Non-Fermi-Liquid and Topological States with Strong Spin-Orbit Coupling

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We argue that a class of strongly spin-orbit-coupled materials, including some pyrochlore iridates and the inverted band gap semiconductor HgTe, may be described by a minimal model consisting of the Luttinger Hamiltonian supplemented by Coulomb interactions, a problem studied by Abrikosov and collaborators. It contains twofold degenerate conduction and valence bands touching quadratically at the zone center. Using modern renormalization group methods, we update and extend Abrikosov's classic work and show that interactions induce a quantum critical non-Fermi-liquid phase, stable provided time-reversal and cubic symmetries are maintained. We determine the universal power-law exponents describing various observables in this Luttinger-Abrikosov-Beneslavskii state, which include conductivity, specific heat, nonlinear susceptibility, and the magnetic Gruneisen number. Furthermore, we determine the phase diagram in the presence of cubic and/or time-reversal symmetry breaking perturbations, which includes a topological insulator and Weyl semimetal phases. Many of these phases possess an extraordinarily large anomalous Hall effect, with the Hall conductivity scaling sublinearly with magnetization $\sigma_{xy} \sim M^{0.51}$.

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Divining the nature of critical non-Fermi-liquid (NFL) phases of electrons is one of the most outstanding problems in correlated electron systems, such as cuprates, pnictides, and heavy fermion materials [1–4]. Motivated by these materials, theoretical research has focused on models with large Fermi surfaces (or Fermi pockets). In spite of the recent technical advances [5], a clear resolution of experimental puzzles awaits deeper understanding.

In this work, we uncover another venue for NFL physics. Recent theory and experiment have revealed a new frontier for correlated phenomena: Mott correlation physics in materials with strong spin-orbit coupling (SOC) [6,7]. Of particular interest in this regard are the $5d$ transition metal oxides, where compelling evidence has been built for Mott phenomena driven cooperatively by SOC and Coulomb interactions [6–8]. This paper explores distinct NFL states that exist only in the strong SOC regime.

We are particularly motivated by the pyrochlore iridates $A_2Ir_2O_7$, where A is a lanthanide element [9,10]. These materials display $T > 0$ metal-insulator transitions, with the metal-insulator transition temperature decreasing with increasing A radius. The progression culminates with $Pr_2Ir_2O_7$, which is a highly unconventional metal down to the lowest temperatures [11,12]. It displays logarithmic NFL behavior of the magnetic susceptibility and a remarkably enormous zero field anomalous Hall effect (AHE) in the absence of any measurable magnetization [11,12].

With these studies as motivation, we utilize prior studies of the electronic structure of pyrochlore iridates [13–15] to show that a minimal description for the electronic states in their paramagnetic phase is a storied Hamiltonian from semiconductor physics: the Luttinger model of inverted band gap semiconductors [16]. This model has gained recent notoriety for its relevance to HgTe, the starting material for some topological insulators [17–20]. While HgTe is a weakly correlated material where band structure alone provides a sufficient description, in the $5d$ materials, the Luttinger Hamiltonian must be supplanted by interactions.

In this Letter, we carry out such an analysis, rediscovering and extending a storied analysis by Abrikosov and Beneslavskii of Coulomb forces on the Luttinger problem [21,22]. Using modern renormalization group (RG) techniques, we confirm Abrikosov's conclusion that long-range Coulomb interactions convert the quadratic band touching into a quantum critical NFL, prove the stability of the state within an ϵ expansion, and calculate the full set of anomalous dimensions characterizing the state. Consequently, we call the resulting phase a Luttinger-Abrikosov-Beneslavskii (LAB) state. While the LAB phase is stable in the presence of time-reversal and cubic symmetries, we show that it is a "parent" state for other exotic states that can be reached by breaking either or both of these: metallic and double-Weyl semimetallic phases with enormous AHEs, and topological insulators. We discuss the implications for the iridates at the end of the Letter.

The LAB phase itself has striking properties. Its NFL nature is revealed directly by algebraic singularities in the electron spectral function (probed in angle-resolved photoemission) and in optical conductivity, as well as indirectly through many power-law thermodynamic and response functions.

We now turn to the exposition of these results. We consider the paramagnetic band structure based on prior work [13–15], which argued that the states at the zone center (Γ point) near the Fermi energy are comprised of the four-dimensional representation, which can be described by "angular momentum" operators $\vec{J}$ (which are $j = 3/2$ matrices) transforming as the T_2 representation of the cubic group. In our minimal model, we assume only these states close to Γ are important. Then, $k \cdot p$ theory and cubic symmetry determine the band structure in their vicinity to be precisely described by the Luttinger Hamiltonian with three effective mass parameters [16,23]

$$\mathcal{H}_0(k) = \frac{k^2}{2\tilde{M}_0} + \frac{\frac{5}{4}k^2 - (\vec{k} \cdot \vec{J})^2}{2m} - \frac{(k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2)}{2M_c}.$$

This describes doubly degenerate bands with energy

$$E_\pm(k) = \frac{k^2}{2M_0} \pm \sqrt{\left(\frac{k^2}{2m}\right)^2 + \frac{m + 2M_c}{4mM_c^2} p_c(k)}, \quad (1)$$

where $p_c(k) = \sum_i k_i^4 - \sum_{i \neq j} k_i^2 k_j^2$ and $M_0 = (4M_c\tilde{M}_0)/(4M_c - 5\tilde{M}_0)$. Henceforth, we assume $M_0 > m$, which describes conduction and valence bands touching quadratically at $E = k = 0$, where the chemical potential for the undoped material crosses.

The LAB is obtained by adding to this the long-range Coulomb interaction. We implement the latter by a scalar potential φ, which in the Euclidean path integral formalism gives the action

$$S_L = \int d\tau d^d x \{\psi^\dagger [\partial_\tau - ie\varphi + \hat{\mathcal{H}}_0]\psi + \frac{c_0}{2}(\partial_i \varphi)^2\}, \quad (2)$$

with $\hat{\mathcal{H}}_0 = \mathcal{H}_0(-i\vec{\nabla})$ and $c_0 = 1/4\pi$. Here, ψ is a four-component spinor, but subsequently we will artificially add an additional $U(N_f)$ flavor index, which allows a check on our calculations by large N_f methods; the physical case is $N_f = 1$. Equation (2) contains, in addition to the three mass parameters, the Coulomb coupling constant e. For $e = 0$, scale invariance is manifest, with the scaling dimensions $[x^{-1}] = 1$, $[\tau^{-1}] = z$, $[\psi] = (d/2)$, $[(1/m)] = z - 2$, and $[\varphi] = (d + z - 2)/2$. Here, we introduce the dynamic critical exponent (z), which is naturally $z = 2$ with $e = 0$ but will become nontrivial with interactions.

Directly in the physical case $d = 3$, the dimension of the coupling constant is $[e^2] = 1$, so Coulomb interactions are strongly relevant. Therefore, we employ the $\varepsilon = 4 - d$ expansion to control the RG analysis. As is familiar from quantum electrodynamics, three one loop Feynman diagrams contribute to leading order in ε: the fermion self-energy, boson self-energy, and vertex correction. Here, we show that the relevance of Coulomb interactions signals, rather than a flow to strong coupling and a symmetry breaking instability, the formation of a new stable interacting fixed point, which describes the critical non-Fermi-liquid LAB state (Abrikosov's analysis tacitly assumes this stability).

The RG is carried out perturbatively in e but nonperturbatively in the mass parameters. Thus, a full treatment gives nontrivial and complete beta functions for the two dimensionless mass ratios m/M_0 and m/M_c; these are given in the Supplemental Material [24]. The analysis of the full RG shows, however, that there is a single stable isotropic fixed point corresponding to $m/M_0 = m/M_c = 0$, so for simplicity, we quote in the main text only the results in the vicinity of this point.

In this limit, the leading contribution to the bosonic self-energy becomes

$$\frac{1}{N_f}\Sigma_\varphi(q, 0) = -(2m)e^2 \left[\int \frac{d^d k}{(2\pi)^d} \frac{1}{k^4}\right] \times q^2, \quad (3)$$

where we took the $\omega \to 0$ limit because frequency dependence is subdominant. The divergence should be absorbed by rescaling the bosonic field $\varphi \to e^{-\eta_b d\ell}\varphi$ upon reduction of the hard momentum cutoff $\Lambda \to e^{-d\ell}\Lambda$, which defines the RG parameter ℓ. This gives the bosonic anomalous dimension $\eta_b = 2N_f u$ [25], where the dimensionless coupling constant is $u = (me^2/8\pi^2 c_0 \Lambda^{4-d})$, which has the physical meaning in $d = 3$ of the ratio of the real space cutoff to the effective Bohr radius. The frequency dependence of the one loop fermionic self-energy and the vertex correction both vanish, the result of a Ward identity. For $k \neq 0$, the fermion self-energy gives mass corrections, e.g., $\delta(1/m) = 8u/(15m) \times d\ell$ to leading order. Detailed analysis is given in the Supplemental Material [24].

Given these calculations, we choose $z = 2 - 8u/15$ to keep the mass m fixed, which gives the RG equations, to lowest order in m/M_c, m/M_0,

$$\frac{d}{d\ell}u = \varepsilon u - \frac{30N_f + 8}{15}u^2, \qquad \frac{d}{d\ell}\left(\frac{m}{M_c}\right) = -0.152u\left(\frac{m}{M_c}\right),$$
$$\frac{d}{d\ell}\left(\frac{m}{M_0}\right) = -\frac{8}{15}u\left(\frac{m}{M_0}\right). \quad (4)$$

From the first equation above, we find the fixed point coupling and hence dynamical exponent

$$u^* = \frac{15}{30N_f + 8}\varepsilon, \qquad z = 2 - \frac{4}{15N_f + 4}\varepsilon, \quad (5)$$

and since $u^* > 0$, the second line in Eq. (4) implies both m/M_0 and m/M_c are irrelevant. This establishes the existence and nature of the stable, isotropic fixed point describing the LAB phase. As a check, we have carried out a large N_f expansion, which gives the same bosonic anomalous dimension as in the ε expansion at the one-loop level, supporting the stability of the LAB phase.

The presence of the stable interacting fixed point can be understood physically as a balance of partial dynamical screening of the Coulomb interactions by electron-hole pairs and mass enhancement of the same quasiparticles by pairs. This situation is in sharp contrast to the case of a vanishing indirect band gap, for which to leading order in the long-range Coulomb interaction electrons and holes are separately conserved, so there is no screening by virtual electron-hole pairs, and exciton formation destabilizes the putative gapless state [26].

Using the RG, we can evaluate the anomalous dimension of any physical operator. By charge conservation, $[\psi^\dagger\psi] = d$. Because of the isotropy of the fixed point, there are only two nontrivial values for the other charge-conserving fermion bilinear operators. We obtain $[\psi^\dagger\Gamma_a\psi] = d + \eta_1$ and $[\psi^\dagger\Gamma_{ab}\psi] = d + \eta_{12}$, where Γ_a are the (time-reversal invariant) Dirac gamma matrices, $\Gamma_{ab} = -(i/2)[\Gamma_a, \Gamma_b]$ are time-reversal odd, and $a, b = 1, 2, \ldots, 5$. Using the standard operator insertion technique, we find $\eta_1 = -(6/15N_f + 4)\varepsilon$ and $\eta_{12} = -(3/15N_f + 4)\varepsilon$. These operators describe many physical observables, e.g., the "angular momentum" operator $J_z \sim \psi^\dagger(-\Gamma_{34} - \frac{1}{2}\Gamma_{12})\psi$. The negative anomalous dimension of these operators suggests a schematic picture of power-law excitons due to electron-hole attraction. For pairing channels, we find positive anomalous dimensions, consistent with this view. The local pairing channel has $\eta_{\text{pairing}} = (u^*/5) = (3/30N_f + 8)\epsilon$.

Using these results, we obtain thermodynamic responses such as the specific heat $c_v \sim T^{d/z} \approx T^{1.7}$ and the spin susceptibility $\chi(T) \sim a + bT^{(d-z+2\eta_{12})/z} \approx a + bT^{0.5}$, with some constants a and b. Interestingly, the nonlinear susceptibility $\chi_3 = \partial^3 M/\partial H^3|_{H=0} \sim T^{-(3z-4\eta_{12}-d)/z} \approx T^{-1.7}$ diverges, as in spin glasses but with completely different physics. Comparing the scaling of current and electric field gives the usual result $[\sigma_{ij}] = d - 2$. Consequently, the temperature and frequency dependence of the conductivity is $\sigma(\omega, T) \sim T^{1/z}\mathcal{F}(\omega/T)$, and a clean, undoped LAB is therefore a power-law insulator, where $\mathcal{F}(x)$ is a scaling function for optical conductivity.

We now turn to the effect of applied strain and Zeeman field upon the LAB. These perturbations break cubic or time-reversal symmetries and thus destabilize the LAB. Because of the isotropic nature of the LAB fixed point, the response to the Zeeman field alone is to leading order independent of its direction (the cubic mass $1/M_c$ can be "dangerously irrelevant," however—see below), so we take it to lie along the (001) direction. We consider for simplicity tetragonal strain which preserves C_4 rotation about this axis (in the absence of Zeeman field, the direction of strain is again unimportant). This leads to the perturbations

$$\mathcal{H}' = -\delta(J_z^2 - \frac{5}{4}) - H[\cos(\theta)J_z + \sin(\theta)J_z^3], \quad (6)$$

where δ parametrizes the strain, H is the Zeeman field, and θ controls the strength of the cubic Zeeman term allowed by the cubic symmetry [27,28]. Using the RG results, the dimensions of these perturbations are $[\delta] = z - \eta_1 \approx 2.1$ and $[H] = z - \eta_{12} \approx 1.9$; i.e., strain is slightly enhanced while the Zeeman field is slightly suppressed by interactions. However, both dimensions are positive and close to 2, so that they are strongly relevant. They flow to strong coupling under the RG, and the fate of the system must be reanalyzed in the limit.

To do so, we assume, and check self-consistently, that interactions have weak effects at strong coupling, and simply solve the quadratic Hamiltonian (with $m/M_0 = m/M_c = 0$) in the presence of the renormalized $\mathcal{H}'$. The result depends upon the dimensionless quantities θ and the renormalized coupling ratio $\Delta = (\delta/H)_R \sim \delta/H^{(z-\eta_1)/(z-\eta_{12})}$. For $H = 0$ ($\Delta = \infty$), we have time-reversal invariance, and we recover the known result that strain $\delta > 0$ induces a gapped, $3d$ topological insulator phase, as observed in HgTe [19]. The situation in an applied Zeeman field is more interesting. Notice that for $\vec{k} = k\hat{z}$, J_z is a good quantum number, and there is no level repulsion between bands of different J_z. This allows (nondegenerate) bands to cross along this axis, which indeed occurs when $|\Delta|$ is not too large. Further analysis in the Supplemental Material [24] shows that these crossings correspond to a pair of double-Weyl points, with linear dispersion along the z axis and quadratic dispersion normal to it. These points are strength ± 2 monopoles in momentum space. Away from the k_z axis, electron and hole pockets may accidentally cross the Fermi energy. If this does not occur, one has a pristine double-Weyl semimetal, which occurs for the angular range $\theta_1 \le \theta \le \theta_2$, where $\theta_1 = -\tan^{-1}[(8 + 4\sqrt{3})/(7\sqrt{3} + 26)]$ and $\theta_2 = \tan^{-1}[(8 - 4\sqrt{3})/(7\sqrt{3} - 26)]$ for $\delta = 0$, as shown in the horizontal axis of Fig. 1.

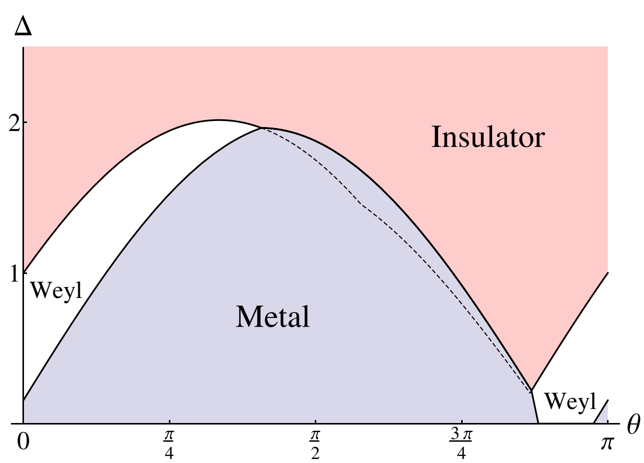

FIG. 1 (color online). Phase diagram of the perturbed LAB in the space of renormalized strain to Zeeman field ratio $\Delta \equiv (\delta/H)_R$ versus cubic Zeeman angle θ. The subscript (R) is for anomalous dimensions of strain and Zeeman field (see the text). "Weyl" denotes the (double-)Weyl semimetal, "Ins." the insulator, and "Metal" a metallic phase which has Weyl points shifted from the Fermi energy in the region below the dashed line. For $H = 0$, the insulator is a topological insulator.

When $0 < |\Delta| < \infty$, we observe insulating, double-Weyl semimetal and Weyl metal (with coexisting electron-hole pockets) phases, as shown in Fig. 1. Note that in all these phases, the Coulomb interactions become either unimportant (in the insulator), screened (in the metal), or marginally irrelevant (in the Weyl semimetal), justifying our treatment of the phase diagram to a first approximation.

More subtle effects may make small modifications to this picture. Coulomb interactions can destabilize some of the quantum phase transitions in Fig. 1, leading to intermediate phases. When the magnetic field is applied along a low symmetry axis, the double-Weyl points can split into multiple single-Weyl points, once the effects of the cubic mass $1/M_c$ are included, which are dangerously irrelevant in this case.

A striking experimental consequence of this phase diagram is the AHE due to the Zeeman field, which could originate either from an external magnetic field or as an exchange field due to local moments in the material. The latter is particularly interesting in light of the experimental results on $Pr_2Ir_2O_7$, which shows a large AHE in a regime where the magnetization M is immeasurably small [11,12]. On symmetry grounds, $\sigma_{xy} \neq 0$ implies $M \neq 0$, but evidently σ_{xy} is unusually large relative to M. This behavior is in fact characteristic of the LAB: since the Hall conductivity has dimensions of inverse length, we expect $\sigma_{xy} \sim H^{1/(z-\eta_{12})} \approx H^{0.51}$. In the situation relevant for $Pr_2Ir_2O_7$, the Zeeman field is generated by Kondo exchange with the Pr moments, so $H \sim J_K M$, with M the (dimensionless) Pr magnetization, which implies a highly unconventional sublinear dependence of σ_{xy} on M for the pristine LAB. If the Fermi level is displaced from the band touching by an amount ϵ_F, then we expect, treating the above power as a square root, $\sigma_{xy} \sim (e^2/h)\sqrt{(mH/\hbar^2)}\mathcal{S}(H/\epsilon_F)$, where $\mathcal{S}$ is a scaling function (see the Supplemental Material [24]). This gives an order of magnitude quantitative estimate

$$\sigma_{xy} \sim 10^3\ \Omega^{-1}\,\mathrm{cm}^{-1} \times \begin{cases} \sqrt{\frac{m}{m_e}}\sqrt{\frac{J_K}{\mathrm{Ry}}}\sqrt{M} & J_K M \gg \epsilon_F \\ \sqrt{\frac{m}{m_e}}\frac{J_K}{\sqrt{\epsilon_F \mathrm{Ry}}} M & J_K M \ll \epsilon_F, \end{cases} \tag{7}$$

where $\mathrm{Ry} = 13.6$ eV is the Rydberg, and m_e is the electron mass. The lower regime gives $\sigma_{xy} \sim 0.1\ \Omega^{-1}\,\mathrm{cm}^{-1}$, within an order of magnitude of observations in $Pr_2Ir_2O_7$ [12], for parameters $m \sim 20 m_e$ (estimated from the calculations in Ref. [15]), $\epsilon_F \sim 10$ meV, $J_K \sim 100$ K (estimated from the measured Curie-Weiss temperature), and $M \sim 0.01$.

Another interesting experimental observation in $Pr_2Ir_2O_7$ is a diverging magnetic Gruneisen number $\Gamma_H = (1/T)(\partial T/\partial H)|_S$ in the zero field limit [29–31]. In a purely electronic system with no local moment contribution to the entropy, we can readily obtain the behavior of the LAB in the low temperature limit

$$\Gamma_H(H,T) = -\frac{d - y_0 z}{y_0(z - \eta_{12})}\frac{1}{H}, \tag{8}$$

which depends upon the exponent y_0 defining the temperature dependence of the specific heat $C \sim T^{y_0}$ of the LAB phase. In the Weyl metal, $y_0 = 1$ and $\Gamma_H < 0$, while for isolated double-Weyl points, $y_0 = 2$ and $\Gamma_H > 0$. Thus, one may imagine a sign change of the Gruneisen number when field or strain is varied. Note that in $Pr_2Ir_2O_7$, there is certainly a large local moment contribution to the entropy, so that Eq. (8) is not literally applicable. Nevertheless, the LAB physics may play some role in this quantity.

In conclusion, we have described a novel NFL phase occurring in correlated strong SOC systems, with a natural connection to the pyrochlore iridates. Even with weak correlation effects, some of the phenomena discussed here can be observed with only minor modifications, and it would be interesting to search for them in HgTe. Future theoretical studies should include a more comprehensive treatment of the breaking of cubic symmetries and the effects of disorder and doping.

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