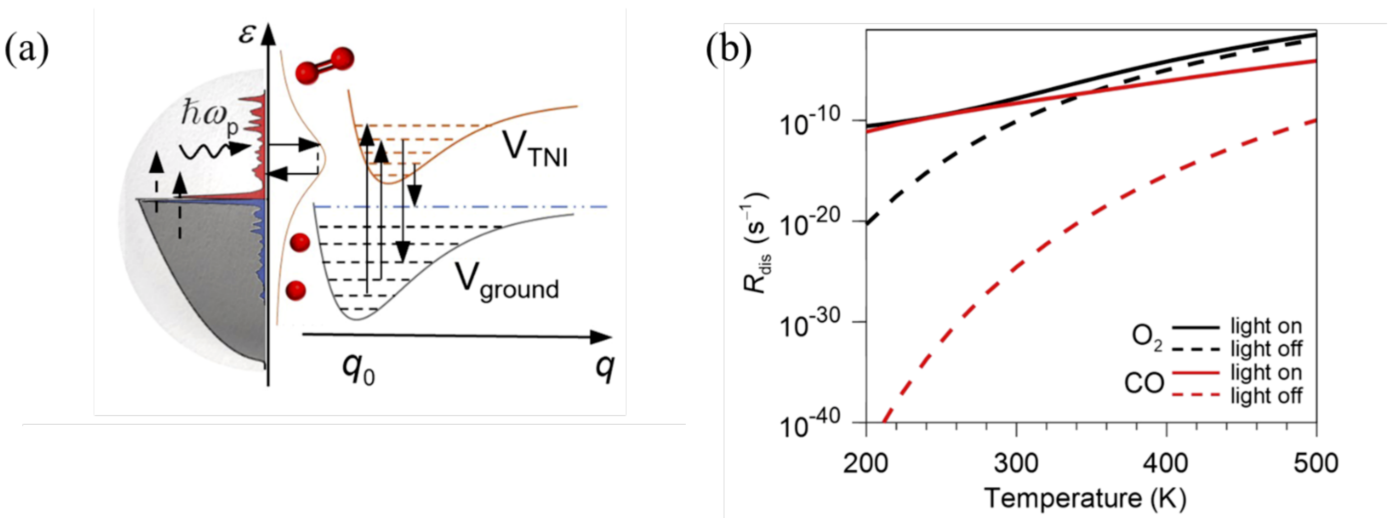


**Fig 1.** (a) Schematic nonthermal carrier transfer and vibrational excitation induced by plasmonic damping. (b) Reaction rates with (solid lines) and without (dashed lines) light of $O_2$ (black) and CO (red) dissociation.

# 等离激元热载流子的光催化反应机理的模型研究

吴盛祥，陈宇，高世武

等离激元弛豫产生的热电子-空穴对为光催化提供了新的可能路径。然而热载流子如何参与分子的振动激发并实现能量传递的微观机理和动力学过程尚不清楚。它与可能的热效应机制的竞争也存在争议。基于热电子-分子散射的理论框架，高世武教授课题组发展了等离激元热载流子诱导的分子振动激发和化学键分解的量子模型。通过对比光照和黑暗下的反应速率，研究发现高能的热电子，虽然其布居数很低，可以为光催化反应提供有效的反应途径，这个过程在低温和量子区间占主导作用。对于 $O_2$ 在银纳米球上分解这一模型体系，理论模型很好地描述了反应速率随波长的依赖关系，计算得到的反应增强因子与实验数据可以定性比拟。这些结果揭示了等离激元光催化反应的热载流子机制和增强效应的基本动力学过程。为进一步探索表面等离激元光催化，及其相关的能源转换过程提供了理论框架和基础。

图 1：(a)等离激元弛豫引起的热载流子转移和振动激发示意图。(b)光照(实线)和黑暗(虚线)情况下 $O_2$ (黑线)和 CO (红线)的分解速率。

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# MACHINE-LEARNING INSPIRED DENSITY-FLUCTUATION MODEL OF LOCAL STRUCTURAL INSTABILITY IN METALLIC GLASSES

By Yicheng Wu, Bin Xu, Xuefeng Zhang, Pengfei Guan*

Predicting the instability of disordered systems from a structural perspective has been a long-standing and highly regarded scientific inquiry. While recently emerged supervised machine learning models have made significant advancements in forecasting instability in disordered systems, challenges persist regarding the generalizability and interpretability of these machine learning models. Furthermore, an additional concern lies in the requirement of incorporating dynamical information during the training process of these recent machine learning models.

Professor Pengfei Guan's research group at the Beijing Computational Science Research Center has employed molecular dynamics simulations to systematically investigate the structural origins of plastic instability in metallic glasses. They have proposed a density-fluctuation model that demonstrates outstanding predictive capabilities for plastic events and generalizability. The research findings have been published under the title "Machine-learning inspired density-fluctuation model of local structural instability in metallic glasses" in the journal Acta Materialia.

The findings of this study reveal that in the context of metallic glass systems, the weighting function used to build the "softness" structural parameter (achieved through machine learning) is remarkably similar to the radial distribution function, as shown in the left panel of Figure 1. This observation has led to the introduction of a novel structural parameter termed "radial softness" ( $S_g$ ), which employs local radial symmetry functions as atomic structural feature descriptors and the modified global RDF as the weighting function. As a result, $S_g$ is a purely structural parameter.

The outcomes indicate that across various metallic glass systems, $S_g$ exhibits predictive capabilities for plastic events comparable to “softness” ( $S_\omega$ , constructed through machine learning). Moreover, $S_g$ significantly outperforms commonly employed pure structural parameters such as local configurational anisotropy ( $|\vec{u}|$ ), structural entropy ( $S_2$ ), and local five-fold symmetry ( $f_5$ ), as shown in the right panel of Figure 1. Consequently, the density-fluctuation model provides fresh insights and understanding into the structure-property relationship of disordered systems.

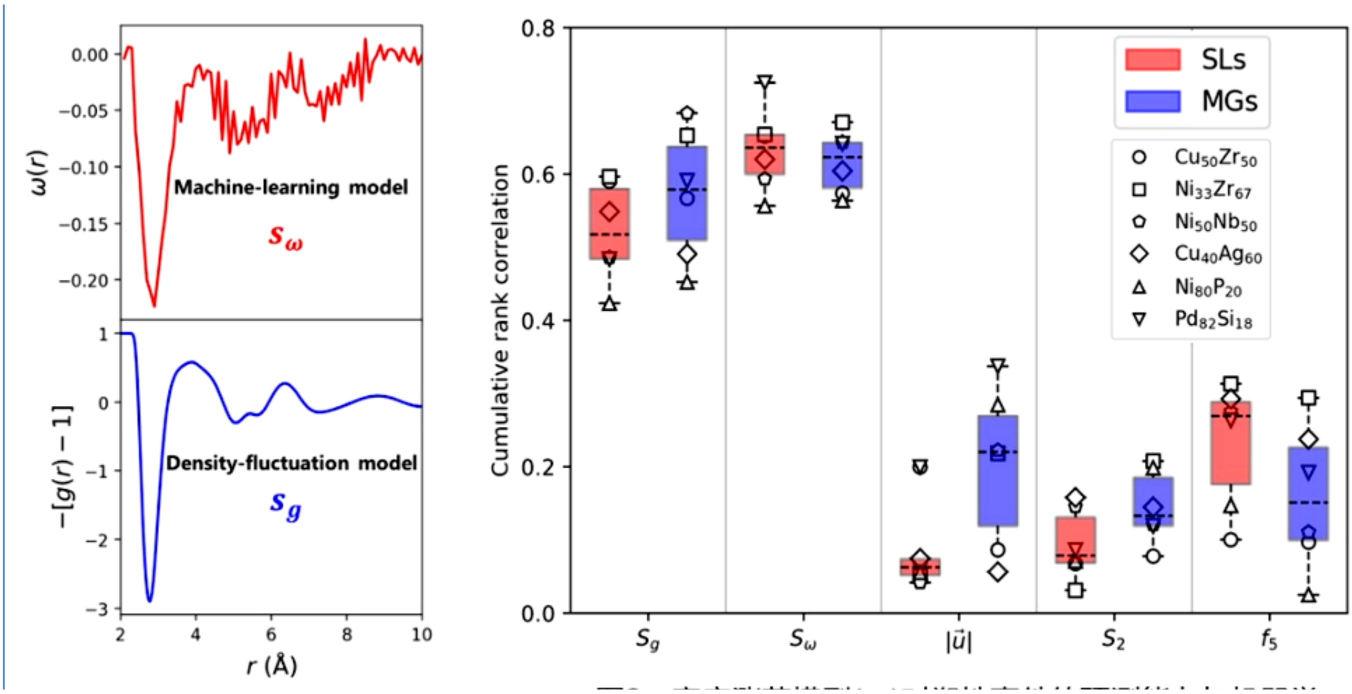


**Fig 1.** (Left) High similarity between machine learning weight and radial distribution function; (Right) Predictive capabilities of the density-fluctuation model ($S_g$) for plastic events compared to the machine learning model ($S_\omega$), significantly outperforming widely utilized pure structural parameters.


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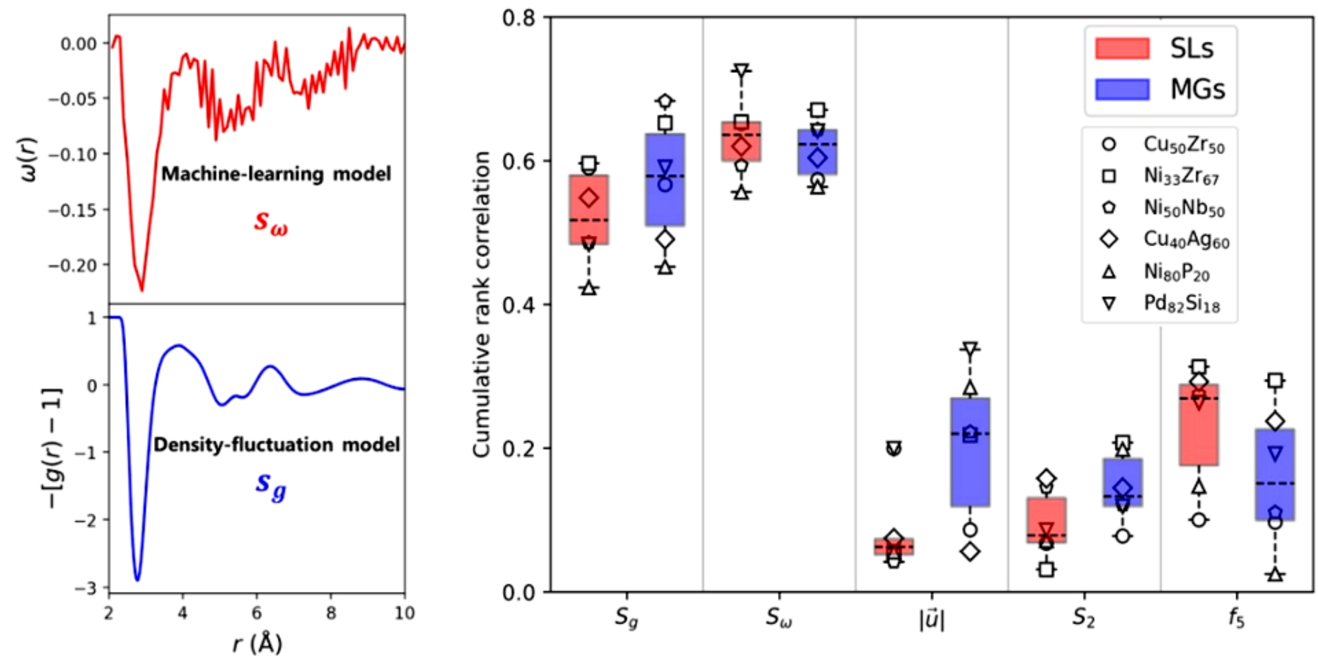


图 1：(左)机器学习权重与径向分布函数高度相似; (右)密度涨落模型($S_g$)对塑性事件的预测能力与机器学习模型($S_\omega$)相比拟，并且显著优于广泛使用的纯结构参数。

# 受机器学习启发的金属玻璃密度涨落结构模型

吴义成，徐斌，张雪峰，管鹏飞*

如何从结构出发预测无序体系失稳是一个长期以来备受关注的科学问题。尽管最近兴起的监督式机器学习模型在预测无序体系失稳方面取得了重要进展，但是机器学习模型的泛化能力以及可解释性依旧存在问题，另外机器学习模型在训练的过程中需要使用动力学信息。

北京计算科学研究中心管鹏飞教授课题组利用分子动力学模拟，系统地研究了金属玻璃塑性失稳的结构起源。提出了密度涨落模型 (density-fluctuation model)，该模型具有优异的塑性事件预测能力以及泛化能力。相关研究成果以“Machine-learning inspired density-fluctuation model of local structural instability in metallic glasses”为题在 Acta Materialia 上发表。

研究人员发现，对于金属玻璃体系，构建软度结构参量所需的权重函数（由机器学习训练得到）与径向分布函数具有很高的相似性（图1左）。从而提出新的结构参量“radial softness”($S_g$)，使用局域径向对称函数作为原子结构特征描述符，整体径向分布函数作为特征权重。因此 $S_g$ 是一个纯结构参量。结果表明在多种金属玻璃体系中，$S_g$ 对塑性事件的预测能力与软度($S_\omega$，机器学习构建)相比拟，并且显著优于广泛使用的纯结构参量，比如各向异性度( $|\vec{u}|$ )、结构熵($S_2$)、局域五次对称性($f_5$)（图1右）。因此，密度涨落模型为无序体系结构-性能关联提供了新的认识与理解。

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# CAPTURING THE MYSTERIOUS MOIRÉ MAGNETIC EXCHANGE INTERACTIONS

By B. Yang, Y. Li, H. J. Xiang, H. Q. Lin, and B. Huang*

Whereas conventional magnets undergo a few simple magnetic exchange interactions, moiré lattices in twisted magnets could induce large-scale periodic magnetic exchange interactions with more than tens of thousands of nonequivalent magnetic parameters, forming complicated moiré magnetic exchange interactions (MMEIs). For instance, to model the moiré magnets at $\theta \sim 1°$, one should account for > 20,000 atoms for a moiré supercell and the resulting number of MMEIs reaches to > 400,000. "More is different", as stated by Philip Anderson in 1972, indicating the uniqueness of MMEIs in generating new magnetic phenomena. Unfortunately, owing to extreme complexity and twist-angle sensitivity, MMEIs in twisted magnets have never been understood. As a result, many puzzling experimental observations have been made on the complex spin textures and magnetic phase transitions in twisted magnets.

In a recent study, B. Huang in collaboration with H. Q. Lin and H. J. Xiang (Fudan University) made a key step towards understanding the long-standing mystery of MMEIs. First, they develop a simple but powerful sliding-mapping approach to effectively capture the MMEIs. Then, they set up a microscopic moiré spin Hamiltonian that enables the description of magnetic structures induced by the MMEIs. Remarkably, they discover that the emergence of MMEIs can create an unprecedented magnetic skyrmion bubble (SkB) with non-conversed helicity. They name it as moiré-type SkB. Interestingly, the SkB can form an unusual frustrated bilayer-lattice, indicating new physics may be generated in this SkB lattice. Importantly, the size and population of SkBs can be finely controlled by twist angle, a key step for skyrmion-based information storage and quantum computing. Finally, they reveal that the MMEIs can be effectively manipulated by the substrate-induced interfacial Dzyaloshinskii-Moriya interaction, modulating the twist-angle-dependent magnetic phase diagram, which solves the outstanding disagreements between prior theories and experiments.

This work has recently been published in Nature Computational Science [1]. Prof. D. Soriano at Universidad de Alicante (Spain) highlights that "*these computational advances are a huge step towards a more realistic picture of the physics of materials*" in the News and Views [2]. In addition, this work is also selected as the cover of the journal and featured by the editors [3].

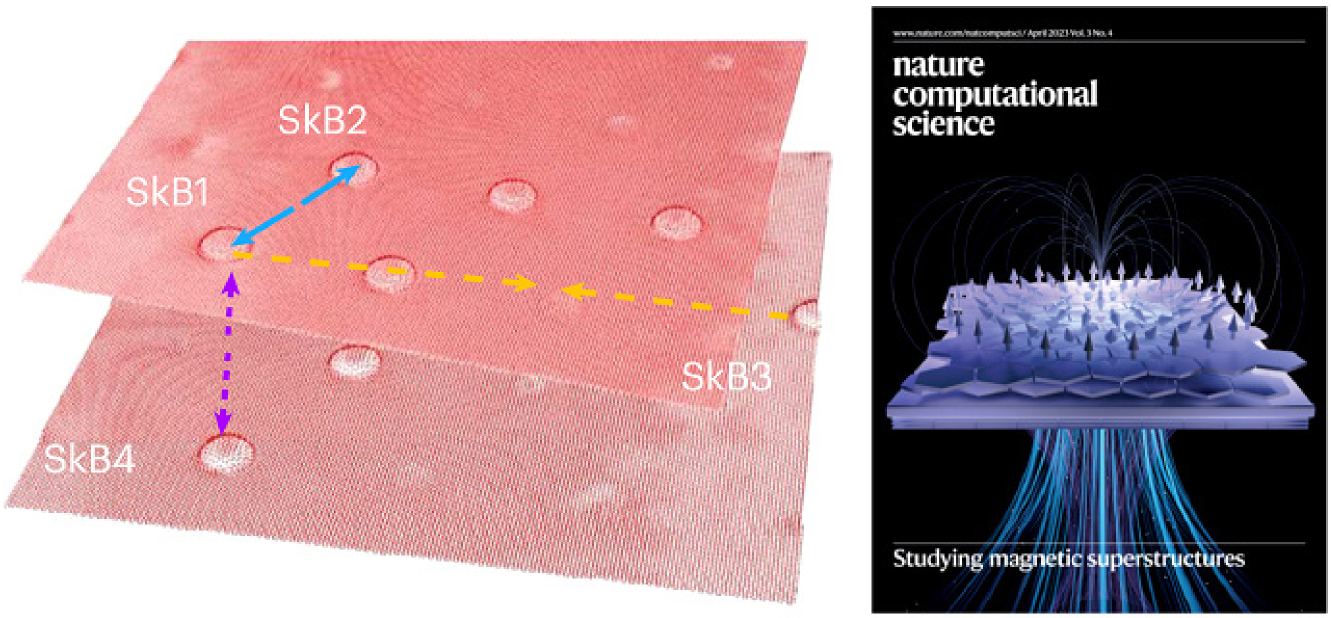


**Fig.** Computationally probing moiré magnets.


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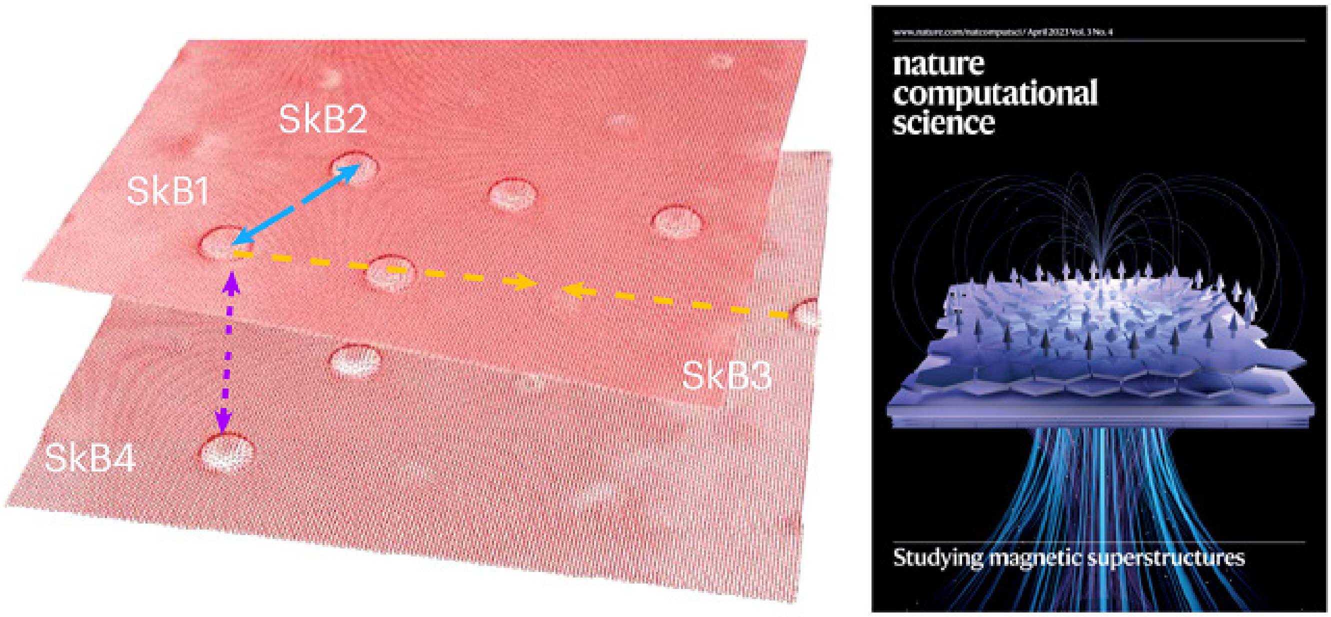


图 摩尔磁体中的复杂磁结构。

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[3] Editorial, Computationally probing moiré magnets, *Nat. Comput. Sci*. 3, 277 (2023).

# 揭开摩尔磁交换相互作用的神秘面纱

杨百顺，李阳，向红军，林海青，黄兵*

在传统磁性体系中只存在一些简单的磁交换相互作用。而在转角磁性体系中，摩尔堆叠结构可以诱导出大规模的周期性磁交换相互作用，其通常具有数万个不等效磁参数，形成复杂的摩尔磁交换相互作用（MMEIs）。例如，在 ~1° 的摩尔转角磁体中，~20,000个磁性原子会产生数量高达 400,000 以上的的 MMEIs。正如菲利普·安德森在1972年所说的，“more is different”，MMEIs会在产生新的磁性物理现象方面起到独特作用。不幸的是，由于其极其复杂庞大的磁参数空间和对转角角度的敏感依赖性，目前我们对转角磁体中的 MMEIs 一直无法理解，也无法理解很多令人困惑的实验观测结果，其中涉及复杂的自旋结构和磁相变现象。

在最近的研究中，北京计算科学研究中心的杨百顺博士、黄兵研究员、林海青教授等与合作者，为揭开 MMEIs 的神秘面纱迈出了重要的一步。首先，他们发展了一种简单但有效的滑动-映射方法，可以有效地计算得到转角磁体中的 MMEIs，并可以追溯其在原胞中的物理起源。然后，他们建立了一个微观摩尔自旋哈密顿量，用于模拟由 MMEIs 引发的磁性结构。他们发现由于 MMEIs 的存在，在转角磁性体系中可以得到一种前所未有的具有非守恒旋度的磁性斯格明子气泡，他们将其命名为摩尔磁性斯格明子气泡。有趣的是，磁性斯格明子气泡之间存在特殊的相互作用，从而最终可以形成一种磁阻挫斯格明子晶格。磁性斯格明子气泡的大小和数量可以通过转角角度进行精细控制，这有利于实现基于斯格明子的信息存储。最后，他们揭示了MMEIs可以通过衬底引起的界面 Dzyaloshinskii-Moriya 相互作用进行有效操控，从而解决了之前理论和实验之间存在的争议。

这项研究最近在《自然计算科学》[1]杂志上发表。西班牙 Universidad de Alicante 的D. Soriano教授在《新闻与观点》[2]中强调“these computational advances are a huge step towards a more realistic picture of the physics of materials”。此外，这项工作还被选为该杂志的封面，并获得编辑们的推荐介绍[3]。

# FIRST-PRINCIPLES CALCULATIONS OF SHALLOW IMPURITY LEVELS IN SEMICONDUCTORS

By Jun Kang, L.-W. Wang

Accurate modeling of shallow impurities in semiconductors through first-principles density functional theory calculations is challenging due to the delocalized nature of the impurity wavefunction. The situation could be more complicated for shallow impurity complexes where the interactions between impurities lead to a large perturbation to the host. In this work [1], the shallow acceptor levels of the group-IIIA acceptor-carbon (A-C, with A=B, Al, Ga, In, Tl) complexes in silicon were studied using a potential patching method combined with a hybrid-functional correction. The potential patching method removes the artificial interaction between periodic images and allows the calculations of large supercells containing over 104 atoms to obtain converged acceptor levels. The correction based on hybrid-functional calculations overcomes the underestimation of the ionization energies predicted by semilocal exchange-correlation functionals, resulting in good agreements with experiments. The A-C complexes are found to have smaller acceptor ionization energies than the corresponding single-A substitutional acceptors. The origin of the ionization energy reduction is further analyzed, and the roles of the chemical electronic effect and the strain field effect are clarified. Our results indicate that the combination of the potential patching method and the hybrid-functional correction could be a feasible approach for accurate simulations of shallow impurities and their complexes.

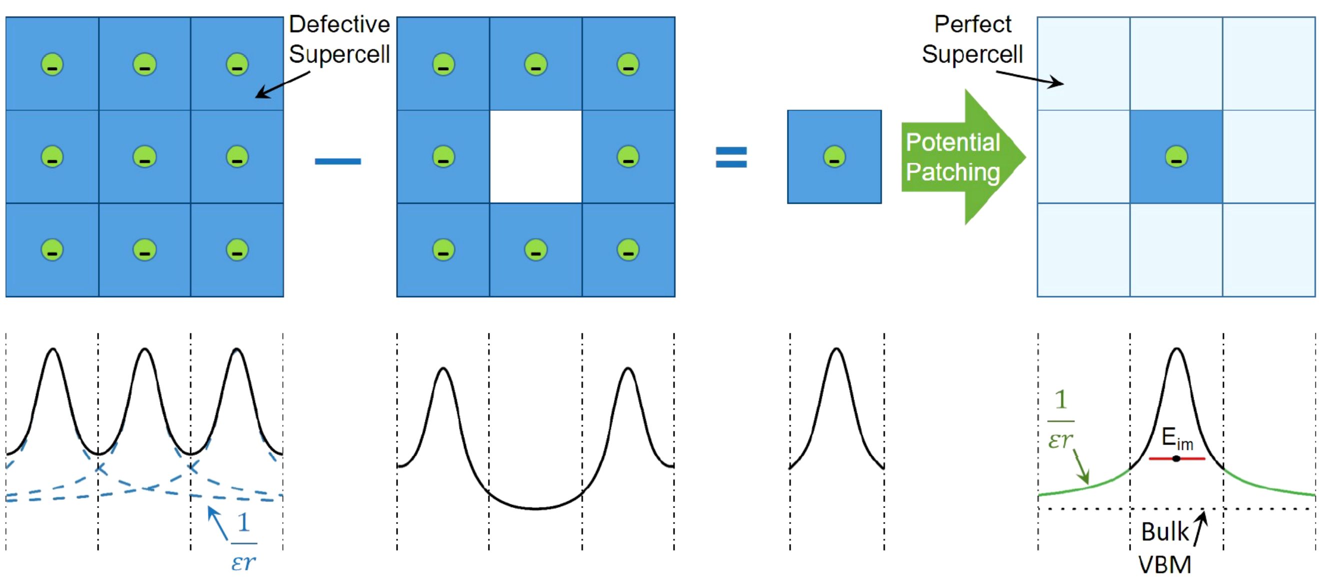


**Fig. 1.** An illustration scheme of the potential patching method.

# 半导体中浅能级缺陷的第一性原理计算

**康俊**，汪林旺

在半导体能源材料中，通常需要引入浅能级的施主或受主产生自由载流子，相应的杂质离化能对载流子浓度有关键影响。受第一性原理计算能力限制，通常的缺陷模拟一般基于包含数百原子的超胞。对于局域的深能级缺陷，这一超胞尺寸可以实现较好效果。然而对于浅能级缺陷，由于缺陷态非常扩展，小的超胞难以包含整个缺陷态波函数，将导致很大的计算误差。在本工作中，基于势能补缀和杂化泛函计算，我们发展了半导体浅能级缺陷的大超胞计算方法。利用势能补缀方法可构建包含数万原子超胞的哈密顿量并实现准线性标度的模拟，有效避免了缺陷态间的镜像作用。同时结合杂化泛函计算，在非局域赝势中引入修正，克服了半局域交换关联泛函的自相互作用误差。二者结合实现了10 meV级别的浅能级离化能计算精度。

图 1：势能补缀法示意图。

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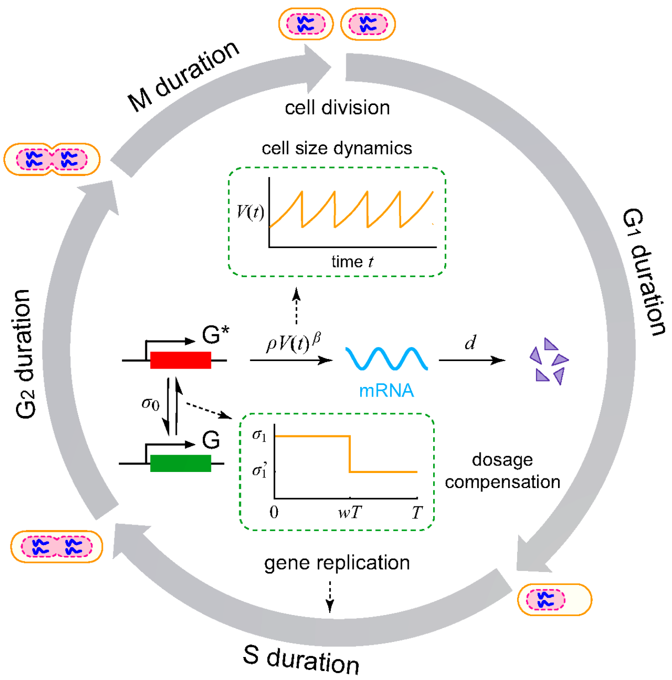
# COUPLED STOCHASTIC DYNAMICS OF GENE EXPRESSION, CELL SIZE, AND CELL CYCLE

By Chen Jia#, Ramon Grima*

The standard model describing the fluctuations of mRNA numbers in single cells is the telegraph model which includes synthesis and degradation of mRNA, and switching of the gene between active and inactive states. While commonly used, this model does not describe how fluctuations are influenced by the cell cycle phase, cellular growth and division, and other crucial aspects of cellular biology. Here we derive the analytical time-dependent solution of an extended telegraph model (Fig. 1) that explicitly considers the doubling of gene copy numbers upon DNA replication, dependence of the mRNA synthesis rate on cellular volume, gene dosage compensation, partitioning of molecules during cell division, cell-cycle duration variability, and cell-size control strategies [1,2]. Based on the time-dependent solution, we obtain the analytical distributions of transcript numbers for lineage and population measurements in steady-state growth and also find a linear relation between the Fano factor of mRNA fluctuations and cell volume fluctuations. We show that generally the lineage and population distributions in steady-state growth cannot be accurately approximated by the steady-state solution of extrinsic noise models, i.e. a telegraph model with parameters drawn from probability distributions. This is because the mRNA lifetime is often not small enough compared to the cell cycle duration to erase the memory of division and replication. Accurate approximations are possible when this memory is weak, e.g. for genes with bursty expression and for which there is sufficient gene dosage compensation when replication occurs.

**Fig 1.** A coupled stochastic model of gene expression dynamics, cell size dynamics, and cell cycle events. This model takes exponential growth of cell volume, volume-dependent transcription, gene replication, gene dosage compensation, and cell division into account. We computed the analytical time-dependent distributions of mRNA numbers across cell cycles. The analytical solution is in full agreement with stochastic simulations obtained using the finite-state projection algorithm.




## reaction scheme

### before gene replication

$$G \xrightarrow{\sigma_1} G^*, \quad G^* \xrightarrow{\sigma_0} G, \quad G^* \xrightarrow{\rho V(t)^\beta} G^* + M, \quad M \xrightarrow{d} \varnothing,$$

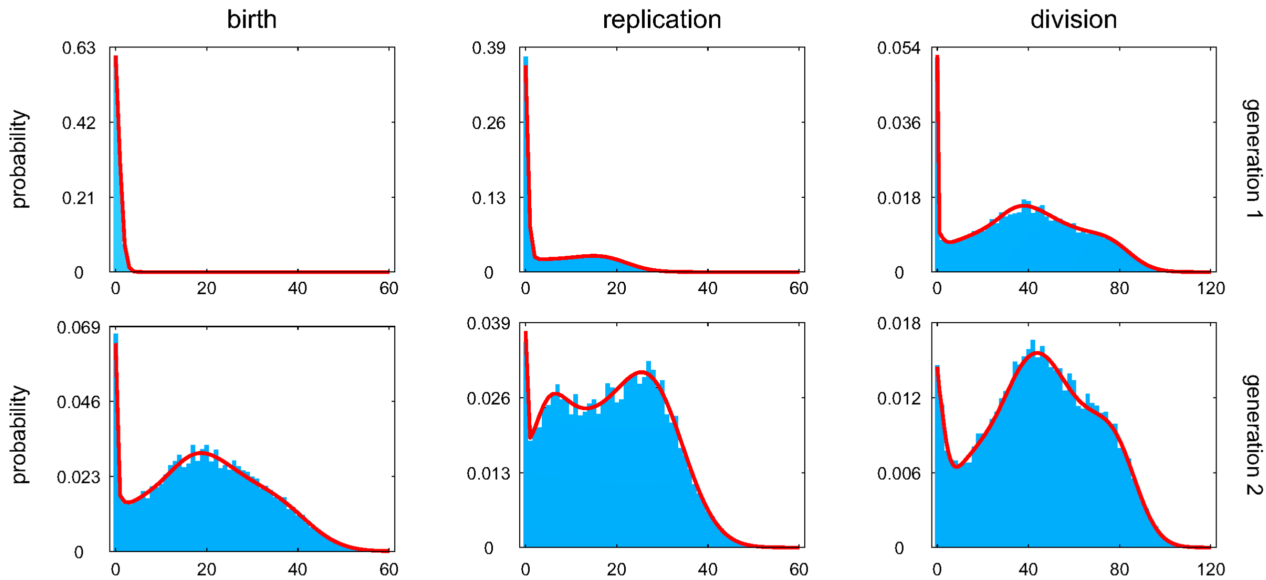
### after gene replication

$$G_A \xrightarrow{\sigma_1'} G_A^*, \quad G_A^* \xrightarrow{\sigma_0} G_A, \quad G_B \xrightarrow{\sigma_1'} G_B^*, \quad G_B^* \xrightarrow{\sigma_0} G_B,$$
$$G_A^* \xrightarrow{\rho V(t)^\beta} G_A^* + M, \quad G_B^* \xrightarrow{\rho V(t)^\beta} G_B^* + M, \quad M \xrightarrow{d} \varnothing,$$

## analytical distribution

$$F(t,z) = \sum_{n=0}^{\infty} p_n(t)(z+1)^n = L_0(t,z)F_0(0, e^{-dt}z) + L_1(t,z)F_1(0, e^{-dt}z),$$

$$L_0(t,z) = \Big[M(1+a-b; 1-b; ue^{-dt}z)M(a; b; ue^{\beta gt}z) + \frac{auz}{b(b-1)}e^{-rt} \times M(1+a; 1+b; ue^{-dt}z)M(1+a-b; 2-b; ue^{\beta gt}z)\Big]e^{-ue^{-dt}z},$$
$$L_1(t,z) = \Big[M(a-b; 1-b; ue^{-dt}z)M(a; b; ue^{\beta gt}z) - \frac{(b-a)uz}{b(b-1)}e^{-rt} \times M(a; 1+b; ue^{-dt}z)M(1+a-b; 2-b; ue^{\beta gt}z)\Big]e^{-ue^{-dt}z}.$$





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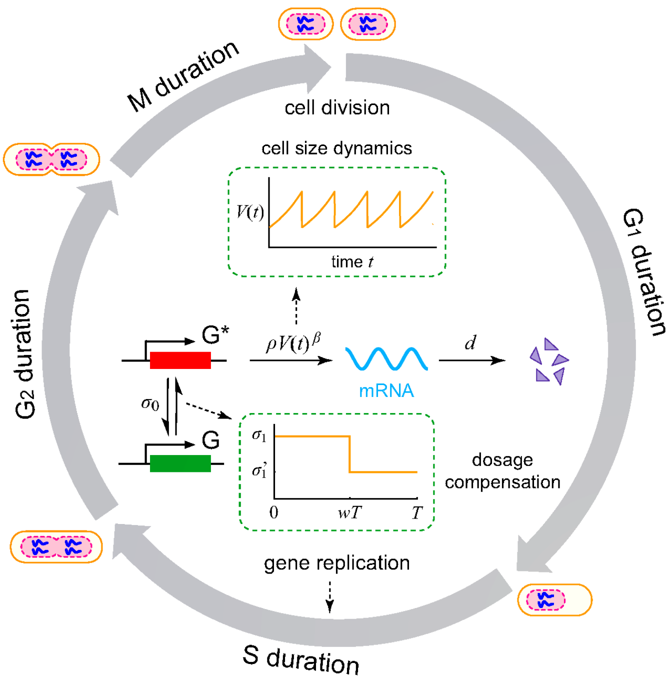


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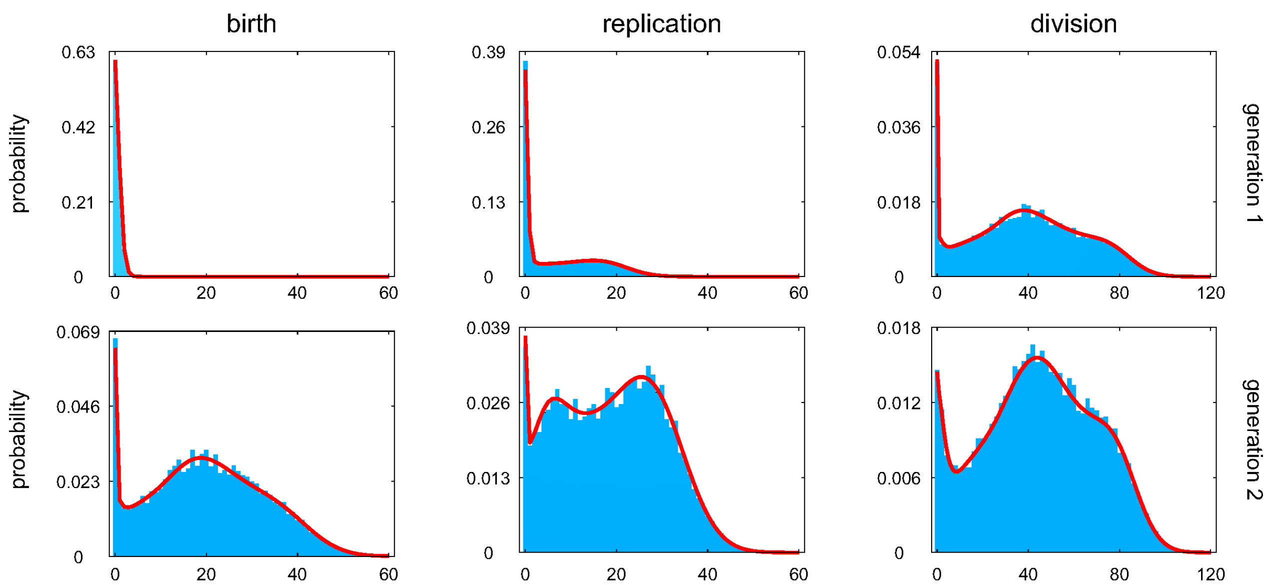
$$L_1(t,z) = \Big[M(a-b; 1-b; ue^{-dt}z)M(a; b; ue^{\beta gt}z) - \frac{(b-a)uz}{b(b-1)}e^{-rt} \times M(a; 1+b; ue^{-dt}z)M(1+a-b; 2-b; ue^{\beta gt}z)\Big]e^{-ue^{-dt}z}.$$



# 基因表达、细胞体积、细胞周期的耦合随机动力学

贾晨#, Ramon Grima*

基因表达的电报模型由 mRNA 的合成与降解以及基因在打开与关闭两个状态下的切换所组成，是刻画单细胞内 mRNA 数量涨落的标准模型。尽管被广泛使用，该模型无法刻画细胞周期阶段，细胞生长与分裂，以及其他细胞生物学中的重要因素对 mRNA 涨落的影响。在本文中[1,2]，我们得到了基因表达广义电报模型（图1）的解析时间依赖解。该模型明确地考虑了基因复制时基因拷贝数的倍增，mRNA 合成速率对细胞体积的依赖，基因计量补偿，细胞分裂时分子的分配，细胞周期时间变异性，以及细胞体积调控策略。基于该时间依赖解，我们得到了稳态生长条件下谱系测量与群体测量的 mRNA 数量的解析分布，并且发现了 mRNA 涨落与细胞体积涨落的 Fano 因子之间的线性关系。我们的结果表明，一般来说，稳态生长条件下的谱系分布与群体分布不能被外部噪声模型（即参数受到外部噪声影响的电报模型）的稳态解所精确地逼近。这是由于 mRNA 的生存时间与细胞周期时间相比并不是非常小的，因此不足以消除系统对基因复制与细胞分裂的记忆。外部噪声模型只有当该记忆很弱时，即基因表达具有爆发性且复制发生时具有足够的基因计量补偿时，才可以提供精确的逼近。

◀ 图 1：基因表达、细胞体积、细胞周期的耦合随机动力学模型。该模型考虑了细胞体积的指数增长，转录对细胞体积的依赖，基因复制，基因计量补偿，以及细胞分裂。我们计算了不同细胞周期下mRNA数量的解析时间依赖分布。该解析解与有限状态投影算法下的随机模拟结果取得了完美的吻合。

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# SUPERCLOSENESS OF THE LOCAL DISCONTINUOUS GALERKIN (LDG) METHOD FOR SINGULARLY PERTURBED CONVECTION-DIFFUSION PROBLEMS WITH EXPONENTIAL AND PARABOLIC LAYERS

By Yao Cheng, Shan Jiang and Martin Stynes*

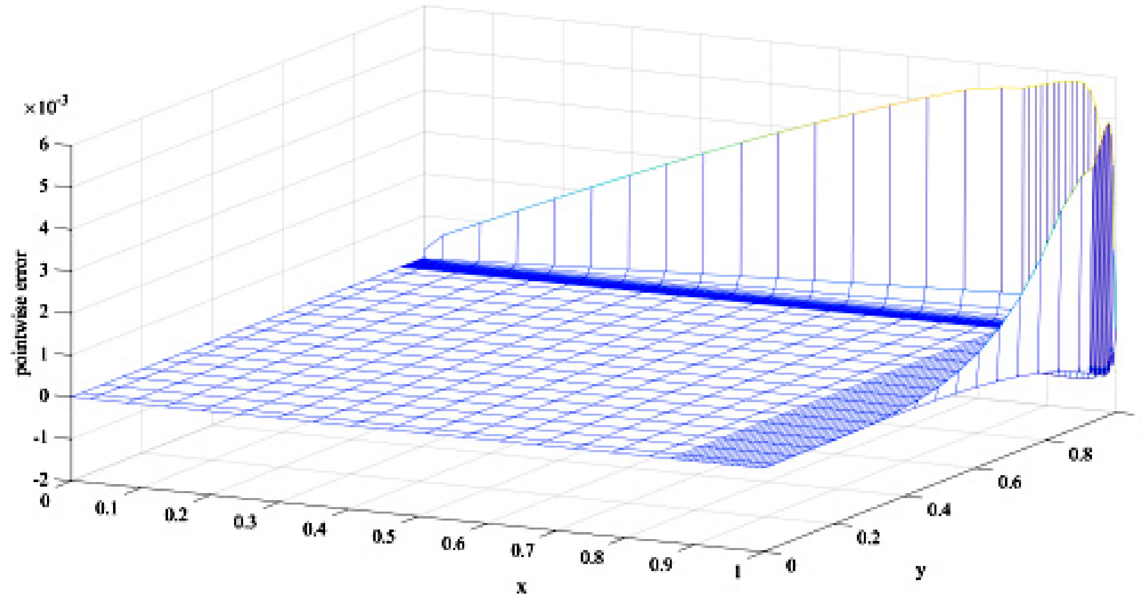
The numerical solution of singularly perturbed differential equations has been studied for many years because these equations have a large variety of applications. Nevertheless many theoretical questions remain unanswered because numerical error analysis in this setting is made difficult by the presence of *layers*: narrow regions where the exact solution changes rapidly. In the work described here, significant new theoretical results are proved for the well-known LDG method.

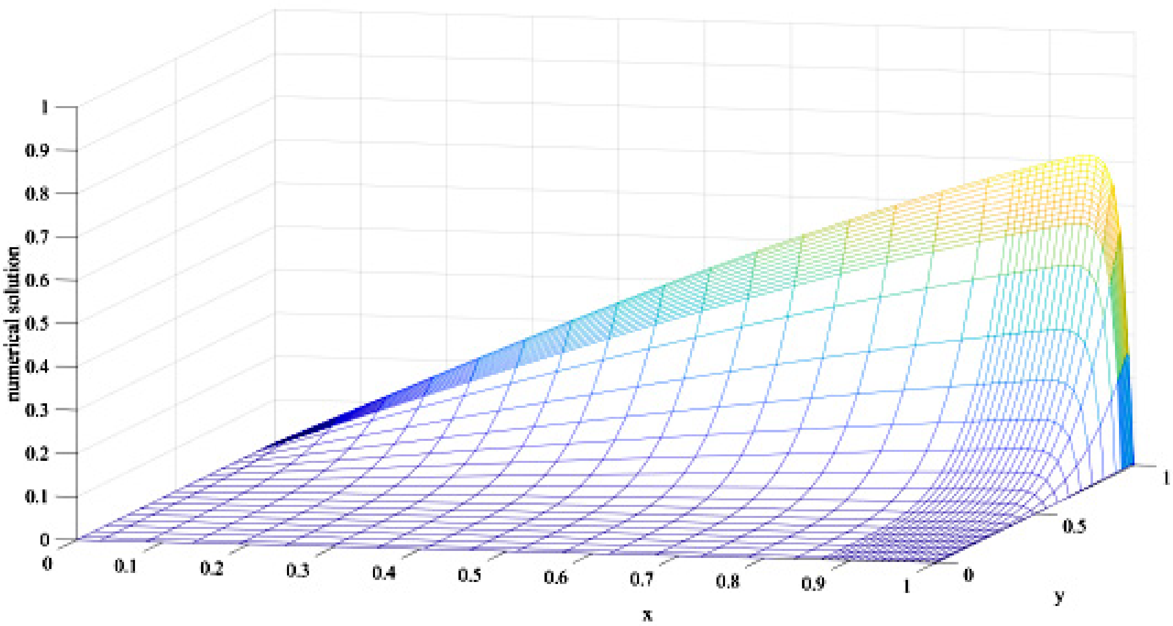
Consider the singularly perturbed convection-diffusion problem $-\varepsilon\Delta u + a\cdot\nabla u + bu = f$ on the unit square $\Omega = (0,1)\times(0,1)$, and satisfying the boundary conditions $u = 0$ on $\partial\Omega$. Here $\varepsilon > 0$ is a small parameter, $a(x,y) = (a_1(x,y), a_2(x,y)) \geq (\alpha_1, \alpha_2) > (0,0)$, and the functions $a, b, f$ are smooth. It is well known that typical exact solutions of this problem have exponential boundary layers along the sides $x = 1$ and $y = 1$ of $\Omega$. To address this difficulty when solving the problem numerically, one uses a tensor-product layer-adapted mesh; Shishkin meshes, Bakhvalov meshes and Bakhvalov-Shishkin meshes are considered in our work.

The problem is solved numerically on one of these meshes by means of a local discontinuous Galerkin (LDG) finite element method. The LDG uses functions $Q_k$ that are polynomials of degree at most $k \geq 1$ in each of the $x$ and $y$ variables on each mesh rectangle, but are not necessarily continuous when one moves from one rectangle to another. The precise LDG formation is complicated; see [1] for details.

A lengthy error analysis (see [1]) proves that, independently of the value of the small parameter ε, the computed solution approximates a local Gauss-Radau projection of the exact solution (into the finite element space) more accurately than it approximates the exact solution. This phenomenon is commonly known as *supercloseness*; it is a desirable property of any numerical solution. It implies higher-order convergence of the computed solution to the exact solution in the $L^2(\Omega)$ norm—a new and sharp result for this method. A typical computed solution on a Shishkin mesh, and the error in this solution, are shown in the figure.

In reference [2] a related problem is considered, where the PDE is replaced by $-\varepsilon\Delta u + au_x + bu = f$; now the exact solution will have an exponential layer along the side $x = 1$ of $\Omega$ and parabolic layers along the sides $y = 0$ and $y = 1$. A similar LDG is used and an energy-norm convergence result, which is again independent of the value of the small parameter ε, is proved; it is the first result of this type in the research literature for the LDG method applied to a parabolic-layer problem.

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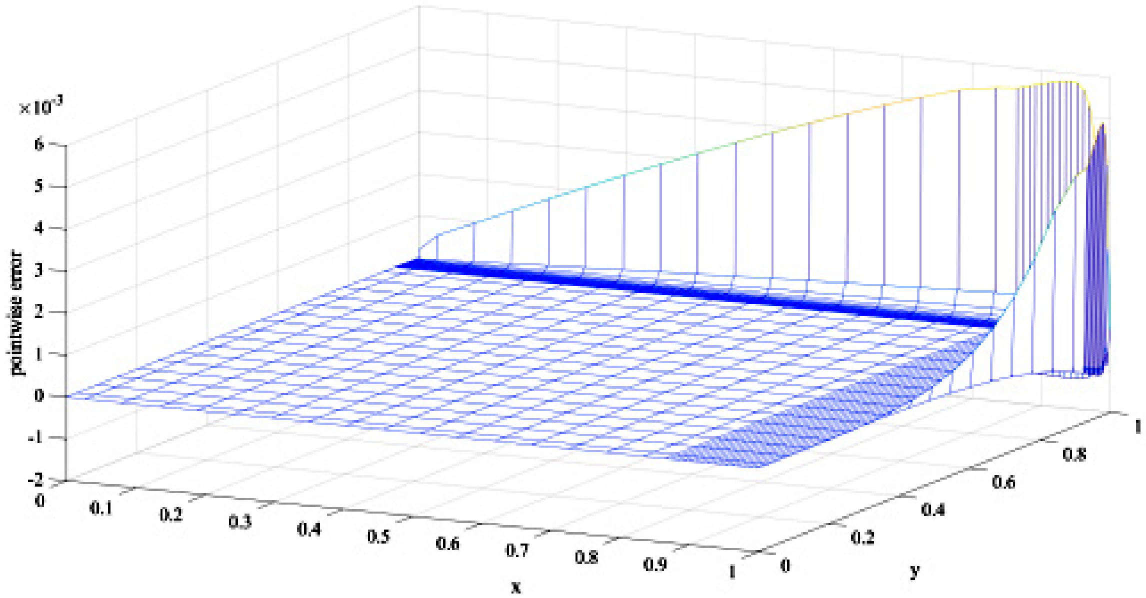


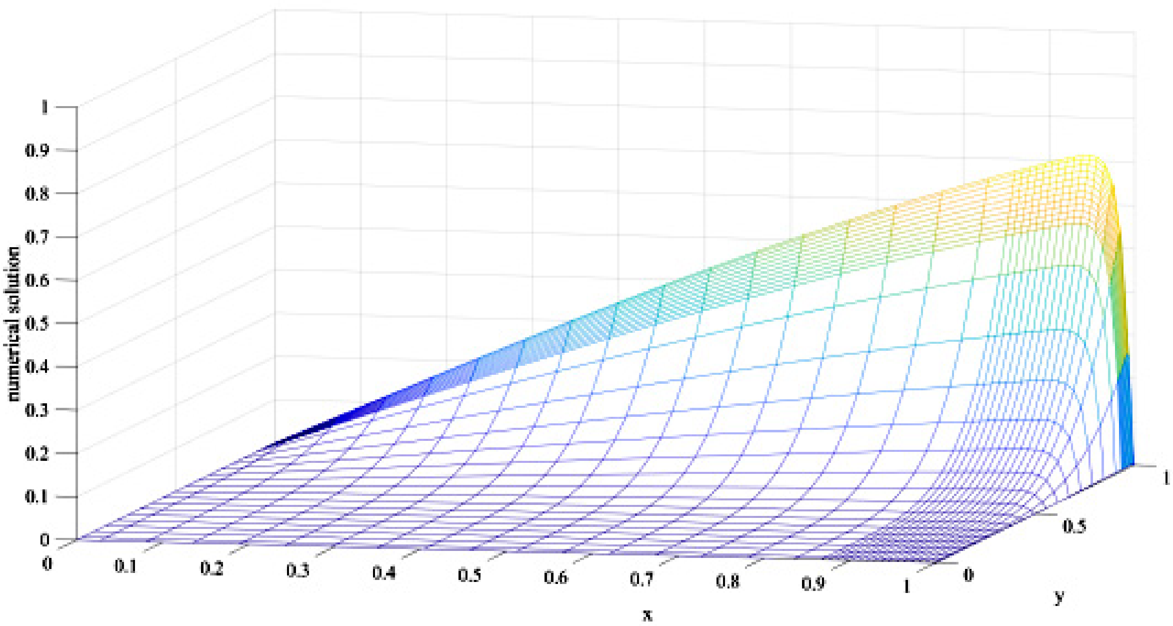



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# 局部间断伽辽金方法求解带有指数及抛物层奇异摄动对流扩散问题的超逼近性

程瑶，江山, Martin Stynes*

奇异摄动微分方程具有广泛的应用范围，关于其数值解的研究已经有很多年的历史。然而，由于解急剧变化的边界层的出现，使得该类方程的数值分析十分困难，许多理论问题仍有待解决。

本工作对众所周知的 LDG 方法证明了一个重要的新的理论结果。

考虑区域$\Omega=(0,1)\times(0,1)$上的奇异摄动对流扩散问题$-\varepsilon\Delta u+a\cdot\nabla u+bu=f$，其在边界$\partial\Omega$上满足条件$u=0$。这里$\varepsilon>0$是一个小参数, $a(x,y)=(a_1(x,y),a_2(x,y))\geq(a_1,a_2)>(0,0)$，函数$a,b,f$是光滑的。众所周知，该问题的典型解在区域 $\Omega$ 的两侧 $x=1$ 和 $y=1$ 处有指数边界层。为了处理数值求解时边界层带来的困难，张量积层适应网格被应用于该问题：本工作分别考虑了 Shishkin 网格, Bakhvalov 网格和 Bakhvalov-Shishkin 网格。

本工作分别利用上述网格构造 local discontinuous Galerkin (LDG) 格式对该问题进行数值求解。其中，LDG 格式使用在每一个矩形网格内x和y变量方向均不超过 $k(k\geq1)$ 次的多项式 $Q_k$，其在矩形网格中间不一定连续。对该 LDG 格式更精确地描述可以参见文献[1]。

一个详尽的误差分析（见[1]）证明了，不依赖于小参数 ε 的值，所得数值解逼近真解的一个局部Gauss-Radau投影（有限元空间投影）比逼近真解本身更为精确。这种现象通常被称为 supercloseness。对任何数值解而言，这都是一个理想的性质。这意味着在 $L^2(\Omega)$ 范数意义下，数值解具有更高的收敛阶--这是一个创新且严格的结果。在Shishkin网格上的一个经典的数值解以及相应的误差见左图。

文献 [2]中考虑了如下这样一个相关的 PDE 问题：$-\varepsilon\Delta u+au_x+bu=f$；该问题的真解会在边界 $x=1$ 处具有指数边界层，在边界 $y=0$ 和 $y=1$ 处具有抛物边界层。类似的 LDG 格式被应用于求解这个问题。在能量范数意义下，不依赖于小参数 ε 的收敛性结果得到了证明。在现有关于 LDG 格式应用到抛物边界层问题的研究中，这是首次给出该类型的结果。

# HIGHLY EFFICIENT ENERGY-CONSERVING MOMENT METHOD FOR THE MULTI-DIMENSIONAL VLASOV-MAXWELL SYSTEM

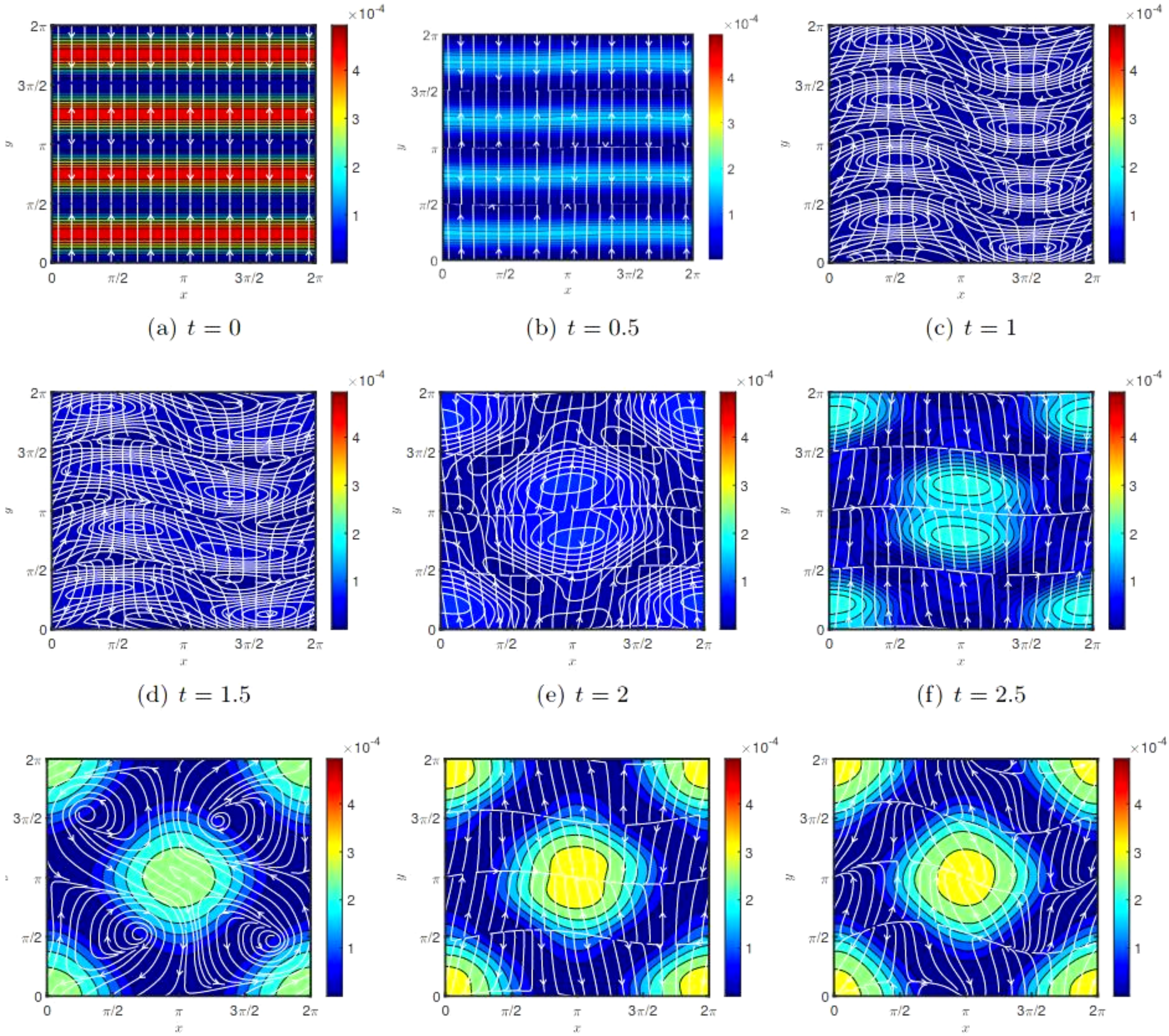
By Tianai Yin, Xinghui Zhong, Yanli Wang*

Plasma, which exists widely in the universe, is the fourth fundamental state of matter after solid, liquid, and gas. Understanding the complex behavior of plasma has led to significant advances ranging from space physics and fusion energy, to high-power microwave generation and large-scale particle accelerators. One of the fundamental models in plasma physics is the Vlasov system, which describes the time evolution of the distribution function of collisionless charged particles with long-range interactions. The long-range interactions may occur under a self-generated electromagnetic field. For example, the evolution of the electromagnetic field can be modeled by Maxwell's equations or Poisson's equation in the zero-magnetic field limit, resulting in the well-known Vlasov-Maxwell (VM) or Vlasov-Poisson (VP) systems.

Numerically solving the VM system is a difficult task. There are several challenges such as the high dimensionality, the conservation of physical quantities due to the Hamiltonian structure of the system, various physical phenomena, nonlinearity.

This work proposes an energy-conserving regularized moment method for the multi-dimensional VM system. The distribution function is expanded by a series of Hermite functions with the expansion center and the scaling factor chosen adaptively. With this specially chosen expansion center, the effect of the Lorentz force from the electromagnetic field can be changed into a linear combination of the moment coefficients, so that the computational cost can be significantly reduced. To design the energy-conserving scheme, the moment system is split into the convection step and the Lorentz force step by the Strang splitting method. Thus, the effect of the Lorentz force term is reduced to several ODEs related to the macroscopic velocity and high-order moment coefficients. Most importantly, an implicit scheme is developed to solve Maxwell's equations and the Lorentz force step simultaneously, enabling the conservation of the mass and total energy for the VM system. Only a small system of linear equations needs to be solved for this implicit scheme.

Several numerical examples of the VM system, such as one-dimensional Landau damping, two-stream instability, Weibel instability, and two-dimensional Orszag-Tang vortex problems, are studied to exhibit the high efficiency of the proposed energy-conserving numerical methods.



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1$

(d) $t = 1.5$ (e) $t = 2$ (f) $t = 2.5$

(g) $t = 3$ (h) $t = 3.5$ (i) $t = 4$

**Fig 1.** Orszag-Tang vortex problem. Time evolution of the magnetic field. Here, the background is the total magnetic energy, and the white line is the magnetic field.

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[1] Z. Cai, Y. Fan, and R. Li. Globally hyperbolic regularization of Grad's moment system.Communications on pure and applied mathematics, 67(3):464–518, 2014.

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[3] C. Liu and K. Xu. Unified gas-kinetic wave-particle methods IV: multi-species gas mixture and plasma transport.Advances in Aerodynamics, 3(9), 2021.

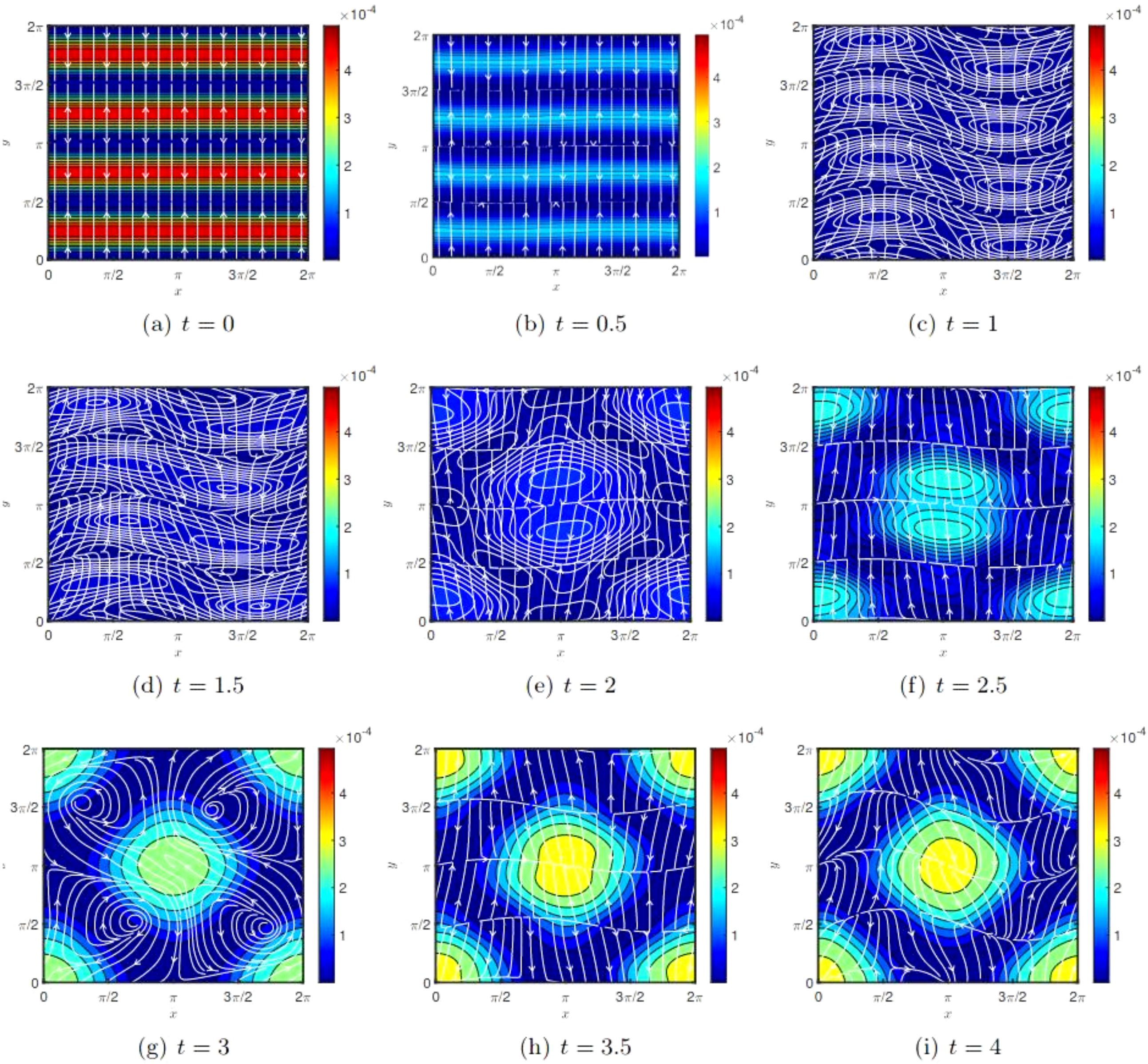


图 1：Orszag-Tang vortex 问题. 电磁场时间演化图，这里背景等高线展示了总电磁能，白色线为磁力线。

# 求解高维 VLASOV-MAXWELL 方程的保能量守恒高效矩方法

尹天爱, 仲杏慧, 王艳莉*

等离子体作为除固体，液体，气体外的第四类物质，在宇宙中广泛存在。理解等离子体的复杂运动体系在空间物理，高能量物理等领域有着重要作用。Vlasov 方程作为等离子物理的基本方程之一，描述了无碰撞带电粒子的长程相互作用。长程相互作用往往伴随着自洽电磁场。当自洽电磁场由 Maxwell 方程或者 Poisson 方程所描述时，我们即可使用 Vlasov-Maxwell (VM) 方程来描述等离子体运动。数值求解VM系统充满挑战，Vlasov 方程自身的高维性，系统的Hamiltonian结构所要求的相关物理量守恒性，非线性性等都导致了数值求解 VM 系统的困难。

该工作针对高维 VM 系统提出了保能量守恒的正则化矩方法。在该方法框架下，分布函数由一系列 Hermite 方程近似，并且近似基函数的展开中心与伸缩因子选取为本地的宏观速度与热温度。在这组特殊选取的展开中心下，由自洽电磁场产生的 Lorentz 力作用可简化为矩系数线性组合，从而大幅减低计算量。为了设计保能量守恒数值格式，数值求解矩系统时，其被分裂为对流步与外力步。因此Lorentz力的作为效果简化为对宏观速度与高阶矩系数的常微分方程。更重要的是，Maxwell 方程与Lorentz外力作用的 ODE 方程通过特殊设计的隐格式同时求解，从而保证了质量和能量守恒。并且，在该隐格式中，仅仅需要求解一个小规模线性方程组。

该工作通过一维线性 Landau 衰减问题，双流不稳定性问题，Weibel 不稳定性问题与二维 Orszag-Tang vortex 问题等基准算例验证了算法的高效性与能量守恒性。

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[1] Z. Cai, Y. Fan, and R. Li. Globally hyperbolic regularization of Grad's moment system.Communications on pure and applied mathematics, 67(3):464–518, 2014.

[2] Y. Cheng, A.J. Christlieb, and X. Zhong. Energy-conserving discontinuous Galerkin methods for the Vlasov-Maxwell system.Journal of Computational Physics, 279:145–173, 2014.

[3] C. Liu and K. Xu. Unified gas-kinetic wave-particle methods IV: multi-species gas mixture and plasma transport.Advances in Aerodynamics, 3(9), 2021.

# SWIMMING MECHANISMS OF THE MIDGE LARVA

By Bowen Jin, Chengfeng Pan, Neng Xia, Jialei Song, Haoxiang Luo, Li Zhang, Yang Ding

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. The midge and mosquito larvae can reach swimming speeds of more than one body length per cycle performing a “figure eight” gait, in which their elongated bodies periodically bend nearly into circles and then fully unfold.

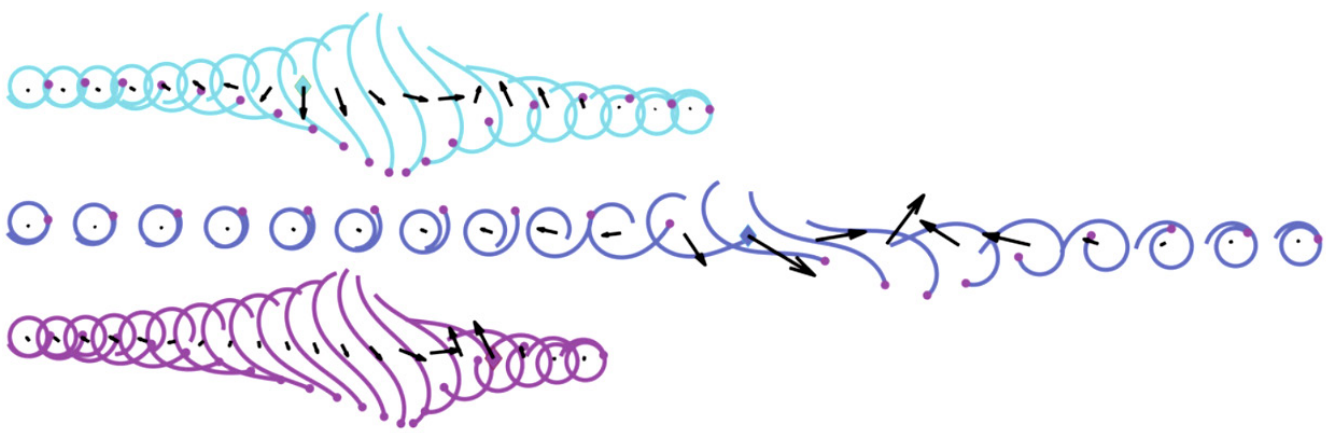

**Fig 1.** Snapshots of the swimmer over a period shows that the speed sensitively depends on the modulation of deformation speed.

To elucidate the propulsion mechanism of this cycle of motion, a team led by Prof. Yang Ding from CSRC and Prof. Li Zhang from CUHK conducted a three-dimensional (3D) numerical study and robotic experiments. They investigated the hydrodynamics of undergoing the prescribed kinematics. They found novel propulsion mechanisms, such as modulating the body deformation rate to dynamically increase the maximum net propulsion force, using asymmetric kinematics to generate torque and the appropriate rotation, and controlling the radius of the curled body to manipulate the moment of inertia. The figure eight gait is found to achieve propulsion at a wide range of Re but is most effective at intermediate Re. The results were further validated experimentally, via the development of a soft millimeter-sized robot that can reach comparable speeds using the figure eight gait.

# 孑孓的“8”字形游动机理

靳博文，潘程枫，夏能，宋加雷，罗浩翔，张立，丁阳

生物的高效运动能力常常是在它们在自然界生存的关键因素。理解动物的运动方式，有助于理解生物行为和身体构造，也为设计制作仿生机器人提供思路和指导。与很多鱼类游动所使用的方式不用，孑孓使用一种“8“字形游动：它们先几乎弯曲成一个圆圈，然后再迅速完全展开。这样，它们能够以一个周期内超过一个身体长度的高速进行，比鱼类一个周期行进速度高得多。

为了阐明这种运动周期的推进机制，由计科中心的丁阳研究员和香港中文大学张立教授领导的团队进行了三维（3D）数值研究和机器人实验。他们发现了新的游动推进机制，包括调节身体变形速率以动态增加最大净推进力，使用不对称运动学来产生扭矩和适当的旋转，并通过控制卷曲体的半径来操纵转动惯量。他们发现“8“字形游动步态能够在广泛的雷诺数范围内实现推进，但在毫米到厘米大小和中等雷诺数下效果最好。通过开发一个能够使用“8“字形步态的机器人，这些结果还在实验上得到了进一步的验证。

◀ 图：数值模拟给出不同身体变形速度时孑孓的游动轨迹

REFERENCES:

[1] Bowen Jin, Chengfeng Pan, Neng Xia, Jialei Song, Haoxiang Luo, Li Zhang, Yang Ding; Swimming of the midge larva: Principles and tricks of locomotion at intermediate Reynolds number. Physics of Fluids 1 March 2023; 35 (3): 031903.

# NONLINEAR COUPLING EFFECTS OF THE THERMOCAPILLARITY AND INSOLUBLE SURFACTANTS TO DROPLET MIGRATION UNDER POISEUILLE FLOW

By Zhenlin Guo #

Under a fully developed Poiseuille flow with nonisothermal condition, it has been widely reported that the thermocapillary effects always strengthen the droplet migration velocity as long as the temperature increases along the direction of Poiseuille flow. The insoluble surfactant, on the other hand, always retards the droplet migration. This is due to the fact that, for most of the models, the Langmuir equation of state for the surface tension is usually simplified under the assumption of low surfactant concentration. The coupling term of temperature and surfactant concentration is dropped, and the thermo-induced and surfactant-induced Marangoni forces are therefore decoupled. In this study, Zhenlin develops a thermodynamically consistent phase-field model for investigating the coupling effects of temperature and surfactant concentration on droplet migration under a fully developed Poiseuille flow. By choosing the interface free energy sophisticatedly, the surface tension of our model consists of not only the classical linear part for the thermocapillary effects but also a nonlinear coupling term of temperature and surfactant concentration that recovers the Langmuir equation of state. This coupling term allows us to investigate the case of high surfactant concentration. Through 3D numerical simulations, Zhenlin finds that this nonlinear coupling term introduces extra thermo-induced and surfactant-induced Marangoni forces to the droplet migration, leading to a competition between the two, especially for the case of high surfactant concentration. In particular, the initial migration velocity of a surfactant-covered droplet is always faster than that of a droplet with a clean interface. The terminal velocity, on the other hand, does not reach its steady state but instead decreases gradually as the droplet moves toward the hotter region, whereas, for the case without this term, the initial migration velocity of a surfactant-covered droplet is always lower than that of a clean interface and the terminal velocity stays steady.

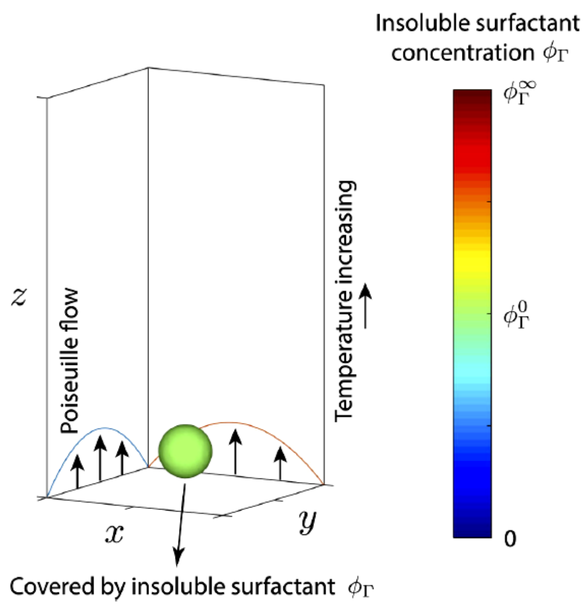


**Fig 1.** Problem setup. A surfactant-covered droplet is initially centered at the centerline of a square microchannel under a fully developed Poiseuille flow. The initial temperature field is assumed to be linearly increasing along the flow direction (z axis).

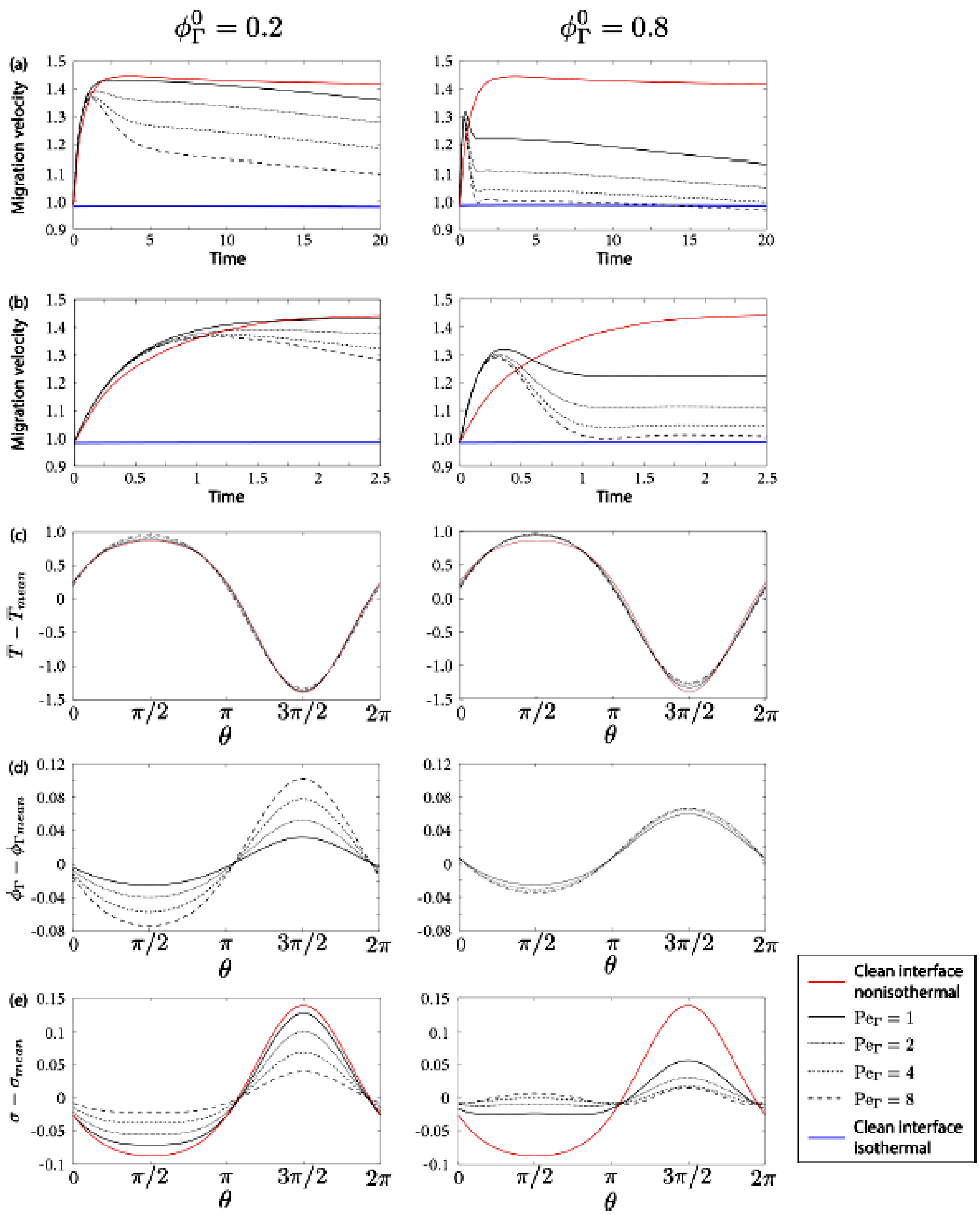


**Fig 2.** Droplets covered by insoluble surfactants migrate under a fully developed Poiseuille flow with a nonisothermal condition. The results for two cases, one with low surfactant concentration ($\phi= 0.2$ left) and one with high concentration ($\phi= 0.8$ right), with various $Pe_\Gamma$ up to (at) time t = 20 are presented. (a) Evolution of migration velocities of droplets covered by surfactant (black lines), a droplet with a clean interface under a nonisothermal condition (red solid line) and a droplet with a clean interface under an isothermal condition (blue line). (b) Zoom in of (a). (c)–(e) Interface surfactant concentration, temperature. and surface tension along the droplet interface, respectively. These quantities are plotted as the functions of an angle $\theta$ the 2D plane (x, y = 0, z) at time t = 20. The angle $\theta$ is obtained anticlockwise while treating the droplet center as the origin, where $\theta = π/2$ stands for the droplet front, and $\theta = 3π/2$ stands for the droplet rear. For simplicity, all quantities in (c–e) are subtracted by their mean values over the interface.

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[1] Zhenlin Guo, Nonlinear coupling effects of the thermocapillarity and insoluble surfactants to droplet migration under Poiseuille flow, Phys. Rev. Fluids, 8, 024001, 2023.

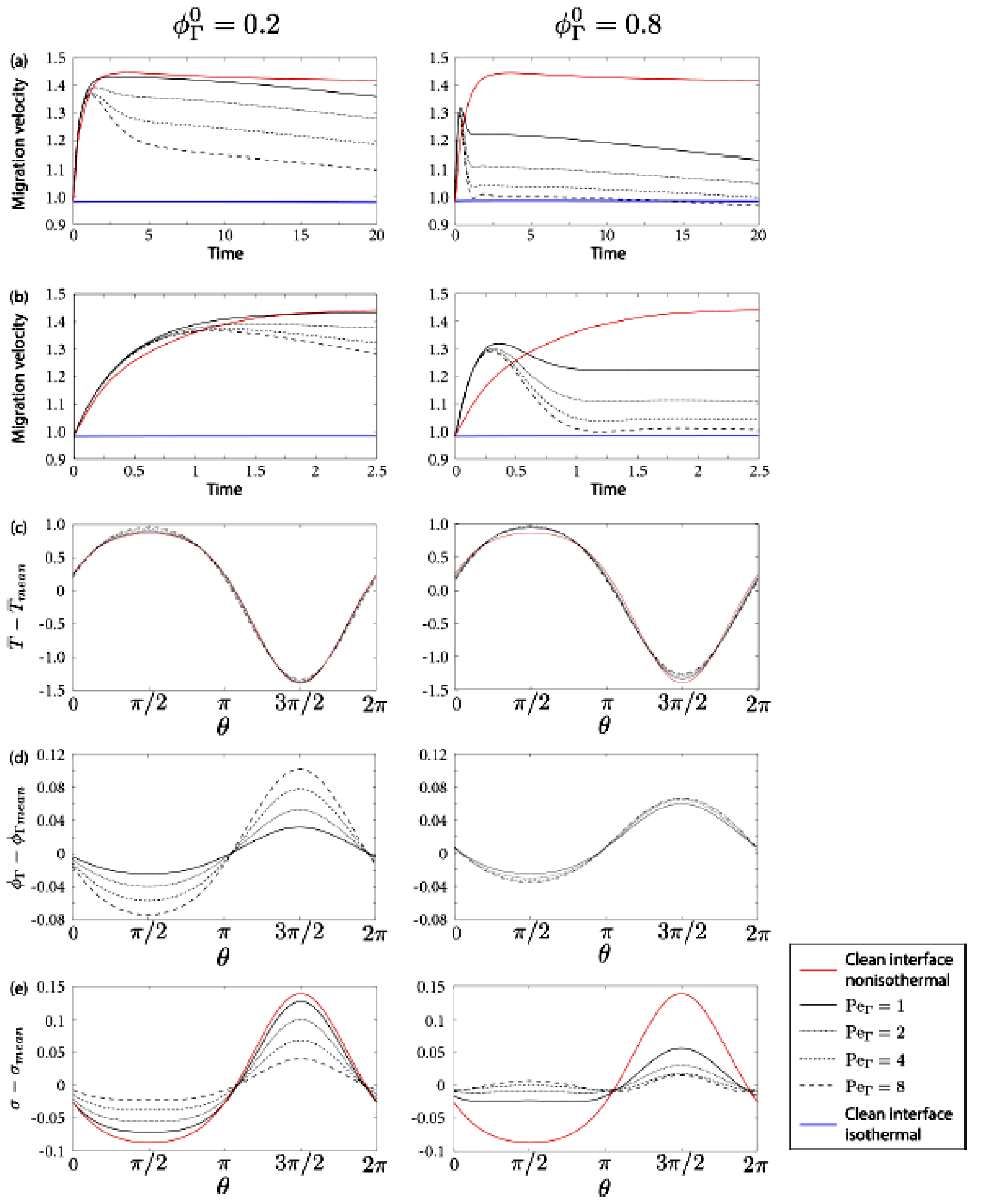


图 2: 非等温条件下充分发展的泊肃叶流动中，初始覆盖表面活性剂的液滴，在不同Pe值下迁移情况。图中展示了在两种表面活性剂初始浓度下的结果，左：$\phi= 0.2$，右：($\phi= 0.8$ right)。 (a)&(b) 液滴迁移速度. (c)–(e) 液滴表面活性剂浓度，温度，以及表面张力沿着液滴界面的分布。

**REFERENCES:**


[1] Zhenlin Guo, Nonlinear coupling effects of the thermocapillarity and insoluble surfactants to droplet migration under Poiseuille flow, Phys. Rev. Fluids, 8, 024001, 2023.

# 泊肃叶流中热毛细现象与不可溶性表面活性剂对液滴迁移的非线性耦合效应

郭震林#

普遍认为，在非等温充分发展的泊肃叶流中，只要温度沿着泊肃叶流动的方向升高，热毛细效应总是会增加液滴的迁移速度，而不可溶表面活性剂则总是阻碍液滴的迁移。这种普遍的认知，是因为在大多数模型中，液滴表面张力的 Langmuir 状态方程通常是在表面活性剂浓度较低的假设下简化得到的。在这种假设下，温度和表面活性剂浓度的耦合项往往被忽略，导致热毛细效应和表面活性剂效应所引发的两种马兰戈尼表面效应是解耦的。在本研究中，郭震林建立了一个满足热力学一致性的多物理场两相流相场模型，用于研究在充分发展的泊肃叶流中，温度和表面活性剂浓度对液滴迁移的耦合效应。通过选择特定的两相流界面自由能，模型中所得表面张力不仅包括热毛细管效应的经典线性部分，还包含了温度场和表面活性剂浓度场的非线性耦合项，该项与经典的 Langmuir 状态方程非线性项一致。而这正是传统模型所忽略的。通过考虑这一非线性耦合项，郭震林研究了在高浓度表面活性剂情况下，热毛细效应和表面活性剂对液滴迁移速度的非线性效应。通过三维数值模拟，他发现这一非线性耦合项为液滴迁移引入了额外的非均匀表面张力效应，且该效应为热毛细效应和表面活性剂效应相互竞争作用的结果。具体来讲，他发现，如果考虑此非线性项，初始覆盖表面活性剂的液滴初始速度，总是高于不含表面活性剂的液滴。同时，覆盖表面活性剂的液滴，在泊肃叶流中，总是无法达到稳态，而是随着液滴向较热区域移动而逐渐减小。另一方面，如果不考虑此非线性项，被表面活性剂覆盖的液滴的初始迁移速度总是低于不含表面活性剂的液滴，且迁移速度可以达到稳态。

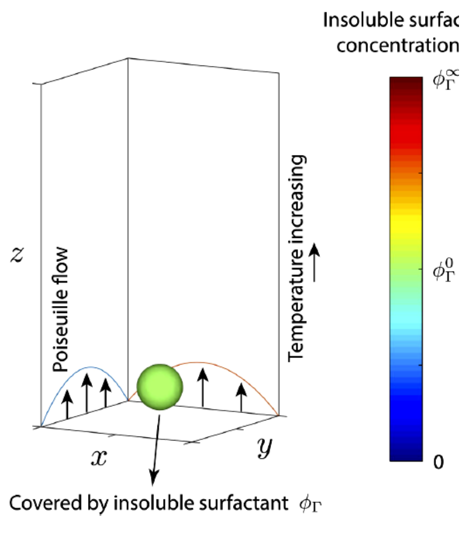


图 1：问题描述. 非等温条件下充分发展的泊肃叶流动中，初始覆盖表面活性剂的液滴。温度场随着泊肃叶流动方向增高。

During the 2022-2023 academic year, CSRC is undertakeing 41 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. 3 projects were concluded during the academic year.

2022-2023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41项，其中年内结题3项。

| 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 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 | 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 |
| 6 | 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 |
| 7 | 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 |
| 8 | 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 |
| 9 | 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 |

| No. | PI<br>项目负责人 | SOURCE<br>经费来源 | CATEGORY<br>项目类别 | PROJECT TITLE<br>项目名称 | FROM AND TO<br>起始时间 |
|---|---|---|---|---|---|
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | 张智民 | 国家自然科学基金委员会 | 数学天元基金项目 | 高阶非线性粘弹性弯曲波问题的高效数值方法及应用 | 2023.01 - 2023.12 |
| 18 | 陈家麒 | 国家自然科学基金委员会 | 理论物理专款 | 费曼积分约化关系的数学结构与算法 | 2023.01 - 2023.12 |
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |

续表

| No. | PI<br>项目负责人 | SOURCE<br>经费来源 | CATEGORY<br>项目类别 | PROJECT TITLE<br>项目名称 | FROM AND TO<br>起始时间 |
|---|---|---|---|---|---|
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | 曲登科 | 中国博士后科学基金会 | 博士后创新人才支持计划 | . | 2023.09 - 2025.08 |
| 30 | 李　培 | 中国博士后科学基金会 | 博士后国际交流计划派出项目 | . | 2021.07 - 2023.07 |
| 31 | 肖　磊 | 中国博士后科学基金会 | 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 |
| 32 | 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 |
| 33 | 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 | 2023.08 - 2025.05 |
| 34 | 邹　芬 | 中国博士后科学基金会 | 面上资助 | 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 - 2023.10 |
| 35 | 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 | 2023.08 - 2025.05 |

| No. | PI<br>项目负责人 | SOURCE<br>经费来源 | CATEGORY<br>项目类别 | PROJECT TITLE<br>项目名称 | FROM AND TO<br>起始时间 |
|---|---|---|---|---|---|
| 36 | 葛　磊 | 中国博士后科学基金会 | 面上资助 | 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 - 2024.05 |
| 37 | 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 |
| 38 | 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 | 2023.08 - 2025.05 |
| 39 | 赵志稳 | 中国博士后科学基金会 | 面上资助 | 复合材料中的椭圆方程和方程组 | 2021.11 - 2023.10 |
| 40 | 聂运欢 | 中国博士后科学基金会 | 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 |
| 41 | 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 |

2022-2023学术年期间，中心合计发表论文约300篇，其中归属中心（包括第一单位及通讯作者第一单位）论文148篇，其他合作论文151篇。

During the 2022-2023 academic year, CSRC has published a total of about 300 papers.

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

| | |
|---|---|
| 1 | WS2-Flake-Sandwiched, Au-Nanodisk-Enabled High-Quality Fabry-Perot Nanoresonators for Photoluminescence Modulation;<br>Huang, He; Wang, Hao; Li, Shasha; Jiang, Jingyao; Liu, Yi; Cai, Mingyang; Shao, Lei; Chen, Huanjun; Wang, Jianfang; ACS NANO (2022) |
| 2 | Routing the Exciton Emissions of WS2 Monolayer with the High- Order Plasmon Modes of Ag Nanorods;<br>Li, Shasha; Ai, Ruoqi; Chui, Ka Kit; Fang, Yini; Lai, Yunhe; Zhuo, Xiaolu; Shao, Lei; Wang, Jianfang; Lin, Hai-Qing; NANO LETTERS, 23, 10 (2023) |
| 3 | Excitation of Chiral Cavity Plasmon Resonances in Film-Coupled Chiral Au Nanoparticles;<br>Wang, Jing; Zheng, Jiapeng; Li, Kwai Hei; Wang, Jianfang; Lin, Hai-Qing; Shao, Lei; ADVANCED OPTICAL MATERIALS (2023) |
| 4 | Nonreciprocity of magnons goes into the quantum region;<br>Pan, Yueting; Xia, Ke; SCIENCE CHINA-PHYSICS MECHANICS & ASTRONOMY, 65, 8 (2022) |
| 5 | Phonon-mediated Migdal effect in semiconductor detectors;<br>Liang, Zheng-Liang; Mo, Chongjie; Zheng, Fawei; Zhang, Ping; PHYSICAL REVIEW D, 106, 4 (2022) |
| 6 | Using Weak Measurements to Synthesize Projective Measurement of Nonconserved Observables of Weakly Coupled Nuclear Spins;<br>Wang, Ping; Yang, Wen; Liu, Renbao; PHYSICAL REVIEW APPLIED, 19, 5 (2023) |
| 7 | Scaling of energy and power in a large quantum battery-charger model;<br>Gao, Lei; Cheng, Chen; He, Wen-Bin; Mondaini, Rubem; Guan, Xi-Wen; Lin, Hai-Qing; PHYSICAL REVIEW RESEARCH, 4, 4 (2022) |
| 8 | Hybrid states of a cavity-photon-vortex coupled system in a superconductive cavity;<br>Wang, Lei; Shang, Xin; Liu, Haiwen; Min, Tai; Xia, Ke; APPLIED PHYSICS LETTERS, 121, 19 (2022) |
| 9 | Higher-order topological insulator in a modified Haldane-Hubbard model;<br>Yi, Tian-Cheng; Lin, Hai-Qing; Mondaini, Rubem; PHYSICAL REVIEW B, 107, 16 (2023) |
| 10 | Fate of the quasicondensed state for bias-driven hard-core bosons in one dimension;<br>Puel, T. O.; Chesi, Stefano; Kirchner, Stefan; Ribeiro, P.; PHYSICAL REVIEW B, 107, 12 (2023) |

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| 11 | Subgap modes in two-dimensional magnetic Josephson junctions;<br>Fang, Yinan; Han, Seungju; Chesi, Stefano; Choi, Mahn -Soo; PHYSICAL REVIEW B, 107, 11 (2023) |
| 12 | Linear response functions respecting Ward-Takahashi identity and fluctuation-dissipation theorem within the GW approximation;<br>Li, Hui; Sun, Zhipeng; Su, Yingze; Lin, Haiqing; Huang, Huaqing; Li, Dingping; PHYSICAL REVIEW B, 107, 8 (2023) |
| 13 | Charge excitations across a superconductor-insulator transition;<br>Jin, Xiaodong; Liu, Yuhai; Mondaini, Rubem; Rigol, Marcos; PHYSICAL REVIEW B, 106, 24 (2022) |
| 14 | Hamming distance and the onset of quantum criticality;<br>Yi, Tian-Cheng; Scalettar, Richard T.; Mondaini, Rubem; PHYSICAL REVIEW B, 106, 20 (2022) |
| 15 | Bilayer Hubbard model: Analysis based on the fermionic sign problem;<br>Mou, Yingping; Mondaini, R.; Scalettar, R. T.; PHYSICAL REVIEW B, 106, 12 (2022) |
| 16 | Compatibility relationships in van der Waals quasicrystals;<br>Yu, Guodong; Wang, Yunhua; Katsnelson, Mikhail I.; Lin, Hai-Qing; Yuan, Shengjun; PHYSICAL REVIEW B, 106, 7 (2022) |
| 17 | Enhancing topological Weyl Semimetals by Janus transition-metal dichalcogenides structures;<br>Griffith, M. A. R.; Rufo, S.; Dias, Alexandre C.; Da Silva, Juarez L. F.; COMPUTATIONAL MATERIALS SCIENCE, 218 (2023) |
| 18 | Nonlinear dynamics of the dissipative anisotropic two-photon Dicke model;<br>Li, Jiahui; Fazio, Rosario; Chesi, Stefano; NEW JOURNAL OF PHYSICS, 24, 8 (2022) |
| 19 | Goos-Hanchen shift of electron waves reflected by 8-Pmmn borophene np junctions;<br>Zhang, Chao; Yang, Jin; Zhang, Shu-Hui; Yang, Wen; JOURNAL OF APPLIED PHYSICS, 132, 18 (2022) |
| 20 | Quantum dynamics of Gaudin magnets;<br>He, Wen-Bin; Chesi, Stefano; Lin, Hai-Qing; Guan, Xi-Wen; COMMUNICATIONS IN THEORETICAL PHYSICS, 74, 9 (2022) |

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

| | |
|---|---|
| 1 | Observation of dark edge states in parity-time-symmetric quantum dynamics;<br>Xue, Peng; Qiu, Xingze; Wang, Kunkun; Sanders, Barry C.; Yi, Wei; NATIONAL SCIENCE REVIEW, 10, 8 (2023) |

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

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| 2 | Synchronous Observation of Bell Nonlocality and State-Dependent Contextuality;<br>Xue, Peng; Xiao, Lei; Ruffolo, G.; Mazzari, A.; Temistocles, T.; Cunha, M. Terra; Rabelo, R.; PHYSICAL REVIEW LETTERS, 130, 4 (2023) |
| 3 | Stable Atomic Magnetometer in Parity-Time Symmetry Broken Phase;<br>Zhang, Xiangdong; Hu, Jinbo; Zhao, Nan; PHYSICAL REVIEW LETTERS, 130, 2 (2023) |
| 4 | Topological Phase Transitions and Mobility Edges in Non-Hermitian Quasicrystals;<br>Lin, Quan; Li, Tianyu; Xiao, Lei; Wang, Kunkun; Yi, Wei; Xue, Peng; PHYSICAL REVIEW LETTERS, 129, 11 (2022) |
| 5 | Enantiodetection of Chiral Molecules via Two-Dimensional Spectroscopy;<br>Cai, Mao-Rui; Ye, Chong; Dong, Hui; Li, Yong; PHYSICAL REVIEW LETTERS, 129, 10 (2022) |
| 6 | On system reliability for time-varying structure;<br>Cui, L. X.; Du, Yi-Mu; Sun, C. P.; RELIABILITY ENGINEERING & SYSTEM SAFETY, 234 (2023) |
| 7 | Experimental witnessing for entangled states with limited local measurements;<br>Zhu, Gaoyan; Zhang, Chengjie; Wang, Kunkun; Xiao, Lei; Xue, Peng; PHOTONICS RESEARCH, 10, 9 (2022) |
| 8 | Experimental demonstration of a quantum engine driven by entanglement and local measurements;<br>Wang, Kunkun; Xia, Ruqiao; Bresque, Lea; Xue, Peng; PHYSICAL REVIEW RESEARCH, 4, 3 (2022) |
| 9 | Enantiodiscrimination of chiral molecules via quantum correlation function;<br>Zou, Fen; Chen, Yu-Yuan; Liu, Bo; Li, Yong; OPTICS EXPRESS, 30, 17 (2022) |
| 10 | Magnetic field constraint for Majorana zero modes in a hybrid nanowire;<br>Qiao, Guo-Jian; Li, Sheng-Wen; Sun, C. P.; PHYSICAL REVIEW B, 106, 10 (2022) |
| 11 | Demonstration of a photonic router via quantum walks;<br>Gao, Huixia; Wang, Kunkun; Qu, Dengke; Lin, Quan; Xue, Peng; NEW JOURNAL OF PHYSICS, 25, 5 (2023) |
| 12 | Laser-assisted in-flight muon-catalyzed deuteron-triton fusion;<br>Liu, Shiwei; Ye, Difa; Liu, Jie; PHYSICAL REVIEW C, 106, 6 (2022) |
| 13 | Demonstration of the charging progress of quantum batteries;<br>Huang, Xiaojian; Wang, Kunkun; Xiao, Lei; Gao, Lei; Lin, Haiqing; Xue, Peng; PHYSICAL REVIEW A, 107, 3 (2023) |
| 14 | Enhancing dissipative cat-state generation via nonequilibrium pump fields;<br>Zhou, Zheng-Yang; Gneiting, Clemens; Qin, Wei; You, J. Q.; Nori, Franco; PHYSICAL REVIEW A, 106, 2 (2022) |

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| 15 | Experimental Detection of Initial System-Environment Entanglement in Open Systems;<br>Zhu, Gaoyan; Qu, Dengke; Xiao, Lei; Xue, Peng; PHOTONICS, 9, 11 (2022) |
| 16 | Fragmentation dynamics of electron-impact double ionization of helium;<br>Liu, Shiwei; Ye, Difa; Liu, Jie; CHINESE PHYSICS B, 32, 6 (2023) |
| 17 | Electron Correlation Momentum and Energy Spectrum in Triple Ionization of Lithium by the Femtosecond Laser Field (Invited);<br>Shiwei, Liu; Difa, Ye; Jie, Liu; ACTA PHOTONICA SINICA, 51, 8 (2022) |

# MATERIALS AND ENERGY DIVISION 材料与能源研究部

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| 1 | Critical role of hydrogen for superconductivity in nickelates;<br>Ding, Xiang; Tam, Charles C.; Sui, Xuelei; Zhao, Yan; Xu, Minghui; Choi, Jaewon; Leng, Huaqian; Zhang, Ji; Wu, Mei; Xiao, Haiyan; Zu, Xiaotao; Garcia-Fernandez, Mirian; Agrestini, Stefano; Wu, Xiaoqiang; Wang, Qingyuan; Gao, Peng; Li, Sean; Huang, Bing; Zhou, Ke-Jin; Qiao, Liang; NATURE, 615, 7950 (2023) |
| 2 | A Unified Understanding of Diverse Spin Textures of Kramers-Weyl Fermions in Nonmagnetic Chiral Crystals;<br>Tan, Wei; Jiang, Xiao; Li, Yang; Wu, Xiaoqiang; Wang, Jianfeng; Huang, Bing; ADVANCED FUNCTIONAL MATERIALS, 32, 49 (2022) |
| 3 | Defect-characterized phase transition kinetics;<br>Zhang, Xie; Zhang, Jian; Wang, Hongcai; Rogal, Jutta; Li, Hong-Yi; Wei, Su-Huai; Hickel, Tilmann; APPLIED PHYSICS REVIEWS, 9, 4 (2022) |
| 4 | Mechanisms of Photothermalization in Plasmonic Nanostructures: Insights into the Steady State;<br>Wu, Shengxiang; Sheldon, Matthew; ANNUAL REVIEW OF PHYSICAL CHEMISTRY, 74 (2023) |
| 5 | First-principles study of the distribution of excess intercalated lithium in Li3V2O5 with a disordered rock-salt structure;<br>Shi, Jing; Lin, Aming; Wu, Xiaowei; Wei, Su-Huai; Sun, Yi-Yang; JOURNAL OF MATERIALS CHEMISTRY A, 11, 27 (2023) |
| 6 | Moire magnetic exchange interactions in twisted magnets;<br>Yang, Baishun; Li, Yang; Xiang, Hongjun; Lin, Haiqing; Huang, Bing; NATURE COMPUTATIONAL SCIENCE, 3, 4 (2023) |
| 7 | Defect modeling and control in structurally and compositionally complex materials;<br>Zhang, Xie; Kang, Jun; Wei, Su-Huai; NATURE COMPUTATIONAL SCIENCE, 3, 3 (2023) |

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| 8 | Machine-learning inspired density-fluctuation model of local structural instability in metallic glasses;<br>Wu, Yicheng; Xu, Bin; Zhang, Xuefeng; Guan, Pengfei; ACTA MATERIALIA, 247, (2023) |
| 9 | Plasmonic Photocatalysis with Nonthermalized Hot Carriers;<br>Wu, Shengxiang; Chen, Yu; Gao, Shiwu; PHYSICAL REVIEW LETTERS, 129, 8 (2022) |
| 10 | Schottky barrier effect on plasmon-induced charge transfer;<br>Wang, Xinxin; Gao, Shiwu; Ma, Jie; NANOSCALE, 15, 4 (2023) |
| 11 | Construction of group III nitride van der Waals heterostructures for highly efficient photocatalyst;<br>Chen, Yingjie; Guan, Xiaoning; Yang, Lingjia; Jia, Baonan; Zhao, Huiyan; Han, Lihong; Guan, Pengfei; Lu, Pengfei; APPLIED SURFACE SCIENCE, 611 (2023) |
| 12 | Intrinsic oxygen defects in UO2 (111) and PuO2 (111) surfaces;<br>Lv, Wenting; Zhao, Zhongwei; Sun, Bo; Guan, Pengfei; Yang, Yu; Zhang, Ping; APPLIED SURFACE SCIENCE, 610 (2023) |
| 13 | Electronic origin of the unusual thermal properties of copper-based semiconductors: The s-d coupling-induced large phonon anharmonicity;<br>Yang, Kaike; Yang, Huai; Sun, Yujia; Wei, Zhongming; Zhang, Jun; Tan, Ping-Heng; Luo, Jun-Wei; Li, Shu-Shen; Wei, Su-Huai; Deng, Hui-Xiong; SCIENCE CHINA-PHYSICS MECHANICS & ASTRONOMY, 66, 7 (2023) |
| 14 | Light-induced magnetic phase transition in van der Waals antiferromagnets;<br>Chen, Jiabin; Li, Yang; Yu, Hongyu; Yang, Yali; Jin, Heng; Huang, Bing; Xiang, Hongjun; SCIENCE CHINA-PHYSICS MECHANICS & ASTRONOMY, 66, 7 (2023) |
| 15 | Editorial;<br>Wei, Su-Huai; You, Jingbi; Yang, Xudong; SCIENCE CHINA-PHYSICS MECHANICS & ASTRONOMY, 66, 1 (2023) |
| 16 | Investigation of Ag(Ga,In)Se-2 as thin-film solar cell absorbers: A first-principles study;<br>Wang, Rong; Dou, Baoying; Zheng, Yifeng; Wei, Su-Huai; SCIENCE CHINA-PHYSICS MECHANICS & ASTRONOMY, 65, 10 (2022) |
| 17 | Enhanced Anharmonicity by Forming Low-Symmetry Off-Center Phase: The Case of Two-Dimensional Group-IB Chalcogenides;<br>Zhou, Ran; Liang, Hanpu; Duan, Yifeng; Wei, Su-Huai; JOURNAL OF PHYSICAL CHEMISTRY LETTERS, 14, 3 (2023) |
| 18 | Doping Limits of Phosphorus, Arsenic, and Antimony in CdTe;<br>Chatratin, Intuon; Dou, Baoying; Wei, Su-Huai; Janotti, Anderson; JOURNAL OF PHYSICAL CHEMISTRY LETTERS, 14, 1 (2023) |
| 19 | Doping Limits of Phosphorus, Arsenic, and Antimony in CdTe;<br>Chatratin, Intuon; Dou, Baoying; Wei, Su-Huai; Janotti, Anderson; JOURNAL OF PHYSICAL CHEMISTRY LETTERS (2023) |

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| 20 | Origin of Structural Anomaly in Cuprous Halides;<br>Wang, Zhi-Hao; Zhang, Xie; Wei, Su-Huai; JOURNAL OF PHYSICAL CHEMISTRY LETTERS, 13, 49 (2022) |
| 21 | Chemical Trend of Nonradiative Recombination in Cu(In,Ga)Se2 Alloys;<br>Dou, Baoying; Falletta, Stefano; Neugebauer, Joerg; Freysoldt, Christoph; Zhang, Xie; Wei, Su -Huai; PHYSICAL REVIEW APPLIED, 19, 5 (2023) |
| 22 | Cation-Disorder-Enhanced Unintentional Doping in MgSnN2;<br>Ning, Feng; Huang, Jing; Kang, Jun; PHYSICAL REVIEW APPLIED, 19, 5 (2023) |
| 23 | Trends in the Electronic Structure and Chemical Bonding of a Series of Porphyrinoid-Uranyl Complexes;<br>Wang, Cong; Hu, Shu-Xian; Zhang, Lu; Wang, Kai; Liu, Hai-Tao; Zhang, Ping; INORGANIC CHEMISTRY, 62, 14 (2023) |
| 24 | First-Principles Calculations of Shallow Acceptor-Carbon Complexes in Si: A Potential-Patching Method with a Hybrid-Functional Correction;<br>Kang, Jun; Wang, Lin -Wang; PHYSICAL REVIEW APPLIED, 18, 6 (2022) |
| 25 | Electronic Structures and Unusual Chemical Bonding in Actinyl Peroxide Dimers [An(2)O(6)](2+) and [(An(2)O(6))(12-crown-4 ether)(2)](2+) (An = U, Np, and Pu);<br>Hu, Shu-Xian; You, Xiao-Xia; Zou, Wen-Li; Lu, Erli; Gao, Xiang; Zhang, Ping; INORGANIC CHEMISTRY, 61, 39 (2022) |
| 26 | Identification of carbon location in p-type GaN: Synchrotron x-ray absorption spectroscopy and theory;<br>Huang, Huayang; Yan, Xiaolan; Yang, Xuelin; Yan, Wensheng; Qi, Zeming; Wu, Shan; Shen, Zhaohua; Tang, Ning; Xu, Fujun; Wang, Xinqiang; Ge, Weikun; Huang, Bing; Shen, Bo; APPLIED PHYSICS LETTERS, 121, 25 (2022) |
| 27 | Verification of the Accuracy and Efficiency of Dispersion-Corrected Density Functional Theory Methods to Describe the Lattice Structure and Energy of Energetic Cocrystals;<br>Liu, Guangrui; Wei, Su-Huai; Zhang, Chaoyang; CRYSTAL GROWTH & DESIGN, 22, 9 (2022) |
| 28 | Local structural power exponent as an indicator of elastic heterogeneity in glasses;<br>Wei, Xuerui; Wang, Weihua; Guan, Pengfei; PHYSICAL REVIEW B, 107, 17 (2023) |
| 29 | Origin of the variation in lattice thermal conductivities in pyrite-type dichalcogenides;<br>Jia, Tiantian; Liu, Xiaobing; Zhang, Yongsheng; Wei, Su-Huai; PHYSICAL REVIEW B, 107, 11 (2023) |
| 30 | Hole doping dependent electronic instability and electron-phonon coupling in infinite-layer nickelates;<br>Sui, Xuelei; Wang, Jianfeng; Chen, Chao; Ding, Xiang; Zhou, Ke-Jin; Cao, Chao; Qiao, Liang; Lin, Haiqing; Huang, Bing; PHYSICAL REVIEW B, 107, 7 (2023) |
| 31 | Bidirectional Transport Phenomenon of Ions in Electric Fields Due to the Cluster Formation in Two-Dimensional Graphene Channels;<br>Zhang, Xinke; Li, Shuang; Gao, Shiwu; Su, Jiaye; JOURNAL OF PHYSICAL CHEMISTRY C, 127, 2 (2023) |

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| 32 | Overcoming the doping limit in semiconductors via illumination;<br>Cai, Xuefen; Luo, Jun-Wei; Li, Shu-She; Wei, Su-Huai; Deng, Hui-Xiong; PHYSICAL REVIEW B, 106, 21 (2022) |
| 33 | Defect and Doping Properties of Two-Dimensional PdSe2;<br>Huang, Jing; Kang, Jun; JOURNAL OF PHYSICAL CHEMISTRY C, 126, 48 (2022) |
| 34 | Role of large Rashba spin-orbit coupling in second-order nonlinear optical effects of polar BiB3O6;<br>Jiang, Xiao; Ye, Liangting; Wu, Xiaoqiang; Kang, Lei; Huang, Bing; PHYSICAL REVIEW B, 106, 19 (2022) |
| 35 | Generating two-dimensional ferromagnetic charge density waves via external fields;<br>Jin, Heng; Chen, Jiabin; Li, Yang; Shao, Bin; Huang, Bing; PHYSICAL REVIEW B, 106, 16 (2022) |
| 36 | What Are the Roles of Hydrogen in Infinite-Layer Nickelates?;<br>Huang, Bing; CHINESE PHYSICS LETTERS, 40, 5 (2023) |
| 37 | Competition between Stepwise Polarization Switching and Chirality Coupling in Ferroelectric GeS Nanotubes;<br>Wang, Hao-Chen; Wang, Zhi-Hao; Chen, Xuan-Yan; Wei, Su-Huai; Zhu, Wenguang; Zhang, Xie; CHINESE PHYSICS LETTERS, 40, 4 (2023) |
| 38 | Profiling the off-center atomic displacements in CuCl at finite temperatures with a deep-learning potential;<br>Wang, Zhi-Hao; Chen, Xuan-Yan; Zhang, Zhen; Zhang, Xie; Wei, Su -Huai; PHYSICAL REVIEW MATERIALS, 7, 3 (2023) |
| 39 | Crystal-liquid duality enhanced dynamical stability of hybrid perovskites;<br>Chen, Xuan-Yan; Zhao, Bai-Qing; Liu, Zheng; Wei, Su-Huai; Zhang, Xie; PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 25, 27 (2023) |
| 40 | Thickness-dependent oxygen chemisorption behaviors on (111) surfaces of two-dimensional FCC metals Al and Cu: First-principles study;<br>Yang, Huanhuan; Guan, Pengfei; COMPUTATIONAL MATERIALS SCIENCE, 219, (2023) |
| 41 | XPu(CO)n (X = B, Al, Ga; n=2 to 4): pi Back-Bonding in Heterodinuclear Plutonium Boron Group Compounds with an End- On Carbonyl Ligand;<br>Hu, Shu-Xian; Zhang, Peng; Cao, Ling-Zhi; Zou, Wen-Li; Zhang, Ping; JOURNAL OF PHYSICAL CHEMISTRY A, (2023) |
| 42 | First-principles study of different oxidation process on Al(111) and Cu (111): Metal pulled-off effect;<br>Yang, Huanhuan; Zhang, Xie; Guan, Pengfei; SURFACE SCIENCE, 731, (2023) |
| 43 | Advances and challenges in DFT-based energy materials design;<br>Kang, Jun; Zhang, Xie; Wei, Su-Huai; CHINESE PHYSICS B, 31, 10 (2022) |
| 44 | Hydrogen bonds determine the nonbonding adhesion at HMX-basedPBX interface;<br>Zhang,Xinke; Li,Shuang; Kang,Jun ; Su,Jiaye; Deng,Kaiming. PHYSICA SCRIPTA 98, 085941 (2023) |

## COMPLEX SYSTEMS DIVISION 复杂系统研究部

| | |
|---|---|
| 1 | Direct experimental observation of blue-light-induced conformational change and intermolecular interactions of cryptochrome;<br>Li, Pei; Cheng, Huaqiang; Kumar, Vikash; Lupala, Cecylia Severin; Li, Xuanxuan; Shi, Yingchen; Ma, Chongjun; Joo, Keehyoung; Lee, Jooyoung; Liu, Haiguang; Tan, Yan-Wen; COMMUNICATIONS BIOLOGY, 5, 1 (2022) |
| 2 | Module intersection and uniform formula for iterative reduction of one-loop integrals;<br>Chen, Jiaqi; Feng, Bo; JOURNAL OF HIGH ENERGY PHYSICS, 2 (2023) |
| 3 | Gluonic evanescent operators: two-loop anomalous dimensions;<br>Jin, Qingjun; Ren, Ke; Yang, Gang; Yu, Rui; JOURNAL OF HIGH ENERGY PHYSICS, 2 (2023) |
| 4 | One-loop diagrams with quadratic propagators from the worldsheet;<br>Feng, Bo; He, Song; Zhang, Yong; Zhang, Yao-Qi; JOURNAL OF HIGH ENERGY PHYSICS, 8 (2022) |
| 5 | Generation function for one-loop tensor reduction;<br>Feng, Bo; COMMUNICATIONS IN THEORETICAL PHYSICS, 75, 2 (2023) |
| 6 | PV-reduction of sunset topology with auxiliary vector;<br>Feng, Bo; Li, Tingfei; COMMUNICATIONS IN THEORETICAL PHYSICS, 74, 9 (2022) |
| 7 | Elucidation of partial activation of cannabinoid receptor type 2 and identification of potential partial agonists: Molecular dynamics simulation and structure-based virtual screening;<br>Uba, Abdullahi Ibrahim; Aluwala, Harika; Liu, Haiguang; Wu, Chun; COMPUTATIONAL BIOLOGY AND CHEMISTRY, 99 (2022) |
| 8 | A scoring function for the prediction of protein complex interfaces based on the neighborhood preferences of amino acids;<br>Nagaraju, Mulpuri; Liu, Haiguang; ACTA CRYSTALLOGRAPHICA SECTION D-STRUCTURAL BIOLOGY, 79 (2023) |
| 9 | X-ray free-electron lasers and their applications in ultrafast structural dynamics research;<br>Liu XinWei; Liu HaiGuang; Zhang WenKai; SCIENTIA SINICA-PHYSICA MECHANICA & ASTRONOMICA, 52, 7 (2022) |

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

| | |
|---|---|
| 1 | Coupling gene expression dynamics to cell size dynamics and cell cycle events: Exact and approximate solutions of the extended telegraph model;<br>Jia, Chen; Grima, Ramon; ISCIENCE, 26, 1 (2023) |

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

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|---|---|
| 2 | Linear energy stable numerical schemes for a general chemo-repulsive model;<br>Jiang, Maosheng; Zhao, Jia; Wang, Qi; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 415 (2022) |
| 3 | Residual-based a posteriori error estimators for mixed finite element methods for fourth order elliptic singularly perturbed problems;<br>Du, Shaohong; Lin, Runchang; Zhang, Zhimin; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 412 (2022) |
| 4 | Superconvergence and fast implementation of the barycentric prolate differentiation;<br>Tian, Yan; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 410 (2022) |
| 5 | FE-holomorphic operator function method for nonlinear plate vibrations with elastically added masses;<br>Pang, Xiangying; Sun, Jiguang; Zhang, Zhimin; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 410 (2022) |
| 6 | A Fast High-Order Predictor-Corrector Method on Graded Meshes for Solving Fractional Differential Equations;<br>Su, Xinxin; Zhou, Yongtao; FRACTAL AND FRACTIONAL, 6, 9 (2022) |
| 7 | Discretised general fractional derivative;<br>Fan, Enyu; Li, Changpin; Stynes, Martin; MATHEMATICS AND COMPUTERS IN SIMULATION, 208 (2023) |
| 8 | Concentration fluctuations in growing and dividing cells: Insights into the emergence of concentration homeostasis;<br>Jia, Chen; Singh, Abhyudai; Grima, Ramon; PLOS COMPUTATIONAL BIOLOGY, 18, 10 (2022) |
| 9 | Large deviations and fluctuation theorems for cycle currents defined in the loop-erased and spanning tree manners: A comparative study;<br>Jiang, Yuhao; Wu, Bingjie; Jia, Chen; PHYSICAL REVIEW RESEARCH, 5, 1 (2023) |
| 10 | A sharp discrete convolution sum estimate;<br>Stynes, Martin; Wang, Dongling; COMMUNICATIONS IN NONLINEAR SCIENCE AND NUMERICAL SIMULATION, 117 (2023) |
| 11 | Band Structure Calculations of Dispersive Photonic Crystals in 3D using Holomorphic Operator Functions;<br>Xiao, Wenqiang; Gong, Bo; Lin, Junshan; Sun, Jiguang; COMMUNICATIONS IN COMPUTATIONAL PHYSICS, 33, 2 (2023) |
| 12 | Quasi-incompressible models for binary fluid flows in porous media;<br>Li, Yakun; Wang, Qi; APPLIED MATHEMATICS LETTERS, 136 (2023) |
| 13 | Some mathematical aspects of Anderson localization: boundary effect, multimodality, and bifurcation;<br>Jia, Chen; Liu, Ziqi; Zhang, Zhimin; COMMUNICATIONS IN THEORETICAL PHYSICS, 74, 11 (2022) |

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| 14 | LINEARLY IMPLICIT INVARIANT-PRESERVING DECOUPLED DIFFERENCE SCHEME FOR THE ROTATION-TWO-COMPONENT CAMASSA-HOLM SYSTEM;<br>Zhang, Qifeng; Liu, Lingling; Zhang, Zhimin; SIAM JOURNAL ON SCIENTIFIC COMPUTING, 44, 4 (2022) |
| 15 | SPECTRAL ELEMENT METHODS FOR EIGENVALUE PROBLEMS BASED ON DOMAIN DECOMPOSITION;<br>Wang, Wei; Zhang, Zhimin; SIAM JOURNAL ON SCIENTIFIC COMPUTING, 44, 2 (2022) |
| 16 | Temperature Patches for a Generalised 2D Boussinesq System with Singular Velocity;<br>Khor, Calvin; Xu, Xiaojing; JOURNAL OF NONLINEAR SCIENCE, 33, 2 (2023) |
| 17 | Finite element method for the stationary dual-porosity Navier-Stokes system with Beavers-Joseph interface conditions;<br>Qiu, Meilan; Qing, Fang; Yu, Xijun; Hou, Jiangyong; Li, Dewang; Zhao, Xiaolong; COMPUTERS & MATHEMATICS WITH APPLICATIONS, 141 (2023) |
| 18 | A FAMILY OF FINITE ELEMENT STOKES COMPLEXES IN THREE DIMENSIONS;<br>Hu, Kaibo; Zhang, Qian; Zhang, Zhimin; SIAM JOURNAL ON NUMERICAL ANALYSIS, 60, 1 (2022) |
| 19 | A C-1 CONFORMING PETROV-GALERKIN METHOD FOR CONVECTION-DIFFUSION EQUATIONS AND SUPERCONVERGENCE ANALYSIS OVER RECTANGULAR MESHES;<br>Cao, Waixiang; Jia, Lueling; Zhang, Zhimin; SIAM JOURNAL ON NUMERICAL ANALYSIS, 60, 1 (2022) |
| 20 | CONVERGENCE OF RENORMALIZED FINITE ELEMENT METHODS FOR HEAT FLOW OF HARMONIC MAPS;<br>Gui, Xinping; Li, Buyang; Wang, Jilu; SIAM JOURNAL ON NUMERICAL ANALYSIS, 60, 1 (2022) |
| 21 | Block generalized St?rmer-Cowell methods applied to second order nonlinear delay differential equations;<br>Li, Cui; Zhou, Yongtao; APPLIED NUMERICAL MATHEMATICS, 178 (2022) |
| 22 | Thermodynamically Consistent Models for Coupled Bulk and Surface Dynamics;<br>Jing, Xiaobo; Wang, Qi; ENTROPY, 24, 11 (2022) |
| 23 | Error Estimates of Finite Difference Methods for the Biharmonic Nonlinear Schrodinger Equation;<br>Ma, Ying; Zhang, Teng; JOURNAL OF SCIENTIFIC COMPUTING, 95, 1 (2023) |
| 24 | High Order Asymptotic Preserving Hermite WENO Fast Sweeping Method for the Steady-State S-N Transport Equations;<br>Ren, Yupeng; Xing, Yulong; Wang, Dean; Qiu, Jianxian; JOURNAL OF SCIENTIFIC COMPUTING, 93, 1 (2022) |
| 25 | An Oscillation-free Discontinuous Galerkin Method for Shallow Water Equations;<br>Liu, Yong; Lu, Jianfang; Tao, Qi; Xia, Yinhua; JOURNAL OF SCIENTIFIC COMPUTING, 92, 3 (2022) |
| 26 | Sharp Error Estimate of an Implicit BDF2 Scheme with Variable Time Steps for the Phase Field Crystal Model;<br>Di, Yana; Wei, Yifan; Zhang, Jiwei; Zhao, Chengchao; JOURNAL OF SCIENTIFIC COMPUTING, 92, 2 (2022) |

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

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| 27 | A Posteriori Error Analysis for Variable-Coefficient Multiterm Time-Fractional Subdiffusion Equations;<br>Kopteva, Natalia; Stynes, Martin; JOURNAL OF SCIENTIFIC COMPUTING, 92, 2 (2022) |
| 28 | Balanced-Norm and Energy-Norm Error Analyses for a Backward Euler/FEM Solving a Singularly Perturbed Parabolic Reaction-Diffusion Problem;<br>Meng, Xiangyun; Stynes, Martin; JOURNAL OF SCIENTIFIC COMPUTING, 92, 2 (2022) |
| 29 | Uniformly Accurate Nested Picard Iterative Integrators for the Klein-Gordon Equation in the Nonrelativistic Regime;<br>Cai, Yongyong; Zhou, Xuanxuan; JOURNAL OF SCIENTIFIC COMPUTING, 92, 2 (2022) |
| 30 | Mesh-Robustness of an Energy Stable BDF2 Scheme with Variable Steps for the Cahn-Hilliard Model;<br>Liao, Hong-lin; Ji, Bingquan; Wang, Lin; Zhang, Zhimin; JOURNAL OF SCIENTIFIC COMPUTING, 92, 2 (2022) |
| 31 | The local discontinuous Galerkin method for a singularly perturbed convection-diffusion problem with characteristic and exponential layers;<br>Cheng, Yao; Stynes, Martin; NUMERISCHE MATHEMATIK, 154, 1-2 (2023) |
| 32 | Numerical computation for rogue waves in the coupled nonlinear Schrodinger equations with the coherent coupling effect;<br>Liu, Lei; Wang, Pengde; INTERNATIONAL JOURNAL OF COMPUTER MATHEMATICS, 99, 12 (2022) |
| 33 | An exponential convergence approximation to singularly perturbed problems by Log orthogonal functions;<br>Chen, Sheng; Zhang, Zhimin; CALCOLO, 59, 3 (2022) |
| 34 | Second-order error analysis of the averaged L1 & nbsp;scheme (L1)over bar for time-fractional initial-value and subdiffusion problems;<br>Shen, Jinye; Zeng, Fanhai; Stynes, Martin; SCIENCE CHINA-MATHEMATICS (2023) |
| 35 | Gradient estimates for the insulated conductivity problem: The case of m-convex inclusions;<br>Zhao, Zhiwen; JOURNAL OF MATHEMATICAL PHYSICS, 64, 3 (2023) |
| 36 | A Survey of the L1 Scheme in the Discretisation of Time-Fractional Problems;<br>Stynes, Martin; NUMERICAL MATHEMATICS-THEORY METHODS AND APPLICATIONS, 15, 4 (2022) |
| 37 | REGULARITY OF THE SOLUTION OF A NONLINEAR VOLTERRA INTEGRAL EQUATION OF THE SECOND KIND;<br>Liang, Hui; Stynes, Martin; DISCRETE AND CONTINUOUS DYNAMICAL SYSTEMS-SERIES B (2022) |
| 38 | FACTORIZATION METHOD FOR INVERSE TIME-HARMONIC ELASTIC SCATTERING WITH A SINGLE PLANE WAVE;<br>Ma, Guanqiu; Hu, Guanghui; DISCRETE AND CONTINUOUS DYNAMICAL SYSTEMS-SERIES B, 27, 12 (2022) |

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| 39 | UNCONDITIONALLY OPTIMAL ERROR ESTIMATE OF A LINEARIZED VARIABLE-TIME-STEP BDF2 SCHEME FOR NONLINEAR PARABOLIC EQUATIONS;<br>Zhao, Chenchao; Liu, Nan; Ma, Yuheng; Zhang, Jiwei; COMMUNICATIONS IN MATHEMATICAL SCIENCES, 21, 3 (2023) |
| 40 | THERMODYNAMICALLY CONSISTENT DYNAMIC BOUNDARY CONDITIONS OF PHASE FIELD MODELS;<br>Jing, Xiaobao; Wang, Qi; COMMUNICATIONS IN MATHEMATICAL SCIENCES, 21, 3 (2023) |
| 41 | Exact solutions for the insulated and perfect conductivity problems with concentric balls;<br>Zhao, Zhiwen; MATHEMATICS IN ENGINEERING, 5, 3 (2023) |
| 42 | ANALYSIS OF THE IMPLICIT-EXPLICIT ULTRA-WEAK DISCONTINUOUS GALERKIN METHOD FOR CONVECTION-DIFFUSION PROBLEMS;<br>Wang, Haijin; Xu, Anping; Tao, Qi; JOURNAL OF COMPUTATIONAL MATHEMATICS (2022) |
| 43 | ANALYSIS OF A FULLY DISCRETE FINITE ELEMENT METHOD FOR PARABOLIC INTERFACE PROBLEMS WITH NONSMOOTH INITIAL DATA;<br>Wang, Kai; Wang, Na; JOURNAL OF COMPUTATIONAL MATHEMATICS, 40, 5 (2022) |
| 44 | Huizhou GDP forecast based on fractional opposite-direction accumulating nonlinear grey bernoulli markov model;<br>Qiu, Meilan; Li, Dewang; Luo, Zhongliang; Yu, Xijun; ELECTRONIC RESEARCH ARCHIVE, 31, 2 (2022) |
| 45 | Local regularity for nonlinear elliptic and parabolic equations with anisotropic weights;<br>Miao, Changxing; Zhao, Zhiwen; PROCEEDINGS OF THE EDINBURGH MATHEMATICAL SOCIETY (2023) |

## MECHANICS DIVISION 力学研究部

| | |
|---|---|
| 1 | Swimming of the midge larva: Principles and tricks of locomotion at intermediate Reynolds number;<br>Jin, Bowen; Pan, Chengfeng; Xia, Neng; Song, Jialei; Luo, Haoxiang; Zhang, Li; Ding, Yang; PHYSICS OF FLUIDS, 35, 3 (2023) |
| 2 | Highly efficient energy-conserving moment method for the multi-dimensional Vlasov-Maxwell system;<br>Yin, Tianai; Zhong, Xinghui; Wang, Yanli; JOURNAL OF COMPUTATIONAL PHYSICS, 475 (2023) |
| 3 | Hermite spectral method for multi-species Boltzmann equation;<br>Li, Ruo; Lu, Yixiao; Wang, Yanli; Xu, Haoxuan; JOURNAL OF COMPUTATIONAL PHYSICS, 471 (2022) |

## MECHANICS DIVISION 力学研究部

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|---|---|
| 4 | Flake Size Limits for Growth of Vertically Stacked Two-Dimensional Materials by Analytical Diffusion-Based Kinetic Model;<br>Ye, Han; Xiang, Xinshuang; Wang, Mingchao; Sun, Naizhang; Wang, Yujing; Quhe, Ruge; Liu, Yumin; Guo, Zhenlin; CRYSTAL GROWTH & DESIGN, 22, 9 (2022) |
| 5 | NUMERICAL SOLVER FOR THE BOLTZMANN EQUATION WITH SELF-ADAPTIVE COLLISION OPERATORS;<br>Cai, Zhenning; Wang, Yanli; SIAM JOURNAL ON SCIENTIFIC COMPUTING, 44, 2 (2022) |
| 6 | Nonlinear coupling effects of the thermocapillarity and insoluble surfactants to droplet migration under Poiseuille flow;<br>Guo, Zhenlin; PHYSICAL REVIEW FLUIDS, 8, 2 (2023) |
| 7 | Q-Tensor Gradient Flow with Quasi-Entropy and Discretizations Preserving Physical Constraints;<br>Wang, Yanli; Xu, Jie; JOURNAL OF SCIENTIFIC COMPUTING, 94, 1 (2023) |
| 8 | Unified Solution of Conjugate Fluid and Solid Heat Transfer-Part I. Solid Heat Conduction;<br>Li, Shujie; Ju, Lili; ADVANCES IN APPLIED MATHEMATICS AND MECHANICS, 15, 3 (2023) |
| 9 | Learning Invariance Preserving Moment Closure Model for Boltzmann-BGK Equation;<br>Li, Zhengyi; Dong, Bin; Wang, Yanli; COMMUNICATIONS IN MATHEMATICS AND STATISTICS, 11, 1 (2023) |
| 10 | Shock-Capturing Exponential Multigrid Methods for Steady Compressible Flows;<br>Li, Shu-Jie; COMPUTATIONAL MATHEMATICS AND MATHEMATICAL PHYSICS, 62, 8 (2022) |
| 11 | Table-Top Platform of a Large Scale Underwater Swarm;<br>Fu, Rong; Ding, Yang; 2023 9TH INTERNATIONAL CONFERENCE ON MECHATRONICS AND ROBOTICS ENGINEERING, ICMRE (2023) |

## ALGORITHMS DIVISION 计算方法研究部

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| 1 | Error Bounds of a Finite Difference/Spectral Method for the Generalized Time Fractional Cable Equation;<br>Ma, Ying; Chen, Lizhen; FRACTAL AND FRACTIONAL, 6, 8 (2022) |
| 2 | Investigation of plasmon relaxation mechanisms using nonadiabatic molecular dynamics;<br>Wu, Xiaoyan; Liu, Baopi; Frauenheim, Thomas; Tretiak, Sergei; Yam, ChiYung; Zhang, Yu; JOURNAL OF CHEMICAL PHYSICS, 157, 21 (2022) |
| 3 | Theoretical prediction and design for chalcogenide-quantum-dot/TiO2 heterojunctions for solar cell applications;<br>Shen, Kangqi; Saranya, Govindarajan; Chen, Mingyang; RSC ADVANCES, 12, 45 (2022) |

# WORKSHOPS & CONFERENCES (2022-2023)

## 中心主办、合办的学术会议

| 时间 Date | 会议名称 Title |
|---|---|
| 2023.7.27-29 | 7th Conference on Numerical Methods for Fractional-derivative Problems<br>第七届分数导数问题数值方法会议 |
| 2023.4.19-23 | Workshop on Modeling, Algorithm and Analysis of Complex Fluid Dynamics<br>复杂流体建模、分析、算法培训班及研讨会 |
| 2023.3.24-26 | Workshop on Modeling & Simulations for Complex System<br>复杂系统建模与数值模拟讨论会 |
| 2022.9.24-25 | 2022年应用与计算数学研讨会第三次会议<br>2022 Third Workshop of the Applied and Computational Mathematics Symposium |
| 2022.8.11-13 | 6th Conference on Numerical Methods for Fractional-derivative Problems<br>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<br>应用与计算数学小型研讨会 |

# TUTORIALS (2022-2023) 培训班

| 时间 Date | 会议名称 Title |
|---|---|
| 2022.11.7-10 | 动力学平均场的基本理论与前沿进展培训班 |
| 2022.10.31-11.3 | “材料与能源前沿科学：能源转换和储存中的基础科学问题”培训班 |

如需了解更多会议详情，请浏览：
For more details about Workshops & Conferences in CSRC, please visit:
http://www.csrc.ac.cn/events/WorkshopsConferences/

# 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。2022-2023学术年期间中心共举办专题讲座68期（总1225期）。

CSRC invites national and overseas leading researchers to give academic seminars. During academic year 2022-2023, CSRC has already held 68 seminars.

| No. | DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|---|
| 1 | 2022-8-1 | 陈掌星<br>Zhangxing Chen | 卡尔加里大学<br>University of Calgary | CCUS（碳捕集、利用与封存）技术现状、进展、挑战及前景 |
| 2 | 2022-8-9 | 杨志坚<br>Zhijian Yang | 武汉大学<br>Wuhan University | 数据与机理融合的可计算建模与高性能计算 |
| 3 | 2022-8-11 | 武振伟<br>Zhen-Wei Wu | 北京师范大学<br>Beijing Normal University | 无序体系拓扑结构与物性关联 |
| 4 | 2022-8-15 | Cheng Wang | 美国马萨诸塞大学达特茅斯分校<br>University of Massachusetts Dartmouth | A BDF2 decoupled numerical scheme for resistive magnetohydrodynamic equations |
| 5 | 2022-8-15 | 黄学海<br>Xuehai Huang | 上海财经大学<br>Shanghai University of Finance and Economics | FINITE ELEMENT COMPLEXES FROM COMPLEXES |
| 6 | 2022-8-18 | 李明星<br>Ming-Xing Li | 中科院物理所<br>Institute of Physics, CAS | 非晶合金的高通量与数据驱动式研发 |
| 7 | 2022-8-22 | 吴朔男<br>Shuonan Wu | 北京大学<br>Peking University | A monotone discretization for integral fractional Laplacian on bounded Lipschitz domains: pointwise error estimates under H\"{o}lder regularity |
| 8 | 2022-8-24 | 郑慧婕<br>Hui-Jie Zheng | 中科院物理所<br>Institute of Physics, CAS | 基于氮空位（NV）色心金刚石的量子传感 |
| 9 | 2022-8-30 | Wanrong Cao | 东南大学<br>Southeast University | On spectral Petrov-Galerkin method for solving optimal control problem governed by fractional diffusion equations with fractional noise |

# CSRC SEMINAR 专题报告

| No. | DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|---|
| 10 | 2022-9-5 | 雍稳安<br>Wen-An Yong | 清华大学<br>Tsinghua University | On dissipativity of moment closure systems for the Boltzmann equation |
| 11 | 2022-9-8 | 杨卫明<br>Wei-Ming Yang | 中国矿业大学<br>China University of Mining and Technology | 金属玻璃物理性质的遗传“基因” |
| 12 | 2022-9-20 | 杨秀峰<br>Xiu-Feng Yang | 北京理工大学<br>Beijing Institute of Technology | 光滑粒子法SPH及其在固体入水中的应用 |
| 13 | 2022-9-22 | 胡　丹<br>Dan Hu | 上海交通大学<br>Shanghai Jiao Tong University | A Non-Gradient Method for Solving Partial Differential Equations with Deep Neural Networks |
| 14 | 2022-9-27 | 蔡振宁<br>Zhen-Ning Cai | 新加坡国立大学<br>National University of Singapore | A Conservative and Entropic Scheme for the Boltzmann Equation |
| 15 | 2022-9-28 | 杨丰玮<br>Feng-Wei Yang | 华威大学<br>University of Warwick | 浅谈虚拟与增强现实在工业4.0中的应用 |
| 16 | 2022-10-9 | 李永海<br>Yonghai Li | 吉林大学<br>Jilin University | (1)有限体积元法的文献历史简介 及(2)四面体二次元有限体积法的构造和分析 |
| 17 | 2022-10-11 | 张　晨<br>Chen Zhang | 北京自动化控制装备研究所<br>Beijing Institute of Automatic Control Equipment | 基于NV色心系综的磁测量: 应用与进展 |
| 18 | 2022-11-15 | 许志钦<br>Zhi-Qin Xu | 上海交通大学<br>Shanghai Jiao Tong University | Simple Implicit Regularizations in Deep Learning |
| 19 | 2022-11-29 | 廖海军<br>Hai-Jun Liao | 中国科学院物理研究所<br>Institute of Physics (CAS) | Spin Excitation Spectra of Anisotropic Spin-1/2 Triangular Lattice Heisenberg Antiferromagnets |
| 20 | 2022-12-11 | 胡　丹<br>Dan Hu | 上海交通大学<br>Shanghai Jiao Tong University | A non-gradient method for solving partial differential equations with deep neural networks |

| No. | DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|---|
| 21 | 2022-12-12 | 蔡振宁<br>Zhen-Ning Cai | 新加坡国立大学<br>National University of Singapore | A conservative and entropic scheme for the Boltzmann equation |
| 22 | 2023-1-30 | 曹外香<br>Wai-Xiang Cao | 北京师范大学<br>Beijing Normal University | A Class of Spectral Volume (SV) Methods for Hyperbolic and Diffusion Equations |
| 23 | 2023-2-3 | 王耀来<br>Yao-Lai Wang | 江南大学<br>Jiangnan University | 转录研究的历史与模型 |
| 24 | 2023-2-3 | 陆　俊<br>Jun Lu | 中国科学院物理研究所<br>Institute of Physics (CAS) | 精准测频式锁相放大器研发的一点新进展 |
| 25 | 2023-2-6 | 李会元<br>Hui-Yuan Li | 中国科学院软件研究所<br>Institute of Software (CAS) | A Fast Maxwell Solver Based on Exact Discrete Eigen-Decompositions |
| 26 | 2023-2-7 | 张　钰<br>Yu Zhang | 北京理工大学<br>Beijing Institute of Technology | 探测并调控二维材料中缺陷诱导的新奇量子物态 |
| 27 | 2023-2-8 | 诸葛昌靖<br>Chang-Jing Zhuge | 北京工业大学<br>Beijing University Of Technology | 新冠病毒传播的动力学模型研究及其应用 |
| 28 | 2023-2-13 | 王志刚<br>Zhi-Gang Wang | 吉林大学<br>Jilin University | 从超原子科学到超原子物理学 |
| 29 | 2023-2-13 | 胡　俊<br>Jun Hu | 北京大学<br>Peking University | High Accurate Algorithms for Eigenvalue Problems Based on Nonconforming Finite Element Methods |
| 30 | 2023-2-15 | 钱　紘<br>Hong Qian | 华盛顿大学<br>University of Washington | Toward a New Mathematical Foundation of Statistical Thermodynamics |
| 31 | 2023-2-20 | 李东方<br>Dong-Fang Li | 华中科技大学<br>Huazhong University of Science and Technology | 高精度线性化算法：构造、分析和应用 |
| 32 | 2023-2-27 | 张继伟<br>Ji-Wei Zhang | 武汉大学<br>Wuhan University | Do We Need Decay-Preserving Error Estimate for Solving Parabolic Equations with the Initial Singularity? |

# CSRC SEMINAR 专题报告

| No. | DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|---|
| 33 | 2023-3-6 | 聂　华<br>Hua Nie | 陕西师范大学<br>Shaanxi Normal University | The Effect of Diffusion on the Dynamics of a Predator-Prey Chemostat Model |
| 34 | 2023-3-6 | 毛士鹏<br>Shi-Peng Mao | 中科院数学与系统科学研究院<br>Academy of Mathematics and Systems Science (CAS) | 基于磁势变量三维磁流体力学数值方法研究 |
| 35 | 2023-3-7 | 邓明华<br>Ming-Hua Deng | 北京大学<br>Peking University | scEMAIL: Universal and Source-free Annotation Method for scRNA-seq Data with Novel Cell-type Perception |
| 36 | 2023-3-10 | 谭　鹏<br>Peng Tan | 复旦大学<br>Fudan University | 玻璃化和非平衡结晶过程的密切联系 |
| 37 | 2023-3-13 | 黄建国<br>Jian-Guo Huang | 上海交通大学<br>Shanghai Jiao Tong University | A Robust Lower Order Mixed Finite Element Method for a Strain Gradient Elastic Model |
| 38 | 2023-3-15 | 敖　平<br>Ping Ao | 上海演化力学研究院(拟建)上海演化力学研究院(拟建) | Third Universal Mechanics: Towards Unifying Non-Equilibrium Processes in Physics and Network Dynamics in Biology |
| 39 | 2023-3-16 | 王大伟<br>Da-Wei Wang | 浙江大学<br>Zhejiang University | Observing the Quantum Topology of Light |
| 40 | 2023-3-20 | 沈　捷<br>Jie Shen | 普渡大学<br>Purdue University | Efficient High-Order Methods for Parabolic PDEs |
| 41 | 2023-3-22 | 王　欢<br>Huan Wang | WileyWiley | Wiley科学期刊论文写作与发表 |
| 42 | 2023-4-10 | 袁　喆<br>Zhe Yuan | 北京师范大学<br>Beijing Normal University | 各向异性磁电阻微观理论研究新进展 |
| 43 | 2023-4-26 | 蓝　可<br>Ke Lan | 北京应用物理与计算数学研究所<br>Institute of Applied Physics and Computational Mathematics | 美国捧得“点火”圣杯——通向可重复、可预测的高增益聚变时代 |
| 44 | 2023-5-8 | 李聪丛<br>Cong-Cong Li | 中国科学技术大学<br>University of Science and Technology of China | 面向脑磁测量的原子磁强计研究 |

| No. | DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|---|
| 45 | 2023-5-10 | 潘　捷<br>Pan Jie | Nature Computational Science, SPRINGER NATURE Nature Computational Science, SPRINGER NATURE | Inside Nature Journals |
| 46 | 2023-5-17 | 肖泽文<br>Ze-Wen Xiao | 华中科技大学<br>Huazhong University of Science and Technology | 金属卤化物半导体光电材料的构效关系与理性设计 |
| 47 | 2023-5-18 | 田矗舜<br>Chu-Shun Tian | 中国科学院理论物理研究所<br>Institute of Theoretical Physics (CAS) | Connecting Maximal and Minimal Chaos: From Perspectives of SYK and String Theory |
| 48 | 2023-5-19 | 彭　毅<br>Yi Peng | 中国科学院物理研究所<br>Institute of Physics (CAS) | Hydrodynamic Effects in Biological Active Fluids |
| 49 | 2023-5-19 | 王　成<br>Cheng Wang | 马萨诸塞大学达特茅斯分校<br>University of Massachusetts Dartmouth | A Positivity Preserving, Energy Stable and Convergent Numerical Scheme for the Poisson-Nernst-Planck System |
| 50 | 2023-5-23 | 刘　畅<br>Chang Liu | 西安交通大学<br>Xi' an Jiaotong University | 大量间隙固溶TiZrNb系多主元合金研发与原子尺度表征 |
| 51 | 2023-5-24 | 经光银<br>Guang-Yin Jing | 西北大学<br>Northwest University | Swimming Bacteria: Individually and Collectively Motion |
| 52 | 2023-5-29 | 周　健<br>Jian Zhou | 西安交通大学<br>Xi' an Jiaotong University | Hidden Modes in Bulk Photovoltaic Effect |
| 53 | 2023-5-31 | 王　勇<br>Yong Wang | 中国科学院数学与系统科学研究院应用数学研究所<br>Institute of Applied Mathematics, AMSS (CAS) | 基因调控网络建模 |
| 54 | 2023-6-5 | 胡一南<br>Yi-Nan Hu | 中国科学院生物物理研究所<br>Institute of Biophysics (CAS) | 小型化光量子磁力计与新型脑功能成像设备 |
| 55 | 2023-6-7 | 陈航晖<br>Hang-Hui Chen | 上海纽约大学<br>NYU Shanghai | Emergent Phenomena in Complex Oxide Thin Films |
| 56 | 2023-6-9 | 司徒国海<br>Guo-Hai Situ | 中国科学院上海光学精密机械研究所<br>Shanghai Institute of Optics and Fine Mechanics (CAS) | 物理融合深度神经网络及其在计算光学成像中的应用 |

# CSRC SEMINAR 专题报告

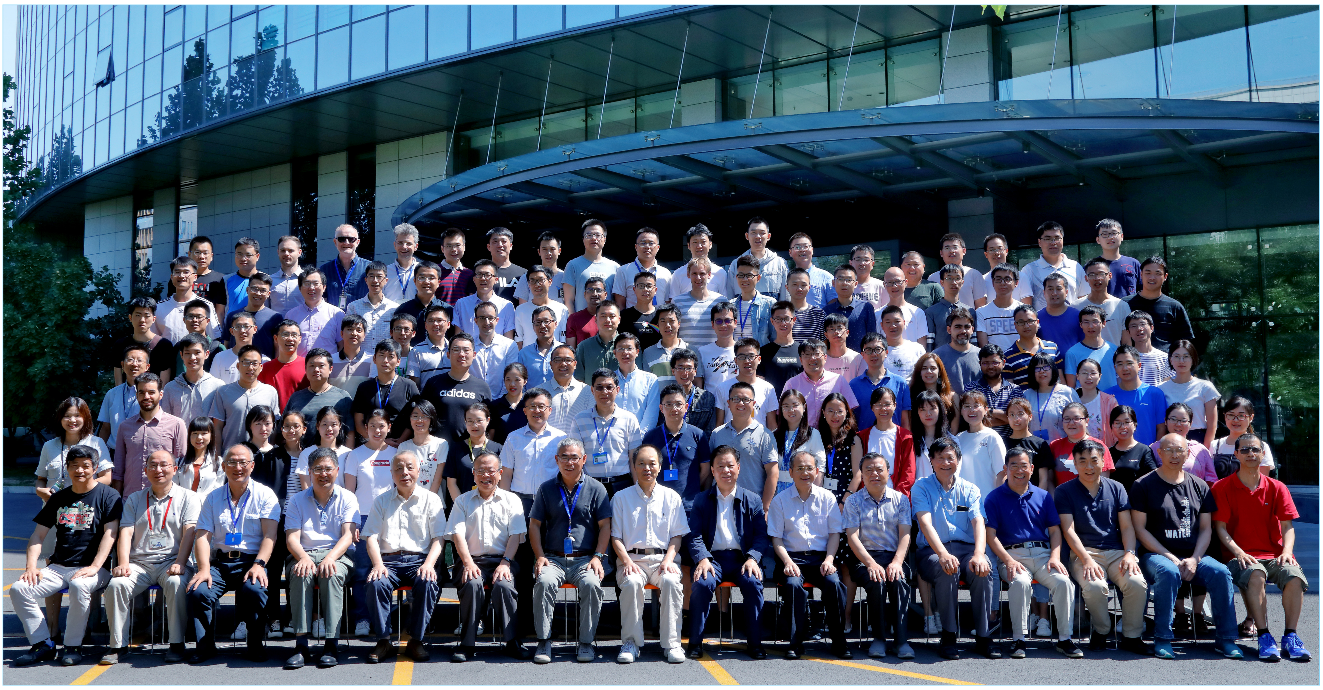
| No. | DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|---|
| 57 | 2023-6-26 | 雷锦志<br>Jin-Zhi Lei | 天津工业大学<br>Tiangong University | Heterogeneity, Plasticity, Entropy, and Waddington Landscape |
| 58 | 2023-6-27 | 徐振礼<br>Zhen-Li Xu | 上海交通大学<br>Shanghai Jiao Tong University | Structure-Preserving Numerical Methods for Plasma Simulations |
| 59 | 2023-6-27 | 陈艳萍<br>Yan-Ping Chen | 华南师范大学<br>South China Normal University | An Adaptive HDG Method for the Pointwise Tracking Optimal Control Problem of Elliptic Equations |
| 60 | 2023-7-6 | 段俊明<br>Jun-Ming Duan | 瑞士洛桑联邦理工学院<br>École Polytechnique Fédérale de Lausanne, EPFL | High-Order Accurate Entropy Stable Adaptive Moving Mesh Methods |
| 61 | 2023-7-6 | 柳天寒<br>Tian-Han Liu | 美国加州大学洛杉矶分校<br>University of California-Los Angeles | Control of Chirality, Spin, and Orbital in Chiral Molecular Devices |
| 62 | 2023-7-10 | 林　平<br>Ping Lin | 英国邓迪大学<br>University of Dundee, UK | A Thermodynamically Consistent Phase-Field Model and an Energy-Law Preserving Finite Element Scheme for Vesicles Motions and Interaction |
| 63 | 2023-7-13 | 谢和虎<br>He-Hu Xie | 中国科学院数学与系统科学研究院<br>Academy of Mathematics and Systems Science (CAS) | 张量神经网络及其应用 |
| 64 | 2023-7-19 | 丁　俊<br>Jun Ding | 西安交通大学<br>Xi'an Jiaotong University | Tuning Order in Disorder: From Metallic Glasses to High-Entropy Alloys |
| 65 | 2023-7-21 | Maxim F. Gelin | 杭州电子科技大学<br>Hangzhou Dianzi University | Novel Simulation Methods in Quantum Dynamics and Femtosecond Spectroscopy |
| 66 | 2023-7-24 | 张力舒<br>Li-Shu Zhang | 德国于利希研究中心<br>Jülich Research Centre, Germany | Current-Driven Magnetic Resistance in Van der Waals Spin-Filter Antiferromagnetic Tunnel Junctions |
| 67 | 2023-7-24 | 陈艺冰<br>Yi-Bing Chen | 北京应用物理与计算数学研究所<br>Institute of Applied Physics and Computational Mathematics | 极端条件下三维多物理多介质数值模拟的若干问题研究 |
| 68 | 2023-7-27 | 赵雁翔<br>Yan-Xiang Zhao | 美国乔治华盛顿大学<br>The George Washington University, USA | Supervised Optimal Transport |

# 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。自开展至今已举办八期。



如需了解更多报告信息，请浏览：
For more details about Seminars in CSRC, please visit:
http://www.csrc.ac.cn/events/seminars/



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 2022-2023, 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。2022-2023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。

## INTERNATIONAL PARTNERSHIP 国际及地区合作伙伴

UNIVERSITY OF GOTHENBURG, SWEDEN
瑞典哥德堡大学

UNIVERSITY OF OSLO, NORWAY
挪威奥斯陆大学

INSTITUTE FOR QUANTUM COMPUTING, UNIVERSITY OF WATERLOO, CANADA
加拿大滑铁卢大学

NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY, NORWAY
法国原子能与可替代能源委员会

UNIVERSITY OF WARWICK, UK
英国华威大学

CENTER FOR SIMULATIONAL PHYSICS, THE UNIVERSITY OF GEORGIA, USA
美国乔治亚大学

NTNU
NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY, NORWAY
挪威科技大学

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY, CHINA
香港科技大学

COLLEGE OF SCIENCES, OLD DOMINION UNIVERSITY, USA
美国奥多明尼昂大学

RIKAGAKU KENKYUSHO/INSTITUTE OF PHYSICAL AND CHEMICAL RESEARCH, JAPAN
日本理化学研究所

DEPARTMENT OF PHYSICS, NATIONAL TAIWAN NORMAL UNIVERSITY, CHINA
国立台湾师范大学

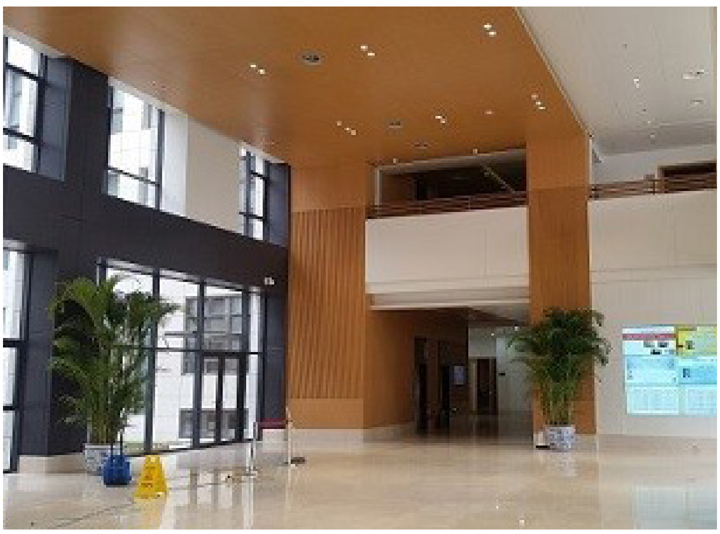
DEPARTMENT OF PHYSICS, THE CHINESE UNIVERSITY OF HONG KONG, CHINA
香港中文大学

HEARNE INSTITUTE FOR THEORETICAL PHYSICS, LOUISIANA STATE UNIVERSITY, USA
美国路易斯安那州立大学

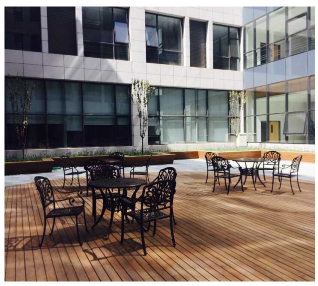
KOREA INSTITUTE FOR ADVANCED STUDY, SOUTH KOREA
韩国高等科学院

〖 中心办公楼效果图 〗 CSRC building

〖 大厅 〗 Lobby



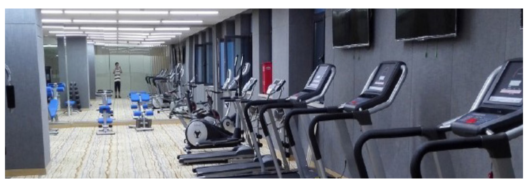
〖 中庭院 〗 Courtyard



〖 学术报告厅 〗 Auditorium

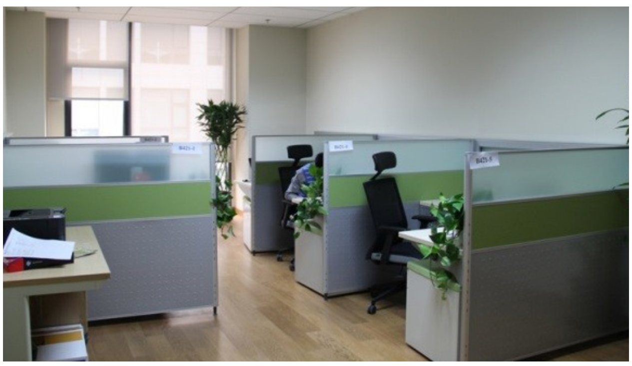
Seminar Rom 〖 学术会议室 〗

Common 〖 学术讨论区 〗

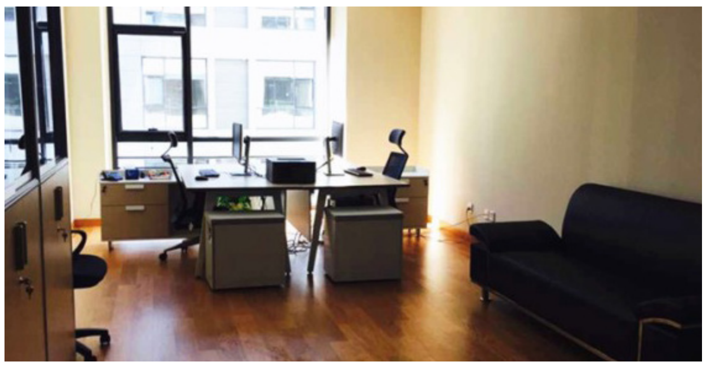


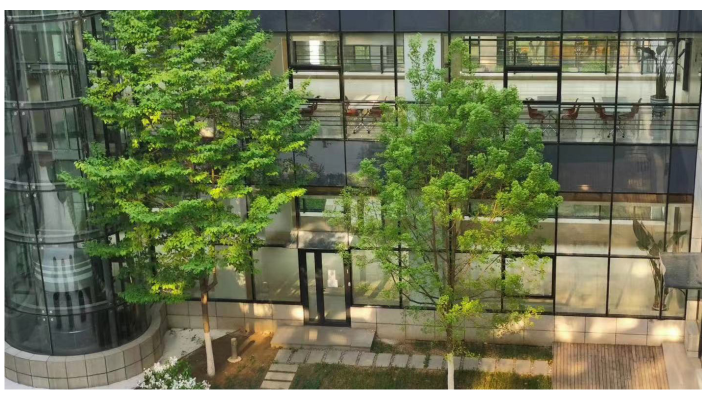

ZPark 〖 中关村软件园一二期鸟瞰图 〗

〖 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

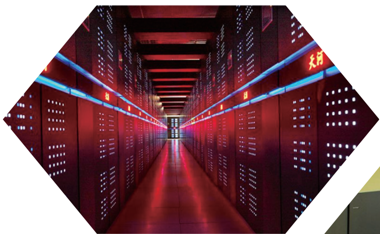
# 天河二号-计科中心集群系统

# 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