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14. ABSTRACT

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RPPR Final Report
as of 18-Apr-2019

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STEM Degrees: 1 **STEM Participants:**

Major Goals: The major goals of the projects are to discover and design new states of matter arising from the strong spin orbit coupling in quantum many-body systems. Specifically we explore the new correlated phases and novel phenomena in two dimensional transition metal dichalcogenides (TMD) and three dimensional Weyl semimetals. Both are characterized by multiple valleys in the energy landscape, with spin split bands possessing nontrivial topological properties. They are representative of a class of materials which hold the promise of new technologies. The challenges are threefold: 1) identify and characterize the thermodynamic and transport properties that can be precisely controlled and widely varied; 2) determine the nature of superconducting phases supported; and 3) find materials that exhibit the novel behavior.

The proposed research investigates new phases and novel phenomena resulting from strong spin orbit coupling in quantum many-body systems. In particular the thrusts are:

1) Explore new states of matter, such as unconventional superconductivity, obtained due to the unusual spin split bands structure in interacting hole doped transition two-dimensional metal dichalcogenides. Exploit valley selective probes, such as circularly polarized light, to investigate the nature of correlated ground states.

2) Characterize the properties of Weyl semimetals, with an emphasis on the topological aspects of transport and thermodynamic response. Determine the possible phases and establish the phase diagram of Weyl semimetals in the presence of electron-electron interaction. Identify symmetry criteria for realization of Weyl semimetals and perform first principle band structure calculations to search for candidate materials.

Accomplishments: A pdf detailing the accomplishments has been uploaded.

Training Opportunities: Graduate Students:

Evan Sosenko and Shima Imani worked on projects supported by the grant. Evan successfully defended his PhD thesis in August 2016.

Postdoctoral Researcher:

Dr. Junhua Zhang worked on projects supported by the grant and also helped in mentoring the graduate students.

Participation and presentations are included under the dissemination section.

Results Dissemination: Journal Publication:

1) Unconventional superconductivity and anomalous response in hole-doped transition metal dichalcogenides, Evan Sosenko, Junhua Zhang, and Vivek Aji, Phys. Rev. B 95, 144508 (2017) - Published 18 April 2017

2) Topological Yu-Shiba-Rusinov chain in monolayer transition-metal dichalcogenide superconductors, Junhua Zhang and Vivek Aji, Phys. Rev. B 94, 060501(R) (2016) - Published 1 August 2016

Presentations:

1) Superconducting phases of monolayer transition-metal dichalcogenides, Evan Sosenko and Vivek Aji, APS March Meeting 2016, Baltimore, USA

2) Magnetic response and pair-breaking effect in superconducting transition metal dichalcogenides, Junhua Zhang, Evan Sosenko and Vivek Aji, APS March Meeting 2016, Baltimore, USA

3) Unconventional superconducting states in strongly spin-orbit coupled monolayer transition-metal dichalcogenides, Junhua Zhang, 03/30/2016, SoCAL Meeting UC Riverside, USA

4) 2D Transition metal dichalcogenides: A platform for new phases and phenomena, Vivek Aji, University of Toronto, Canada, 09/28/2016

5) 2D Transition metal dichalcogenides: A platform for new phases and phenomena, Vivek Aji, University of Waterloo, Canada, 09/29/2016

6) Topological Yu-Shiba-Rusinov chain in monolayer transition-metal dichalcogenide superconductors, Junhua Zhang and Vivek Aji, APS March Meeting 2017, New Orleans, USA

7) 2D Transition metal dichalcogenides: A platform for new phases and phenomena, Vivek Aji, University of California Berkeley, USA, 04/19/2017

8) Unconventional superconducting phases in hole doped two dimensional transition metal dichalcogenides, Vivek Aji, The 12th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors, August 2018, Beijing China (Invited in January 2018)

Thesis:

Spin and valley physics in two dimensional systems: Graphene and superconducting transition metal dichalcogenides, Evan Sosenko, 2016

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

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as of 18-Apr-2019

PARTICIPANTS:

Participant Type: Graduate Student (research assistant)
Participant: Evan Sosenko
Person Months Worked: 9.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Junhua Zhang
Person Months Worked: 15.00 **Funding Support:**
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Other Collaborators:

Participant Type: Graduate Student (research assistant)
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ACCOMPLISHMENTS

I. TRANSITION METAL DICHALCOGENIDES

Two dimensional TMDCs have a honeycomb lattice structure like graphene, but the two inequivalent sites are occupied by different atoms. The breaking of inversion opens up a gap at the two valleys. In addition the heavy transition metal causes spin splitting of the bands as a result of spin orbit coupling. For MoS$_2$, the band structure is shown in Fig.1. To a first approximation the band structure consists of Mo d bands lying between the Mo-S s-p bonding and anti bonding bands. In the vicinity of $\pm\vec{K}$ (valleys), the symmetry adapted basis states are d_z^2 and $d_{x^2-y^2} + i\tau d_{xy}$ where $\tau = \pm$ is the valley index. The Hamiltonian is

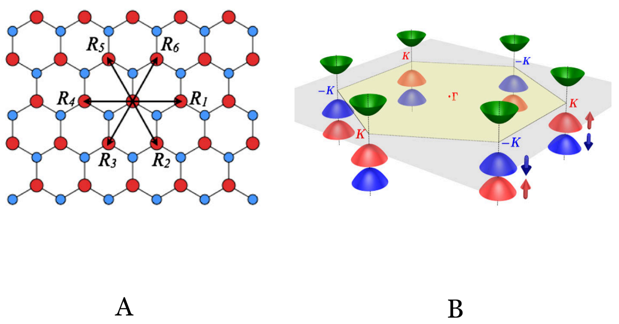

Fig. 1: Crystal structure and low energy bands of MoS$_2$[1]. Red and blue label Mo and S respectively. Mo atoms form a triangular lattice, and their d orbitals make up the low energy theory near $\pm\vec{K}$.

$$H = H_0 + H_{soc}, \quad H_0 = at(\tau k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + \frac{\Delta}{2}\hat{\sigma}_z, \quad H_{soc} = \lambda\tau\frac{\hat{\sigma}_z - 1}{2}\hat{s}_z \tag{1}$$

where $\vec{\sigma}$ denotes the pauli matrices for the basis states, a is the lattice parameter, t the effective hopping integral, Δ is the energy gap, 2λ is the spin splitting and $\hat{s}_z$ is the spin pauli matrix.

There are three aspects of these systems that make them particularly interesting[1]:

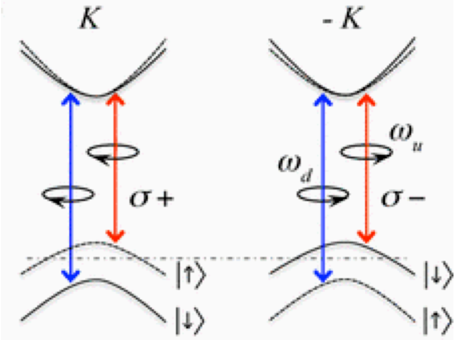

Fig. 2: Optical transitions in TMDs. Depending on the polarization, light causes transitions in one valley or the other[1].

- The spins in the valence band have valley specificity. In a hole doped system, there are two inequivalent fermi surfaces with one valley having spins up while the other having spin down states. The quantization axis is perpendicular to the plane of the crystal. The spin splitting is very large (0.15 $\sim$ 0.46 eV) and there is a significant window in doping where the singly degenerate bands occur at the chemical potential.
- The bands have nontrivial Berry curvature ($\vec{\Omega}$) associated with them, with the sign on the two valleys being opposite of each other. One of the consequences is that the velocity of the electrons

has a term of the form $\vec{\Omega} \times \vec{E}$ in the presence of an external electric field. Since the signs are opposite not only between the two valleys, but also between the conduction and valence bands in the same valley, electron and holes move in opposite directions transverse to an applied electric field.

An alternate view of the topological nature of the band structure is to recognize that associated with each state $(\vec{k}, E_{n\tau}(\vec{k}))$, where $E_{n\tau}(\vec{k})$ is the energy of the state in band n and valley τ, is an angle $\theta_{n\tau\vec{k}}$ which only depends on $|\vec{k}|$ and τ. The angle parametrizes the mixing of the two basis orbitals. The mapping $(\vec{k}, E_{n\tau}(\vec{k})) \rightarrow (\theta_{n\tau\vec{k}}, \phi_{n\tau\phi_{\vec{k}}})$, where $\phi_k = \tan^{-1}(k_y/k_x)$, wraps the band n onto the Bloch sphere. The resulting texture is of a hedgehog reflecting the skymionic nature of the bands. While this is the property of the linearly dispersing physics extrapolated to all energies, the picture is a useful reference to understand the structure of the low energy theory.

• The orbital content of the bands allow for valley selectivity[1–4]. The optical matrix elements connecting the valence and conduction band are such that only one circular polarization of light couples to a given valley. It is important to emphasize that the optical activity comes not from the orbital magnetic moments of the atomic orbitals but the orbital moments of the Bloch state[5]. The spin splitting also implies that magnetic coupling to individual valley is possible. Both these abilities allow for, not only new ways to probe correlated phases, but also control of the valley degree of freedom.

1. *Superconductivity*

Given the valley structure of the energy landscape, two classes of superconducting states are generically allowed. For attractive interaction and proximity to s-wave superconductor the Cooper pairs are made up of electrons from different valleys and have a net zero center of mass momentum. The lack of inversion and spin splitting implies that these states are admixtures of spin singlets and triplets with nontrivial orbital structure. This allows for the realization of Majorana fermions on a ferromagnetic chain placed in proximity to the unconventional superconductor. A rather remarkable aspect is that valley selective probes couple to one of the electrons of the pair, an ability not available in other superconductors. Consequently, the pair breaking due to circularly polarized light is valley discriminating leading a new type of anomalous Hall effect of the qausi-particles[6].

We demonstrated that attractive interactions and proximity to an s-wave superconductor leads to an inter-valley paired state (type A in Fig.3). The superconducting state is unconventional in that the spin-valley locking leads cooper pairs which are equal mixture of spin singlet and m=0 triplet states. Moreover the pairs live on different Fermi surfaces, one in each valley. Such configuration, in conjunction to strong spin splitting of the hole bands and non zero Berry curvature (nonzero Ω_z in Fig.4) engenders the superconducting state with a number of anomalous properties. We showed that the state is stable against large in-plane magnetic fields. In particular, for ultra-clean

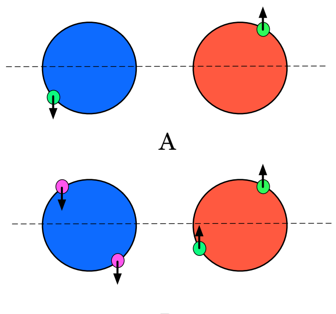

Fig. 3: Two classes of superconductors in TMDS: A) Intervalley paired state, and B) Intravalley paired state.

systems there is no pair breaking effect of the magnetic field and the transition temperature is weakly suppressed due to change in the effective interaction strength. Inter-valley scattering is necessary for the in plane fields to have a pair breaking effect.

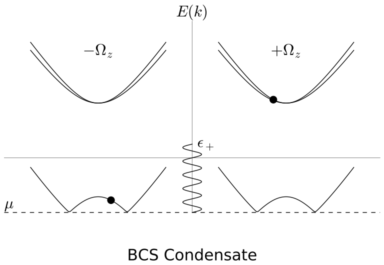

Fig. 4: Pair breaking excitations due to circularly polarized light. For a given polarization a quasipartilce(hole) is generated in the valence band in one valley and the conduction band in the other.

The Berry curvature allows for valley specific particle hole excitations in the normal state. Depending on the polarization light couples preferentially to one valley or the other. One of the questions we aimed to answer is whether the property extended to pair breaking in the superconducting state. Our analysis shows that that this indeed is the case. Fig.4 depicts the pair breaking response for right circularly polarized light where the two quasiparticle generated occupy different valleys and different bands. For opposite polarization the valleys and bands are switched[6].

Another phenomena enabled by the symmetries is the possibility of generating Majorana particles. The system has two of the three needed ingredients namely spin splitting due to large spin orbit coupling and an odd parity component to the superconductivity. If we can also break time reversal symmetry all the necessary ingredients are available to create topological superconductivity. To this end we considered a system where we place a chain of magnetic atoms on the superconducting TMDC. (see Fig.5)

Depending on the relative orientation of the chain with respect to the two dimensional crystal, the spacing between the magnetic atoms, and direction of the spin a large space in parameter exists where majorana bound states appear at the end (see Fig.6). Thus the superconducting state in TMDCs offers a new system for generating topological excitation adding to the list of potential platforms for quantum computation[7].

A key question that arises is what new phenomena is enabled due to valley specific excitations and whether defects such as vortices acquire nontrivial topological character. A related question is whether or not the existence of two fermi surfaces leads to Leggett modes (internal Josephson effect) and how they can be detected if allowed. Our work has uncovered a number of new phenomena. They result from two observations: 1) intra valley pairing involves cooper pairing at finite center of mass momentum and 2) the pair breaking for such superconductors also is valley specific (i.e. addressable by the polarity of incident light). Remarkably the pair breaking at energies corresponding to the superconducting gap (unlike the intervalley case where the energy is of order the band gap) is itself valley selective.

Repulsive interactions tend to stabilize intra-valley paired superconducting states. Since the momentum of the cooper pairs is associated with the K and K' points of the Brillouin

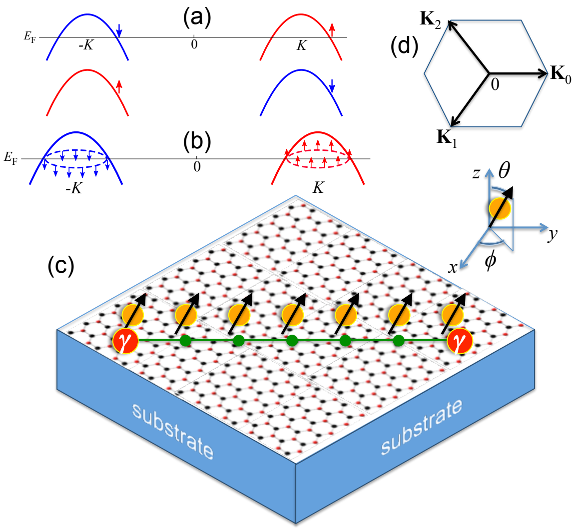

Fig. 5: Schematic illustrations of (a) the lightly-hole doped system and (b) its disconnected Fermi surface pieces with opposite spin directions. (c) Schematic setup of the proposed magnetic moments form a ferromagnetic chain on the monolayer TMD superconductor. We show that Majorana zero modes γ can be realized at the ends of the chain induced by the magnetic moments. (d) Schematic illustration of the three momenta $\mathbf{K}_n$, $n = 0, 1, 2$, associated with the valley centers.

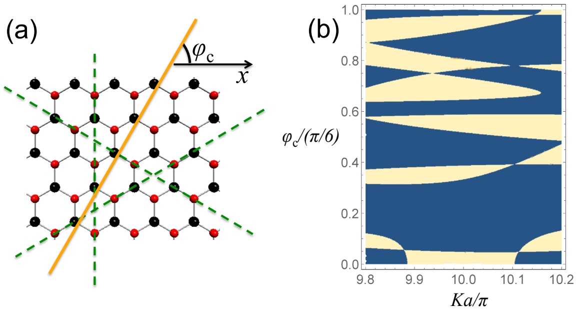

Fig. 6: (a) Schematic illustration of the chain orientation relative to the 2D crystal structure characterized by the angle φ_c. The dash lines correspond to the mirror-plane directions along which the bands are gapless. (b) Calculated topological phase diagram as a function of $\varphi_c \in (0,\ \pi/6)$ and Ka ($K = |\mathbf{K}_n|$ and a is the spacing between magnetic atoms) for the magnetic moments aligning in the crystal plane, i.e., $\theta = \pi/2$. The dark color represents topological phase characterized by an odd number of Majoranas at its ends, whereas the light color refers to non topological phase.

zone, with the net momentum zero, the state is characterized by finite supercurrents which form closed loops within the unit cell. The flux pattern generated by one of the valleys is shown in Fig.7. The supercurrent from the other valley has the opposite chirality and the net flux cancels. This is reminiscent of the FFLO[8,9] phase, except here multiple wave vectors are involved. The fact that that superfluid density of one of the valleys can be depleted by circularly polarized light implies that the flux patterns are revealed under illumination. Currently we are still analyzing if these currents are an artifact of the approximation scheme implemented and that the only effect is to generate a modulated pair density wave. Either

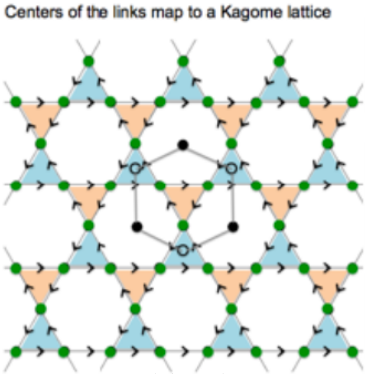

Fig. 7: Intraunitcell flux patterns generated by the supercurrents associated with the Cooper pairs of one of the two valleys. The flux has opposite polarity from the other valley resulting in net zero flux.

result is of great interest and will lead to a publication of signifiant impact.

In addition to phenomena associated with the geometric pattern, these unconventional states also have a nontrivial superconducting phase. The lack of spin degeneracy (and inversion) leads to both chiral and non-chiral order parameters which are/nearly are degenerate within mean field or perturbative renormalization group analysis[10]. As such TMDCs are a rare example where one can study the interplay of the two sectors namely spatial and internal.

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