“Dirac and Weyl Fermions in Topological Semimetals”

POSTER SESSION ABSTRACTS

9-11 March 2016
Jadwin Hall, Room 407

Workshop Organizers
B. Andrei Bernevig
M. Zahid Hasan
Yi Li
Titus Neupert
N. Phuan Ong

This workshop is supported in part by PCCM, MRSEC, and the Gordon and Betty Moore Foundation.
Title: A new form of (unexpected) Dirac fermions in the strongly-correlated cerium monopnictides

Abstract: Discovering Dirac fermions with novel properties has become an important front in condensed matter and materials sciences. Here, we report the observation of unusual Dirac fermion states in a strongly-correlated electron setting, which are uniquely distinct from those of graphene and conventional topological insulators. In strongly-correlated semimetallic cerium monopnictides, we find two sets of highly anisotropic Dirac fermions that interpenetrate each other with negligible hybridization, and show a peculiar four-fold degeneracy where their Dirac nodes overlap. Despite the lack of protection by crystalline or time-reversal symmetries, this four-fold degeneracy is robust across magnetic phase transitions. Comparison of these experimental findings with our theoretical calculations suggests that the observed surface Dirac fermions arise from bulk band inversions at an odd number of high-symmetry points, which is analogous to the band topology which describes a Z2-topological phase. Our findings open up an unprecedented and long-sought-for platform for exploring novel Dirac fermion physics in a strongly-correlated semimetal.
Title: Bosonic Dirac materials in two dimensions

Abstract: We examine the low energy effective theory of phase oscillations in a two-dimensional granular superconducting sheet where the grains are arranged in honeycomb lattice structure. Two different types of collective phase oscillations are obtained, which are analogous to the massive Leggett and massless Bogoliubov-Anderson-Gorkov modes in a two-band superconductor. It is shown that the spectra of these collective bosonic modes cross each other at the K and K points in the Brillouin zone and form a Dirac node. Dirac node dispersion of bosonic excitations is representative of Bosonic Dirac Materials (BDM). We show that the Dirac node is preserved in presence of an inter-grain interaction, despite induced changes of the qualitative features of the two collective modes. Finally, breaking the sublattice symmetry by choosing different on-site potentials for the two sublattices leads to a gap opening near the Dirac node, in analogy with Fermionic Dirac materials.
The discovery of Weyl fermions as quasiparticles in the crystal TaAs provides the first observation of a Weyl fermion in nature and offers a beautiful example of emergence in science. Such crystals, Weyl semimetals, also offer access in condensed matter to fascinating phenomena associated with Weyl fermions in quantum field theory. One important example is the chiral anomaly, where the classical conservation law for the chiral charge of a Weyl fermion is violated by quantum fluctuations. The chiral anomaly in a Weyl semimetal is predicted to give rise to an unusual transport response where the resistance decreases under parallel electric and magnetic fields, called negative longitudinal magnetoresistance (LMR). Crucially, a Weyl semimetal is expected to exhibit the chiral anomaly in a semiclassical transport regime, relevant for device applications. We present our recent magnetoresistance measurements on TaAs, where we observe negative LMR in a semiclassical regime with a characteristic dependence on chemical potential and direction of the applied fields which is the hallmark of the chiral anomaly [1]. Our data strongly supports observation of the chiral anomaly in a Weyl semimetal.

Abstract:

Topological Nodal-line Fermions in PbTaSe2 and TlTaSe2

Topological semimetals can support one-dimensional Fermi lines or zero-dimensional Weyl points in momentum space, where the valence and conduction bands touch. While the degeneracy points in Weyl semimetals are robust against any perturbation that preserves translational symmetry, nodal lines require protection by additional crystalline symmetries such as mirror reflection. Here we report, based on a systematic theoretical study and experimental characterizations, the existence of topological nodal-line states in the non-centrosymmetric compound Pb(Tl)TaSe2 with strong spin-orbit coupling [1,2]. Remarkably, the spin-orbit nodal lines in Pb(Tl)TaSe2 are not only protected by the reflection symmetry but also characterized by an integer topological invariant. Our detailed angle-resolved photoemission measurements, first-principles simulations and theoretical topological analysis illustrate the physical mechanism underlying the formation of the topological nodal-line states and associated surface states for the first time, thus paving the way towards exploring the exotic properties of the topological nodal-line fermions in condensed matter systems.

References:
   Topological Nodal-Line Fermions in Spin-Orbit Metal PbTaSe2, Nature Commun. 7:10556 (2016)

ABSTRACT: We will provide an answer to the question: “What kind of observations and assumptions are minimally needed to formulate a physical theory?” Our answer to this question leads to the new systematic approach of Operational Dynamical Modeling (ODM), which allows to deduce equations of motions from time evolution of observables. Using ODM, we are not only able to re-derive well-known physical theories, but also infer novel physical dynamics (and solve open problems) in the realm of non-equilibrium quantum statistical mechanics.
Effects of the environment on relativistic quantum systems described by the Dirac equation

We present a relativistic formalism of open quantum dynamics in order to take into account effects of the environment that induce decoherence and energy dissipation for systems that are otherwise described by the Dirac equation. We apply this formalism to study an ensemble of relativistic quantum systems considering more realistic conditions in the laboratory. In particular we introduce new Lindbladian equations of motion through a systematic procedure to ensure the validity of physical conditions such as translation invariance and proper Ehrenfest theorems consistent with energy dissipation.

--Renan Cabrera
Princeton University
Jennifer Cano and Barry Bradlyn

"New Fermions"

We explore the types of crystal symmetry-protected free fermionic excitations that can occur in condensed matter systems, going beyond the classification of Majorana, Weyl, and Dirac particles. We exhaustively classify linear and quadratic 3-, 6-, and 8- band crossings stabilized by space group symmetries in solid state systems with spin-orbit coupling and time-reversal symmetry. For each new class of fermion, we analyze its topological properties by constructing low-energy effective Hamiltonians and comment on any possible experimental signatures. In addition, for each space group, we present candidate materials which should realize these exotic fermions, as verified by ab-intio calculations. Finally, we comment on experimental investigations that are currently underway.
Abstract: As opposed to ordinary metals, whose Fermi surfaces are two dimensional, topological (semi-)metals can exhibit protected one-dimensional Fermi lines or zero-dimensional Fermi points, which arise due to an intricate interplay between symmetry and topology of the electronic wavefunctions. Here, we study how reflection symmetry, time-reversal symmetry, SU(2) spin-rotation symmetry, and inversion symmetry lead to the topological protection of line nodes in three-dimensional semimetals. We obtain the crystalline invariants that guarantee the stability of the line nodes in the bulk and show that a quantized Berry phase leads to the appearance of protected surfaces states, which take the shape of a drumhead. By deriving a relation between the crystalline invariants and the Berry phase, we establish a direct connection between the stability of the line nodes and the drumhead surface states. As a representative example of a topological semimetal, we consider Ca$_3$P$_2$, which has a line of Dirac nodes near the Fermi energy.
Boundary effects on Bose-Einstein condensation in ultra-static space-times

The boundary effects on the Bose-Einstein condensation with a non-vanishing chemical potential on an ultra-static space-time are studied. High temperature regime, which is the relevant regime for the relativistic gas, is studied through the heat kernel expansion for both Dirichlet and Neumann boundary conditions. The high temperature expansion in the presence of a chemical potential is generated via the Mellin transform method as applied to the harmonic sums representing the free energy and the depletion coefficient. The effects of boundary conditions on the relation between the depletion coefficient and the temperature are analyzed. Both charged and neutral bosons are considered.
Uncovering new analytical solutions to the Dirac equation.

In this work we provide a new inversion technique developed to find new analytical solutions to the Dirac equation. Given the desired form of the Dirac spinor, which can also be time-dependent and designed such that the particle density follows a predefined and nontrivial trajectory, we can solve for the full vector potential whose solution is the given Dirac spinor. Moreover, the calculated electromagnetic fields satisfy Maxwell's equations. Our technique provides a powerful method to find new analytical solutions for the Dirac equation as well as to design physical realizable fields for practical applications.

Andre Gontijo Campos, Princeton University
Title: A 3+1D fractional chiral metal at the surface of a 4+1D fractional quantum Hall state constructed with coupled-wires.

Abstract: Formulating consistent theories describing strongly correlated metallic topological phases is an outstanding problem in condensed matter. In this work we derive a theory defining a fractionalized analogue of the Weyl semimetal state: the fractional chiral metal. Our approach is to construct a 4+1D quantum Hall insulator by stacking 3+1D Weyl semimetals in a magnetic field. In a strong enough field the low-energy physics is determined by the lowest Landau level of each Weyl semimetal, which is highly degenerate and chiral, motivating us to use a coupled-wire approach. The one-dimensional dispersion of the lowest Landau level allows us to model the system as a set of degenerate 1+1D quantum wires that can be bosonized in the presence of electron-electron interactions and coupled such that a gapped phase is obtained, whose response to an electromagnetic field is given in terms of a Chern-Simons field theory. At the boundary of this phase we obtain the field theory of a 3+1D gapless fractional chiral state, which we show is consistent with a previous theory for the surface of a 4+1D Chern-Simons theory. The boundary’s response to an external electromagnetic field is determined by a chiral anomaly with a fractionalized coefficient. We suggest that such anomalous response can be taken as a working definition of a fractionalized strongly correlated analogue of the Weyl semimetal state.
Title: "Electronic Properties of High-Quality Epitaxial Topological Dirac Semimetal Thin Films"

Abstract:
Topological Dirac semimetals (TDS) are three-dimensional analogues of graphene, with linear electronic dispersions in three dimensions. Thin films of TDSs are a necessary step toward observing the conventional-to-topological quantum phase transition (QPT) with increasing film thickness, and could be interfaced with superconductors (realizing a host for Majorana fermions) or ferromagnets (realizing Weyl fermions or T-broken topological states). Here we report structural and electrical characterization of large-area epitaxial thin films of TDS Na$_3$Bi on single crystal Al$_2$O$_3$[0001] substrates. Charge carrier mobilities exceeding 6,000 cm$^2$/Vs and carrier densities below 1 $\times $10$^{18}$ cm$^{-3}$ are comparable to the best single crystal values. Perpendicular magnetoresistance at low field shows the perfect weak anti-localization behaviour expected for Dirac fermions in the absence of intervalley scattering. At higher fields up to 0.5 T anomalously large quadratic magnetoresistance is observed, indicating that some aspects of magnetotransport in this TDS are yet to be explained.
Motoaki Hirayama

Title:
Topological Dirac Nodal Lines in fcc Calcium, Strontium, and Ytterbium

Abstract:
In nodal-line semimetals, which are among the classes of topological semimetals, the gap closes along loops in k space, which are not at high-symmetry points. We show by ab initio calculations that fcc Ca, Sr, and Yb have topological nodal lines near the Fermi level when the spin-orbit interaction is neglected. These nodal lines do not originate from mirror symmetry, and are purely topological. In the materials having the nodal lines, both the large polarization e/2 and the emergent surface states enhance the Rashba splitting, as we show in Bi/Sr(111) and in the well-known giant Rashba system Bi/Ag(111).
Title: Optical conductivity of disordered Weyl semimetals in collisionless regime

Abstract: We study transport in the disordered Weyl semimetals by considering point-like impurity potentials, which can drive a phase transition from the WSM phase into an exotic diffusive metallic phase. We compute the leading correction due to disorder to the noninteracting collisionless conductivity at zero temperature. As a result, we find that all eight possible types of the point-like disorder potentials give rise to a correction to the optical conductivity and the dielectric constant that is universal up to a sign. We also discuss scaling of the optical conductivity in different phases across the phase diagram of a disordered Weyl semimetal.

Vladimir Juricic
Assistant Professor
NORDITA, Nordic Institute for Theoretical Physics
Roslagstullsbacken 23
10691 Stockholm
Email: juricic@gmail.com; juricic@nordita.org
Emergent spinless Weyl semimetals between the topological crystalline insulator and normal insulator phases with glide symmetry

Heejae Kim$^1$ and Shuichi Murakami$^{1,2}$

$^1$Dept. of Phys., Tokyo Inst. of Tech., $^2$TIES, Tokyo Inst. of Tech.

A topological crystalline insulator (TCI) is one of the symmetry protected topological phases protected by crystalline symmetries such as rotational symmetry, mirror symmetry etc. In recent works, a new class of three-dimensional (3D) Z2 TCI with a nonsymmorphic glide symmetry is theoretically predicted both for spinless and spinful systems [1, 2]. In our presentation, a spinless Weyl semimetal (WSM) phase always emerges between a normal insulator (NI) and TCI phases transition in general glide symmetric spinless systems. In particular, we find how the Z2 topological invariant is changed by the trajectories of Weyl nodes (Figure). Furthermore, we introduce a simple spinless tight-binding model on a 3D orthorhombic lattice with two sublattices and two orbitals with glide symmetry. Using this model, we show that the spinless WSM phase emerges between the NI and TCI phases, and the change of the Z2 topological invariant is related with the motions of Weyl nodes. Our numerical calculation also shows that surface Fermi arcs in the spinless WSM phase evolve into a surface Dirac cone in the TCI phase.

Figure. The trajectories of Weyl nodes within the WSM phase.

Weyl semimetal phase in Pb$_{1-x}$Sn$_x$Te

Jinwoong Kim and Nicholas Kioussis
Department of Physics and Astronomy, California State University

For materials possessing topological phase transition, the Weyl semimetal phase can be induced by breaking either the time-reversal or inversion symmetry. The topological crystalline insulator, Pb$_{1-x}$Sn$_x$Te exhibits topological phase transition upon the band inversion strength which can be tailored by the substitutional mixing ratio, strain, thermal expansion, ferroelectric displacement, and/or material thickness via quantum confinement effect. The SnTe, building block of the compound, is also known to have a ferroelectric transition at low temperature which leads to inversion symmetry breakdown. Therefore Pb$_{1-x}$Sn$_x$Te is a potential Weyl semimetal and diverse topological phases are expected. In this study, using density functional calculations we explored the parameter space associated with both band inversion and ferroelectric displacement by. Due to the subtle change of the band gap, tight-binding model calculations have been carried out within the virtual crystalline approximation where the tight-binding parameters are extracted from ab-initio calculations via the Wannierization procedure. The evolution of Weyl points with pressure and the consequent Fermi arc emerging on the surface will be discussed.
Title: Spectroscopic signatures of Weyl semimetals beyond photoemission

Abstract: Weyl semimetals constitute a newly discovered class of three-dimensional topological materials with linear touchings of valence and conduction bands in the bulk. The defining spectroscopic characteristics of Weyl semimetals --- open Fermi surfaces at the boundary (Fermi arcs) and linear band touchings in the bulk (Weyl nodes) --- have so far only been observed in angle-resolved photoemission experiments. I will present how Fermi arcs and Weyl nodes manifest themselves in two alternative probes that measure exclusively either the surface or the bulk, namely, scanning tunnelling spectroscopy and resonant inelastic x-ray scattering, respectively. For the latter, I will show how the topological charge of a Weyl node can be inferred from experimentally obtained spectra.

Rex Lundgren, University of Texas

Title: Electronic cooling in Weyl and Dirac semimetals

Abstract:

Energy transfer from electrons to phonons is an important consideration in any Weyl or Dirac semimetal based application. In this work, we analytically calculate the cooling power of acoustic phonons, i.e. the energy relaxation rate of electrons which are interacting with acoustic phonons, for Weyl and Dirac semimetals in a variety of different situations. For cold Weyl or Dirac semimetals with the Fermi energy at the nodal points, we find the electronic temperature, $T_e$, decays in time as a power law. In the heavily doped regime, $T_e$ decays linearly in time far away from equilibrium. In a heavily doped system with short-range disorder we predict the cooling power of acoustic phonons is drastically increased because of an enhanced energy transfer between electrons and phonons. When an external magnetic field is applied to an undoped system, the cooling power is linear in magnetic field strength and $T_e$ has square root decay in time, independent of magnetic field strength over a range of values.

Magnetotransport in Dirac metals: Chiral magnetic effect and quantum oscillations

Dirac metals are characterized by the linear dispersion of fermionic quasiparticles, with the Dirac point hidden inside a Fermi surface. We study the magnetotransport in these materials using chiral kinetic theory to describe within the same framework both the negative magnetoresistance caused by the chiral magnetic effect and quantum oscillations in the magnetoresistance due to the existence of the Fermi surface. We also consider the role of Fermi Arcs and their contribution for the SdH modes. We discuss the relevance of obtained results to recent measurements on $Cd_3As_2$. 
Lukas Muechler
PhD student Car Lab
Department of Chemistry
151 Frick Laboratory
Princeton University
http://chemists.princeton.edu/car/

Title: Type-II Dirac fermions in the topological semimetals WTe$_2$ and MoTe$_2$
Abstract: We introduce the notion of a band-inverted, topological semimetal, in two-dimensional non-symmorphic crystal structures with a glide mirror symmetry. This concept is materialized in the monolayers of WTe$_2$ and MoTe$_2$ without spin-orbit coupling. We characterize the Dirac band touching topologically via a non-Abelian Wilson-loop invariant. An additional feature of the Dirac cone in monolayer WTe$_2$ and MoTe$_2$ is that it tilts over in a Lifshitz transition to produce electron and hole pockets -- a type II Dirac cone. These pockets, together with the pseudospin structure of the Dirac electrons, suggest a unified, topological explanation for the recently-reported, non-saturating magnetoresistance in WTe$_2$, as well as its circular dichroism in photoemission.
We complement our analysis and first principle band structure calculations with an \{it ab-inito\}-derived tight-binding model for the mono- and bilayer of WTe$_2$. 
Jedediah H. Pixley and David A. Huse

Avoided quantum criticality in disordered three-dimensional Dirac and Weyl semi-metals

We study the effects of short-range random potential disorder on three-dimensional Dirac and Weyl semi-metals. We focus on the proposed quantum critical point (QCP) separating a semi-metal and diffusive metal phase driven by disorder. We will briefly review the existing evidence of such a QCP. We will then explore the non-perturbative effects of rare regions using Lanczos and the kernel polynomial method, from which we establish the existence of two distinct types of excitations in the weak disorder regime. The first are perturbatively renormalized dispersive Dirac states and the second are weakly dispersive quasi-localized “rare” eigenstates. We establish that these rare eigenstates contribute an exponentially small but non-zero density of states at zero energy, thus converting the semi-metal to diffusive metal transition into an avoided quantum critical point.
**Title:** Multi-polar orders and Weyl fermions in pyrochlore iridates.

**Poster presenter:** Bitan Roy, University of Maryland.

**Abstract:** Presently the notion of Weyl fermions is placed at the center stage of condensed matter physics due to recent discovery of Weyl semimetals in many gapless semiconductors. Among several interesting physical properties, perhaps the most tantalizing one is the possibility of observing a large anomalous Hall effect in this system. A question of fundamental importance then arises quite naturally whether the notion of Weyl fermions can provide resolution to an outstanding problem in strongly correlated materials where emergent Hartree-Fock quasiparticles inside a magnetically ordered broken symmetry phase leads to linear touching among Kramers non-degenerate valence and conduction bands at few isolated points in the Brillouin zone. I will argue that an itinerant $3$-in $1$-out order in the pyrochlore lattice of $227$ iridate, which is a linear combination of dipolar and octupolar quantities and built out of spin-ice manifold, can support such exotic broken symmetry phase and lead to a large anomalous Hall effect despite a tiny magnetic moment in the system, when the onsite Hubbard repulsion is sufficiently strong. Such magnetic order can explain multiple enigmatic experimental observation in $\text{Pr}_2\text{Ir}_2\text{O}_7$ at low temperature. I will also address the competition between the $3$-in $1$-out and all-in all-out orders, the later one being a purely octupolar object that also gives birth to Weyl fermions (but does not support anomalous Hall effect), and propose the global phase diagram of $227$ pyrochlore iridates. The variation of anomalous Hall effect across various phases will be highlighted and the effects of an external strain that in turn can boost the anomalous Hall signal will be discussed.
Title: Topological Massive Dirac Edge Modes and Long-Range Superconducting Hamiltonians.

Abstract: I will present a generalisation of the one-dimensional Kitaev chain modified by long-range Hamiltonian deformations in the hopping and pairing terms. This class of models display symmetry-protected topological order measured by the Berry phase of the ground state and the winding number of the Hamiltonians. For exponentially-decaying hopping amplitudes, the topological sector can be significantly augmented as the penetration length increases, something experimentally achievable in synthetic many-body systems.

For power-law decaying superconducting pairings, the massless Majorana modes at the edges get paired together into a massive non-local Dirac fermion localised at both edges of the chain: a new topological quasiparticle that we call topological massive Dirac fermion. This topological phase has fractional topological numbers as a consequence of the long-range couplings. Possible applications to current experimental setups and topological quantum computation will be also discussed.

Double Dirac Semimetals in Three Dimensions

Benjamin J. Wieder, Youngkuk Kim, A. M. Rappe, C. L. Kane

We study a class of Dirac semimetals that feature an eightfold-degenerate double Dirac point. We show that 7 of the 230 space groups can host such Dirac points and argue that they all generically display linear dispersion. We introduce an explicit tight-binding model for space groups 130 and 135, showing that 135 can host an intrinsic double Dirac semimetal -- one with no additional degeneracies at the Fermi energy. We consider symmetry-lowering perturbations and show that uniaxial compressive strain in different directions leads to topologically distinct insulating phases. In addition, the double Dirac semimetal can accommodate topological line defects that bind helical modes. Potential materials realizations are discussed.

If you find it helpful when considering our poster, you can find additional information about this project from our paper on the arxiv:

http://arxiv.org/abs/1512.00074
Title: Disorder driven superconducting phases in a three-dimensional spinless $p+ip$ superconductor

Abstract: We study the effects of quenched disorder on the three dimensional spinless $p+ip$ superconductor. The relevant clean BCS Hamiltonian in class D supports a trivial thermal insulator and a thermal Hall/Chern insulator which are separated by two distinct Majorana-Weyl thermal Hall semimetals. By using kernel polynomial method we compute average and typical density of states for constructing the global phase diagram in the presence of disorder. The gross features of the phase diagram are consistent with the perturbative stability of the Majorana-Weyl phase for weak disorder, but the nonperturbative effects actually convert the thermal Hall semimetal to a thermal Hall metal. Consequently in the presence of disorder, a class D model only supports two insulating or localized phases separated by a metallic one. We discuss various crossover regimes obtained from our extensive numerical results which we justify through analytical calculations.

Justin H. Wilson, CalTech
Weyl fermion materials may open a new era in condensed matter physics and materials science. They are semimetals, metals, photonic crystals and superconductors whose quasiparticle excitation is the Weyl fermion, a particle that is well-known in the standard model but has not been observed in vacuum. Such a fermion carries an unusual charge, the chiral charge, but, unlike other fermions, must be massless. These properties of the elusive particle in high energy physics have direct analogs in its low-energy solid-state counterpart, leading to wild ranging new physics. We present our theoretical prediction (Huang et al. Nature Commun. 6, 7373 (2015)) and experimental discovery of the first Weyl fermion semimetal state with topological Fermi arcs in the tantalum arsenide, TaAs class of materials (Xu et al. Science 349, 613 (2015); Xu et al. Science 347, 294 (2015)), which also includes NbAs (Xu et al. Nature Phys. 11, 748 (2015)), TaP (Xu et al. Science Advances 1, e1501092 (2015)) and NbP (Belopolski et al. Phys. Rev. Lett. 116, 066802 (2016); Zheng et al. ACS Nano 10, 1378 (2016)). We hope that our discovery can pave the way for realizing the many predicted new physics associated with Weyl fermions.
Quasiparticle interference on Weyl semimetal NbP(001)

Hao Zheng
Princeton University

Weyl semimetals may be the next research focus in condensed matter physics, materials science, and nanotechnology after graphene and topological insulators. We represent the first atomic scale view of the surface states of a Weyl semimetal NbP(001) using scanning tunneling microscopy/spectroscopy[1]. We observe quantum interference patterns that arise from the scattering of quasiparticles near point defects on the surface. The measurements reveal the surface electronic structure both below and above the chemical potential. Moreover, the interference maps uncover the scattering processes of NbP's exotic surface states. Through comparison between experimental data and theoretical calculations, we further discover that the orbital and/or spin texture of the surface bands may suppress certain scattering channels on NbP[2]. These results provide a comprehensive understanding of electronic properties on Weyl semimetal surfaces.

ACS Nano 10, 1378 (2016)