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Helical Quantum Edge Gears in 2D Topological Insulators

Yang-Zhi Chou¹, Alex Levchenko², Matthew S. Foster^{1,3}

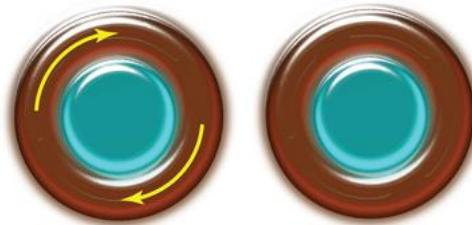
¹*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*

²*Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA*

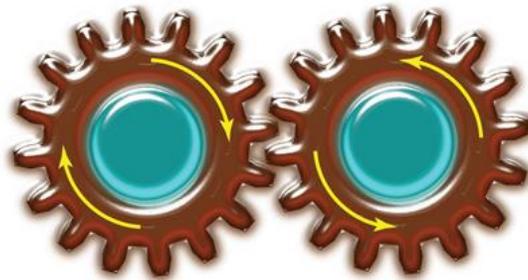
³*Rice Center for Quantum Materials, Rice University, Houston, Texas 77005, USA*

A remarkable and as-yet-unexploited aspect of topological insulator (TI) physics is the topology of the edge states, i.e. the fact that the edge liquid of a 2D TI forms a closed, unbreakable loop in the absence of electrical contacts or magnetic fields. We propose a novel experimental setup in which edge loops rotate as interlocking “gears” through Coulomb drag, in TIs with Rashba spin-orbit coupling. We show that two-terminal transport can measure the Luttinger liquid parameter K , a quantity that is otherwise notoriously difficult to measure. In the low-temperature ($T \rightarrow 0$) perfect drag regime, the conductance is $(e^2/h)(2K + 1)/(K + 1)$. At higher T we predict a conductivity $\sim T^{-4K+3}$. Our results should trigger new experiments and may open a new venue for edge gear-based electronic devices.

Helical edges states with
conserved spin: No drag



With Rashba spin-orbit coupling:
Locking drag due to spin-flip scattering



References:

[1] Yang-Zhi Chou, Alex Levchenko, and Matthew S. Foster, *Phys. Rev. Lett.* **115**, 186404 (2015)

Evolution of the Magnetic Ordering in $\text{CeCu}_{6-x}\text{T}_x$ ($\text{T} = \text{Ag, Pd}$)

L. Poudel^{1,2}, V. O. Garlea², A. E. Taylor², W. Tian², M. Matsuda², T. Hong², M. D. Lumsden², D. Mandrus^{1,2,3}, A. D. Christianson^{1,2}

¹*Department of Physics & Astronomy, the University of Tennessee, Knoxville, TN-37966*

²*Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN*

³*Department of Material Science & Engineering, the University of Tennessee, Knoxville, TN-37966*

The nature of the quantum critical points (QCPs) in many heavy-fermion systems can be interpreted in terms of the Landau-Ginzburg approach provided by Hertz, Millis and Moriya (HMM) [1, 2]. A few of the heavy fermion QCPs, however, deviate from the prediction of the HMM model, but can be described within the framework of the Local-Moment-Magnetic (LMM) model [3, 4]. The heavy fermion series, $\text{CeCu}_{6-x}\text{Au}_x$ ($x = 0.1$) is often considered as a prototype of the LMM QCP [4, 5]. In $\text{CeCu}_{5.9}\text{Au}_{0.1}$, an anomalous scaling exponent ($\alpha = 0.75$) is observed in the dynamic and static magnetic susceptibilities, which is often understood in terms of the LMM model [5]. We study the related systems, $\text{CeCu}_{6-x}\text{Ag}_x$ and $\text{CeCu}_{6-x}\text{Pd}_x$ to add greater breadth to the understanding of LMM QCPs. In $\text{CeCu}_{6-x}\text{Pd}_x$ and $\text{CeCu}_{6-x}\text{Ag}_x$, the magnetic QCP occurs at $x = 0.05$ and $x = 0.2$, respectively [6,7,8]. The magnetic structure of $\text{CeCu}_{6-x}\text{Au}_x$ and $\text{CeCu}_{6-x}\text{Pd}_x$ is composed of a sinusoidal modulation of the Ce-moments pointed along the c -axis of the orthorhombic structure [8]. The magnetic structure propagates with an incommensurate wavevector $(\delta_1 \ 0 \ \delta_2)$, where $\delta_1 \approx 0.64$, $\delta_2 \approx 0.3$ for $\text{CeCu}_{6-x}\text{Ag}_x$ and $\delta_1 = 0.62$, $\delta_2 = 0.25$ for $\text{CeCu}_{6-x}\text{Pd}_x$ series [8].

References:

- [1] J. A. Hertz, Phys. Rev. B **14**, 1165(1976)
- [2] H. v. Löhneysen *et al.*, Rev. Mod. Phys. **79**, 1015 (2007).
- [3] S. Friedemann *et al.*, PNAS, **107**, 14547 (2010).
- [4] Q. Si *et al.*, Nature **413**, 804-808 (2001)
- [5] A. Schröder *et al.*, Nature **407**, 351 (2000).
- [6] M. Sieck *et al.*, Physica B: Condensed Matter 223–224, 325 (1996).
- [7] E.-W. Scheidt *et al.*, Physica B 321 (2002) 133–137
- [8] L. Poudel *et al.*, arXiv:1510.00363

Lie Algebraic Similarity Transformations

Jacob M. Wahlen-Strothman¹, Carlos A. Jiménez-Hoyos², Thomas M. Henderson^{1,2},
Gustavo E. Scuseria^{1,2}

¹*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA;* ²*Department of Chemistry, Rice University, Houston, Texas 77005, USA*

We present a class of Lie algebraic similarity transformations generated by exponentials of two-body, hermitian operators whose Hausdorff series can be summed exactly without truncation. The correlators are defined over the entire basis and include the Gutzwiller factor $n_{i\uparrow}n_{i\downarrow}$, and two-site products of density ($n_{i\uparrow} + n_{i\downarrow}$) and spin ($n_{i\uparrow} - n_{i\downarrow}$) defined as a general diagonal operator. The resulting non-hermitian many-body Hamiltonian can be solved in a biorthogonal mean-field approach with polynomial computational cost. Jastrow factors such as these are commonly used in quantum Monte-Carlo [1] and other applications. We demonstrate an alternative approach by transforming the Hamiltonian and solving a projected system of equations with no stochastic error. The proposed similarity transformation generates locally weighted orbital transformations of the reference determinant. Although the energy of the model is unbound, projective equations in the spirit of coupled cluster theory [2] lead to well-defined solutions, and properties can be calculated with response equations. Accurate results are produced for 1D and 2D systems in both the strong and weak correlation regimes. We seek to extend the method to general Hamiltonians to test and study molecules and crystals.

References:

- [1] B. Edegger, V. N. Muthukumar, and C. Gros, *Adv. Phys.* **56**, 927 (2007).
- [2] R. J. Bartlett and M. Musial, *Rev. Mod. Phys.* **79**, 291 (2007).

Non-Fermi Liquid Behavior Close to a Quantum Critical Point in a Ferromagnetic State without Local Moments

E. Svanidze,¹ L. Liu,² B. Frandsen,² B. D. White,³ T. Besara,⁴ T. Goko,² T. Medina,⁵ T. J. S. Munsie,⁵ G. M. Luke,⁵ D. Zheng,⁶ C. Q. Jin,⁶ T. Siegrist,⁴ M. B. Maple,³ Y. J. Uemura,² and E. Morosan¹

¹*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*

²*Department of Physics, Columbia University, New York, New York 10027, USA*

³*Department of Physics, University of California, San Diego, La Jolla, California 92093, USA*

⁴*National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA*

⁵*Department of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S 4M1, Canada*

⁶*Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

A quantum critical point occurs upon chemical doping of the weak itinerant ferromagnet $\text{Sc}_{3.1}\text{In}$. Remarkable for a system with no local moments, the quantum critical point is accompanied by non-Fermi liquid behavior, manifested in the logarithmic divergence of the specific heat both in the ferro- and the paramagnetic states, as well as linear temperature dependence of the low-temperature resistivity. With doping, critical scaling is observed close to the quantum critical point, as the critical exponents δ , γ , and β have weak composition dependence, with δ nearly twice and β almost half of their respective mean-field values. The unusually large paramagnetic moment $\mu_{\text{PM}} \sim 1.3 \mu_{\text{B}}/\text{F.U.}$ is nearly composition independent. Evidence for strong spin fluctuations, accompanying the quantum critical point at $x_c = 0.035 \pm 0.005$, may be ascribed to the reduced dimensionality of $\text{Sc}_{3.1}\text{In}$, associated with the nearly one-dimensional Sc-In chains.

Multi-Branch Spin Chain Models for Strongly interacting Spinor Fermi and Bose gases in One-Dimension

Li Yang¹, Han Pu¹

¹*Department of Physics and Astronomy, and Rice Quantum Institute,
Rice University, Houston, TX 77251, USA*

By mapping a 1D spinor Fermi or Bose gases wavefunction to a direct product of a spinless fermion wavefunction and a spin chain wavefunction, we obtain a spin-charge coupling Hamiltonian which is a multi-branch spin chain model. The charge part of this model are p-wave pseudo potential interactions. The spin part of this model are spin parity projection operators. Previously obtained spin chain models [1,2,3] are first order perturbation of this multi-branch spin chain model. With this model, for particles in a harmonic trap in strongly interacting regime, we study breathing mode frequencies and the system's response to a spin dependent magnetic gradient and quench dynamics.

References:

- [1] A. G. Volosniev, D. V. Fedorov, A. S. Jensen, M. Valiente and N. T. Zinner, *Nature Commun.* **5**, 5300 (2014).
- [2] F. Deuretzbacher, D. Becker, J. Bjerlin, S. M. Reimann, and L. Santos, *Phys. Rev. A* **90**, 013611 (2014).
- [3] L. Yang, L. Guan, and H. Pu, *Phys. Rev. A* **91**, 043634 (2015).

Global phase diagram of the Ising-anisotropic Kondo lattice

Kevin Ingersent¹, Emilian Marius Nica², and Qimiao Si²

¹*Department of Physics, University of Florida, P.O. Box 118440, Gainesville, Florida 32611*

²*Department of Physics and Astronomy, Rice University, Houston, Texas 77005*

In recent years, a significant amount of work has been dedicated to understanding heavy-fermion quantum criticality. What has emerged is a proposed global phase diagram [1] meant to capture the interplay between Kondo singlet formation, magnetic ordering and intrinsic fluctuations associated with the quantum-mechanical nature of the local moments. Using an Extended Dynamical Mean-Field Theory (EDMFT) approach, we study a prototypical Ising-anisotropic Kondo lattice model in the presence of a transverse field that provides a way of controlling the quantum fluctuations of the local moments. We show that the transverse field opens up a line of continuous transitions directly from an antiferromagnetic phase with Kondo destruction (and, hence, a small Fermi surface) to a paramagnetic heavy-fermion state (with a large Fermi surface). We show that the critical scaling characteristics along this line are the same as for the previously studied zero-transverse field case, indicating the robustness of the Kondo-destruction scenario with respect to enhanced quantum fluctuations. General implications of our results for the global phase diagram and heavy-fermion quantum criticality will be discussed.

References:

[1] “Kondo Destruction and Quantum Criticality in Kondo Lattice Systems,” Q. Si, J. H. Pixley, E. Nica, S. J. Yamamoto, P. Goswami, R. Yu, and S. Kirchner, *J. Phys. Soc. Jpn.* **83**, 061005 (2014).

Low energy spin excitations in charge-compensated $\text{Ba}_{0.67}\text{K}_{0.33}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$

R. Zhang¹, M. Stone², P. Dai¹

¹*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*

²*Neutron Scattering Sciences Division, Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, Tennessee 37831, USA*

The low energy spin excitations and spin resonance in iron pnictide superconductors are crucial in understanding the mechanism of superconductivity. In hole doped $\text{Ba}_{0.67}\text{K}_{0.33}\text{Fe}_2\text{As}_2$, the low energy spin excitation at $(\pi, 0)$ is longitudinally elongated, while in electron doped $\text{BaFe}_{2-x}\text{TM}_x\text{As}_2$ (TM=Ni, Co), it is transversely elongated. Since RPA calculation shows that such different wave vector dependence could result from different carriers in the systems, we studied the low energy spin excitations in charge-compensated $\text{Ba}_{0.67}\text{K}_{0.33}(\text{Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$. Upon doping Co into optimally doped $\text{Ba}_{0.67}\text{K}_{0.33}\text{Fe}_2\text{As}_2$, T_c has been suppressed from 37K to 28K, and the low energy spin excitation around 12meV has changed from longitudinal elongated to almost isotropic. Such doping dependence is strong evidence for coupling between low energy spin excitation and itinerant electrons in iron pnictides.

Ising-Nematic Order and Spin Excitations in the bilinear-biquadratic model for the Iron Pnictides

Patricia Bilbao Ergueta¹, Andriy Nevidomskyy^{1,2}

¹*Department of Physics and Astronomy, Rice University, 6100 Main St., Houston, TX* ²*Rice Center for Quantum Materials*

Motivated by the recent inelastic neutron scattering (INS) measurements in the iron pnictides which show a strong anisotropy of spin excitations even above the magnetic transition temperature T_N ^[1], we study the spin dynamics within the frustrated Heisenberg model with biquadratic spin-spin exchange interactions. Using the Dyson-Maleev (DM) representation, which proves appropriate for all temperature regimes, we find that the spin-spin dynamical structure factors are in excellent agreement with experiment, exhibiting breaking of the C_4 symmetry even into the paramagnetic region $T_N < T < T_\sigma$, which we refer to as the Ising-nematic phase. In addition to the Heisenberg spin interaction, we include the biquadratic coupling $-K (\mathbf{S}_i \cdot \mathbf{S}_j)$ its effect on the dynamical temperature range $T_\sigma - T_N$ of the Ising-nematic phase. We find that this range reduces dramatically when even small values of the interlayer exchange J_c and biquadratic coupling K are included. To supplement our analysis, we benchmark the results obtained using full decoupling in the DM method against those from different nonlinear spin-wave theories, including the recently developed generalized spin-wave theory^[2] (GSWT), and find good qualitative agreement among the different theoretical approaches as well as experiment for both the spin-wave dispersions and the dynamical structure factors. For details, see Ref. [3].

References:

- [1] X. Lu, J. T. Park, R. Zhang, H. Luo, A. H. Nevidomskyy, Q. Si, and P. Dai, *Science* **345**, 657 (2014).
- [2] R. A. Muniz, Y. Kato, and C. D. Batista, *Prog. Theor. Exp. Phys.* (2014) 083I01.
- [3] P. Bilbao Ergueta, and A. H. Nevidomskyy, *Phys. Rev. B* **92**, 165102 (2015).

Quantum phase transitions and anomalous Hall effect in a pyrochlore Kondo lattice

Sarah E. Grefe¹, Wenxin Ding², Qimiao Si¹

¹*Department of Physics and Astronomy, Rice University, Houston, TX USA, sarah.e.grefe@rice.edu*

²*Department of Physics and Astronomy, University of California Santa Cruz, Santa Cruz, CA USA*

The metallic variant of the pyrochlore iridates $\text{Pr}_2\text{Ir}_2\text{O}_7$ has shown characteristics of a possible chiral spin liquid state [1, 2, 3] and evidence of quantum criticality [4]. An important question surrounding the significant anomalous Hall response observed in this compound is the nature of the f-electron local moments, including their Kondo coupling with the conduction d-electrons. The heavy effective mass and related thermodynamic characteristics point towards the involvement of the Kondo effect in this system's electronic properties. In this work, we study the effects of Kondo coupling on candidate time-reversal-symmetry-breaking spin liquid states on the pyrochlore lattice. Representing the f-moments as slave fermions Kondo-coupled to conduction electrons, we study the competition between Kondo-singlet formation and chiral spin correlations and determine the zero-temperature phase diagram. We derive an effective chiral interaction between the local moments and the conduction electrons and calculate the anomalous Hall response across the quantum phase transition from the Kondo destroyed phase to the Kondo screened phase. We discuss the results of our study as well as their implications for $\text{Pr}_2\text{Ir}_2\text{O}_7$ and related frustrated Kondo-lattice systems.

References:

- [1] S. Nakatsuji, Y. Machida, Y. Maeno, T. Tayama, T. Sakakibara, J. van Duijn, L. Balicas, J. N. Millican, R. T. Macaluso, and Julia Y. Chan, *Phys. Rev. Lett.* **96** 087204 (2006)
- [2] Y. Machida, S. Nakatsuji, Y. Maeno, T. Tayama, T. Sakakibara, and S. Onoda, *Phys. Rev. Lett* **98**, 057203 (2007)
- [3] Y. Machida, S. Nakatsuji, S. Onoda, T. Tayama and T. Sakakibara, *Nature* **463**, 210 (2010)
- [4] Y. Tokiwa, J. J. Ishikawa, S. Nakatsuji and P. Gegenwart, *Nat. Mater.* **13**, 356 (2014)

Superconducting Pairing Correlations near a Kondo-destruction Quantum Critical Point in Cluster Impurity Models

Ang Cai^{1*}, J. H. Pixley², Qimiao Si¹

¹*Department of Physics and Astronomy, Rice University, Houston, Texas, 77005, USA;* ²*Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA; *ac58@rice.edu*

There is considerable interest in superconductivity driven by quantum criticality. It is natural to explore this issue in heavy fermions, given that they represent a canonical system to study both quantum criticality and unconventional superconductivity. The quantum critical point (QCP) observed in heavy fermion system has been classified based on whether the Fermi surface volume jumps across the transition. In the conventional spin density wave (SDW) scenario, the heavy quasi-particles stay intact through the magnetic instability, while in the unconventional type, the Kondo coupling itself become critical at the QCP. In the latter case it remains an open question as to whether Kondo destruction type QCP can also promote superconductivity. Particularly motivated by the properties of CeRhIn₅, which shows the characteristic features of a Kondo destruction quantum critical point in its normal state, and has one of the highest T_c's among the heavy fermion superconductors, we address this problem within a cluster-EDMFT approach [1]. As a first step we analyze a four-site Anderson impurity model with the antiferromagnetic spin component of the cluster coupled to a sub-Ohmic bosonic bath. We find a QCP that belongs to the same universality class as the single-site Bose-Fermi Anderson model. Together with previous work on a two-site model [2], our result suggests that the Kondo destruction QCP is robust as cluster size increases. More importantly, we are able to calculate the d-wave pairing susceptibility, which we find to be enhanced near the QCP. Implications of our results for the superconductivity in the case of the Kondo lattice model will be discussed.

References:

- [1] J. H. Pixley, A. Cai, Q. Si, Phys. Rev. B 91, 125127 (2015)
- [2] J. H. Pixley, L. Deng, K. Ingersent, Q. Si, Phys. Rev. B 91, 201109 (2015)

Quadrupolar Orders in FeSe

Zhentao Wang¹, Andriy H. Nevidomskyy¹

¹*Department of Physics and Astronomy, Rice University, Houston, Texas 77005*

Motivated by the absence of long-range magnetic order and the strong spin fluctuations observed in the Fe-based superconductor FeSe, we study spin-1 model on a square lattice up to next-nearest neighbor Heisenberg and biquadratic spin exchanges. The zero-temperature variational phase diagram gives the conventional antiferromagnetic order and also more exotic quadrupolar spin phases. These quadrupolar phases do not host long-range magnetic order and preserve time-reversal symmetry, but break the spin $SU(2)$ symmetry. In particular, we observe a robust ferroquadrupolar order (FQ) in immediate proximity to the columnar AFM phase. We envision that FeSe may be positioned within the FQ phase close to the phase boundary. Using the flavor-wave technique, we calculate the structure factor inside the FQ phase and find a Goldstone mode emerging from $\mathbf{Q}=(0,0)$, which however bears zero spectral weight at $\omega=0$ due to time reversal symmetry. At the same time, we observe strong spin fluctuations near $(\pi,0)/(0,\pi)$, which agrees with the recent neutron scattering experiments. Further, we calculate the higher order interactions between the $(\pi,0)$ and $(0,\pi)$ spin fluctuations inside the FQ phase, which may shed light on the C_4 symmetry breaking in the nematic phase of FeSe.

Intermediate valence in single crystals of $(\text{Lu}_{1-x}\text{Yb}_x)_3\text{Rh}_4\text{Ge}_{13}$ ($0 \leq x \leq 1$)

Binod K Rai¹, Emilia Morosan¹

¹*Department of Physics and Astronomy, Rice University, Houston TX 77005 USA*

The hybridization of transition metal or rare earth localized d or f -electrons with conduction electrons often gives rise to exotic electronic properties such as intermediate valence (IV) states, Kondo insulator, pseudogap, superconductivity, heavy fermion (HF), and quantum criticality.[1-5] Intermediate valence states generally form with electronically unstable rare earths like Ce, Yb, Eu, and Sm. Two competing energy scales in such materials, the Ruderman-Kittel-Kasuya-Yosida (RKKY) $T_{\text{RKKY}} \propto 1/JN(E_{\text{F}})$ and the Kondo energy $T_{\text{K}} \propto e^{-1/JN(E_{\text{F}})}$ (where J is the spin coupling constant and $N(E_{\text{F}})$ is the density of states at the Fermi level), give rise to either Kondo, heavy fermion when $T_{\text{K}} \gg T_{\text{RKKY}}$ or magnetic when $T_{\text{RKKY}} \gg T_{\text{K}}$. In this presentation, I will discuss the physical properties a continuous solid solution $(\text{Lu}_{1-x}\text{Yb}_x)_3\text{Rh}_4\text{Ge}_{13}$ displays a continuous evolution from superconductivity in a disordered metal close to $x = 0$ [5] to Kondo to intermediate valence regimes for low ($x \leq 0.3$) and high ($0.3 \leq x \leq 1$) Yb compositions.

References:

- [1] C. M. Varma, *Rev. Mod. Phys.* 48, 219 (1976).
- [2] G. R. Stewart, *Rev. Mod. Phys.* 56, 755 (1984).
- [3] J. H. Pixley, S. Kirchner, K. Ingersent, and Q. Si, *Phys. Rev. Lett.* 109, 086403 (2012).
- [4] Q. Si and F. Steglich, *Science* 329, 1161 (2010).
- [5] B. K. Rai, I. W. H. Oswald, J. Wang, G. T. McCandless, J. Y. Chan, and E. Morosan, *Chem. Mater.* 27, 2488 (2015).

Large-N Schwinger Boson Approach to the Multiple Impurity Kondo Problem

Patricia Bilbao Ergueta¹, Andriy Nevidomskyy^{1,2}

¹*Department of Physics and Astronomy, Rice University, 6100 Main St., Houston, TX* ²*Rice Center for Quantum Materials*

Motivated by the studies of one^[1] and two-impurity^[2] multichannel Kondo model using the bosonic impurity spin representation, we investigate the effect that adding a third impurity has on the properties of the system. We use a Schwinger boson representation for the spin operators, resulting in coupled integral equations for self-energies, to be solved iteratively. Our method differs from that employed in earlier works, which used the real frequency spectral representation of the Green's functions. Here instead, we use the imaginary frequency representation. We calculate physical quantities, such as magnetic susceptibility and scattering phase shift, which we benchmark against existing results for the one and two-impurity Kondo model. The results for three-impurities show a qualitatively similar susceptibility behavior and phase diagram to those of the two-impurity case, due to the fact that the ground state of a 3 spins problem is dimerized. We are presently extending our formalism to study the interplay of magnetic frustrations and Kondo screening on the triangular lattice.

References:

- [1] O. Parcollet and A. Georges, *Phys. Rev. Lett.* **79**, 4665 (1997).
- [2] J. Rech, P. Coleman, G. Zarand, and O. Parcollet, *Phys. Rev. Lett.* **96**, 016601 (2006).

Two branches of high energy spin excitations in $\text{LiFe}_{1-x}\text{Co}_x\text{As}$ induced by orbital differentiation

Yu Li¹, Xiancheng Wang², David Tam¹, Zhiping Yin³, Meng Wang², D.L. Abernathy⁴, A. Podlesnyak⁴, Thomas A. Maier⁵, Kritjan Haule³, Gabriel Kotliar³, Lingyi Xing², Changqing Jin², Pengcheng Dai^{1,*}

¹*Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*

²*Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

³*Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA*

⁴*Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

⁵*Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6494, USA*

The ultimate role of the orbital degrees of freedom on the magnetism and superconductivity in Fe-pnictides materials remains an unsolved puzzle. It was proposed^[1,2] that in iron based material the orbital differentiation enhanced by Hund's coupling decouples the bands and leads to orbital-selective physics. This was supported by the ARPES experiment^[3] which shows the renormalization factor of each band corresponding to different orbital, is quite different. In this manuscript, we report our neutron scattering measurements on the spin excitation spectra in electron doped $\text{LiFe}_{1-x}\text{Co}_x\text{As}$ system. At the low energy part of the spin excitation, we observed a doping dependence of the incommensurability of low energy spin fluctuations which is completely different from that in BaFe_2As_2 system^[4]. More importantly, we found strong evidences that suggest the high energy spin excitations in LiFeAs system actually split into two branches corresponding to distinct orbital components. Fascinatingly, our results are in good agreement with our DMFT calculations. The orbital projection of the calculated dynamic spin susceptibility suggests that the "two branches" are actually dominated by different orbital- d_{xy} and $d_{xz/yz}$. Our results can be well explained by the orbital differentiation due to the Hund's coupling pointing to an orbital selective Mott physics in iron based superconductors. Our results can also cast light on understanding the origin of magnetism in other multi-orbital correlated systems.

References:

- [1] Luca de' Medici, Gianluca Giovannetti, and Massimo Capone, Phys. Rev. Lett. 112, 177001 (2014)
- [2] Z. P. Yin, K. Haule and G. Kotliar, Nat. Mater. 10, 932 (2011)
- [3] M. Yi, Z-K Liu, Y. Zhang, R. Yu, J.-X. Zhu, J. J. Lee, R. G. Moore, F. T. Schmitt, W. Li, S. C. Riggs, J.-H. Chu, B. Lv, J. Hu, M. Hashimoto, S.-K. Mo, Z. Hussain, Z. Q. Mao, C. W. Chu, I. R. Fisher, Q. Si, Z.-X. Shen, and D. H. Lu, Nat. Commun. 6, 7777 (2015)
- [4] Pengcheng Dai, Rev. Mod. Phys. 87, 855 (2015)

Variational Monte Carlo study of gapless spin liquid in the spin-1/2 XXZ antiferromagnetic model on the kagome lattice

Wen-Jun Hu¹, Shou-Shu Gong¹, Federico Becca², and D. N. Sheng¹

¹*Department of Physics and Astronomy, California State University, Northridge, California 91330, USA*

²*Democritos National Simulation Center, Istituto Officina dei Materiali del CNR, and SISSA-International School for Advanced Studies, Via Bonomea 265, I-34136 Trieste, Italy*

By using the variational Monte Carlo technique, we study the spin-1/2 XXZ antiferromagnetic model (with easy-plane anisotropy) on the kagome lattice. A class of Gutzwiller projected fermionic states with a spin Jastrow factor is considered to describe either spin liquids (with U(1) or Z_2 symmetry) or magnetically ordered phases (with $\mathbf{q}=(0,0)$ or $\mathbf{q}=(4\pi/3,0)$). We find that the magnetic states are not stable in the thermodynamic limit. Moreover, there is no energy gain to break the gauge symmetry from U(1) to Z_2 within the spin-liquid states, as previously found in the Heisenberg model. The best variational wave function is therefore the U(1) Dirac state, supplemented by the spin Jastrow factor. Furthermore, a vanishing S=2 spin gap is obtained at the variational level, in the whole regime from the XY to the Heisenberg model.

References:

- [1] W. Zhu, S.S. Gong, and D.N. Sheng, *Phys. Rev. B* **92**, 014424 (2015)
- [2] W.-J. Hu, S.S. Gong, F. Becca, and D.N. Sheng, arXiv:1505.06276

Neutron scattering resonance mode in $\text{Ce}_{1-x}\text{Yb}_x\text{CoIn}_5$ as a paramagnon

Yu Song¹, John Van Dyke², I. K. Lum^{3,4,5}, B. D. White^{4,5}, L. Shu^{6,7}, S. Jang^{3,4,5}, A. Schneidewind⁸, P. Čermak⁸, Y. Qiu⁹, M. B. Maple^{3,4,5}, D. K. Morr² and Pengcheng Dai¹

¹*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*

²*Department of Physics, University of Illinois at Chicago, Chicago, Illinois 60607, USA*

³*Materials Science and Engineering Program, University of California, San Diego, La Jolla, California 92093, USA*

⁴*Department of Physics, University of California, San Diego, La Jolla, California 92093, USA*

⁵*Center for Advanced Nanoscience, University of California, San Diego, La Jolla, California 92093, USA*

⁶*State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, China*

⁷*Collaborative Innovation Center of Advanced Microstructures, Fudan University, Shanghai 200433, China*

⁸*Jülich Center for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, D-85747, Garching, Germany*

⁹*NIST center for Neutron Research, National Institute of Standard and Technology, Gaithersburg, Maryland 20899, USA*

The resonance mode seen by in unconventional superconductors is typically interpreted as a spin-exciton [1]. In the case of CeCoIn_5 , an intense resonance mode has been observed [2] and interpreted as either a spin exciton [3] or a paramagnon [4]. We have systematically investigated the dispersion of the resonance mode in $\text{Ce}_{1-x}\text{Yb}_x\text{CoIn}_5$ ($x = 0, 0.05, 0.30$) and found, (a) the resonance disperses upwards in all investigated compounds, (b) the dispersion is ring-like in the $[\text{H},\text{K}]$ plane and (c) both superconductivity and dispersion of the resonance mode are robust against the dramatic change in Fermi surface that happens between ($x = 0.1$ and $x = 0.2$) [5]. Our results suggest that the resonance mode in CeCoIn_5 should be interpreted as a paramagnon rather than a spin-exciton.

References:

- [1] D. Scalapino, *Rev. Mod. Phys.* **84**, 1383 (2012); M. Eschrig, *Adv. in Phys.* **55**, 47 (2006)
- [2] C. Stock *et al.*, *Phys. Rev. Lett.* **100**, 087001 (2008)
- [3] I. Eremin *et al.*, *Phys. Rev. Lett.* **101**, 187001 (2008)
- [4] A. Chubukov *et al.*, *Phys. Rev. Lett.* **101**, 147004 (2008)
- [5] H. Kim *et al.*, *Phys. Rev. Lett.* **114**, 027003 (2015)

Orbital-selective pairing: a $\tau_3 B_{1g}$ pairing candidate state for the alkaline iron selenides

Emilian Marius Nica¹, Rong Yu², and Qimiao Si¹

¹*Department of Physics and Astronomy, Rice University, Houston, Texas 77005*

²*Department of Physics, Renmin University of China, Beijing 100872, China*

The iron-based unconventional superconductors are inherently multi-orbital systems and show remarkable variation in the Fermi-surfaces and pairing symmetries. In the alkaline iron selenides cases, ARPES experiments indicate fully gapped superconducting states, which suggests s-wave pairing, while neutron-scattering studies show resonances in the spin-spectrum with wave vectors across the electron Fermi pockets, suggesting d-wave pairing. We propose a novel superconducting state composed of a direct product of an s-wave form factor and a rotational symmetry-breaking orbital matrix in the $d_{xz/yz}$ sectors [1]. It belongs to the B_{1g} representation of the D_{4h} point group, allowing for the overall change in sign between the pairing field at the electron pockets close to the 1-Fe BZ edge. While it supports a spin resonance, it also produces a fully gapped quasiparticle spectrum, making it a candidate pairing state for the alkaline iron selenide compounds. Our results also show how such a state can become energetically competitive in the regime of quasi-degeneracy between the s and d-wave pairing states. In a broader context, this pairing provides an alternative to the $s+id$ to reconstruct the degenerate pairing states, while preserving the time-reversal symmetry. We discuss possible analogs in other multi-band strong-coupling superconductors such as the heavy fermions.

References:

[1] "Emergent superconducting state from quasi-degenerate s- and d-wave pairing channels in iron-based superconductors," E. M. Nica, R. Yu, and Q. Si, arXiv:1505.04170v1 (2015).

High T_c Superconductivity, Structure, Magnetic, Transport Properties, Lower Critical Field, Penetration Depth, Anisotropy and Gap Evidences of Electron-Doped $\text{Ca}_{10}(\text{Pt}_n\text{As}_8)[(\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2]_5$ ($n = 3 \ \& \ 4$) Single Crystals

Kalyan Sasmal¹ and Ching-Wu (Paul) Chu¹

¹Texas Center for Superconductivity & Department of Physics, University of Houston, Houston, TX, USA,
ksasmal@uh.edu

Platinum iron arsenides $\text{Ca}_{10}(\text{Pt}_n\text{As}_8)[(\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2]_5$ with $n = 3 \ \& \ 4$ are the first Fe based superconductors [1] with metallic PtAs intermediary layers in Ca-Fe-Pt-As system [2,3,4]. Superconducting single crystals have been grown and characterized by X-ray diffraction, wavelength-dispersive spectroscopy electron probe microanalysis, magnetization, transport and thermodynamic measurements. Crystal structure has stacks of Ca (Pt_nAs_8) Ca (Fe_2As_2) consists of superconducting Fe_2As_2 layers alternating with Pt_nAs_8 layers, forming a triclinic PI , “10-3-8” phase with $n = 3$ (β - phase) and tetragonal $P4/n$, (“10-4-8” phase) with $n = 4$ (α -phase). In comparison with other pnictides the difference lies in structural & electronic characters of metallic intermediary PtAs layers rather than insulating intermediary layers and the difference in T_c arises because intermediary layer is semiconducting in 10-3-8 phase but metallic in 10-4-8 phase. Also both metal-like (Pt_4As_8) and (Fe_2As_2) blocks in $\text{Ca}_{10}(\text{Pt}_4\text{As}_8)(\text{Fe}_2\text{As}_2)_5$ phase make significant contributions to total density of states on Fermi level E_F . This leads to greater interactions between blocks and increased T_c in this system. Pt-substitution is detrimental to higher T_c , which increases up to 38 K only by charge doping of pure FeAs layers. Two different negatively charged layers $[(\text{FeAs})_{10}]^{n-}$ and $(\text{Pt}_{3+y}\text{As}_8)^{m-}$ compete for electrons provided by Ca^{2+} -ions. In parent compound $\text{Ca}_{10}(\text{FeAs})_{10}(\text{Pt}_3\text{As}_8)$, no excess charge dopes FeAs-layer, and superconductivity has to be induced by Pt-substitution, although below 15 K. In contrast, additional Pt in Pt_4As_8 layer shifts charge balance between layers equivalent to charge doping by 0.2 electrons per FeAs. Only in this case T_c raises to 38 K, but decreases again if additionally Pt is substituted for Fe. Charge doping is supported by $T_c \approx 30$ K in electron-doped RE(La, Pr)-1038, $x = 0.2$ $(\text{Ca}_{1-x}\text{RE}_x)_{10}(\text{Pt}_3\text{As}_8)(\text{Fe}_2\text{As}_2)_5$ without significant Pt-substitution. With La/Pr doping, the structural/magnetic phase transitions are suppressed [5]. Magnetic properties are explored [6]. Magnetization measurements reveal fish-tail hysteresis loop and relatively high critical current density at low T . Exponential T dependence of J_c arises from nonlinear effective flux-creep activation energy, also suggests that the anisotropy is much larger than that of 122-FeSC's [7]. Normal-state magnetic susceptibility with characteristic T -linear dependence in a wide temperature range is indicative of strong spin / magnetic fluctuations as in most of the Fe-pnictide superconductors. Ginzburg-Landau parameters extracted from reversible magnetizations of single crystal data. Resistive transition for H/c axis shows modest broadening. Upper critical field determined by resistive transition along c and ab directions, shows a relatively large mass anisotropy. Anisotropic Ginzburg-Landau scaling parameter γ increases with decreasing temperature and is much larger than that of other FeSCs. This strong 2D character may lead to the absence of long-range AFM magnetic order. Lower critical field, H_{c1} deduced from vortex penetration into single crystals with a temperature dependence closer to that of two-gap (s-wave) superconductors [8]. T -dependency of the H_{c1} is compared with BCS-gap models and anisotropy of H_{c1} are calculated. Anisotropic superconducting gap possibly due to multiband physics of the superconducting pairing.

References:

- [1] Kamihara Y, Watanabe T, Hirano M and Hosono H 2008 J. Am. Chem. Soc. 130 3296
- [2] N. Ni, J. M. Allred, B. C. Chan, and R. J. Cava, Proc. Natl. Acad. Sci. (USA) 108, E1019 (2011).
- [3] C. Lohnert, T. Sturzer, M. Tegel, R. Frankovsky, G. Friederichs, and D. Johrendt, Angew. Chem. Int. Ed. 50, 9195 (2011).
- [4] S. Kakiya, K. Kudo, Y. Nishikubo, K. Oku, E. Nishibori, H. Sawa, T. Yamamoto, T. Nozaka, and M. Nohara, J. Phys. Soc. Jpn. 80, 093704 (2011).
- [5] Tobias Stürzer, Gerald Derondeau, and Dirk Johrendt Phys. Rev. B 86, 060516(R) – (2012)
- [6] K. Sasmal, B. Lv, Z. J. Tang, F. Chen, Y. Y. Xue, B. Lorenz, A. M. Guloy, and C. W. Chu Phys. Rev. B 79, 184516 (2009)
- [7] Kalyan Sasmal, Bing Lv, Bernd Lorenz, Arnold M. Guloy, Feng Chen, Yu-Yi Xue, and Ching-Wu (Paul) Chu Phys. Rev. Lett. 101, 107007 (2008)
- [8] K. Sasmal, B. Lv, Z. Tang, F. Y. Wei, Y. Y. Xue, A. M. Guloy, and C. W. Chu Phys. Rev. B 81, 144512 (2010)

Skyrmion defects of antiferromagnet and competing singlet orders of a Kondo-Heisenberg model on honeycomb lattice

Chia-Chuan Liu¹, Pallab Goswami², Qimiao Si¹

¹*Department of Physics and Astronomy, Rice University, Houston*

²*Condensed Matter Theory Center, University of Maryland, College Park*

The competition between antiferromagnetism and proximate singlet orders is the common feature of many heavy fermion compounds. Depending on the context, the singlet order can be described by static Kondo singlets, unconventional superconductivity, site or bond centered charge orders, or more exotic density waves. It is a fundamentally important but challenging problem to develop a general scheme for identifying the competing singlet orders from the antiferromagnetically ordered side and vice versa. We are interested in studying this problem on Kondo honeycomb lattice model, and approach it starting from the Kondo-destroyed antiferromagnetic phase [1].

By virtue of honeycomb lattice, the low energy effective model can be described as two species Dirac fermion, one for conduction electron and the other for local moment. The loss of the Neel order will make the skyrmion defects proliferate, which could induce different orders [1]. By solving the Dirac equation in a skyrmion background field, we compute the different order parameters. Following this approach, firstly we have proven that for the case of one species of Dirac fermions, the valence bond solid indeed gain most enhancement near the core of skyrmion defect of Neel order. We outline how to determine the Kondo singlet and related order parameters for the Kondo-Heisenberg model within the same approach.

References:

[1] P. Goswami and Q. Si, “Topological defects of Neel order and Kondo singlet formation for Kondo-Heisenberg model on a honeycomb lattice”, *Phys. Rev. B* **89**, 045124 (2014).

Local Density of States of Impurities in Mott Insulators

Wenxin Ding¹ and Qimiao Si¹

¹*Department of Physics and Astronomy, Rice University, Houston*

Motivated by recent scanning tunneling microscope measurements of local density of states on impurities in parent compounds and very lightly doped, insulating compounds^{1,2}, we start with the slave rotor description of a Mott insulator, and study the local density of states of the impurities sites. Excellent qualitative agreement with the experimental results is found. The important, local features of the impurity-induced in-gap spectrum are already captured within the theory. We find that the suppression of density of states at the Fermi energy is a generic feature of a Mott insulator due to the structure of its Green's function. The spectral weight transfer from the upper Hubbard band to the lower Hubbard band, and the correlation between spectral weights and the bound states energies, are also both described by our calculation.

Itinerant chiral ferromagnetism in a trapped Rashba spin-orbit coupled Fermi gas

Shang-Shun Zhang^{1,2}, Wu-Ming Liu¹, and Han Pu²

¹*Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

²*Department of Physics and Astronomy, and Rice Center for Quantum Materials, Rice University, Houston, Texas 77251, USA*

We consider a repulsive two-component Fermi gas confined in a two dimensional isotropic harmonic potential and subject to a large Rashba spin-orbit coupling. The single-particle dispersion can be tailored by the spin-orbit coupling term, which provides an opportunity to study itinerant ferromagnetism in this system. We show that the interplay among spin-orbit coupling, correlation effect and mean-field repulsion leads to a competition between ferromagnetic and non-magnetic phases. The weakly correlated non-magnetic and the ferromagnetic phases can be well described by the mean-field Hartree-Fock theory, while the transition between the ferromagnetic and a strongly correlated non-magnetic phase is driven by beyond-mean-field quantum correlation effect. Furthermore, the ferromagnetic phase of this system possesses a chiral current density induced by the Rashba spin-orbit coupling, whose experimental signature is investigated.

References:

- [1] S.-S. Zhang, W.-M. Liu, and H. Pu, arXiv:1509.04095
- [2] H. Hu, B. Ramachandhran, H. Pu, and X. -J. Liu, *Phys. Rev. Lett.* **108**, 010402 (2012)
- [3] G. J. Conduit, *Phys. Rev. A* **82**, 043604 (2010)