2023 - 2024 年度报告 ANNUAL REPORT

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本册所列所有信息为2023年8月1日至2024年7月31日学术年期间

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

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

As of August 2024, CSRC has 29 faculty members, 2 engineers, 25 postdoctoral fellows and 115 students. With its talented research staff, CSRC has established the following seven divisions: Simulation of Physical Systems, Quantum Physics and Quantum Information, Materials and Energy, Complex Systems, Applied and Computational Mathematics, Mechanics, and Algorithms. In research performance, CSRC has published 146 papers, organized 8 academic conferences and workshops, 8 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.

**Mission of CSRC**

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

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

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

CSRC

## 中心定位与目标

**1．开展科学前沿研究**

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

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

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

**2．发挥科学支撑效能**

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

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

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

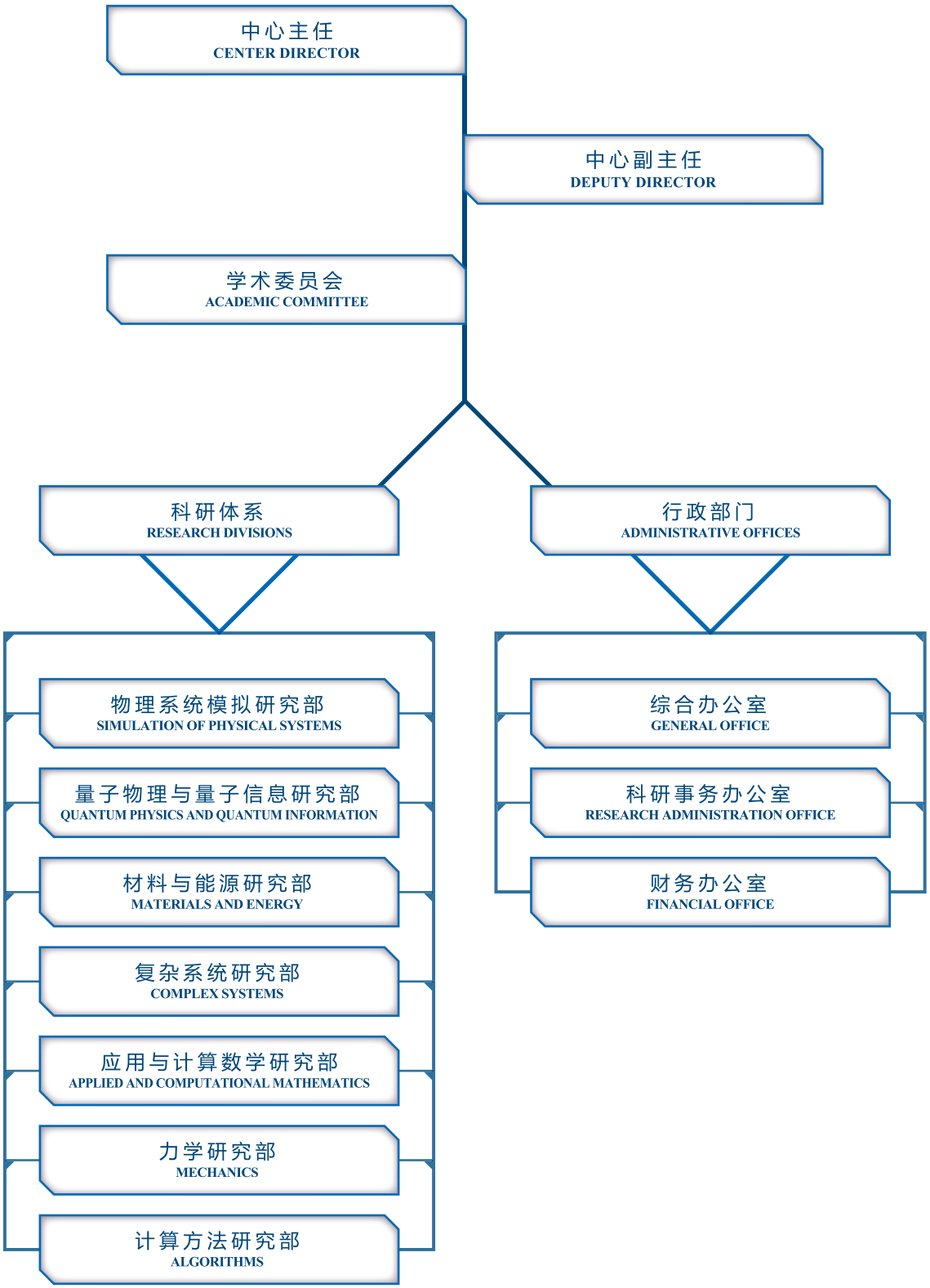
**北京计算科学研究中心**（以下简称中心）是隶属于中国工程物理研究院的独立法人单位，是以计算科学为牵引的多学科基础研究机构。中心成立于2009年8月。中心的定位是开展计算科学研究，促进科技发展，打造一个国际一流的开展计算科学及相关学科交叉研究的综合平台。

中心积极引进高层次人才，努力开展计算科学相关学科的交叉和创新研究，共有七个研究部：物理系统模拟研究部、量子物理与量子信息研究部、材料与能源研究部、复杂系统研究部、应用与计算数学研究部、力学研究部、计算方法研究部。截至2024年8月，中心的科研人才队伍包括11位讲座教授、3位教授、6位副教授、6位特聘研究员、3位特聘副研究员、2位工程师和25位博士后。另外，中心还有博士/硕士研究生115位。他们的研究领域涵盖了数学、力学、物理学、化学、材料科学、计算机科学等多个基础、前沿领域。

2023-2024学术年期间，中心公开发表国际学术论文146篇，主办合办国内外学术会议8场，开设培训班8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。

# ORGANIZATION 中心组织构架



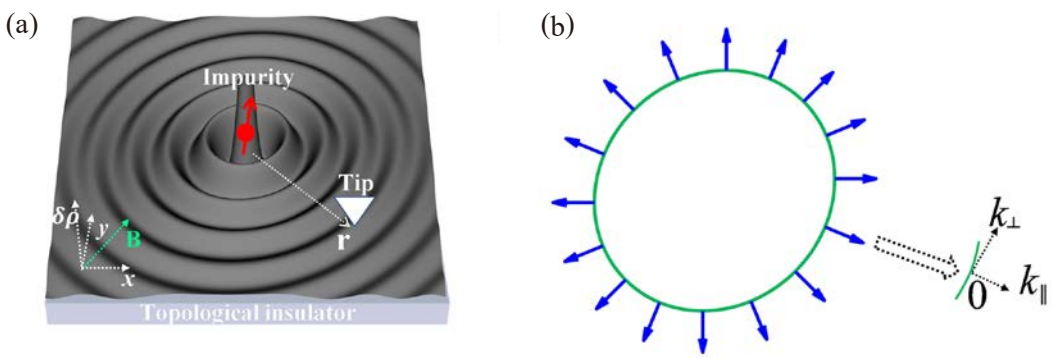
# SPIN TEXTURE AND RIEMANN CURVATURE FROM SPIN-POLARIZED QUASI-PARTICLE INTERFERENCE

By Shu-Hui Zhang*, Jin Yang, Ding-Fu Shao, Jia-Ji Zhu, Wen Yang*, and Kai Chang*

The energy band dispersion and corresponding eigenstates are key quantities in electronic band theory. The former has been widely recognized to control the physical properties of crystalline materials, whereas the latter are not valued until the accompanying geometric phase is identified. The geometric phase has become an essential component of modern band structure theory and generates various remarkable phenomena. However, the geometric aspect of the energy dispersion remains unexplored.

In this study, we derived a neat, universal formula for the real-space Green's function in any 2D system with translational symmetry. It shows that each part of the Green's function is determined by a single property of a particular point (determined by the propagation direction of the Green's function) on the Fermi contour, hence allowing us to extract its information from spin-polarized quasi-particle interference (QPI) measurements: (1) The phase part reveals the Fermi momentum; (2) The magnitude part reveals the Riemann curvature; (3) The matrix part reveals the spin texture or spinor wave function.

Recognition of (1) several decades ago triggered intensive research activities to reconstruct the Fermi contour and energy dispersion, forming a fruitful research field – "QPI in the Fourier space". However, points (2) and (3) have not been recognized yet. Here we demonstrate the possibility to make direct, momentum-resolved detection of the Riemann curvature and spin texture using the QPI in real space. This makes a basic step in STM technology. To our knowledge, only one geometric quantity– the Berry phase/curvature – has been recognized so far. Our work adds a new geometrical quantity – the Riemann curvature □ of the Fermi contour – to this toolkit, by showing that □ deeply influences the Green's function and hence various physical properties. Therefore, our work also makes a step in exploring the interplay between geometry, topology, and physics. It may trigger new theoretical and experimental efforts in searching for related effects.



# 自旋极化准粒子干涉揭示自旋纹理及费米面曲率

张书辉*, 杨锦, 绍定夫, 朱家骥, 杨文*, 常凯*

在电子能带理论中, 能带色散和相应的本征态是关键物理量。前者已被广泛认为控制着晶体材料的各种物理性质, 而后者直到发现几何相位有关的效应后才受到重视, 目前几何相位已成为现代能带结构理论的重要组成部分。然而, 对能带色散中的几何量对物理性质的影响尚未见到报导。

在本研究中, 我们推导出了一个简洁的通用公式用于描述具有平移对称性的任意二维系统中的实空间格林函数。它表明, 格林函数的每一个因子都由费米面上的特定点(由格林函数的传播方向确定)的单个性质决定，因此允许我们从自旋极化准粒子干涉(QPI)测量中提取其信息: (1) 相位部分揭示了费米动量; (2) 幅度部分揭示了黎曼曲率; (3) 矩阵部分揭示了自旋纹理或旋量波函数。

目前对第一点的相关研究已经形成一个以重建费米面轮廓和能量色散为目标的研究领域: “傅里叶空间中的准粒子干涉(QPI)”。然而, 对后两点的研究尚未开展。我们基于上述公式, 理论展示了利用实空间中 QPI对黎曼曲率和自旋纹理进行直接的、运量分辨的测量的可能性, 推动了扫描隧道显微镜技术的发展。据我们所知, 到目前为止, Berry相位/曲率是目前唯一一个被广泛认识到对物理性质有深刻影响的几何量, 而我们的工作表明费米面的黎曼曲率这个新的几何量同样对各种物理性质有重要影响, 从而在探索几何、拓扑和物理的互动方面迈出了重要的一步。

**REFERENCES:**

[1] Shu-Hui Zhang*, **Jin Yang**, Ding-Fu Shao, Jia-Ji Zhu, **Wen Yang***, and Kai Chang*, Phys. Rev. Lett. 133, 036204 (2024)

# DISCRETE TIME CRYSTAL IN AN OPEN OPTOMECHANICAL SYSTEM

By Dongni Chen, Zhenyang Peng, Jiahui Li, Stefano Chesi, and Yingdan Wang

A time crystal is a system where time-translational invariance is spontaneously broken. While this type of collective dynamics is impossible in equilibrium, the realization of time crystals in periodically driven systems has recently attracted great interest. In these discrete time crystals, the system observables show persistent and robust oscillations, with a period which is a multiple (typically 2T) of the period T of the external drive. Proposals are mostly based on the collective dynamics of certain interacting spin systems, while realizations in other types of quantum systems are much less explored. In a recent study, however, a collaboration between the research groups of Prof. Stefano Chesi (Beijing Computational Research Center) and Prof. Yingdan Wang (Institute of Theoretical Physics, CAS) has extended the applicability of the time crystal concept, by proposing the first realization with optomechanical systems [1].

The specific setup is based on two mechanical elements interacting with the discrete mode of a quantum cavity. As a first step, Dr. Dongni Chen and colleagues find a suitable working point where the optomechanical system can be mapped to the well-known Dicke model, in which a superradiant phase takes place. Afterwards, they devise a special periodic modulation of the optical drive which can switch between the two broken-symmetry states of the superradiant phase, with periodicity 2T. The theoretical analysis shows that the period-doubling dynamics is robust to variations of system's parameters and is compatible with currently available optomechanical technology, paving the way for the realization of discrete time crystals with a new class of quantum devices.

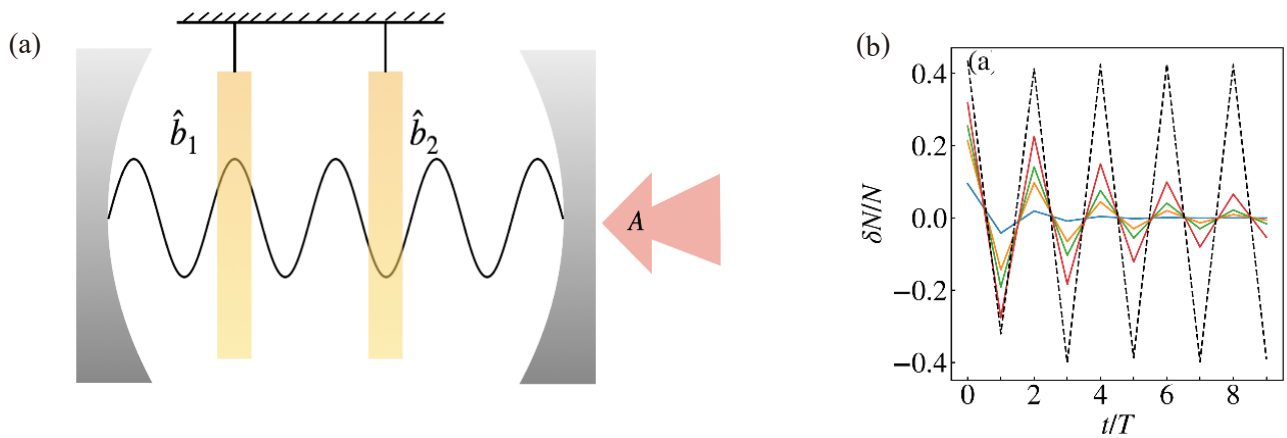



**Fig.** (a) Schematics of the optomechanical system. (b) Oscillations in the difference between the number of phonons of the two mechanical elements. The oscillations are damped when the total number of phonons ***N*** is finite but survive for arbitrarily long times in the thermodynamic limit (dashed curve). These oscillations with ***2T*** periodicity are the main signature of a discrete time-crystal.

# 开放光力学系统中的离散时间晶体

陈冬妮, 彭振阳, 李佳慧, Stefano Chesi, 王颖丹

时间晶体是一种由时间平移对称性自发破缺导致的现象。然而, 这种集体动力学在平衡状态下无法实现, 因此在周期性驱动系统中实现离散时间晶体最近引起了人们的广泛关注。在这些离散时间晶体中, 系统观测量会持续且稳定地振荡, 其振荡周期是外部驱动周期 T 的倍数(通常为 2T)。目前为止, 大多数实现方案都基于相互作用自旋系统的集体动力学, 而对其他类型量子系统的研究则较少。最近, 北京计算科学研究中心的Stefano Chesi团队和中国科学院理论物理研究所的王颖丹团队首次提出了在光力学系统中实现离散时间晶体的方案[1], 这项理论研究拓展了时间晶体概念的适用性。

研究的模型基于两个机械振子与量子光腔相互作用的光力学系统。首先, 研究团队在特定的参数条件下, 将光力学系统映射到Dicke模型中, 从而产生超辐射相。接着, 他们设计了一种周期为T的光驱动调制方案, 使系统在超辐射相的两个对称性破缺态之间以2T的周期来回切换。研究表明, 这种离散时间晶体对系统参数的变化具有很强的鲁棒性, 并且可以通过现有的光力学技术实现。这一研究为探索离散时间晶体在新型量子器件中的应用奠定了基础。

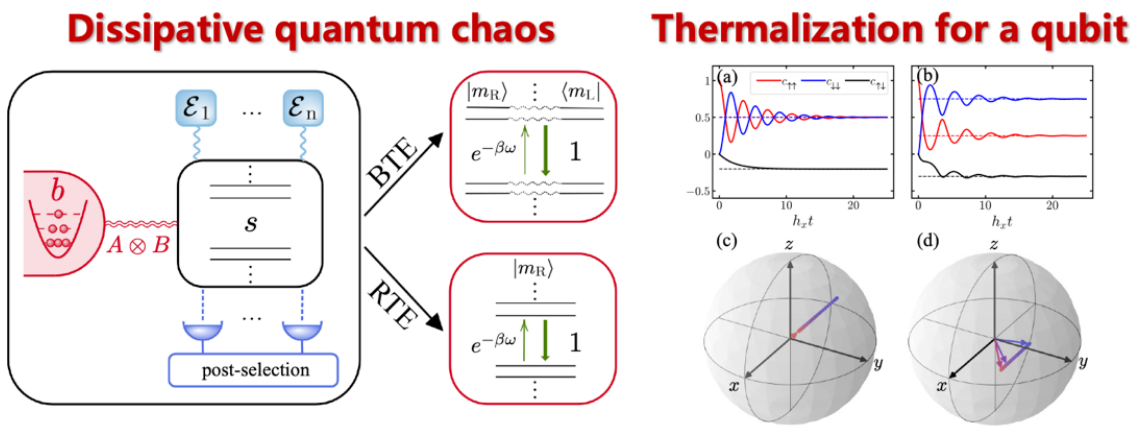
◀ 图 (a)光力学系统的示意图。 (b)两个力学模声子数差异的振荡。当总声子数 N 有限时, 振荡会逐渐衰减, 但在热力学极限下(虚线)可以持续无限长时间。这些具有 2T 周期的振荡是离散时间晶体的主要特征。

**REFERENCES:**

[1] D. Chen, Z. Peng, J. Li, **S. Chesi***, and Y. Wang*, Phys. Rev. Res. 6, 013130 (2024)

# DIAGNOSING THERMALIZATION DYNAMICS OF NON-HERMITIAN QUANTUM SYSTEMS VIA GKSL MASTER EQUATION

By Yiting Mao, Peigeng Zhong, Haiqing Lin, Xiaoqun Wang, and Shijie Hu




Chaos systems are renowned for their high sensitivity to initial conditions and unpredictable long-term behavior. In non-Hermitian chaotic systems, such as dissipative quantum systems described by Lindbladian or non-Hermitian Hamiltonian-dominated non-unitary quantum dynamics, level statistics are predicted to follow the Ginibre distribution, exhibiting significant cubic-level repulsion. Despite the establishment of these theoretical frameworks, the potential relationship between dissipative quantum chaos and thermalization in open quantum systems remains unclear and has thus been widely studies in recent years. Over the past year, the construction of eigenstate thermalization hypotheses based on non-Hermitian random matrix theory and dissipative quantum chaos has become a contentious focus, aimed at describing thermalization phenomena in general non-Hermitian systems. The process of thermalization is exceptionally complex, involving the mutual influence of multiple time-evolution trajectories of the system in a reduced Hilbert space.

The research team derived two versions of the Gorini–Kossakowski–Sudarshan–Lindblad master equation by considering the time evolution of density matrices for biorthogonal and right states, to describe the coupling of non-Hermitian systems with a thermal equilibrium bosonic heat bath. Solving these equations identified sufficient conditions for thermalization under two types of time evolution and yielded corresponding statistics for biorthogonal and right eigenstates in Boltzmann form. This finding clearly indicates flaws in recently proposed biorthogonal random matrix theory and emphasizes the necessity for its correction.

# 通过GKSL主方程诊断非厄米量子系统的热化动力学

毛奕廷, 钟佩耕, 林海青, 王孝群, 胡时杰

混沌系统以其对初始条件的高度敏感性和不可预测的长时间行为而闻名。在非厄米混沌系统中, 例如由Lindbladian描述的耗散量子系统或由非厄米哈密顿量主导的非幺正量子动力学中, 能级的统计被预测遵循Ginibre分布, 并表现出显著的立方级能级斥力。尽管已经建立了这些理论框架, 耗散量子混沌与开放量子系统中的热化之间的潜在关系仍不明确, 因此近年来受到广泛研究。在过去一年中, 关于非厄米随机矩阵理论和耗散量子混沌的基础上构建本征态热化假设已成为一个争论的焦点, 用以描述一般非厄米系统中的热化现象。热化过程异常复杂, 涉及系统在约化希尔伯特空间中多条时间演化轨迹的相互影响。

研究团队通过考虑双正交和右本征态时间演化的密度矩阵, 推导出了两个版本的Gorini–Kossakowski–Sudarshan–Lindblad主方程, 用以描述非厄米系统与热平衡玻色子热浴的耦合。通过解方程确定了两种时间演化下热化的充分条件, 并得出了相应的玻尔兹曼双正交和右本征态的统计。这一发现明确指出了最近提出的双正交随机矩阵理论存在缺陷, 并强调了其需要进行修正的必要性。

**REFERENCES:**

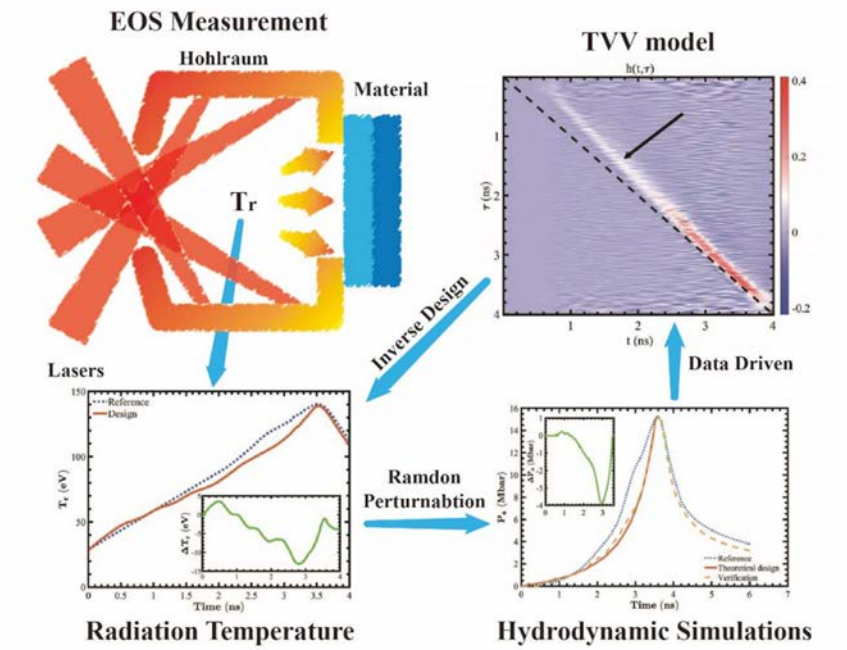
[1] **Yiting Mao**, **Peigeng Zhong**, **Haiqing Lin***, Xiaoqun Wang*, and **Shijie Hu***, "Diagnosing thermalization dynamics of non-Hermitian quantum systems via GKSL master equations", Chin. Phys. Lett. DOI: 10.1088/0256-307X/41/7/07030141, 070301 (2024).

# INVERSE DESIGN OF THE RADIATION TEMPERATURE FOR INDIRECT LASER-DRIVEN EQUATION-OF-STATE MEASUREMENT

By Lingrui Liao, Jingxiang Shen, Liang Sun, Chongjie Mo, Wei Kang

Measurement of the equation of state (EOS) for matter under extreme conditions is of great significance to a variety of research fields of planetary physics, geophysics, high-pressure science, and inertial confinement fusion. Owing to the advent of high-power laser facilities, the difficulty of generating such a laser-driven extreme state under laboratory conditions has been much relieved and laser-driven EOS measurement for the generated matter begins to attract particular interest. The theoretical design for the time profile of radiation temperature plays an important role in indirect laser-driven EOS measurement, which severely relies on a large number of radiation hydrodynamic simulations.

In this work, we provide a concise data-driven method to optimize the radiation temperature profile, which combines a time-varying Volterra model with data generated by radiation hydrodynamic simulations utilizing random perturbations as inputs. We find that the time-varying Volterra model can be used to investigate the time-dependent relationship between the radiation temperature and the key physical quantities of interest, such as shock-wave velocity and ablation drive pressure. With this method, we realize the inverse designs of the radiation temperature profiles for dynamic shock and ramp compression in planar geometry according to the desired shock-wave velocity and drive pressure respectively (shown in the Figure), which shows the advantage of practical application in experiments.



# 激光间接驱动状态方程测量的辐射温度逆向设计

廖棱锐, 沈靖翔, 孙亮, 莫崇杰, 康炜

精确测量物质在极端条件下的状态方程(EOS)对于地球物理学、行星物理学、高压科学以及惯性约束聚变等多个前沿领域的研究具有举足轻重的意义。随着高功率激光技术的飞速发展, 实验室中通过激光驱动的方式产生极端条件下的物质状态已逐渐变得可行, 这使科学家们进一步对极端条件EOS得测量产生兴趣。在激光间接驱动EOS测量领域, 辐射温度演化曲线的理论设计占据着核心地位, 但其设计过程高度依赖于大规模的辐射流体力学模拟。

在本工作中, 我们创新性地引入了一种简明的数据驱动方法用于辐射温度演化曲线的优化。该方法巧妙融合了时变Volterra模型与基于随机扰动输入的辐射流体动力学模拟数据, 能有效揭示辐射温度与关键物理参数(例如冲击波速度和烧蚀驱动压力)之间复杂的时间动态关联。在该方法的基础上, 我们进一步实现了辐射温度的逆向设计, 针对平面动态冲击与斜坡压缩两种典型场景, 分别定制了符合特定冲击波速度和烧蚀驱动压力需求的辐射温度演化曲线, 具体流程如图所示。这一成果揭示了数据驱动方法在实际实验应用中的优势。

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[1] Lingrui Liao, Jingxiang Shen, Liang Sun, **Chongjie Mo***, Wei Kang*, " Inverse design of the radiation temperature for indirect laser-driven equation-of-state measurement", *Physics of Fluids* DOI: /10.1063/5.0206321.

# GENERALIZED QUANTUM MEASUREMENTS ON A HIGHER-DIMENSIONAL SYSTEM VIA QUANTUM WALKS

By Xiaowei Wang#, Xiang Zhan#, Yulin Li, Lei Xiao, Gaoyan Zhu, Dengke Qu, Quan Lin, Yue Yu, Peng Xue*

Quantum measurements play a fundamental role in quantum mechanics. Especially, generalized quantum measurements provide a powerful and versatile tool to extract information from quantum systems. However, how to realize them on an arbitrary higher-dimensional quantum system remains a challenging task. Here this work proposes a simple recipe for the implementation of a general positive-operator valued measurement (POVM) on a higher-dimensional quantum system via a one-dimensional discrete-time quantum walk with a two-dimensional coin. Furthermore, as an application, using linear optics, this work realizes experimentally a symmetric, informationally complete (SIC) POVM on a three-dimensional system with high fidelity. The study paves the way to explore physics and information in higher-dimensional quantum systems and finds applications in various quantum information processing tasks that rely on generalized quantum measurements.

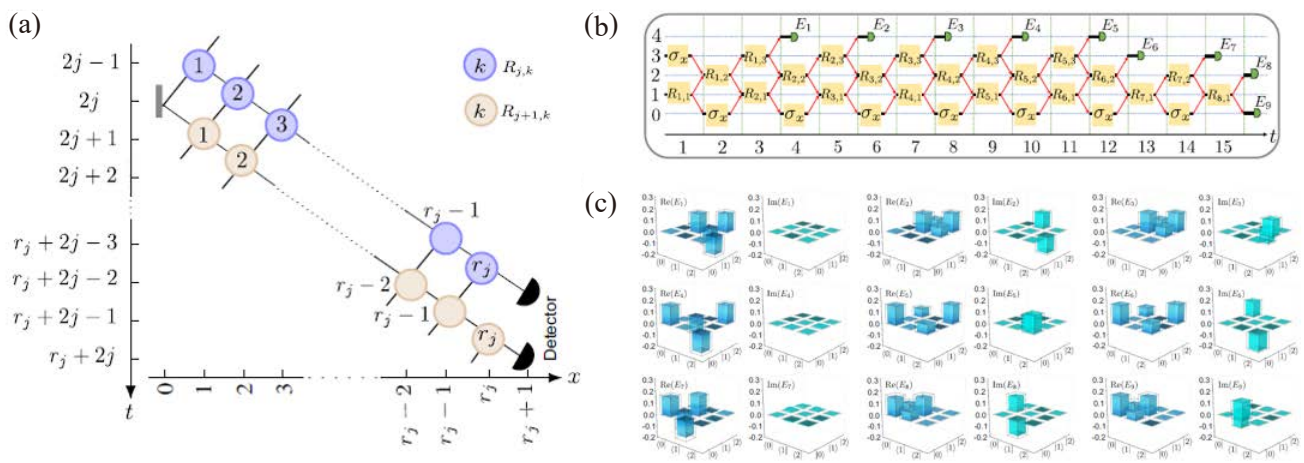


**Fig.** (a)Illustration of the algorithm for the generation of an arbitrary rank-1 POVM on a qudit, where $R_{j,k}$ denotes coin operation. (b) Realization of a qutrit SIC-POVM via QWs. The coin qubit and the walker in positions are taken as a qutrit of interest, whereas the other positions of the walker act as ancillae. Position-dependent coin operations are specified based on the algorithm. The 9 detectors $E_j$ correspond to the 9 outcomes of the qutrit SIC-POVM. (c) Matrix forms of the elements $E_j$ of a qutrit SIC-POVM. Real and imaginary parts of the matrix forms of the 9 reconstructed elements are plotted by solid bars, while hollow bars represent their theoretical predictions.

# 基于量子行走实现高维系统的广义量子测量

王小威#, 詹翔#, 李昱霖, 肖磊, 朱高岩，曲登科，林泉，虞悦，薛鹏*

量子测量在量子力学中起着基础性的作用，特别是广义量子测量。广义测量为从量子系统中提取信息提供了一个强大而通用的工具选择。然而，如何在高维量子系统上实现广义测量，这仍然是一个具有挑战性的任务。这篇工作提出了一种程序化的方法，通过利用基于二维硬币操作的一维离散时间量子行走，在高维量子系统上实现一般的正算子值测量 (也就是广义POVM测量)。此外，作为一个应用, 利用线性光学，这篇工作在实验上实现了高保真度的在三维系统上的对称、信息完备的测量（即SIC- POVM测量）。这篇工作的研究为探索高维量子系统中的物理问题和信息提取铺平了道路，并可以在依赖于广义量子测量的各种量子信息处理任务中找到对应的应用。

◀ 图 (a)在Qudit上生成任意秩为1的 POVM所对应硬币操作$R_{j,k}$的算法示意图。 (b) 通过量子行走实现qutrit SIC-POVM的实验方案图。硬币比特和行走者的位置比特被视为感兴趣的量子比特，而行走者的其他位置则作为辅助比特，位置相关的硬币操作是基于算法指定的。这9个探测器$E_j$对应于qutrit SIC-POVM的9个探测结果。(c) Qutrit SIC-POVM的元素$E_j$的矩阵形式。9个根据实验重构的POVM元素的矩阵形式的实部和虚部用实条表示，空心条表示它们的理论预测。

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[1] X. Wang, # X. Zhan, # Y. Li, L. Xiao, G. Zhu, D. Qu, Q. Lin, Y. Yu, and P. Xue, * Generalized quantum measurements on a higher-dimensional system via quantum walks, Phys. Rev. Lett. 131, 150803(2023).

# MANIPULATING PHOTONIC QUANTUM WALKS UNDER SYNTHETIC MAGNETIC FIELDS

By Quan Lin, Wei Yi*, Peng Xue*

This study [1] explores the dynamic control of photonic quantum walks using synthetic magnetic fields. The manipulation of photonic paths through non-Hermitian skin effects (NHSE) and geometric phases offers a groundbreaking approach to influence the flow of light in novel photonic devices. The following figures demonstrate the critical aspects of the findings.

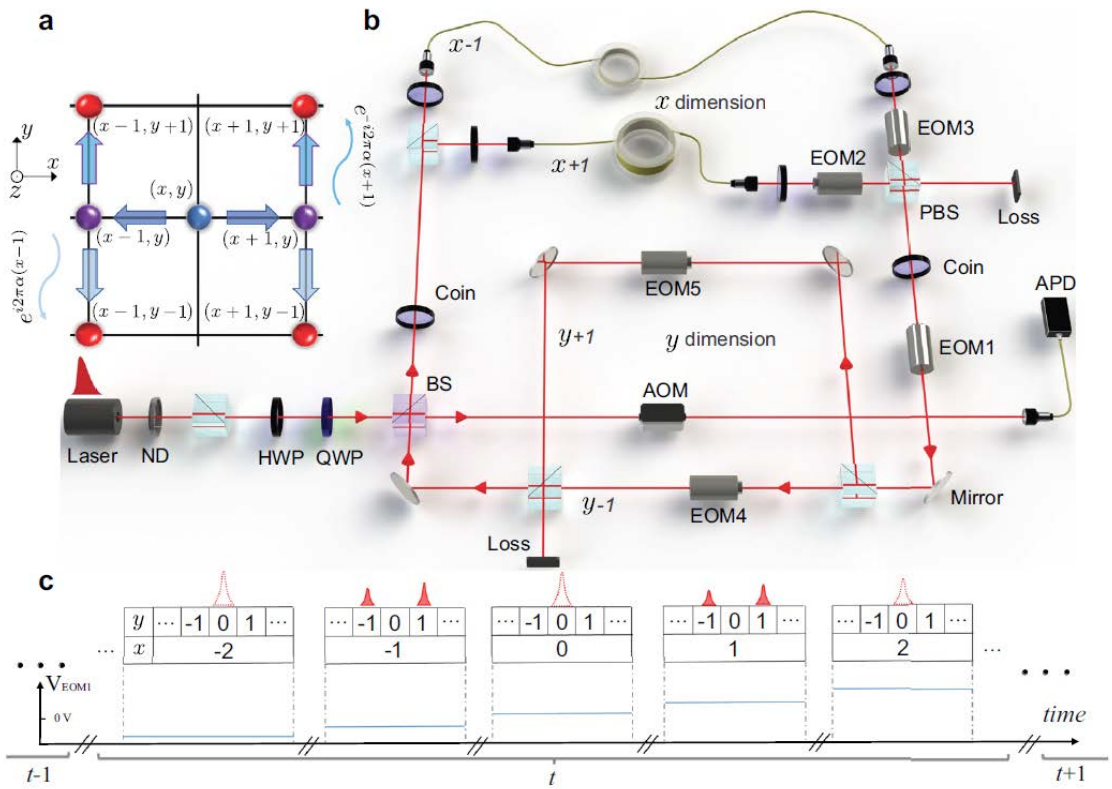
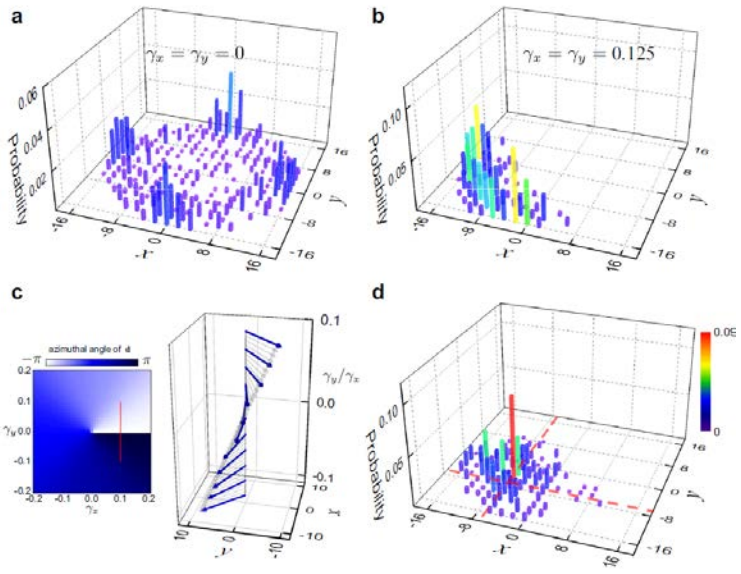



**Fig. 1** Two-Dimensional Non-Hermitian Quantum Walk with a Synthetic Gauge Field

Figure 1 schematically represents the setup for a quantum walk in a two-dimensional photonic system, illustrating how synthetic gauge fields dynamically direct photon movement. The manipulation through geometric phases is fundamental for understanding and controlling quantum states in photonic structures.




◀ **Fig. 2** NHSE and Tunable Photon Transport

Building on Figure 1, Figure 2 demonstrates the effects of the non-Hermitian skin effect (NHSE) on photon distribution in a lattice, showing the asymmetric propagation that results from engineered losses and phase shifts. The control over the flow direction is depicted quantitatively, emphasizing its potential applications in photonic circuits.

▼ **Fig. 3** Magnetic Suppression of the Directional Transport

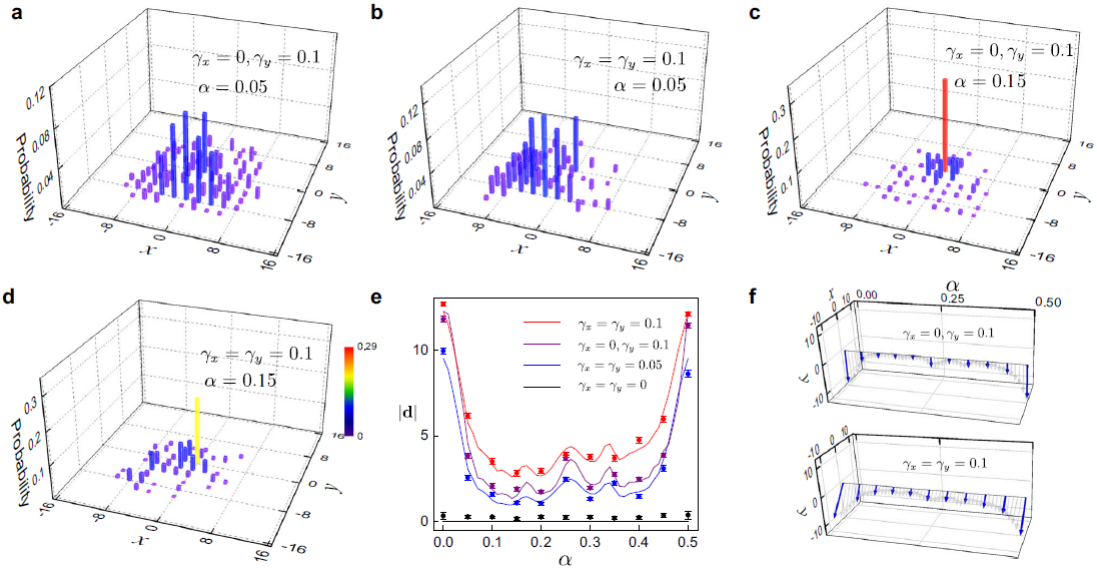



Figure 3 illustrates how introducing a synthetic magnetic field influences the photonic transport, effectively suppressing the NHSE-induced directional flow. This effect is critical for designing devices where control of photon flow is necessary without physical barriers.

The results showcase the flexibility of photonic quantum walks in manipulating light transport through non-Hermitian effects and synthetic dimensions, presenting a novel approach for developing advanced optical devices.

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[1] Quan Lin, Wei Yi*, Peng Xue*, Manipulating Photonic Quantum Walks Under Synthetic Magnetic Fields, *Nat.Commun.*14: 6283 (2023).

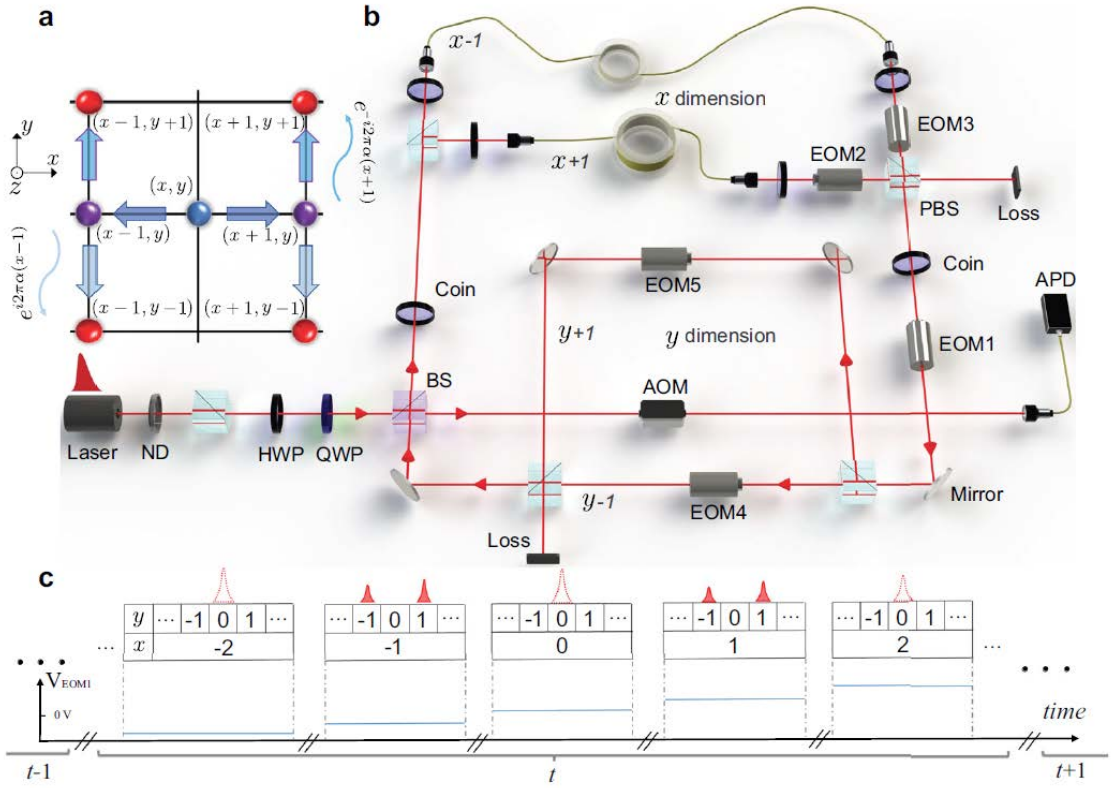


图 1　在合成规范场下的二维非厄米量子行走实验装置

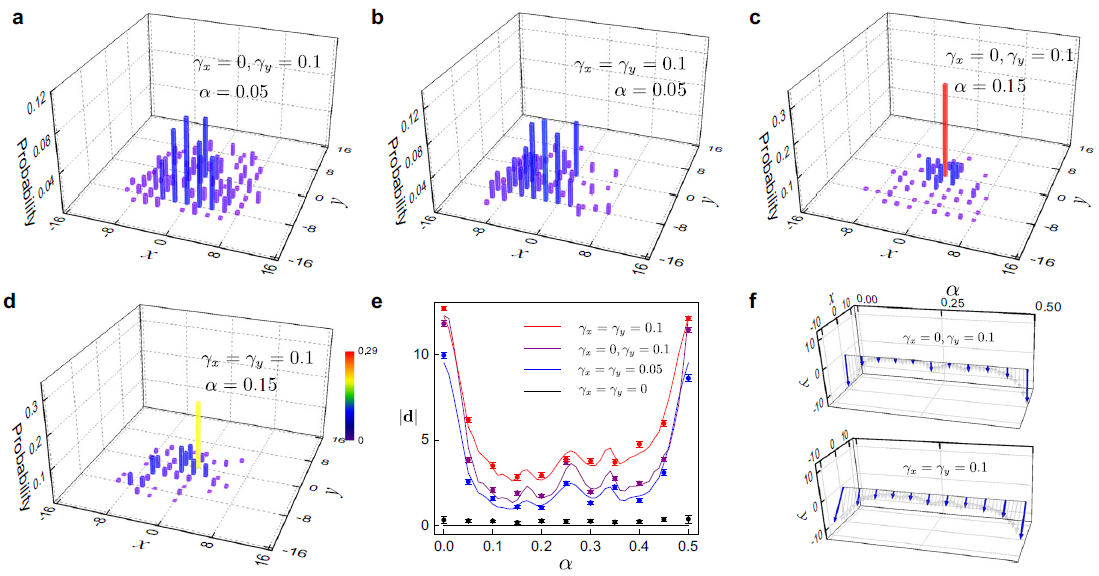


图 3　光子定向传输的磁抑制

# 合成磁场中光子量子行走的操纵

林泉，易为*，薛鹏*

在本研究中[1]，我们探讨了使用合成磁场动态控制光子量子行走的新方法。通过非厄米趋肤效应（NHSE）和几何相位操纵光子路径的方法为在新型光子设备中影响光流提供了开创性的途径。以下各图展示了研究的关键方面。

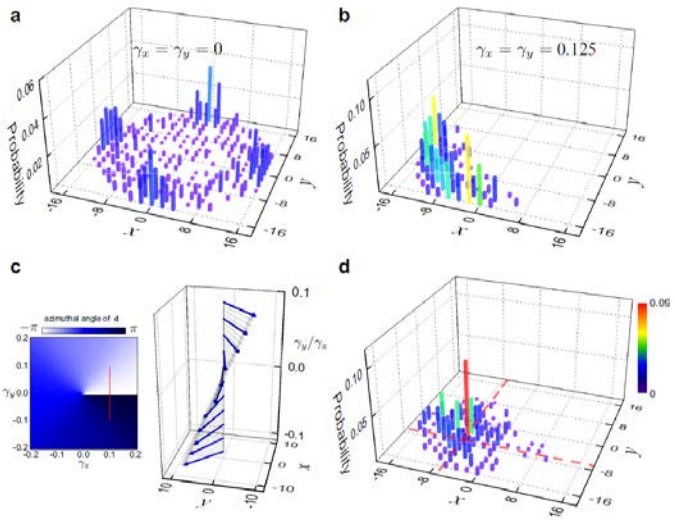


图 2　NHSE与可调谐光子传输

图1展示了在二维光子系统中进行量子行走的实验装置，说明了合成规范场如何动态地影响光子移动。通过几何相位的操控对于理解和控制光子晶体中的量子态至关重要。

基于图1，图2展示了非厄米趋肤效应（NHSE）对晶格中光子分布的影响，显示了由损耗和相移导致的非对称传播。图中定量描述了对光子流向的控制，强调了其在光子电路中的潜在应用。

图3说明了引入合成磁场如何影响光子传输，有效抑制NHSE引起的方向流。这一j结果对于设计需要无物理屏障控制光子流的设备至关重要。

研究结果展示了光子量子行走在通过非厄米效应和合成维度操纵光传输方面的灵活性，为开发先进的光学设备提供了一种新的方法。

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[1] Quan Lin, Wei Yi*, Peng Xue*, Manipulating Photonic Quantum Walks Under Synthetic Magnetic Fields, *Nat.Commun.*14: 6283 (2023).

# STABILITY IMPROVEMENT OF NUCLEAR MAGNETIC RESONANCE GYROSCOPE

By Guoping Gao, Jinbo Hu, Feng Tang, Wenhui Liu, Xiangdong Zhang, Baoxu Wang, Dongge Deng, Mingzhi Zhu, and Nan Zhao

In the field of nuclear magnetic resonance gyroscope (NMRG) research, enhancing stability has always been a goal for scientists. The paper titled "Stability improvement of nuclear magnetic resonance gyroscope with self-calibrating parametric magnetometer" by Prof. Nan Zhao's group of CSRC and the team from Institute of Systems Engineering of CAEP, published in the journal Physical Review Applied, introduces significant academic innovations in this domain.

The paper's central contribution is the proposal of a self-calibrating method to compensate for the NMR phase drift during the measurement by a rubidium (Rb) parametric magnetometer (Rb PM). The authors conducted a comprehensive analysis of various control parameters affecting the stability of the NMR phase, including the DC magnetic field, the frequency and phase of the modulation field, and the Rb resonance linewidth. Through theoretical analysis and experimental verification, they demonstrated how these parameters influence system stability and proposed the self-calibration method based on these insights.

The implementation of the self-calibrating Rb PM markedly improved the bias instability of the NMRG. Experimental data revealed that with the self-calibrating Rb PM, the bias instability of the NMRG was improved from 1 degree per hour to 0.2 degrees per hour for datasets spanning 8 hours, and even to 0.02 degrees per hour for the best approximately 5000-second dataset. This enhancement is crucial for high-precision inertial measurement over extended integration periods.

Moreover, the paper provides a thorough analysis of system errors and measurement methods for key physical parameters, such as the drift of the Rb linewidth. These achievements are essential for further performance improvements in the future. The authors also established a theoretical framework for the NMRG system, focusing particularly on the low-frequency phase noise introduced by the Rb atomic spins under parametric modulation.

Overall, this paper makes a substantial contribution to the improvement of NMRG stability, not only by significantly enhancing measurement precision through the self-calibrating technique but also by providing new theoretical and experimental tools for future research in the fields of quantum measurement and inertial sensing.

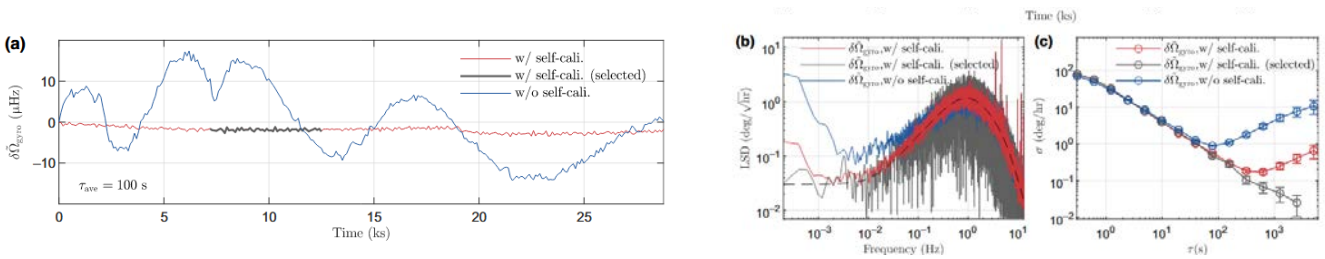


**Fig.** (a)The gyroscope signal with and without applying the self-calibrating Rb PM. The red curve depicts the gyroscope signal drift with a self-calibrating process, and the gray curve is data from a selected segment of the red curve, whereas no self-calibrating method is employed for the blue curve. (b) The noise spectrum of the gyroscope signal with and without the self-calibrating Rb PM. (c) The Allan deviation of the gyroscope signal with and without the self-calibrating Rb PM.

# 核磁共振陀螺仪稳定性的提升

高国平，胡锦波，汤丰，刘文慧，张祥栋，汪宝旭，邓东阁，朱明智，赵楠

在核磁共振陀螺仪（NMRG）的研究领域，稳定性的提升一直是科研人员追求的目标。近期赵楠研究组发表在Physical Review Applied期刊上的相关研究工作，提出了一种自校准方法，用于补偿在铷（Rb）参数磁力计测量过程中的核磁共振（NMR）相位漂移。研究团队深入分析了影响NMR相位稳定性的多种控制参数，包括直流磁场、调制场的频率和相位，以及铷共振线宽等。通过理论分析和实验验证，他们展示了这些参数如何影响系统的稳定性，并基于此提出了自校准方法。

自校准的Rb参数磁力计（Rb PM）的实现，显著提高了NMRG的偏置不稳定性。实验数据显示，使用自校准Rb PM，可以将NMRG的偏置不稳定性从1度/小时改进到0.2度/小时（对于8小时数据集），甚至对于最佳的约5000秒数据集，可以进一步降低到0.02度/小时。这一改进对于长时间积分的高精度惯性测量具有重要意义。

此外，论文还提供了对系统误差和关键物理参数测量方法的全面分析，如铷线宽的漂移。这些成果对于未来性能的进一步提升至关重要。研究团队还建立了一个NMRG系统的理论框架，特别关注由Rb原子自旋在参数调制下引入的低频相位噪声。

总体而言，这篇论文在提高NMRG稳定性方面做出了重要贡献，不仅通过自校准技术显著提升了测量精度，而且为未来在量子测量和惯性传感领域的研究提供了新的理论和实验工具。

◀ 图 1 (a) 应用和不应用自校准铷参数磁力计的陀螺仪信号。红色曲线描绘了采用自校准过程的陀螺仪信号漂移，灰色曲线是红色曲线中选定部分的数据，而蓝色曲线则没有采用自校准方法。 (b) 采用和不采用自校准方法的陀螺仪信号的噪声谱。 (c) 采用和不采用自校准方法的陀螺仪信号的阿伦偏差。

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[1] Gao, G. et al. Stability improvement of nuclear magnetic resonance gyroscope with self-calibrating parametric magnetometer. *Phys. Rev. Applied* 21, 014042 (2024).

# DUAL-LEVEL ENHANCED NONRADIATIVE CARRIER RECOMBINATION IN WIDE-GAP SEMICONDUCTORS

By Chen Qiu, Yu Song*, Hui-Xiong Deng*, Su-Huai Wei*

The conventional single-defect-mediated Shockley–Read–Hall model suggests that the nonradiative carrier recombination rate in wide-band gap (WBG) semiconductors would be negligible because the single-defect level is expected to be either far from valence-band-maximum (VBM) or conduction-band-minimum (CBM), or both. However, this model falls short of elucidating the substantial nonradiative recombination phenomena often observed experimentally across various WBG semiconductors. Owing to more localized nature of defect states inherent to WBG semiconductors, when the defect charge state changes, there is a pronounced structural relaxation around the local defect site. This suggests that a defect at each charge state may exhibit a few distinct local configurations, namely, a stable configuration and a few metastable/transit state configurations. Consequently, a dual-level nonradiative recombination model should more realistically exist in WBG semiconductors. In this model, through the dual-level mechanism, electron and hole trap levels are different from each other and could be closer to the CBM for the electron trap and closer to the VBM for the hole trap, respectively; therefore, significantly increasing the corresponding electron and hole capture rates, enhancing the overall process of nonradiative recombination, and explains the experimental observations. In this work, taking technically important $SiO_2$ as an illustrative example, we introduce the dual-level mechanism to elucidate the mechanism of nonradiative carrier recombination in WBG semiconductors. Our findings demonstrated strong alignment with available experimental data, reinforcing the robustness of our proposed dual-level model. Our fundamental understanding, therefore, provides a clear physical picture of the issue and can also be applied to predict the defect-related nonradiative carrier recombination characteristics in other WBG materials.[1]

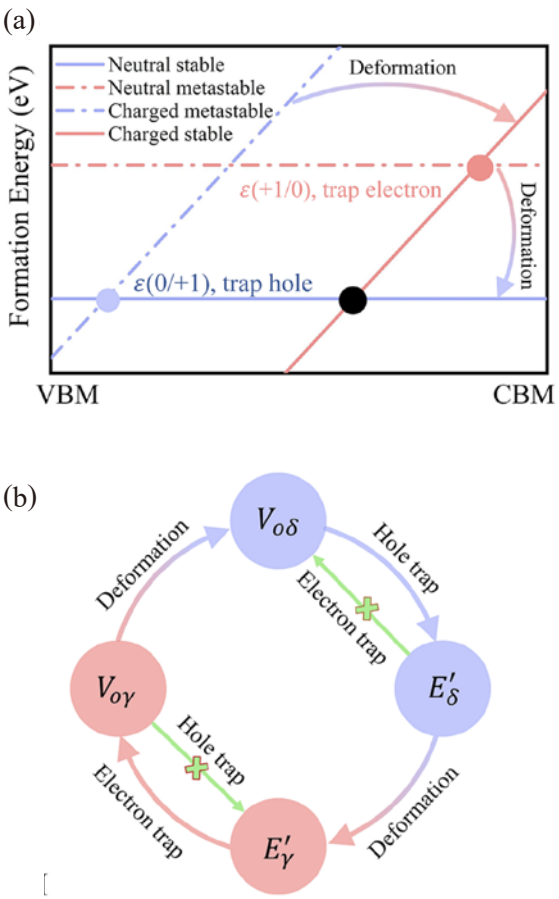


**Fig 1.** (a) Schematic plot of dual-metastable defect configurations enhanced nonradiative carrier recombination. (b) Nonradiative recombination processes of oxygen vacancy in amorphous $SiO_2$, involving four distinct processes: (i) $V_{o\delta}$ captures a hole from the valence band, forming the metastable state $E'_{\delta}$ , (ii) the metastable $E'_{\delta}$ relaxes to stable $E'_{\gamma}$ after overcoming a small energy barrier, (iii) the $E'_{\gamma}$ captures an electron from the conduction band to form the metastable state $V_{o\gamma}$, and (iv) a small energy barrier can be overcome to transfer from the metastable $V_{o\gamma}$ to the stable $V_{o\delta}$ configuration.

# 宽禁带半导体中双能级增强载流子非辐射复合的物理机制

邱晨，宋宇*，邓惠雄*，魏苏淮*

一般来说，半导体中载流子的非辐射复合速率正比于缺陷能级与相应带边的能量差。在宽禁带半导体中，由于大的禁带宽度，缺陷能级要么远离价带顶，要么远离导带底，或者两者同时远离。因此经典的单缺陷导致的Shockley-Read-Hall模型预测宽禁带半导体中载流子的非辐射复合速率可以忽略不计。然而，目前的实验研究已经在多种宽禁带半导体中观察到显著地非辐射复合现象，这一实验事实与Shockley-Read-Hall模型相矛盾，表明应该存在新的非辐射复合机制。我们发现由于宽禁带半导体中缺陷态的局域化特性，当缺陷电荷状态改变时，缺陷周围的结构会发生显著地结构畸变。这表明，每个电荷状态下的缺陷可能表现出几种不同的局部构型，即存在一个稳定结构和几个亚稳态或过渡态构型。因此，在宽禁带半导体中应该存在双能级载流子非辐射复合。在这个模型中，通过双能级复合机制，电子和空穴的俘获能级彼此不同，并且电子俘获能级更接近导带底，而空穴俘获能级更接近价带顶。这极大地增加了相应的电子和空穴俘获速率，增强了整个非辐射复合过程，能够很好地解释目前的实验观察。在本研究中，以技术上重要的非晶二氧化硅为例，我们基于双能级机制阐明了宽禁带半导体中载流子强非辐射复合的物理机制。我们的研究结果与现有的实验数据吻合的非常好，证实了我们提出的双能级载流子非辐射复合模型的可靠性。我们的模型也为理解宽禁带半导体中载流子非辐射复合提供了一个清晰的物理图像，并可以应用于预测其它宽禁带材料中缺陷相关的载流子非辐射复合特性。

◀ 图 1 a) 宽禁带半导体中双亚稳缺陷结构增强载流子非辐射复合的示意图。b) 非晶态二氧化硅中的氧空位的双能级非辐射复合过程，涉及四个不同的过程：(i) 中性稳态结构 $V_{O\delta}$ 从价带俘获一个空穴，形成正一价亚稳态结构 $E'_{\delta}$，(ii) 亚稳态构型 $E'_{\delta}$ 能够迅速地跨越势垒后弛豫至稳态构型 $E'_{\gamma}$，(iii) $E'_{\gamma}$ 从导带俘获一个电子形成中性亚稳态构型 $V_{O\gamma}$，(iv) 亚稳态 $V_{O\gamma}$ 能够迅速跨越势垒结构弛豫到稳态构型 $V_{O\delta}$。

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# HYBRID VAN DER WAALS EPITAXY

By L. Hu, D. Liu, F. Zheng, X. Yang, Y. Yao, B. Shen, and B. Huang*

Nobel Prize winner in Physics, H. Kroemer, said "The interface is the device." Therefore, interfaces hold significant research value in material growth and property control. For traditional thinfilm growth, it can be classified into Frank-Van der Merwe (FV), Volmer-Weber (VW), and Stranski-Krastanov (SK) modes, mainly based on the interaction strength between thinfilm and substrate. In the FV mode, due to the lattice matching between the thinfilm and substrate, in-plane growth is dominant. In contrast, in the VW mode, there is a significant lattice mismatch, which results in a larger resistance to in-plane growth, replaced by an out-of-plane growth. The SK mode is a growth mode that lies between these two. Over the past century, these three growth modes have been able to describe the growth mechanism of almost all the thinfilms on substrates. Recently, experiments have shown that by using two-dimensional materials, such as graphene, as a buffer layer, it is possible to grow high-quality nitride thinfilms on van der Waals substrate. However, this growth mode cannot be simply explained by these three established modes mentioned above, which has also sparked debates in the field.

In a recent study, Prof. Huang in collaboration with the other researchers made a key step towards understanding this puzzling growth mechanism. Taking the growth of aluminum nitride (AlN) thinfilm on graphene as an example, they have used multiscale computation to study the growth of AlN thinfilm on graphene. Simulations revealed a new type of bonding at the interface between the AlN and graphene: only the corners have strong chemical bonds, while the center has weak van der Waals interactions. Interestingly, this hybrid bonding mode makes the growth mode distinct from the traditional FV mode, named as hybrid van der Waals epitaxy (HVE). In this new growth mode, growth in-plane and out-of-the plane are strongly coupled and satisfies certain physical constraints. To confirm the validity of HVE, we have performed experiments. Importantly, experimental collaborators have also verified the correctness of this growth mode through multiple experimental methods, such as AFM and SEM. Overall, this work expands the traditional growth modes and proposes a new growth mechanism beyond the current category of material growth, which may be adopted design high-quality nitride semiconducting thinfilms with different height-size-shape correspondence.

This work has recently been published in Physical Review Letters [1]. In addition, this work is also selected as the Editors' Suggestion.

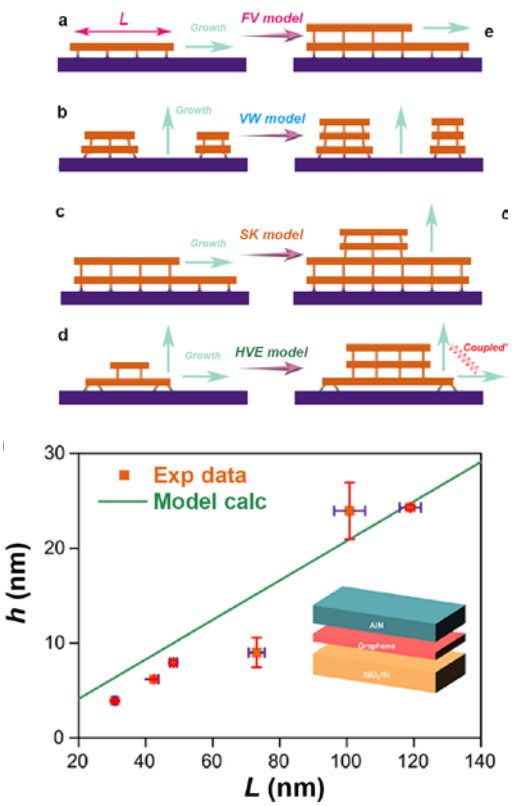


**Fig .** A new growth model: hybrid van der Waals epitaxy (HVE). HVE is fundamentally different from other known growth models, in which the in-plane and out-of-plane growth is strongly coupled.

# 杂化范德华外延生长：一种薄膜生长的新范式

胡麟，刘丹烁，郑法伟，杨学林，姚裕贵，沈波，黄兵*

凝聚态物理中新奇物理现象的研究和信息科学中电子器件的制备都极大依赖于高质量薄膜材料的制备。因此，如何在衬底上外延生长出高质量的薄膜材料是凝聚态物理、材料科学和表面化学等众多研究领域中长期存在的一个焦点问题。在长达将近一个世纪的研究基础上，人们逐步总结出三种普适的薄膜生长模型，它们被称之为FV (Frank-van der Merew)，VW (Volmer-Weber) 和SK (Stranski-Krastanow) 模型。FV模型描述的是一种面内生长模式。与之相反，VW模型则描述的是一种面外垂直生长模式。SK模型则是介于FV和VW之间的一种生长模式。在已知的这三种生长模型中，面内和面外生长是基本解耦的，它们可以描述几乎所有已知薄膜材料在衬底上的外延生长过程。最近，人们发现可以在二维范德华衬底上可以生长出高质量的非范德华氮化物半导体薄膜。这一突破性发现不但开启了一种全新的半导体生长模式，同时也引发了人们对其生长机制的激烈争论。

为了解决这一争议，北京计算科学研究中心的黄兵研究员和北京理工大学的胡麟研究员（原中心博士后成员）等合作，为揭开这一神秘的生长机制迈出了重要的一步。他们以氮化铝薄膜生长在石墨烯上为例，利用多尺度的理论计算和连续介质模型推导，系统研究了氮化铝薄膜在平面内和垂直于平面方向生长动力学过程。有趣的是，他们发现氮化铝与石墨烯的界面存在一种新型的成键方式，即杂化范德华相互作用。这样一种独特的成键方式使得薄膜生长呈现出显著区别于传统模式的新范式，被命名为HVE模型。在HVE模型下，材料平面内和平面外的生长会较强的耦合在一起，并满足一定的物理约束条件，而这个约束条件也受到界面相互作用的影响。为了验证理论提出的这一新生长模型的可靠性，北京大学杨学林研究员等进行了实验验证，初步验证了该生长模式的可靠性。这一发现不但为材料生长领域提供了一种全新的模型，同时也为进一步优化外延氮化物薄膜生长过程提供了理论基础，助力于其在后硅基信息时代发挥更加关键性的作用。

这项研究最近在《物理评论快报》[1]杂志上发表。此外，这项工作还被选为该杂志的编辑们推荐介绍。

◀ 图 杂化范德华外延生长（HVE），一种薄膜外延生长的新范式。

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# MANIPULATION OF NONLINEAR OPTICAL RESPONSES IN LAYERED FERROELECTRIC NIOBIUM OXIDE DIHALIDES

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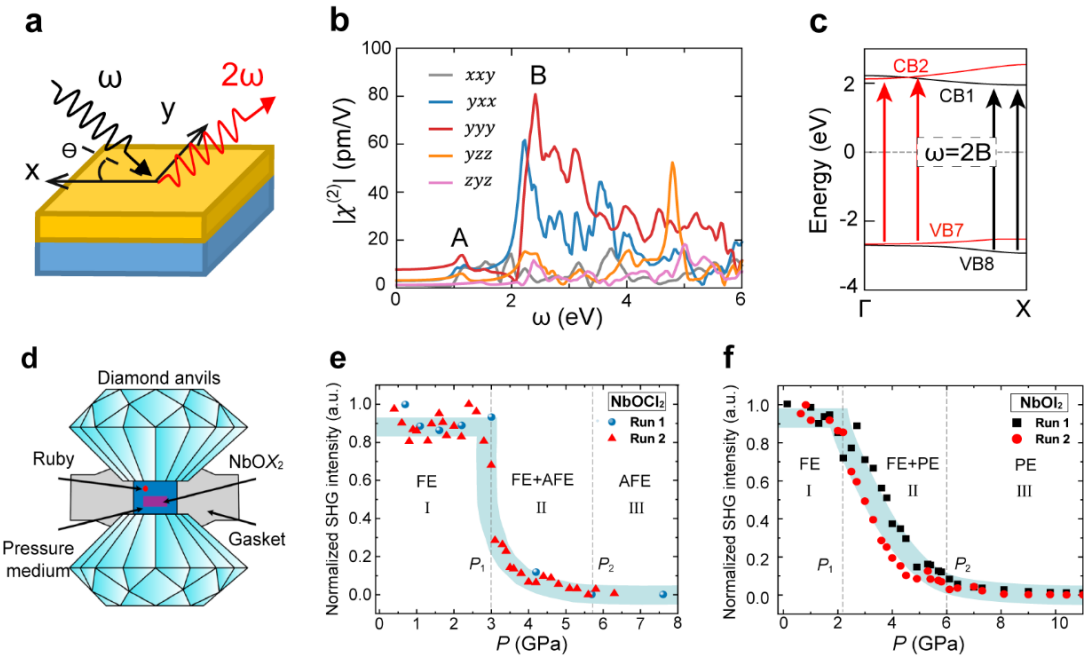


**Fig. 1.** Second-harmonic generation (SHG) response in $NbOX_2$ (X = Cl, I) and its tunability by external field.

Nonlinear optics, a study of the interaction of intense laser light with matter, provides theoretical support and experimental results for applications such as laser frequency conversion, optical switching, and so on. Realization of highly tunable second-order nonlinear optical responses, e.g., second-harmonic generation (SHG) and bulk photovoltaic effect, is critical for developing modern optical and optoelectronic devices. Recently, the van der Waals niobium oxide dihalides are discovered to exhibit unusually large second-harmonic generation [1-2]. However, the physical origin and possible tunability of nonlinear optical responses in these materials remain to be unclear.

In this article, we reveal the mechanism of large second-harmonic generation in $NbOX_2$ (X = Cl, Br, and I) and observe tunable SHG by structural phase transition [3]. By density functional theory, we analyze optical transitions under specific polarization of incident light and find the large band nesting effect in the Brillouin zone. Using the advanced experiment technique, the single-crystal X-ray diffraction analysis technique under high-pressure conditions, aided with extra SHG spectra, we discover the intralayer ferroelectric-to-antiferroelectric phase transition in NbOCl2 and ferroelectric-to-paraelectric phase transition in $NbOI_2$ under certain pressures, accompanied by the greatly tunable nonlinear optical responses but with different microscopic mechanisms. Our study establishes the interesting external-field tunability of $NbOX_2$ for nonlinear optical device applications.

# 层状铁电材料
# 铌氧二卤化物中非线性光学响应的调控

叶良婷#, 周文居#, 姜肖, 李阳*, 缑慧阳*, 黄兵* 等人

非线性光学是一门研究强激光与物质相互作用的学科，为激光频率转换、光开关等应用提供理论支撑和实验结果。实现高度可调的二阶非线性光学响应，例如二次谐波生成和体光伏效应，对于发展现代光学和光电子设备至关重要。最近，范德瓦耳斯材料铌氧二卤化物中存在较大的二次谐波生成效应。然而，这些材料中非线性光学响应的物理起源和可调性仍然不明确[1-2]。

本文揭示了NbOX2（X = Cl, Br, I）中二次谐波生成效应的机制，并通过结构相变观察到了可调的二次谐波生成[3]。通过密度泛函理论，我们分析了不同偏振方向的入射光对光学跃迁的影响，发现了能带嵌套效应。利用高压条件下的单晶X射线衍射分析技术和SHG光谱测量，我们在一定的外部压强范围内实现了NbOCl2的层内铁电至反铁电相变和NbOI2的铁电至顺电相变，并且这两种相变是可逆的，伴随着不同微观机制的可调控非线性光学响应。我们的研究为$NbOX_2$在非线性光学器件应用中的外场可调性奠定了基础。

◀ 图 1：$NbOCl_2$ 和 $NbOI_2$ 中的二次谐波生成效应和外场下的调控机制。

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# IONIC HUBBARD MODEL IN TRILAYER MOIRÉ SUPERLATTICES OF $MOS_2$

By Hongzhen Zhong, Zhixin Su, Jun Kang*

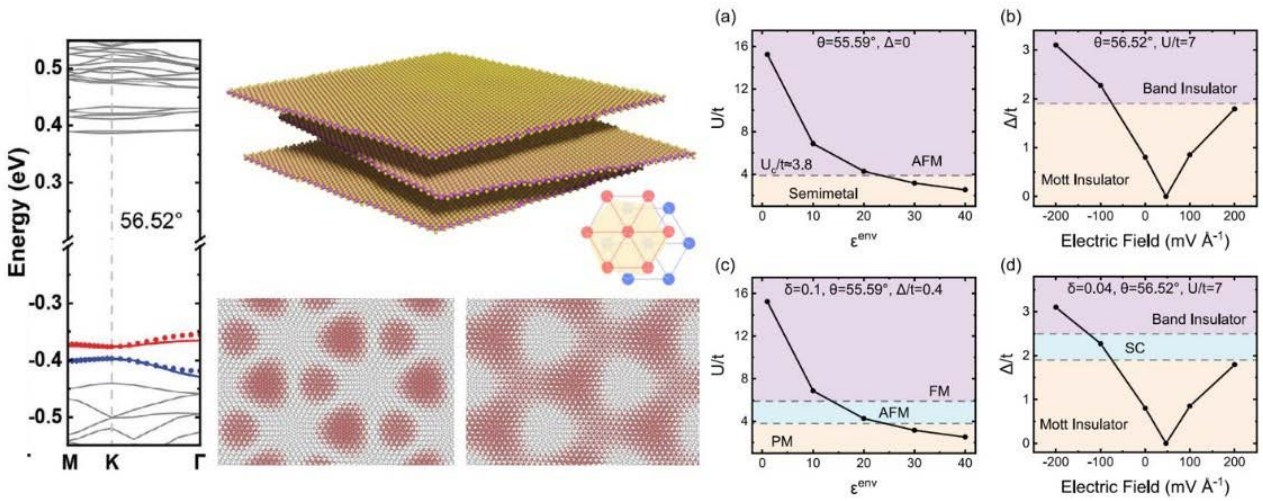


**Fig 1.** Ionic Hubbard model in trilayer moiré superlattices of $MoS_2$

Recently, the electronic properties in moiré superlattices, which consist of two-dimensional van der Waals materials, have become a topic of great interest. The moiré potential with long periodicity results in the formation of flat bands and strongly correlated states, making moiré superlattices a good platform to study strong-correlation physics. The realization of different lattice model Hamiltonians in moiré superlattices has become the focus of researches. Here, it shows that, compared to bilayer moiré superlattices where there is only one interface, the interference between moiré patterns at different interfaces in 2D multilayer structures allows the physical realization of more complicated lattice models. The concept is demonstrated by trilayer moiré superlattices (TMSLs) of $MoS_2$, where it finds that isolated flat moiré bands appear near the valence band edge, and they can be described by the honeycomb lattice ionic Hubbard model. More importantly, the hopping strength, the on-site Coulomb repulsion, and the staggered potential in the TMSLs are highly tunable through the control of the twist angle, the dielectric environment, and the perpendicular electric field. It is possible to achieve various transitions between distinct quantum phases in the TMSLs, spanning from weak to strong correlation regimes. Therefore, the proposed TMSLs can serve as a good platform to study the strong correlation physics in the honeycomb lattice ionic Hubbard model.

# 三层$MoS_2$摩尔超晶格中的离子哈伯德模型

钟泓臻，苏志鑫，康俊*

图 1 ：三层$MoS_2$摩尔超晶格中的离子哈伯德模型

在摩尔超晶格中实现不同的格点模型哈密顿量当前已成为研究的焦点。与仅有一个界面的双层摩尔超晶格相比，在二维多层结构中，通过不同界面多重摩尔图案之间的叠加，有可能实现更复杂的格点模型。本工作在三层$MoS_2$摩尔超晶格(TMSL)验证了这一思路。从完全对齐的AAA堆叠三层$MoS_2$出发，对中间层进行接近60度的旋转，同时底层沿Armchair方向进行适当的滑移，便可构建一种特殊的双重摩尔超晶格。在这种TMSL中，价带边缘附近将出现的局域化平带电子态，其来源于两重摩尔超晶格的两套三角子晶格间的叠加，从而形成六角晶格。由于堆叠方式和局域结构的差异，两套三角子晶格间存在一个等效的离子势差，因此，整个体系可由六角晶格上的Ionic Hubbard模型来描述。特别地，体系的关键参数可大范围独立调控。格点间的跃迁强度随着转角靠近60度而不断减小。格点上的库仑排斥强度可通过改变周围介电环境进行控制，大的环境介电常数将导致小的库伦排斥。最后，由于两个三角子晶格上局域电子态在z方向上分布存在差异，子晶格间的离子势差可通过z方向上的电场进行调控。通过改变电场的强度和方向，离子势差可以增加，减小或消失。基于这些调控策略，以及已报道的Ionic Hubbard模型相图，我们具体研究了不同条件下TMSL中可能存在的强关联物相，发现体系可呈现半金属、铁磁、反铁磁、能带绝缘体、莫特绝缘体、超导等丰富的物相。因此，TMSL可以作为研究六角晶格上的离子Hubbard模型中强关联物理的良好平台。

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# ARTIFICIAL INTELLIGENCE ASSISTED AMORPHOUS ALLOY SIMULATION AND DESIGN

By Pengfei Guan's Group

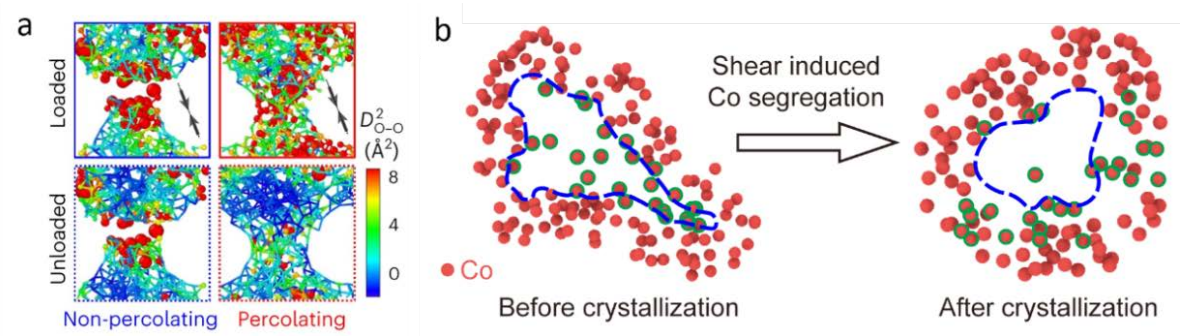


**Fig 1.** (a) Illustration of the oxide network in loaded and unloaded samples [1]; (b)Shear induced segregation of Co out of the ordering region [2]

In the realm of material science, artificial intelligence-assisted machine learning multi-component potential functions are revolutionizing high-precision property predictions and material design. The research team led by Pengfei Guan has made significant strides in developing machine learning potential functions that enable molecular dynamics simulations of multi-component amorphous systems at unprecedented time scales. (1) Zr-Cu-O Machine Learning Potential Function: By constructing a machine learning potential function with first-principles accuracy, the team elucidated the effects of oxygen on the properties of metallic glasses. This research revealed that low-dimensional oxidized metallic glasses can form unique oxygen-rich topological networks. By facilitating elemental exchanges within the metallic glass spectrum, this network exhibits exceptional elastic properties, guiding the synthesis of related materials and introducing a novel elastic recovery mechanism. (2) TiZrHfCo Machine Learning Potential Function: The development of a first-principles-accurate TiZrHfCo machine learning potential function led to groundbreaking findings in shear processes. The rapid diffusion and uneven distribution of cobalt (Co) promote atomic rearrangement, interrupting the typical softening process and enhancing hardening. In contrast, traditional metallic glasses often face conflicts between volume shrinkage due to atomic rearrangement and expansion from deformation, leading to cracks and fractures. However, the newly developed multi-principal element metallic glass achieves deformation-induced expansion through rearrangement, effectively preventing crack formation. This innovation results in processing hardening behavior and intrinsic tensile plasticity, fundamentally addressing the strain softening issue in amorphous alloys. The collaborative research team introduced a substantial amount of Co into conventional TiZrHf alloys, resulting in the creation of $Ti_{25}Zr_{25}Hf_{25}Co_{25}$ multi-component metallic glass. Remarkably, this material exhibits a macroscopic tensile plasticity of up to 2% at room temperature, with processing hardening approaching double the yield strength. Both tensile plasticity and fracture strength surpass currently reported values for metallic glasses, achieving a remarkable combination of high plasticity and high strength. This work provides a practical design framework for developing more high-strength and tough metallic glasses. The advancement of AI-assisted machine learning potential functions will serve as a valuable tool in our ongoing research into the effects of trace elements in disordered alloys and the challenges of simulating amorphous soft magnetic properties.

# 人工智能辅助非晶合金模拟与设计

管鹏飞课题组

人工智能辅助的机器学习多组元势函数可以用于高精度性质预测、材料设计等领域。管鹏飞课题组通过机器学习势函数的开发，实现多元非晶体系秒量级时间尺度分子动力学模拟和设计：（1）基于第一性原理精度Zr-Cu-O机器学习势函数的构建，阐明了非晶合金物性的氧元素效应。从原子尺度揭示这类低维氧化金属玻璃可以形成特殊的富氧拓扑网络结构的现象，并通过和金属玻璃区间的元素交换，来实现该网络的超大弹性，指导了相关材料的合成，并提出了该类材料独特的弹性回复机制。（2）开发了第一性原理精度的TiZrHfCo机器学习势函数，基于分子动力学模拟发现在剪切过程中，钴 (Co) 的快速扩散和不均匀分布有利于原子重排，从而中断通常的软化过程并促进硬化。相比之下，传统的金属玻璃经常面临原子重排引起的体积收缩和变形引起的膨胀之间的冲突，导致裂纹和断裂。然而，研究团队开发的新型多主元金属玻璃通过重排实现形变诱导膨胀，避免了裂纹的形成，从而导致加工硬化行为和本征的拉伸塑性，从根本上解决了非晶合金应变软化问题。合作研究团队通过在传统的TiZrHf合金中引入大量Co元素，制备出$Ti_{25}Zr_{25}Hf_{25}Co_{25}$多组元金属玻璃，实现了室温下的宏观拉伸塑性可以达到2%，加工硬化更是接近屈服强度的一倍。拉伸塑性和断裂强度均超过了目前已报道的金属玻璃，实现了高塑性和高强度的结合。该工作为设计更多高强高韧金属玻璃提供了切实可行的设计思路。人工智能辅助的机器学习势函数开发将为我们后续研究无序合金中微量元素效应、非晶软磁特性等无序合金模拟中的挑战问题提供了有利工具。

图 1: a)加载和卸载过程中的氧化物网络以及[1]；(b)剪切诱导晶化中Co的偏析[2].

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# STICKY BACTERIA ARE HOT

By P. Leishangthem, and X. L. Xu*

Swimming microorganisms are constantly influenced by the presence of boundary surfaces in their natural habitat, giving rise to rich swimming behaviors. However, despite of the fact that interactions between microswimmers and nearby boundary surfaces are vital to many biological functions and industrial applications, little is known about the mechanism responsible for the surface entrapment of microswimmers. After six decades of active research, the mechanism responsible for the surface entrapment of microswimmers is still under heated debate.

In a recent theoretical study led by Prof. Xinliang Xu at Beijing CSRC, the dynamical behaviors of flagellar bacteria near surfaces are investigated. By relating surface entrapment to a fixed point in bacterial dynamics, it is proved that a commonly neglected thermodynamic effect is essential for bacterial entrapment. Using Escherichia coli as an example where experimental data are abundant, it is demonstrated that the incorporation of this thermodynamic effect to even a simplified model of each bacterium as two spherical beads is capable to quantitatively reproduce all existing experimental observations, including two key features that previous theories/simulations fail to resolve: The bacterial "nose-down" configuration, and the anticorrelation between the pitch angle and the wobbling angle. Furthermore, the theory makes the following important predictions that motivate future experiments for further verification: boundary entrapment of bacteria is governed by two analytic relationships, which only exists within an entrapment zone dictated by two dimensionless parameters: $\alpha_1$ the ratio of thermal energy to self-propulsion, and $\alpha_2$ a bacterial intrinsic shape factor. These results provide guidelines for controlling biological and engineering active swimmers near surfaces, and the manuscript summarizing these results authored by Dr. Premkumar Leishangthem (postdoc at CSRC) and Prof. Xinliang Xu is accepted at Phys. Rev. Lett.

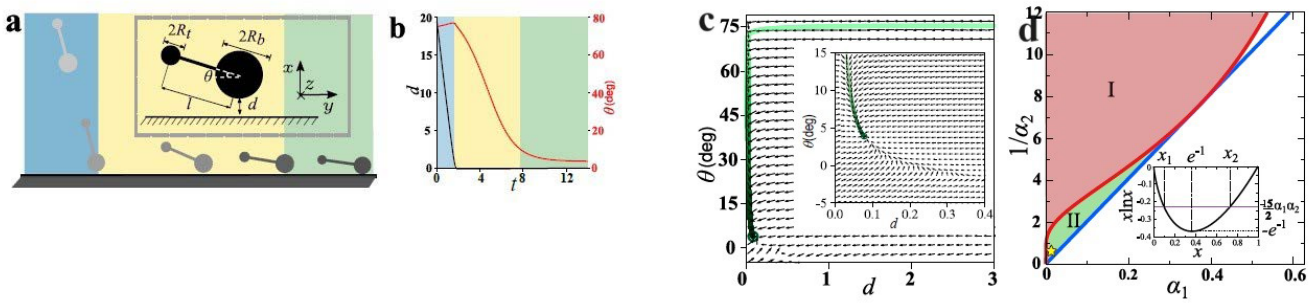


**Fig 1.** Bacterial entrapment. Bacterial trajectory near a planar boundary in physical space (a), and in phase space defined by surface distance $d$ and pitch angle $\theta$ (c). In (b) the temporal evolution of d and $\theta$ is illustrated. In (d) it is illustrated that entrapment only exists when system parameters $\alpha_1 \equiv \frac{k_B T}{F_{act} R_b}$ and $\alpha_2 \equiv \frac{R_t l}{R_b^2}$ fall within region II (the green shaded area).

# 边界吸附的细菌热力非凡

P. Leishangthem & 徐辛亮*

微生物的生存环境中充斥着各种边界，在这些边界的影响下微生物表现出丰富的运动模式。微生物和这些边界的相互作用一方面对其自身的很多生物功能至关重要，同时在很多工程问题中也有很重要的应用场景。然而在长达60年的持续研究后，我们对这些边界附近的细菌行为依然缺乏一个统一的理论认知。

最近，北京计算科学研究中心由徐辛亮教授领导的理论小组对边界附近的细菌运动行为进行了研究。通过将细菌被长期吸附在边界附近的运动与相空间中的一个不动点联系起来，该研究组从理论上证明了热力学效应在其中的必要性。对于大肠杆菌这种实验数据丰富的研究对象，考虑了该热力学效应的一个简单流体相互作用模型定量的解释了所有已有相关实验数据，包括之前所有理论模型/计算模拟都无法解释的两个关键性质：细菌被吸附时的运动步态为“头冲表面”；细菌身体和表面的pitch angle和wobbling angle表达出一种明显的反相关关系。在此基础上，该研究组的这套简单理论还提出了两个重要预言，以供未来的实验来验证。第一，边界吸附的细菌的形态由pitch angle和表面间距决定，而理论预言了这两个物理量满足的两个解析关系式。这两个解析关系式是否有解取决于两个无量纲参数：$\alpha_1$热能/自驱动能的比例，$\alpha_2$细菌尺寸因子。第二，细菌表面吸附现象仅出现于温度低于某个特征温度时（往往远大于室温），但是在绝对零度该解析式无解，无法出现吸附现象。这证明来源于环境的热力学效应是必要的，换言之，表面吸附的细菌都热力非凡。该研究由北京计算科学研究中心博士后Premkumar Leishangthem和徐辛亮教授共同完成，成果于最近在《物理评论快报》杂志成文发表【1】。

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# OPTIMAL LONG-TIME DECAY RATE OF NUMERICAL SOLUTIONS FOR NONLINEAR TIME-FRACTIONAL EVOLUTIONARY EQUATIONS

By Dongling Wang, Martin Stynes*

Fractional-order differential equations offer modeling properties that are superior to classical integer-order differential equations in many physical processes with non-local effects or generic memory characteristics. The exact solutions of these differential equations are of particular interest for large values of time t, as then they behave very differently from the solutions of integer-order differential equations. Despite the significance of the long-time regime (i.e., when $t \to \infty$ ), the behaviour of computed approximate solutions as $t \to \infty$ has not been extensively investigated, in part because there are serious difficulties obstructing its numerical analysis. In the paper [1], the following nonlinear initial-value problem is considered: $\mathcal{D}_t^\alpha y(t) = -\lambda y(t)^\gamma$ for $t > 0$ with $y(0) > 0$ , where $\mathcal{D}_t^\alpha$ is the Caputo derivative of order $\alpha \in (0,1)$ while $\lambda, \gamma$ are positive parameters. Its exact solution $y(t)$ is known to exhibit $O(t^{-\alpha/\gamma})$ decay as $t \to \infty$ , but no corresponding decay result for any discretisation of this problem has previously been proved. In [1] it is established that for the class of Complete Monotonicity-preserving ($\mathcal{CM}$-preserving) schemes (which include the well-known L1 and Grünwald-Letnikov schemes) on uniform meshes $\{t_n := nh\}_{n=0}^{\infty}$ , the discrete solution also has $O(t^{-\alpha/\gamma})$ decay as $t_n \to \infty$ . This striking new result is then extended to $\mathcal{CM}$-preserving discretisations of certain time-fractional nonlinear subdiffusion initial-boundary value problems of parabolic type, such as the time-fractional porous media and p-Laplace equations. Furthermore, for the L1 scheme the $O(t^{-\alpha/\gamma})$ decay result is proved to remain valid on a very general class of nonuniform meshes.

The analysis of [1] uses a discrete comparison principle with discrete subsolutions and supersolutions that are carefully constructed to give tight bounds on the discrete solution. Numerical experiments are provided to confirm the sharpness of the theoretical analysis.

It is expected that in the future, the innovative theory of this paper will be a significant contribution to the numerical analysis of long-time behaviour of solutions of time-fractional differential equations that are computed by various numerical methods.

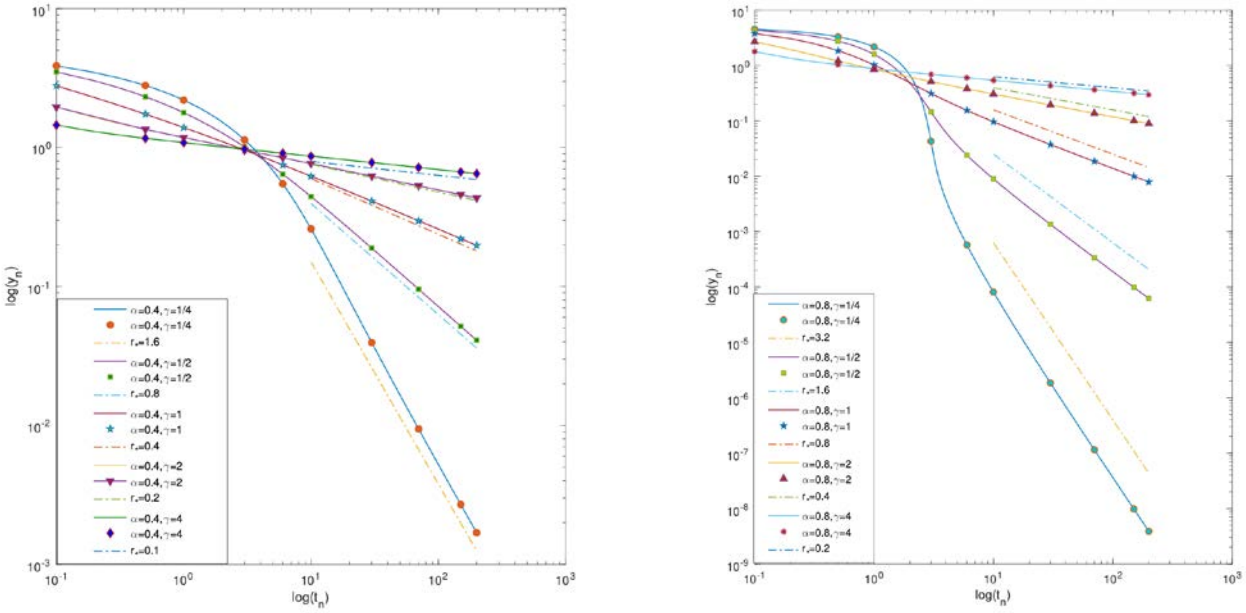


**Fig 1.** Log-log plot of numerical solutions of the nonlinear initial value problem, computed using the Grünwald-Letnikov scheme with $\alpha = 0.4$ (top) and $\alpha = 0.8$ (bottom) and parameter $\gamma = 1/4,1/2,1,2,4$.

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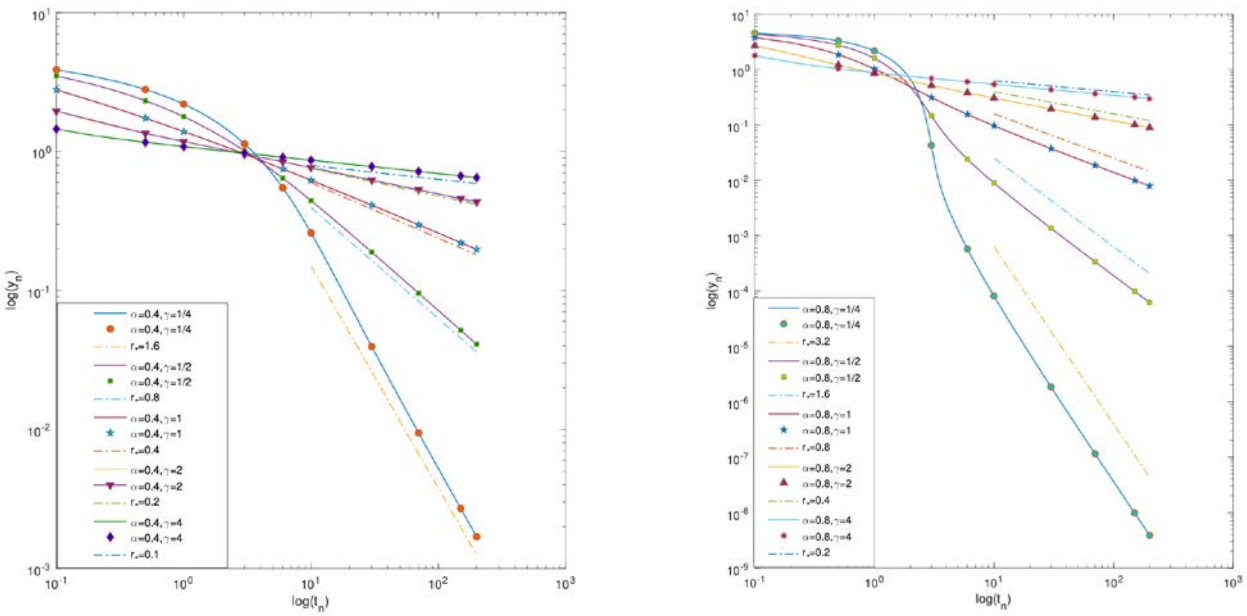


图 1 ：使用Grünwald-Letnikov格式求解非线性初值问题所得数值解的log-log图像，其中分别取 $\alpha=0.4$（上）和 $\alpha=0.8$（下），在每个图像中参数 $\gamma$ 分别取为 $\gamma=1/4,1/2,1,2,4$。每个数值解的衰减速率与我们的理论预测完全一致。

# 非线性分数阶发展方程数值解的最优长时间衰减速率

王冬岭, Martin Stynes*

在许多具有非局部效应或一般记忆特性的物理过程中，分数阶微分方程表现出优于经典整阶微分方程的建模特性。这类微分方程的精确解在时间t较大时表现出有趣的性质，它们的行为与整阶微分方程的解有很大的差异。尽管解的长时状态（即当 $t\to\infty$ 时）具有重要意义，但该类问题的近似解在 $t\to\infty$ 时的行为尚未得到广泛研究，部分原因是其数值理论分析中存在严重的阻碍。在[1]中，我们考虑下述非线性初值问题：$D_t^\alpha\, y(t)=-\lambda y(t)^\gamma$，$t>0$，其初值$y(0)>0$，其中$D_t^\alpha$是$\alpha$阶Caputo导数，$\alpha\in(0,1)$，$\lambda,\gamma$ 是正参数。该问题的精确解$y(t)$在$t\to\infty$时表现出$O(t^{(-\alpha/\gamma)})$的衰减，但是对于这个问题的任何离散化，以前都没有相应的衰减结果的证明。在[1]中，我们证明了对一类在一致网格$\{t_n:=nh\}_{n=0}^\infty$上的保完全单调（CM-preserving）格式（包括众所周知的L1和Grünwald-Letnikov格式），离散解在$t_n\to\infty$时也表现出$O(t_n^{(-\alpha/\gamma)})$的衰减。 这一突出的新结果被推广到一些抛物型时间分数阶非线性次扩散初边值问题的CM-preserving离散，例如时间分数多孔介质和p-Laplace方程。此外，对于L1格式，在非常一般的非一致网格上也证明了离散解具有$O(t_n^{(-\alpha/\gamma)})$的衰减。

在[1]中，采用了离散比较原理进行理论分析，其中非常精细地构造了离散上解和下解以给出离散解严格的上下界。数值实验验证了理论分析的准确性。

预计在未来，在对各种数值方法得到的时间分数阶微分方程解的长时行为数值分析中，本文的创新理论将起到重要的作用。

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# HOLIMAP: AN ACCURATE AND EFFICIENT METHOD FOR SOLVING STOCHASTIC GENE NETWORK DYNAMICS

By Chen Jia#, Ramon Grima*

Gene-gene interactions are crucial to the control of sub-cellular processes but our understanding of their stochastic dynamics is hindered by the lack of simulation methods that can accurately and efficiently predict how the distributions of gene product numbers for each gene vary across parameter space. To overcome these difficulties, here we present Holimap (high-order linear-mapping approximation), an approach that approximates the protein or mRNA number distributions of a complex gene regulatory network by the distributions of a much simpler reaction system (Fig. 1) [1]. We demonstrate Holimap's computational advantages over conventional methods by applying it to predict the stochastic time-dependent dynamics of various gene networks, including transcriptional networks ranging from simple autoregulatory loops to complex randomly connected networks, post-transcriptional networks, and post-translational networks. Compared with the conventional stochastic simulation algorithm, Holimap reduces the CPU time by 70 fold, and within the same CPU time, Holimap elevates the accuracy by 3 fold. Holimap is ideally suited to study how the intricate network of gene-gene interactions results in precise coordination and control of gene expression.

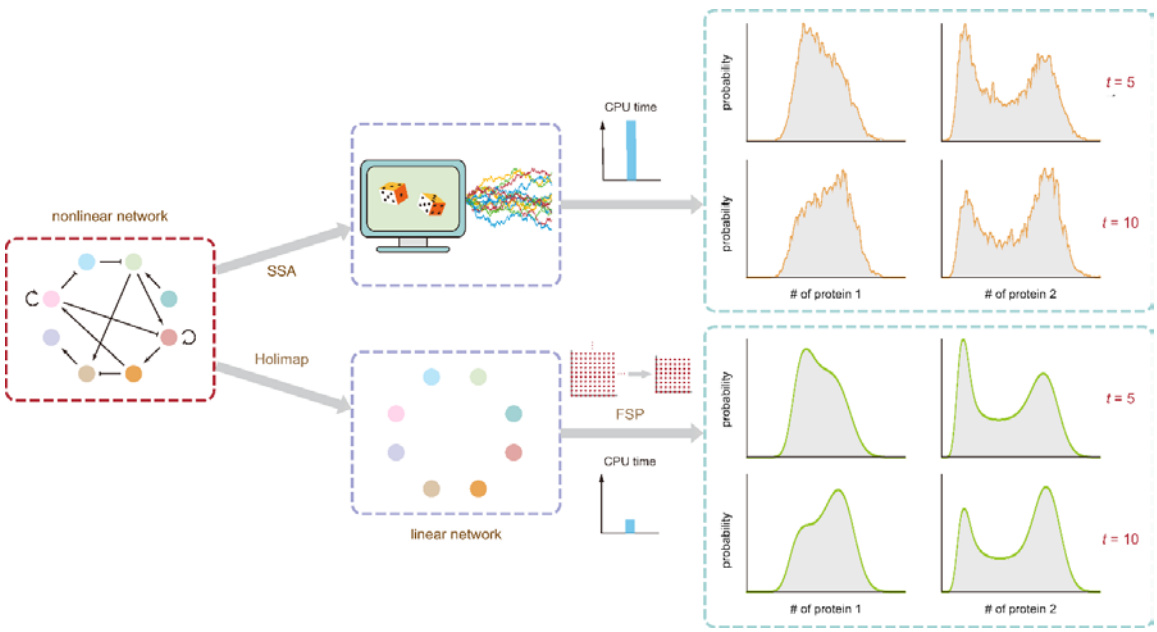


**Fig 1.** Illustration of Holimap and its advantages over the stochastic simulation algorithm (SSA). Holimap decouples gene-gene interactions in a nonlinear regulatory network and transforms it into a linear network with multiple effective parameters, some of which may be time-dependent. The time evolution of protein number distributions (for all genes) of the nonlinear network can be approximately predicted by solving the dynamics of the effective linear network using, e.g., FSP. Compared with the conventional SSA approach, Holimap not only significantly reduces the CPU time, but it also yields an accurate, noise-free prediction of the protein number distributions.

# Holimap:
# 随机基因网络动力学的高效高精度计算方法

Chen Jia#, Ramon Grima*

基因间的相互作用对于亚细胞过程的调控至关重要，但我们对于基因调控网络随机动力学的理解是不够的。这是由于我们缺乏精确地预测基因产物数量分布如何随参数变化的高效模拟方法。为了克服这些困难，在本工作中我们提出了Holimap（高阶线性映射近似）方法。该方法通过一个简单线性反应系统的分布来近似一个复杂基因调控网络的蛋白或mRNA 数量分布（图 1）[1]。我们将Holimap应用于预测各种复杂基因调控网络的随机动力学（包括转录网络、转录后网络以及翻译后网络），并证明了其相对于传统方法的计算优势。相比于传统的随机模拟算法，Holimap可以提升70倍的计算速度，在相同计算时间下可以提升3倍的计算精度。Holimap非常适合研究复杂的基因间相互作用如何实现基因表达的精准协调与控制。

◀ 图 Holimap方法及其相对于随机模拟算法的优势。Holimap将非线性调控网络中基因间的相互作用进行解耦，并将其转换为具有多个等效参数的线性网络，其中一些参数可能依赖于时间。非线性网络中蛋白数量分布的时间演化可以利用等效线性网络的动态行为来进行预测。与传统的随机模拟算法相比，Holimap不仅显著减少了CPU时间，而且还能对蛋白数量分布进行精确的预测。

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# BOOSTING ROBOTIC ARM RELIABILITY WITH ARTIFICIAL TENDONS

By Qiang Yue, Yang Ding*

Robotic arms are essential for tasks in tough and hazardous environments, but they often face challenges when a joint fails and starts swinging freely. Our team has developed an innovative solution to this problem using artificial tendons [1].

In our study, we introduced elastic strings, or artificial tendons, to help robotic arms maintain their function even when a joint fails. These tendons create the necessary force to control the failed joint, ensuring the arm can still reach most of its intended positions. Our approach has significantly increased the arm's operational area compared to traditional methods, which often rely on locking the joint in place.

Our design features retaining rings and elastic strings running along both sides of the robotic arm. These strings, fixed at both the base and the end segment, slide through the intermediate segments, allowing the arm to stay functional by controlling the failed joint through tension.

This innovative method provides more stability and a larger operational area than older techniques. It offers a promising solution for improving the reliability of robotic arms, especially in fields like medicine, space exploration, deep-sea exploration, and nuclear industries.

Our work highlights the potential of artificial tendons to make robotic arms more resilient and reliable in hazardous conditions. This research opens up new possibilities for developing advanced fault-tolerant robotic systems.

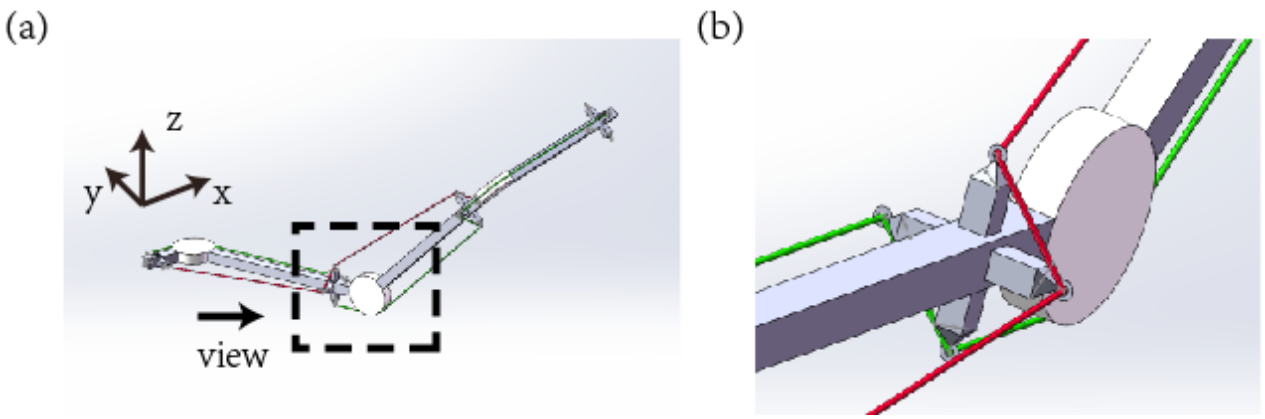


**Fig. 1.** (a) The configuration of a spatial manipulator with elastic ropes. The discs in the figure are the joints, and the first joint is on the left. The gray part is the arm, and the red and green lines on both sides of the manipulator are elastic ropes. (b) The crossed support arm holding rings where the elastic ropes pass through.

# 通过人工肌腱提高机械臂的可靠性

岳强，丁阳*

机械臂在恶劣和危险环境中的任务中起着至关重要的作用，但它们经常面临关节失效并自由摆动的挑战。我们的团队开发了一种利用人工肌腱来解决这一问题的创新解决方案[1]。

在我们的研究中，我们引入了弹性绳索或人工肌腱，以帮助机械臂即使在关节失效时也能保持功能。这些肌腱产生必要的力量来控制失效的关节，确保机械臂仍然可以到达其大部分预定位置。与通常依赖锁定关节位置的传统方法相比，我们的方法显著增加了机械臂的操作区域。我们的设计在机械臂的两侧安装了保持环和弹性绳索。这些绳索固定在基座和末端段，但可以滑过中间段，从而通过张力来控制失效的关节，保持机械臂的功能。

这种创新方法比旧技术提供了更大的稳定性和更广泛的操作区域。它为提高机械臂的可靠性提供了一个有前景的解决方案，特别是在医学、太空探索、深海探索和核工业等领域。

我们的工作展示了人工肌腱在使机械臂在恶劣条件下更具弹性和可靠性的潜力。这项研究为开发先进的容错机械系统开辟了新的可能性。

◀ 图 1： (a) 空间机械手配置有弹性绳索。图中的圆盘是关节，第一个关节在左侧。灰色部分是机械臂，机械手两侧的红线和绿线是弹性绳索。(b) 弹性绳索通过的交叉支撑臂上的保持环。

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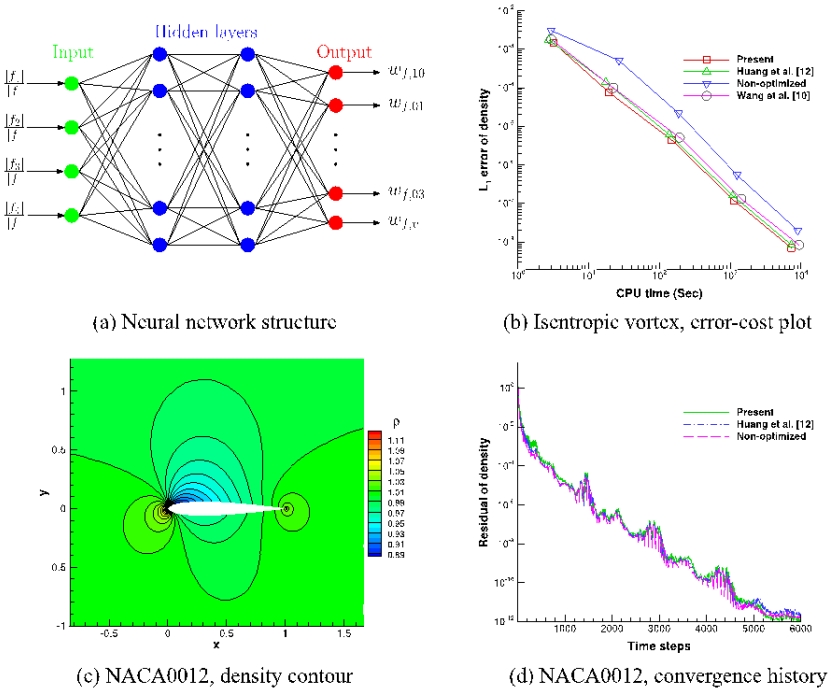
# MACHINE LEARNING OPTIMIZATION OF COMPACT FINITE VOLUME METHODS ON UNSTRUCTURED GRIDS

By Chong-Bo Zhou, Qian Wang*, Yu-Xin Ren

Fourier analysis based optimization techniques have been developed for numerical schemes on structured grids and result in significant performance improvements. However, there lacks an effective optimization technique for numerical schemes on general unstructured grids, due to the mesh geometry complexity that makes Fourier transformation infeasible. To address this issue, an optimization framework based on machine learning is developed in this paper for numerical schemes on unstructured grids [1]. The optimization of a compact high-order variational reconstruction [2] on triangular grids is performed to illustrate the framework. An artificial neural network (ANN) is used to predict the optimal values of the derivative weights on cell interfaces that are the free parameters of the variational reconstruction, given the local geometry as input. The ANN is trained by minimizing the solution errors of a linear advection equation on a set of generated compact stencils, with a set of sampled sine waves as initial conditions. The developed optimization framework is applicable to general numerical schemes on unstructured grids as the training does not require explicit computation of dispersion or dissipation. Numerical results for inviscid flow problems show that the optimized variational finite volume scheme is remarkably more accurate and efficient than its non-optimized counterpart, demonstrating the effectiveness of the machine learning optimization.




(a) Neural network structure

(b) Isentropic vortex, error-cost plot

(c) NACA0012, density contour

(d) NACA0012, convergence history

**Fig 1.** (a) ANN for prediction of optimal parameter values of the variational reconstruction; (b) Error-cost plot of the isentropic vortex problem, which demonstrates that the optimized scheme has remarkably higher efficiency than its non-optimized counterpart; (c) Computed density contour of the subsonic flow around a NACA0012 airfoil; (d) Convergence history of the NACA0012 problem, indicating that the optimized scheme has close convergence property to its non-optimized counterpart.

# 非结构网格紧致高精度有限体积方法的机器学习优化

周崇博, 王乾*, 任玉新

针对结构网格数值方法，人们已经发展了若干种基于傅里叶分析的优化方法，并取得了显著的优化效果。而对于非结构网格数值方法，由于其网格的几何复杂性，致使傅里叶分析无法进行，因此尚缺乏有效的优化方法。本文采用机器学习这一新型研究手段，克服非结构网格的几何复杂性，发展了一种适用于一般非结构网格数值方法的优化框架[1]。本文通过对非结构网格紧致高精度变分有限体积方法[2]的优化，来验证所提出的机器学习优化框架。变分有限体积方法的重构格式包含定义在网格单元交界面上的自由参数，这些参数的最优取值依赖于单元的模板几何信息。本文采用人工神经网络，根据模板几何信息，预测参数的最优取值。通过极小化线性对流方程的数值解误差，来训练神经网络。对于线性对流方程，我们生成一系列不同几何的模板作为计算域，并将一系列不同波数的正弦函数作为这些模板上的初值，形成一个训练数据集，从而可以将数据集上的数值解误差范数作为损失函数。数值测试结果表明，机器学习优化显著提升了变分有限体积方法的精度和效率，从而证明了本文所发展的机器学习优化技术的有效性。需要说明的是，本文所发展的机器学习优化技术无需理论计算格式色散或耗散误差，因而适用于一般的非结构网格数值方法。

◀ 图 1： (a) 变分重构最优参数取值预测网络; (b) 等熵涡问题的计算误差-计算时间曲线，表明机器学习优化格式的计算效率显著高于未优化格式; (c) NACA0012翼型亚声速绕流问题的密度等值线图; (d) NACA0012翼型亚声速绕流问题的收敛历史，机器学习优化格式的残差曲线和未优化格式非常接近，表明其收敛性非常接近。

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# MACHINE LEARNING ENHANCED REAL-TIME AERODYNAMIC FORCES PREDICTION BASED ON SPARSE PRESSURE SENSOR INPUTS

By Junming Duan, Qian Wang*, Jan S. Hesthaven

Accurate real-time prediction of aerodynamic forces is crucial for navigation of unmanned aerial vehicles (UAVs). This paper presents a data-driven aerodynamic force prediction model based on a small number of pressure sensors located on the surface of UAV [1]. The model is built on a linear term that can make a reasonably accurate prediction and a nonlinear correction for accuracy improvement. The linear term is based on a reduced basis reconstruction of surface pressure, with the basis extracted from simulation data and basis coefficients determined by solving linear pressure reconstruction equations at a set of optimal sensor locations, which are obtained by using the discrete empirical interpolation method (DEIM) [2]. The nonlinear term is an artificial neural network (NN) that is trained to bridge the gap between the DEIM prediction and the ground truth, especially when only low-fidelity simulation data is available. The model is tested on numerical and experimental dynamic stall data of a 2D NACA0015 airfoil [3], and numerical simulation data of dynamic stall of a 3D drone. Numerical results demonstrate that the machine learning enhanced model is accurate, efficient and robust, even for the NACA0015 case in which the simulations do not agree well with the wind tunnel experiments.

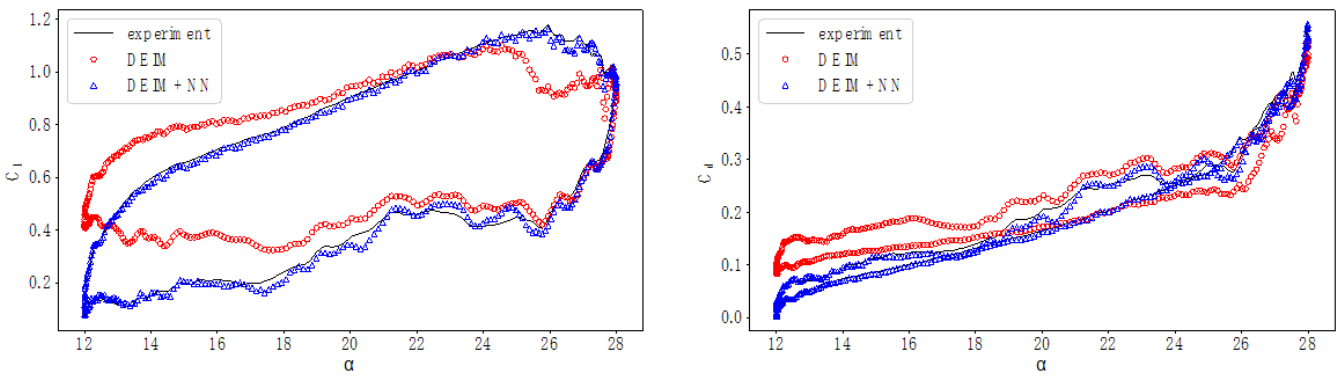


**Fig 2.** Prediction results for the dynamic stall of a NACA0015 airfoil.

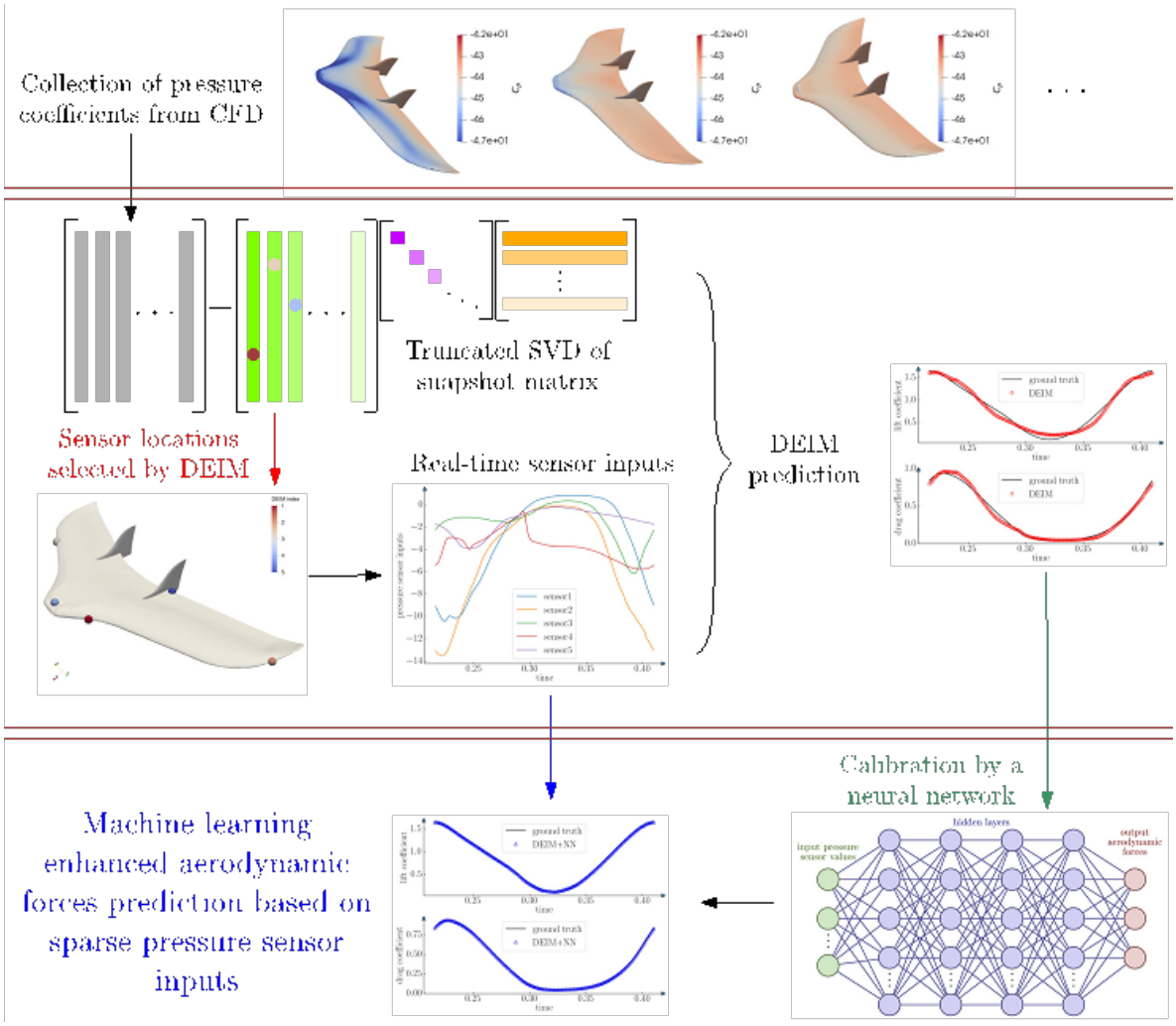


**Fig 1.** Procedures to build machine learning enhanced aerodynamic forces prediction model.

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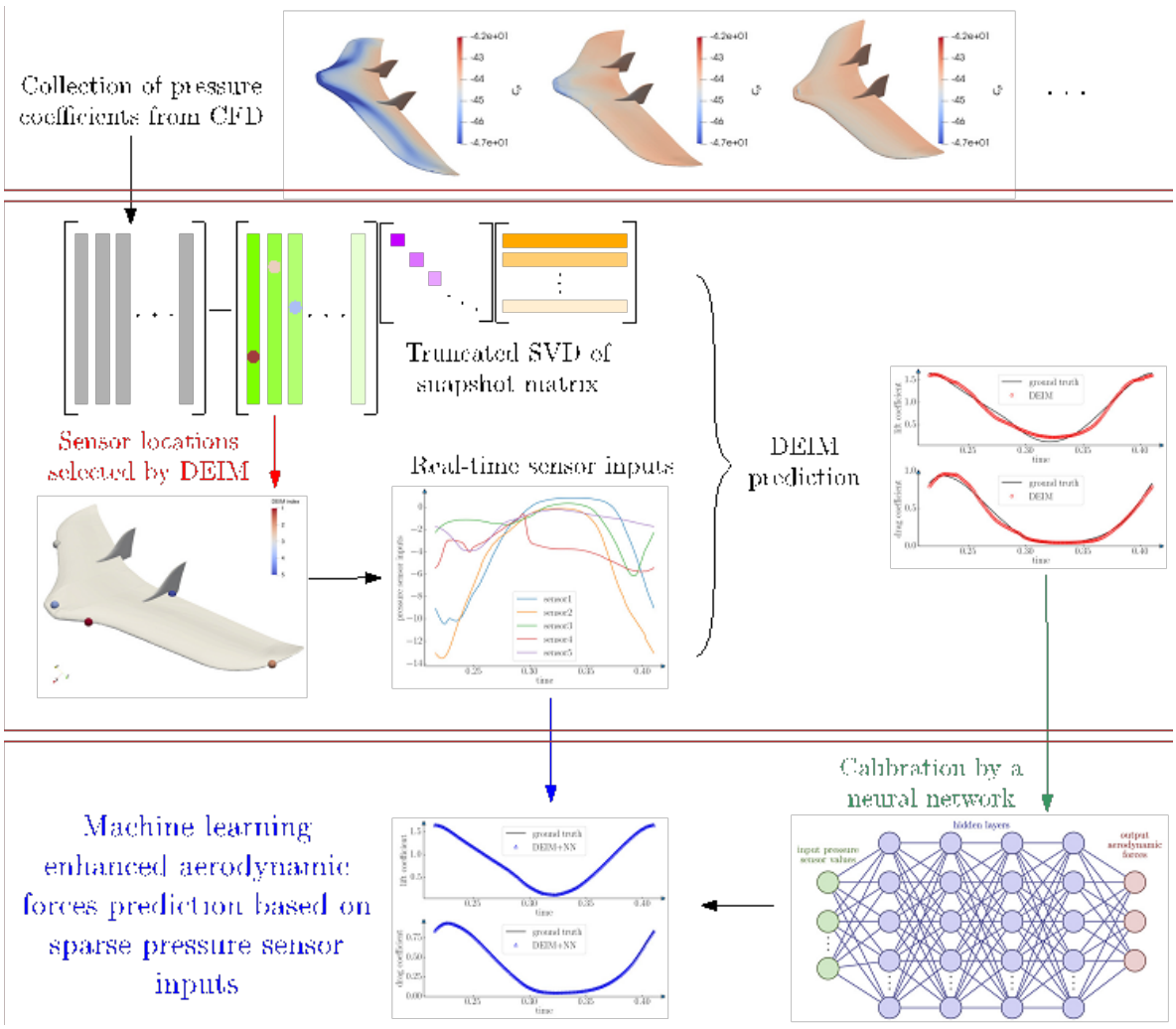


图 1 ： 基于降阶模型和机器学习的气动力模型构建流程.

# 基于降阶模型和机器学习的气动力模型

段俊明，王乾*, Jan S. Hesthaven

气动力模型可应用于无人机导航，准确高效的气动力模型是保证导航精度和可靠性的关键。本文基于降阶模型和机器学习，构造了一种能够根据飞行器表面若干压力传感器值实时计算气动力的模型[1]。这个模型包含一个线性项和一个非线性项。线性项的构造基于降阶模型方法，即构造飞行器表面压力分布的降阶模型，将压力分布表示为若干个主要模态的线性组合，模态系数根据压力传感器值来求解。压力传感器的最优位置通过DEIM算法[2]确定。非线性项是一个修正项，其作用是弥合线性项和真实气动力之间的差距，尤其是在只有低保真度数值模拟结果可用于构建降阶模型的情形。本文采用人工神经网络来作为非线性项。我们用二维NACA0015翼型动态失速的实验[3]和模拟数据，以及三维无人机的动态失速模拟数据，对本文设计的气动力模型进行验证。测试结果表明，两种工况下，气动力模型预测准确、高效，并且对传感器的扰动不敏感，即鲁棒性强。

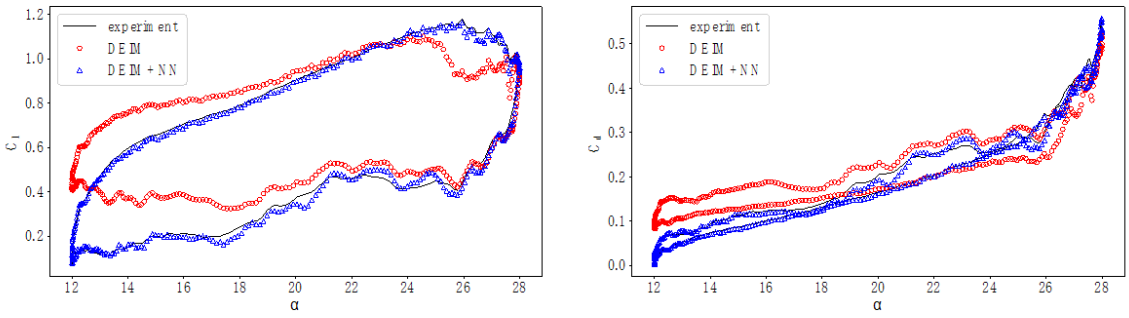


图 2：NACA0015翼型动态失速的预测结果.

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# SOLVING THE BOLTZMANN EQUATION WITH A NEURAL SPARSE REPRESENTATION

By Zhengyi Li, Yanli Wang*, Hongsheng Liu, Zidong Wang, Bin Dong

Interests in the simulating the kinetic theory has grown significantly due to its extensive applications in the engineering fields such as aerospace, plasma, and micro-electro-mechanical systems. However, solving the Boltzmann equation, one of the most critical governing equations in kinetic theory, poses significant challenges. These challenges primarily stem from the high dimensionality of the problem, which includes dimensions in time, physical space, and microscopic velocity space. Additionally, the Boltzmann equation involves complex quadratic collisions with high-dimensional integrals and singular collision kernels.

In this work, we introduce a novel ansatz, called Neural Sparse Representation (NSR), for efficiently solving the Boltzmann equation using neural networks. NSR proves to be a promising approach for both the BGK and quadratic collision models, allowing us to represent the distribution function with significantly fewer degrees of freedom compared to traditional methods. Within the NSR framework, we build networks based on the Discrete Velocity Method (DVM), with input parameters being physical position and time, and the output being the distribution function at discrete velocity points. This eliminates the need for discretization in time and space, thus reducing the degree of freedom and overcoming the curse of dimensionality. This flexibility allows us to extend the NSR method to high-dimensional problems effortlessly. To further reduce the degrees of freedom within the microscopic velocity space, we leverage the low-rank property of the distribution function. Different approximation methods are proposed for the BGK and quadratic collision models. In the BGK model, we approximate using the Canonical Polyadic Decomposition (CPD), a technique widely used in solving Partial Differential Equations (PDEs) and accelerating deep learning. For the complex quadratic collision model, we employ the BGK solution to construct a series of data-driven bases using Singular Value Decomposition (SVD) to approximate the quadratic collision terms. Furthermore, we leverage prior knowledge of the Boltzmann equation to implement multi-scale inputs by scaling time and physical space with parameters at varying magnitudes. This approach aligns with the multi-scale properties inherent in the Boltzmann equation. We also utilize the Maxwellian splitting strategy to process the distribution function, making it easier to capture the behavior of macroscopic variables. To enhance the approximation efficiency of NSR, an adaptive-weighted loss function is designed for the network. In addition to the typical PDE residual loss found in most loss functions, we include a loss term related to macroscopic variables, aligning with the properties of the Boltzmann equation, such as the requirement that the density of the PDE residual should be zero. Moreover, we account for the varying contribution of different microscopic velocity points by adding adaptive weights to the errors associated with each velocity point. These techniques collectively accelerate the process and improve the overall approximation efficiency of NSR.

The effectiveness of the proposed neural network-based methods is validated through a series of numerical experiments. These experiments encompass one-dimensional problems, including cases with both continuous and discontinuous initial conditions, as well as a two-dimensional wave problem.

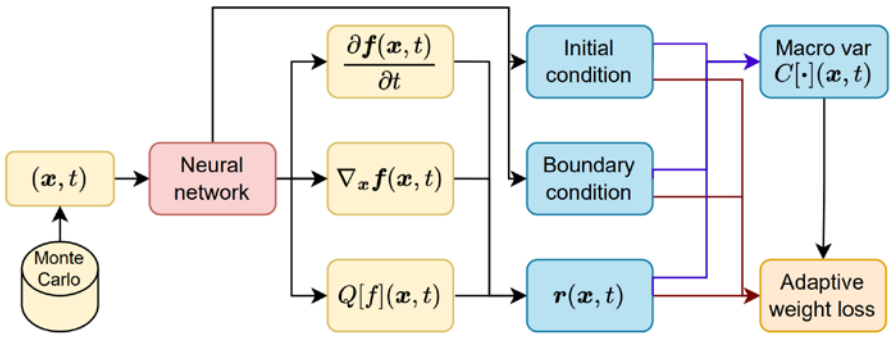


**Fig 1.** Network structure

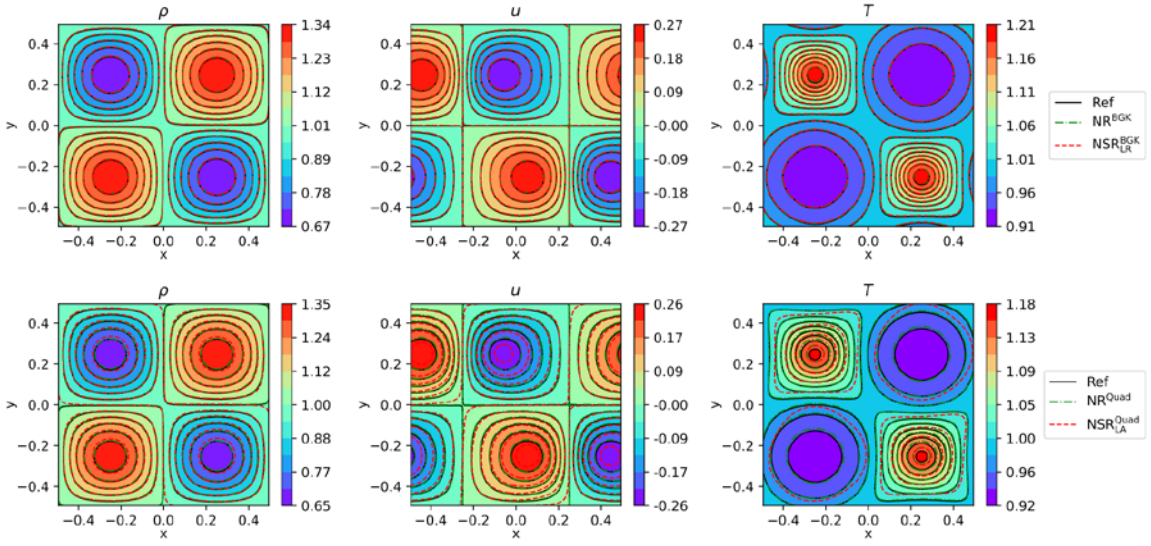


**Fig 2.** The numerical solution of the NR/NSR method for Kn = 0.01 at t = 0.1, The top row displays the solution for the BGK model, and the bottom row represents the solution for the quadratic model.

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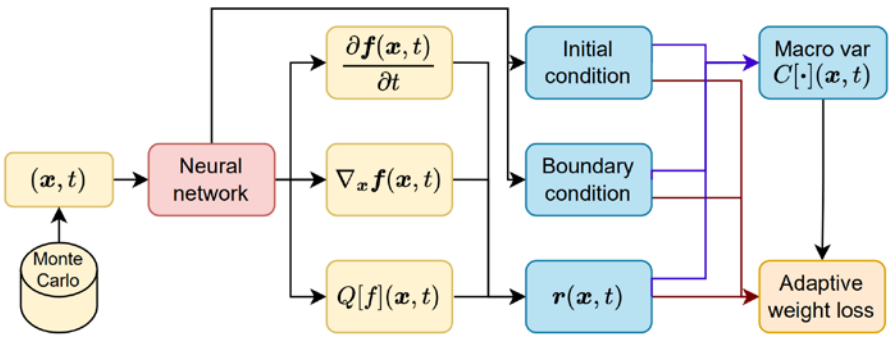


图 1：网络结构

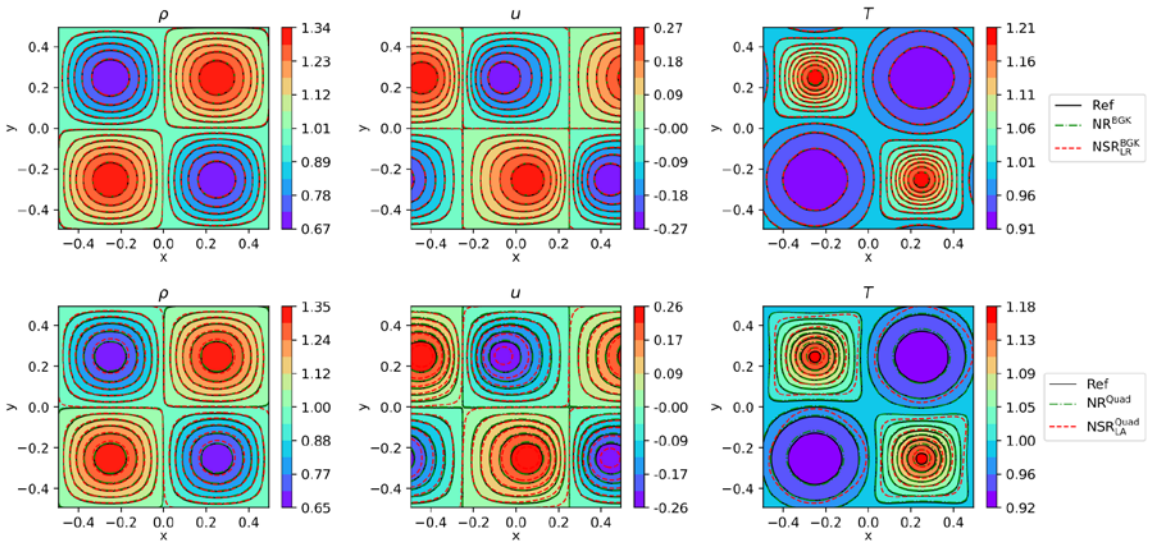


图 2：使用 NR/NSR方法求解Boltzmann方程的数值解图像。
第一行为BGK方程结果，第二行为二元碰撞模型的结果。

# 求解玻尔兹曼方程的稀疏表达方法

李正一，王艳莉*，刘洪生，王子东，董彬

由于动理学在在航空航天、等离子体和微电机电系统等工程领域中的广泛应用，人们对动理学理论模拟的兴趣显著增长。然而，玻尔兹曼方程作为动理学理论中最重要的控制方程之一，其数值模拟面临显著的挑战。这些挑战主要源于问题的高维度，包括时间、物理空间和微观速度空间的维度。此外，玻尔兹曼方程涉的复杂二元碰撞模型涉及高维积分和奇异碰撞核等，使得数值模拟更加充满挑战。

在该项工作中，我们引入了一种新颖的假设，称为神经稀疏表示（Neural Sparse Representation, NSR），通过神经网络高效地数值求解玻尔兹曼方程。数值实验表明该方法对BGK模型和二次碰撞模型都是一种有前途的方法，它使我们能够用比传统方法显著更少的自由度来表示分布函数。在NSR框架下，我们基于离散速度方法 （Discrete Velocity Method, DVM）构建网络，输入参数为物理位置和时间，输出参数为离散速度点处的分布函数。该操作大幅减少了自由度并克服了维度灾难。这种灵活性使我们将NSR方法毫不费力地扩展到高维问题。为了进一步减少微观速度空间中的自由度，我们利用分布函数的低秩特性，并对BGK模型和二次碰撞模型，提出了不同的近似方法。在BGK模型中，我们使用典型的多项式分解（Canonical Polyadic Decomposition, CPD）进行近似。对于复杂的二次碰撞模型，我们采用BGK模型的数值解构建一系列基于数据驱动的基函数，通过奇异值分解（Singular Value Decomposition, SVD）来近似二次碰撞项。此外，我们利用玻尔兹曼方程的先验知识，通过对时间和物理空间进行不同量级的参数缩放来实现多尺度输入，并利用麦克斯韦分裂策略处理分布函数，从而更容易捕捉宏观变量信息。此外，我们考虑了不同微观速度点对误差的不同贡献，对每个速度点上的误差添加自适应权重。这些技术共同提高了NSR 的整体近似效率。

通过一系列数值实验验证了所提出的基于神经网络的方法的有效性。这些数值模拟实验包括一维问题，包括连续和不连续初始条件的情况，以及二维波动问题。

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| 7 | Liu, Chang; Li, Weiming; **Wang, Yanli**; Song, Peng; Xu, Kun, An implicit unified gas-kinetic wave-particle method for radiative transport process, Phys. Fluids, NOV, 2023, 35, 11, 112013. |
| 8 | Ye, Yong-Jin; Han, Ying; Liu, Yang; **Guo, Zhen-Lin**; Huang, Ming-Wei, Utilizing deep learning for automated detection of oral lesions: A multicenter study, Oral Oncol., AUG, 2024, 155, 106873. |
| 9 | Lihua Shao , **Zhenlin Guo** and Yanxiao Sun; A linear mass and energy conserving numerical scheme for two-phase flows with thermocapillary effects, International Journal of Modern Physics C (IJMPC), 2024, 35, 03, 10.1142/S0129183124500359. |
| 10 | Rashid Alavi, **Qian Wang**, Hossein Gorji, and Niema M. Pahlevan. A machine learning approach for computation of cardiovascular intrinsic frequencies." Plos one 18.10 (2023): e0285228. |

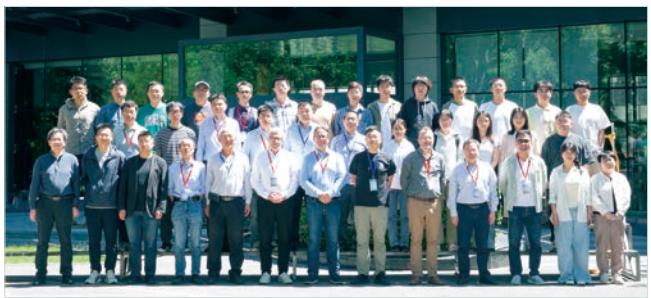
## ALGORITHMS DIVISION 计算方法研究部

| | |
|---|---|
| 1 | **Chen, Lizhen**; Ma, Ying; Ren, Bo; Zhang, Guohui, Numerical Approximations of Diblock Copolymer Model Using a Modified Leapfrog Time-Marching Scheme, Computation, NOV, 2023, 11, 11 , 215. |
| 2 | Saranya, Govindarajan; Bandaru, Sateesh; **Shen, Kangqi**; Jayabal, Subramaniam; Chen, Mingyang, Theoretical Designing of Atomically Precise MgO/$TiO_2$(001) Quantum Dot-Sensitized Solar Cell for High Visible Light Absorption and Fast Charge Injection, J. Phys. Chem. C, JAN 12, 2024, 128, 3, 1222, 1229. |
| 3 | **Dong, Shenghao**; Sarwono, Yanoar Pribadi; Zhang, Rui-Qin, An efficient finite difference approach to solutions of Schrödinger equations of atoms in non-linear coordinates, Phys. Scr., DEC 1, 2023, 98, 12, 125409. |

# WORKSHOPS & CONFERENCES
## (2023-2024) 中心主办、合办的学术会议

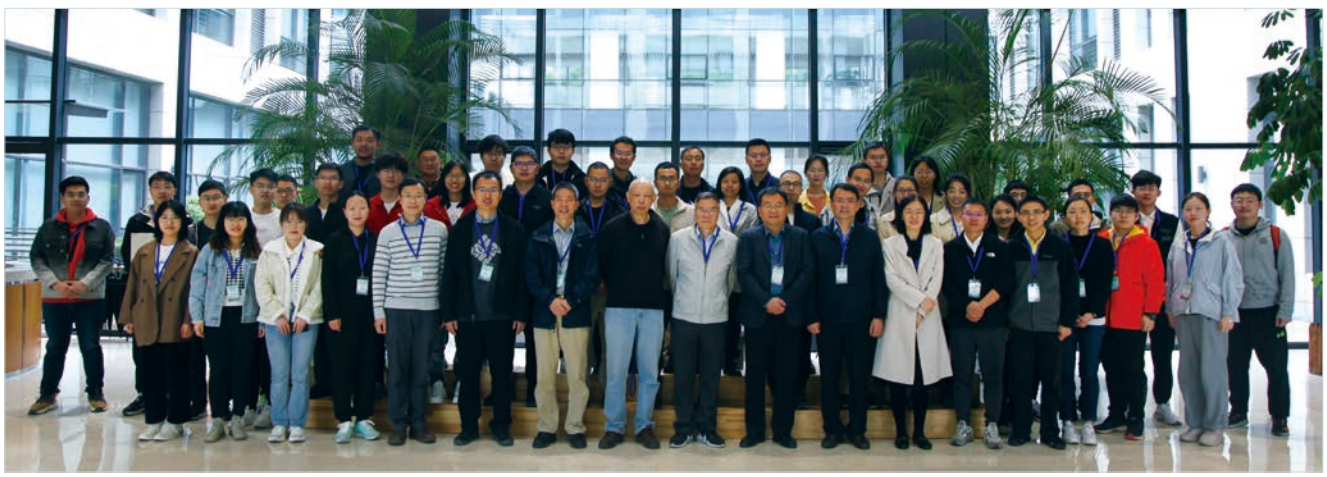
| 时间 Date | 会议名称 Title |
|---|---|
| 2024.7.15 - 19 | ² International Conference on Scientific Computation and Differential Equations<br>科学计算与微分方程国际会议 |
| 2024.7.8 - 11 | 8th Conference on Numerical Methods for Fractional-derivative Problems<br>第八届分数导数问题数值方法会议 |
| 2024.5.15 - 16 | International (CECAM-CN) Workshop on Excited States and Dynamics in Condensed Phases<br>凝聚相激发态和动力学国际（CECAM-CN）研讨会 |
| 2024.4.22 - 26 | Active Matter: Interfaces and Boundaries<br>“活性物质：界面和边界"研讨会 |
| 2024.4.10 - 11 | 科学计算前沿论坛<br>Scientific Computing Frontier Forum |
| 2023.10.27 - 29 | 建模与模拟前沿论坛<br>Frontier Forum on Modeling and Simulation |
| 2023.12.14 - 16 | Workshop on Radiation Detection Technology and New Detector Materials<br>辐射探测技术与探测器新材料研讨会 |
| 2023.8.14 - 16 | 第三届量子场论及其应用研讨会<br>3rd Workshop on Quantum Field Theory and Applications |

第八届分数导数问题数值方法会议
8th Conference on Numerical Methods for Fractional-derivative Problems



凝聚相激发态和动力学国际（CECAM-CN）研讨会
International (CECAM-CN) Workshop on Excited States and Dynamics in Condensed Phases

原子量子精密测量培训班

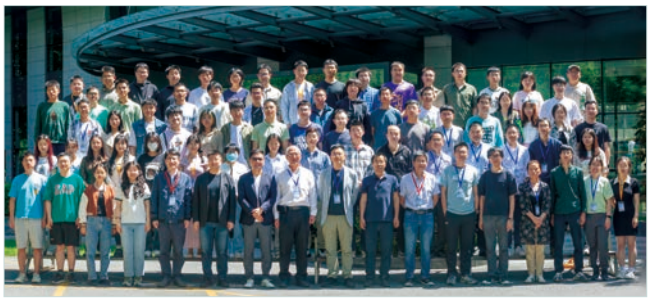


建模与模拟前沿论坛
Frontier Forum on Modeling and Simulation

建模与模拟前沿论坛
Frontier Forum on Modeling and Simulation

辐射探测技术与探测器新材料研讨会
Workshop on Radiation Detection Technology and New Detector Materials

激光惯性约束聚变应用基础及前沿物理研修班



“材料与能源前沿科学：强外场下的结构和物态调控”培训班

非厄米物理及其在精密测量中的应用培训班

第三届量子场论及其应用研讨会

3rd Workshop on Quantum Field Theory and Applications

“活性物质：界面和边界"研讨会
Active Matter: Interfaces and Boundaries

# TUTORIALS (2023-2024) 培训班

| 时间 Date | 会议名称 Title |
|---|---|
| 2024.6.12-14 | 量子磁性与多体计算培训班 |
| 2024.5.13-14 | “材料和能源科学前沿：激发态动力”培训班 |
| 2024.4.26-28 | 非厄米物理及其在精密测量中的应用培训班 |
| 2024.4.22-23 | “活性物质：界面与边界”培训班 |
| 2023.11.29-12.1 | 量子开放系统理论培训班 |
| 2023.10.25-27 | “材料与能源前沿科学：强外场下的结构和物态调控”培训班 |
| 2023.9.15-17 | 激光惯性约束聚变应用基础及前沿物理研修班 |
| 2023.8.23-26 | 原子量子精密测量培训班 |

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# CSRC SEMINAR 专题报告

中心积极邀请国内外相关领域重要学者举行专题报告，活跃学术氛围，激发学术思维。2023-2024学术年期间中心共举办专题讲座68期（总1295期）。

CSRC invites national and overseas leading researchers to give academic seminars. During academic year 2023-2024, CSRC has already held 68 seminars.

| DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|
| 2023-8-30 | 王其星<br>Qi-Xing Wang | 厦门大学<br>Xiamen University | 二维材料中的能量上转化及应用 |
| 2023-8-30 | 王中长<br>Zhong-Chang Wang | 国际伊比利亚纳米技术实验室<br>International Iberian Nanotechnology Laboratory (INL) | Atomic-Scale Analysis and Dynamic Observation of 2D Layered Materials |
| 2023-9-7 | 颜子翔<br>Zi-Xiang Yan | 北京邮电大学<br>Beijing University of Posts and Telecommunications | 社会传播现象的动力学研究简介 |
| 2023-9-11 | 张　科<br>Ke Zhang | 德国联邦物理技术研究院<br>Physikalisch-Technische Bundesanstalt, Germany | Th-229核光钟的研究进展 |
| 2023-9-12 | 黄政宇<br>Zheng-Yu Huang | 北京国际数学研究中心<br>Beijing International Center for Mathematics Research | Modeling and Simulation of the Inflation of Supersonic Parachutes for Mars Landing |
| 2023-9-14 | 张桦森<br>Hua-Sen Zhang | 北京应用物理与计算数学研究所<br>Institute of Applied Physics and Computational Mathematics | 高能量密度下的流体不稳定性研究 |
| 2023-9-15 | Stefan BlügelStefan Blügel | Peter Grünberg Institute and Institute for Advanced Simulation (Germany) Peter Grünberg Institute and Institute for Advanced Simulation (Germany) | Recent Progress of the Full-Potential Linearized Augmented Plane-Wave (FLAPW) Method |
| 2023-9-25 | 刘茂省<br>Mao-Xing Liu | 北京建筑大学<br>Beijing University of Civil Engineering&Architecture | Dynamical Analysis of The Infectious Disease Based on Scale-Free Networks and Higher-Order Networks |
| 2023-10-12 | 徐　宁<br>Ning Xu | 中国科学技术大学<br>University of Science and Technology of China | 非晶固体的负载不稳定性 |

# CSRC SEMINAR 专题报告

| DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|
| 2023-10-13 | 付敬原<br>Jing-Yuan Fu | 北京应用物理与计算数学研究所<br>Institute of Applied Physics and Computational Mathematics | 高能量密度下Rayleigh-Taylor不稳定性尖钉和气泡混合宽度的非线性演化研究 |
| 2023-10-16 | 陈　娜<br>Na Chen | 清华大学<br>Tsinghua University | 源于非晶合金的新型非晶材料 |
| 2023-10-18 | 张又升<br>You-Sheng Zhang | 北京应用物理与计算数学研究所<br>Institute of Applied Physics and Computational Mathematics | 界面不稳定性及其湍流混合研究进展 |
| 2023-10-18 | 詹　翔<br>Xiang Zhan | 南京理工大学<br>Nanjing University of Science and Technology | 量子互文性的测量、诠释与应用 |
| 2023-10-20 | 张文清<br>Wen-Qing Zhang | 南方科技大学<br>Southern University of Science and Technology | Modeling Complex Materials with Chemical Bond Hierarchy: A Machine-Learning Interatomic Potential Approach |
| 2023-10-24 | 杨　硕<br>Shuo Yang | 清华大学<br>Tsinghua University | Non-Hermitian Parent Hamiltonian and Composite Quantum Phases |
| 2023-10-24 | 边志浩<br>Zhi-Hao Bian | 江南大学<br>Jiangnan University | 线性光学体系中高维宇称时间对称的量子信息动力学模拟和守恒量的观测 |
| 2023-10-24 | 王坤坤<br>Kun-Kun Wang | 安徽大学<br>Anhui University | 实验模拟非厄米系统中的高阶奇异点 |
| 2023-11-3 | Iannis Kominis<br>Iannis Kominis | 希腊克里特理工大学<br>University of Crete (Greece) | The Scientific and Technological Promise of Quantum Biology |
| 2023-11-21 | Abolfazl BayatAbolfazl Bayat | 电子科技大学<br>University of Electronic Science and Technology of China | Quantum Many-Body Probes |
| 2023-11-27 | 郑　文<br>Wen Zheng | 太原理工大学<br>Taiyuan University of Technology | 基于下一代人工智能的非晶固体结构特征研究 |
| 2023-11-28 | 倪　冉<br>Ran Ni | 新加坡南洋理工大学<br>Nanyang Technological University (Singapore) | Stable and Metastable Non-equilibrium Hyperuniform Fluids |

| DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|
| 2023-11-30 | 郎兴友<br>Xing-You Lang | 吉林大学<br>Jilin University | 纳米多孔金属间化合物水分解电催化材料 |
| 2023-12-4 | 王　评<br>Ping Wang | 北京师范大学珠海校区<br>Beijing Normal University at Zhuhai | 时序关联表征方法的应用 |
| 2023-12-8 | Giovanni RussoGiovanni Russo | 意大利卡塔尼亚大学<br>University of Catania (Italy) | Weakly Non-Linear Shallow Water Equations Over Periodic Bathymetry |
| 2023-12-8 | Francis FilbetFrancis Filbet | 法国图卢兹第三大学<br>Université Toulouse III - Paul Sabatier | On the Convergence of Discontinuous Galerkin/Hermite Spectral Methods for the Vlasov-Poisson System |
| 2023-12-11 | 张春一<br>Chui-Yi Zhang | 美国普林斯顿大学<br>Princeton University (USA) | 从原子尺度理解水、溶液以及固液界面: 机器学习驱动的第一性原理分子动力学模拟 |
| 2023-12-15 | 蔡　子<br>Zi Cai | 上海交通大学<br>Shanghai Jiaotong University | Fractal Quantum Matters |
| 2023-12-25 | 张永亮<br>Yong-Liang Zhang | 中科院半导体所<br>Institute of Semiconductors (CAS) | 光学连续介质的几何理论 |
| 2023-12-30 | 祁　宏<br>Hong Qi | 山西大学复杂系统研究所<br>Complex Systems Research Center, Shanxi University | 正反馈与双稳态 |
| 2024-1-4 | 马　恩<br>Evan Ma | 西安交通大学<br>Xi'an Jiaotong University | 如何写好科学论文 |
| 2024-1-18 | 王利近<br>Li-Jin Wang | 安徽大学<br>Anhui University | 玻璃低频过剩模式态密度研究 |
| 2024-1-26 | 杜金锦<br>Jin-Jin Du | 沖縄科学技術大学院大学<br>Okinawa Institute of Science and Technology Graduate University (Japan) | Fast Single-Shot Imaging of Individual Impurities in Cold Atomic Gas |
| 2024-3-11 | 边志浩<br>Zhi-Hao Bian | 江南大学<br>Jiangnan University | 基于fine-grained不确定关系的量子导引对两体纠缠纯态的self-test的实验验证 |

# CSRC SEMINAR 专题报告

| DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|
| 2024-3-12 | 詹　翔<br>Xiang Zhan | 南京理工大学<br>Nanjing University of Science and Technology | 一维量子行走中拓扑边界态的局域开关 |
| 2024-3-15 | 陈　立<br>Li Chen | 山西大学<br>Shanxi University | Imaginary-Temperature Zeros for Quantum Phase Transitions |
| 2024-3-18 | 易　为<br>Wei Yi | 中国科学技术大学<br>University of Science and Technology of China | Quantum Stochastic Resonance in a Dissipative Rydberg Gas |
| 2024-3-19 | 袁璐琦<br>Lu-Qi Yuan | 上海交通大学<br>Shanghai Jiaotong University | 合成频率维度原理以及其中的光物理现象 |
| 2024-3-26 | 许振朋<br>Zhen-Peng Xu | 安徽大学<br>Anhui University | Quantum Network-Entanglement: Detection, Measures and Applications |
| 2024-3-27 | 刘永椿<br>Yong-Chun Liu | 清华大学<br>Tsinghua University | 基于非厄米原子系综的精密测量 |
| 2024-3-28 | 刘金明<br>Jin-Ming Liu | 华东师范大学<br>East China Normal University | 优化控制场作用下基于极性分子的量子信息处理 |
| 2024-4-1 | 何杨辉<br>Yang-Hui He | 伦敦数学科学研究所<br>The London Institute for Mathematical Sciences | The AI Mathematician |
| 2024-4-2 | 王书林<br>Shu-Lin Wang | 华中科技大学<br>Huazhong University of Science and Technology | 合成时域光子晶格中的等效电场调控 |
| 2024-4-2 | 秦承志<br>Cheng-Zhi Qin | 华中科技大学<br>Huazhong University of Science and Technology | 合成维度光子规范势及其光场调控 |
| 2024-4-7 | 伏吉庆<br>Ji-Qing Fu | 中国计量科学研究院<br>The National Institute of Metrology (China) | 磁感应强度量值的复现和计量技术 |
| 2024-4-9 | 何凌冰<br>Ling-Bing He | 清华大学<br>Tsinghua University | Global-in-time Stability of the Non-negativity Property in the Spatially Homogeneous Landau Equation with Soft Potentials |

| DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|
| 2024-4-9 | 王振富<br>Zhen-Fu Wang | 北京国际数学研究中心<br>Beijing International Center for Mathematical Research | Entropic Propagation of Chaos for 2D Viscous Vortex Model |
| 2024-4-17 | 罗会仟<br>Hui-Qian Luo | 中国科学院物理研究所<br>Institute of Physics (CAS) | 超导材料探索启示——炒菜、调味、搭积木与原子智造 |
| 2024-4-17 | 尹璋琦<br>Zhang-Qi Yin | 北京理工大学<br>Beijing Institute of Technology | 迈向多体的悬浮光力学 |
| 2024-4-17 | 贾凤东<br>Feng-Dong Jia | 中国科学院大学<br>University of Chinese Academy of Sciences | 辅助微波场修饰增强的里德堡原子微波电场计 |
| 2024-4-19 | 尚江伟<br>Jiang-Wei Shang | 北京理工大学<br>Beijing Institute of Technology | Estimating Many Properties of a Quantum State via Quantum Reservoir Processing |
| 2024-4-19 | 徐大智<br>Da-Zhi Xu | 北京理工大学<br>Beijing Institute of Technology | 基于压缩感知技术的量子系统时变动力学参数测量 |
| 2024-4-25 | 尚　策<br>Ce Shang | 中国科学院空天信息创新研究院<br>Aerospace Information Research Institute (CAS) | 实投射平面中倒易空间和实空间中的拓扑物理 |
| 2024-4-30 | 李纪伟<br>Ji-Wei Li | 北京应用物理与计算数学研究所<br>Institute of Applied Physics and Computational Mathematics | 激光惯性约束聚变混合驱动点火物理 |
| 2024-5-8 | 黄瑞珍<br>Rui-Zhen Huang | 根特大学<br>Ghent University (Belgium) | Symmetric Deformation and Finite Entanglement Scaling |
| 2024-5-17 | 马万彪<br>Wan-Biao Ma | 北京科技大学<br>University of Science and Technology Beijing | 一类刻画微生物连续培养与絮凝/收集问题的时滞微分方程模型的全局动力学 |
| 2024-5-22 | 万　林<br>Lin Wan | 中国科学院数学与系统科学研究院<br>Academy of Mathematics and Systems Science (CAS) | 最优传输框架下的生物复杂数据的建模与计算 |

# CSRC SEMINAR 专题报告

| DATE\日期 | SPEAKER\报告人 | INSITUTE\单位 | TITLE/报告题目 |
|---|---|---|---|
| 2024-5-26 | 周正威<br>Zheng-Wei Zhou | 中国科学技术大学<br>University of Science and Technology of China | 在量子主方程中的非厄米性与拓扑稳定性 |
| 2024-5-26 | 周志远<br>Zhi-Yuan Zhou | 中国科学技术大学<br>University of Science and Technology of China | 量子非线性光场调控研究进展 |
| 2024-6-6 | 邱建贤<br>Jian-Xian Qiu | 厦门大学<br>Xiamen University | High Order Finite Volume Method for Solving Compressible Multicomponent Flows |
| 2024-6-14 | 冯万祥<br>Wan-Xiang Feng | 北京理工大学<br>Beijing Institute of Technology | 磁性拓扑材料非常规反常输运性质的第一性原理研究 |
| 2024-6-14 | 路翠翠<br>Cui-Cui Lu | 北京理工大学<br>Beijing Institute of Technology | 基于合成维度和人工规范场的拓扑物理及器件应用 |
| 2024-6-26 | 薛晓峰<br>Xiao-Feng Xue | 北京交通大学<br>Beijing Jiaotong University | A Survey of Limit Theorems of the Tagged Particle in the SSEP |
| 2024-6-26 | 彭志超<br>Zhi-Chao Peng | 香港科技大学<br>The Hong Kong University of Science and Technology | A Reduced Order Model Enhanced Iterative Solver for Parametric Radiative Transfer Equation |
| 2024-7-10 | Pedro RibeiroPedro Ribeiro | 葡萄牙里斯本大学<br>University of Lisbon (Portugal) | Universal Features of Quantum Dissipative Dynamics |
| 2024-7-10 | 罗明星<br>Ming-Xing Luo | 西安交通大学<br>Southwest Jiaotong University | Quantumness of Energy-Storing Quantum Systems |
| 2024-7-16 | 高　畅<br>Chang Gao | 武汉理工大学<br>Wuhan University of Technology | 典型温稠密物质状态方程的第一性原理研究 |
| 2024-7-19 | 张　续<br>Xu Zhang | 美国加州州立大学北岭分校<br>California State University, Northridge (USA) | First-Principles Study of Excitons and Their Dynamics in 2D Materials |
| 2024-7-26 | 邵　磊<br>Lei Shao | 中山大学<br>Sun Yat-sen University | Photoluminescence Modulation of 2D Semiconductors by Plasmonic Metal Nanostructures |

# 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。

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Since its establishment, more than 5000 visiting scholars from over 20 countries and regions have visited CSRC. CSRC faculty members went out for academic eschange for more than 2000 times. During the academic year 2023-2024, 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。2023-2024学术年期间，中心接待来访学者超过200人次。

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

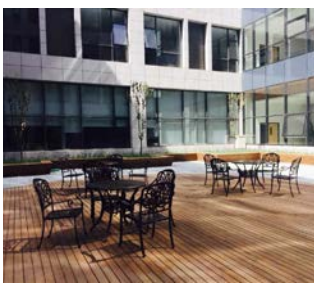
To facilitate scientific interactions between CSRC scientists and scientists elsewhere, CSRC has developed partnerships with several universities and research institutions around the world. Besides engaging in long-term scientific collaborations, CSRC staff also host conferences, workshops, and seminars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

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

〖 中心办公楼效果图 〗 CSRC building

〖 大厅 〗 Lobby

〖 中庭院 〗 Courtyard



〖 学术报告厅 〗 Auditorium

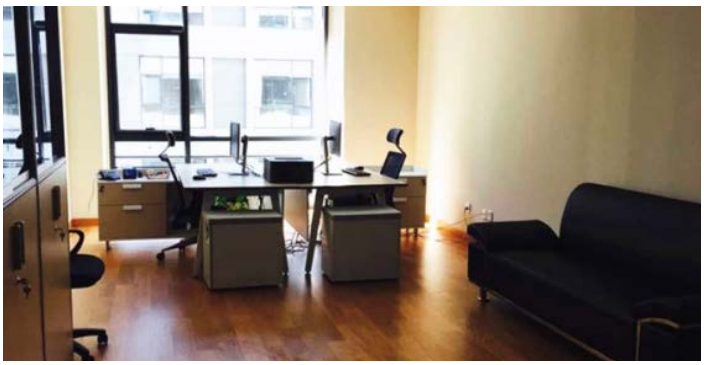
Seminar Rom 〖 学术会议室 〗

Common 〖 学术讨论区 〗


ZPark 〖 中关村软件园一二期鸟瞰图 〗

〖 博士后办公室 〗 Postdoc Office

Visitor Office 〖 客座教授办公室 〗



〖 访问学者办公室 〗 Visitor Office

# 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