Electron fluctuation and superconducting mechanism in 3R-WS2 based on first-principles calculation

Yu Wang
Niigata University

Recently, superconductivity has been discovered in WS_2, which exhibits the highest superconducting transition temperature among transition-metal dichalcogenides, T_c = 8.8 K [1], and has also attracted attention as a candidate topological superconductor [2,3]. In the low-pressure 2M-WS_2 phase, Tc decreases with increasing pressure to 3.5 K at 18 GPa, above which superconductivity disappears, whereas the high-pressure 3R-WS_2 phase shows superconductivity with T_c~2.5 K almost independent of pressure up to 65GPa [4]. In our previous work, we have studied the electronic and phonon states of WS_2 based on the first-principles calculations (Quantum ESPRESSO) and examined the pressure dependence of Tc using the McMillan equation [5]. In 2M-WS_2, it has been found that Tc decreases with increasing pressure as observed in the experiments although the values of Tc are about 1/3~1/6 of the experimental values [5]. On the other hand, Tc is estimated to be zero independent of pressure in 3R-WS_2[5], where the conventional BCS phonon mechanism is considered to fail to account for the superconductivity.

As shown in Fig. 1 (left), the Fermi surface of 3R-WS_2 obtained from the first-principles calculations (WIEN2k) exhibits nesting between the hole pocket at the G point and the six electron pockets located near the midpoint between G and S. Based on the effective 11-band d-p model derived by the maximally-localised Wannier functions, we calculate the bare susceptibilities which show peaks around the H-L and S-F points corresponding to the nesting vector as shown in Fig. 1 (right). Taking into account the Coulomb and the electron-phonon interactions within the random phase approximation (RPA), a possible superconductivity mediated by spin/charge and orbital fluctuations is discussed.

*Numerical calculations were performed using Research Center for Computational Science, Okazaki, Japan (Project: 24-IMS-C315).

[1] Y. Fang et al., Adv. Mater. 31, 1901942 (2019)
[2] Y. Yuan et al., Nature Physics 15, 1046 (2019)
[3] Y. W. Li et al., Nature Communications 12, 2874 (2021)
[4] W. Zhang et al., J. Phys. Chem. Lett. 12, 3321 (2021)
[5] Y. Wang, T. Sekikawa, K. Sano and Y. Ōno, The 24th Asian Workshop on First-Principles Electronic Structure Calculations, Oct. 30-Nov. 1, 2023, Fudan University, Shanghai, China

Hydrodynamic modes and operator spreading in a long-range center-of-mass-conserving Brownian SYK model

Bai-Lin Cheng
Peking University

We study a center-of-mass-conserving Brownian complex Sachdev-Ye-Kitaev model with long-range (power-law) interactions characterized by $1/r^\eta$. The kinetic constraint and long-range interactions conspire to yield rich hydrodynamics associated with the conserved charge, which we reveal by computing the Schwinger-Keldysh effective action. Our result shows that charge transport in this system can be subdiffusive, diffusive, or superdiffusive, with the dynamical exponent controlled by η. We further employ a doubled Hilbert space methodology to derive an effective action for the out-of-time-ordered correlator (OTOC), from which we obtain the phase diagram delineating regimes where the lightcone is linear or logarithmic. Our results provide a concrete example of a quantum many-body system with kinetic constraint and long-range interactions in which the emergent hydrodynamic modes and OTOC can be computed analytically.

Quantum Griffiths singularity in a three-dimensional superconductor to insulator transition

Yi Liu
Renmin University of China

Disorder is ubiquitous in real materials and can have dramatic effects on quantum phase transitions. Originating from the disorder enhanced quantum fluctuation, quantum Griffiths singularity (QGS) has been revealed as a universal phenomenon in quantum criticality of low-dimensional superconductors [1-3]. However, due to the weak fluctuation effect, QGS is very challenging to detect experimentally in three-dimensional(3D) superconducting systems. Here we report the discovery of QGS associated with the quantum phase transition from 3D superconductor to Anderson critical insulator in a spinel oxide $MgTi_2O_4$ (MTO) [4]. Under both perpendicular and parallel magnetic field, the dynamical critical exponent diverges when approaching the quantum critical point, demonstrating the existence of 3D QGS. Among 3D superconductors, MTO shows a relatively strong fluctuation effect featured as a wide superconducting transition region. The enhanced fluctuation, which may arise from the mobility edge of Anderson localization, finally leads to the occurrence of 3D quantum phase transition and QGS. Our findings offer a new perspective to understand quantum phase transitions in strongly disordered 3D systems.

References

[1] Yi Liu#, Ziqiao Wang#, Pujia Shan, Yue Tang, Chaofei Liu, Cheng Chen, Ying Xing, Qingyan Wang, Haiwen Liu*, Xi Lin, X. C. Xie and Jian Wang*, Anomalous quantum Griffiths singularity in ultrathin crystalline lead films, Nature Communications 10, 3633 (2019)

[2] Yi Liu#, Shichao Qi#, Jingchao Fang, Jian Sun, Chong Liu, Yanzhao Liu, Junjie Qi, Ying Xing, Haiwen Liu*, Xi Lin, Lili Wang, Qi-Kun Xue, X.C. Xie and Jian Wang*, Observation of in-plane quantum Griffiths singularity in two-dimensional crystalline superconductors, Physical Review Letters 127, 137001 (2021)

[3] Ziqiao Wang#, Yi Liu#, Chengcheng Ji and Jian Wang*, Quantum phase transitions in two-dimensional superconductors: 37a review on recent experimental progress, Reports on Progress in Physics 87, 014502 (2024)

[4] Shichao Qi#, Yi Liu#, Ziqiao Wang#, Fucong Chen#, Qian Li, Haoran Ji, Rao Li, Yanan Li, Jingchao Fang, Haiwen Liu*, Fa Wang, Kui Jin*, X.C. Xie and Jian Wang*, Quantum Griffiths singularity in a three-dimensional superconductor to Anderson critical insulator transition, Physical Review Letters 133, 226001 (2024)

Spin-charge-entangled Kondo effect induced by a side-coupled Majorana zero mode

Haojie Shen

Shanghai Jiao Tong University

We investigate Kondo physics in a quantum dot side coupled to a Majorana zero mode, where the Majorana coupling induces both spin and charge fluctuations that determine low-energy behavior. Using a wave-function-based Schrieffer-Wolff transformation combined with numerical renormalization group calculations, we discover an $\times$ (2) spin-charge-entangled Kondo state, in which conduction electrons screen the spin-charge-entangled degrees of freedom of the Majorana-quantum dot subsystem. We show that the parity degeneracy of this state gives rise to spin-resolved Andreev-normal boundary conditions, resulting in non-Fermi-liquid behavior. Density matrix renormalization group simulations directly resolve a hallmark of these boundary conditions—a subleading even-odd effect in the screening cloud. Our framework bridges strongly correlated and topological phenomena, and naturally extends to $\mathbb{Z}$ parafermions and $\times$ ( ) Kondo systems.

Identification of gapless phases by twisting operators

Yuan Yao
上海交通大学

We propose a general necessary condition for a spin chain with SO(3) spin-rotation symmetry to be gapped. Specifically, we prove that the ground state(s) of an SO(3)-symmetric gapped spin chain must be spin singlet(s), and the expectation value of a twisting operator asymptotically approaches unity in the thermodynamic limit, where finite-size corrections are inversely proportional to the system size. This theorem provides (i) supporting evidence for various conjectured gapped phases, and (ii) a sufficient criterion for identifying gapless spin chains. We verify our theorem by numerical simulations for a variety of spin models and show that it offers a novel efficient way to identify gapless phases in spin chains with spin-rotation symmetry.

This talk is based on arXiv:2506.02496.

From the Shastry-Sutherland model to the $J_1 - J_2$ Heisenberg model

Xiangjian Qian
Shanghai Jiao Tong University

We propose a generalized Shastry-Sutherland (SS) model which bridges the SS model and the $J_1 - J_2$ Heisenberg model. By employing large-scale density matrix renormalization group and fully augmented matrix product state calculations, combined with careful finite-size scaling, we find the phase transition between the plaquette valence bond state (pVBS) and Néel antiferromagnetic (AFM) phase in the pure SS model is a weak first one. This result indicates the existence of an exotic tricritical point in the pVBS to AFM transition line in the phase diagram, as the transition in the $J_1 - J_2$ Heisenberg model was previously determined to be continuous. We determine the location of the tricritical point in the phase diagram at which the first-order transition turns continuous. Our generalized SS model provides not only a valuable platform to explore exotic phases and phase transitions but also more realistic description of SS materials like $SrCu_2(BO_3)_2$.

Origin of robust Z_2 topological phases in stacked Hermitian systems: Non-Hermitian level repulsion

Zhiyu Jiang[1], Masatoshi Sato[2], Hideaki Obuse[3,4,5,6]
1. The University of Osaka
2. Yukawa Institute for Theoretical Physics, Kyoto University
3. Department of Applied Physics, Hokkaido University
4. Institute for Frontier Education and Research on Semiconductors, Hokkaido University
5. Institute of Industrial Science, The University of Tokyo
6. The Institute for Solid State Physics, The University of Tokyo

The quantum spin Hall insulator [1] with Z_2 topology has attracted great interest since its discovery. There is a widely accepted belief for Z_2 topological phases that a system composed of stacking two layers, where each layer has Z_2 non-trivial topology, should be topologically trivial. However, several research reports that the Z_2 topological phase survives in certain parameter regions in such stacked systems [2,3], while the reason has not yet been clarified.

In this work, we provide a systematic understanding that the robust Z_2 topological phase in a Hermitian system with chiral symmetry originates from level repulsions in the corresponding non-Hermitian system derived from Hermitization. We demonstrate this by treating a class DIII superconductor with Z_2 topology and the corresponding non-Hermitian system in $\mathrm{AII}^\dagger$ with Z_2 point-gap topology as an example. For the latter system, in the case of stacking two layers, the four-fold degeneracy of the spectrum breaks down to two-fold degeneracy due to the level repulsion between two Kramers pairs as expected. Remarkably, Z_2 point-gap topology at the energy E in point gaps emerges as the level repulsion remains non-trivial. Moreover, through Hermitization, the energy E of the non-Hermitian system takes the role of the chemical potential μ of the Hamiltonian for the DIII superconductors. Due to this correspondence, the energy region for the non-trivial Z_2 point-gap topology coincides with the range of μ where Z_2 topological phase of DIII stacked superconductor is non-trivial and zero-energy states appear. Our result provides the systematic understanding of robust Z_2 topology in Hermitian systems with chiral symmetry, as the level repulsion in the corresponding non-Hermitian systems. Moreover, this work provides an important example to clarify an advantage of viewing the Hermitian world from the non-Hermitian perspective.

[1] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
[2] B. Zhou and S.-Q. Shen, Phys. Rev. B 84, 054532 (2011).
[3] Y. Yoshimura, W. Onishi, K. Kobayashi, T. Ohtsuki, and K.-I. Imura, Phys. Rev. B 94, 235414 (2016).

First-Principles Study of Transverse Thermoelectric Anisotropy and Spin reorientation in Rare-Earth Transition Metal Compound

Shibo Wang[1], Leonard Hörnis[1,2], Hiroki Tsuchiura[1], Nobuaki Terakado[1,3]
1. Tohoku University
2. Heidelberg University
3. Kyoto University

Recent advances in spin-caloritronics have highlighted the transverse thermoelectric effects (TTEs), as promising routes for harvesting thermal energy and realizing intelligent thermal control[1]. Particularly in topological magnetic materials with spin-orbit coupling (SOC) and broken time-reversal symmetry, the large anomalous Hall effect (AHE) and TTEs arise from the Berry curvature of the electronic structure, and are closely linked to the direction of magnetization **M**. In this context, rare-earth intermetallics such $DyCo_5$ offer a unique opportunity as $DyCo_5$ exhibits a spin-reorientation transition (SRT), wherein the magnetization direction spontaneously rotates from the (100) direction to the (001) direction at around 350K[2].

In this study, we perform first-principles calculations by the WIEN2k code[3] based on the full-potential linearized augmented plane-wave (FP-LAPW) method combined with LDA+U, and compute the anomalous Hall conductivity σ_{xy} and the transverse thermoelectric conductivity α_{xy} for both magnetization states, here only α_{xy} is shown in Fig.1. We also estimate the anomalous Nernst coefficient S_{ANE} and the anomalous Ettingshausen coefficient Π_{AEE} (Tab.1), which quantify the transverse thermoelectric voltage and transverse heat current, respectively, induced by a longitudinal temperature gradient or electric current. The longitudinal conductivity σ_{xx} of $DyCo_5$ (Fig.2) is calculated by fitting the relaxation time τ using experimental σ_{xx} data for $SmCo_5$ reported by Miura et al.[4] and applying it to our BoltzTraP2 transport calculations[5]. This procedure yields a reasonable approximation of DyCo5's σ_{xx}, enabling a semi-quantitative estimation of its transverse thermoelectric response.

In this study, we also discuss a novel intelligent temperature control device utilizing both the SRT and the AEE with highly anisotropic α_{xy} and Π_{AEE}.

Reference

[1] K. Uchida and R. Iguchi J. Phys. Soc. Jpn. **90**, 122001 (2021)
[2] T. Tsushima and M. Ohokoshi J. Magn. Magn. Mater. **31** Part1 (1983)
[3] P. Blaha et al. An augmented plane wave+ local orbitals program for calculating crystal properties **60**, 2001
[4] A. Miura et al. Appl. Phys. Lett. **115**, 222403 (2019)
[5] Georg K. H. Madsen et al. Comput. Phys. Commun. **231**, 140-145 (2018)

Nanoscale visualization of nematic-to-superconducting phase transition in ferropnictides

Qiangjun Cheng
清华大学

The inherently strong electronic correlations and localized electron pairing in high-temperature superconductors necessitate unraveling the microscopic origin of superconductivity. In iron-based superconductors, extensive studies have established that superconductivity commonly develops upon the suppression of nematic order, yet its microscopic evolution remains elusive. Here, we employ representative $Ca(Fe_{1-x}Co_x)_2As_2$ (CFCA) films as a prototype to preform our microscopic study on FeAs plane. In the undoped CFCA, nematicity manifests as $8a_{Fe-Fe}$ dumbbell-shaped defect states which will develop into $4a_{Fe-Fe}$ charge stripe via slightly Co doping, indicating the emergence of smectic phase. Meanwhile, nanoscale superconducting puddles emerge in the strained region, where smectic phase is suppressed, demonstrating their intrinsic competition. With further Co doping, smectic phase disappears and global superconductivity is established. Quasiparticle interference analysis reveals that the nematic scattering along Fe‑Fe direction is progressively suppressed by Co doping, eventually giving way to isotropic scattering in the superconducting state. Our results provide direct experimental evidence for the emergence of high-temperature superconductivity and establish a paradigm for microscopically tuning superconductivity in iron-based families.

Carbon Nanostructure Synergy for Ultralow Thermal Conductivity Thermal Insulation Materials Under Extreme Temperatures over 2600℃

Zi Yuan
清华大学

We report a novel high-performance thermal insulation material based on stackable super-aligned carbon nanotube films (SACNT-SF), which exhibits exceptional thermal insulation across an extreme temperature range from room temperature to 2600° C, with an ultralow effective thermal conductivity of 0.004 $W \cdot m^{-1} \cdot K^{-1}$ at room temperature and 0.03 $W \cdot m^{-1} \cdot K^{-1}$ at 2600° C under vacuum, significantly outperforming conventional thermal insulation materials such as graphite felt; this superior performance is attributed to the multi-scale structural design of SACNT-SF, which synergistically suppresses all three heat transfer pathways—solid conduction through its nanometer-scale tube diameter and highly anisotropic porous network, radiation conduction via the high extinction coefficient of sp^2 carbon and van Hove singularity-enhanced photon absorption, and gas conduction via Knudsen effect dominance in its nanoporous architecture—while also demonstrating remarkable mechanical flexibility, conformability to complex surfaces, excellent thermal stability in inert environments, and flame retardancy, making it a promising candidate for next-generation thermal management applications in aerospace, energy systems, and high-temperature industrial processes.