A new route to relativistic insulators: Lifshitz transition driven by spin fluctuations and spin-orbit renormalization in NaOsO$_3$

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In systems where electrons form both dispersive bands and small local spins, we show that changes of the spin configuration can tune the bands through a Lifshitz transition, resulting in a continuous metal-insulator transition associated with a progressive change of the Fermi surface topology. In contrast to a Mott-Hubbard and Slater pictures, this spin-driven Lifshitz transition appears in systems with small electron-electron correlation and large hybridization. We show that this situation is realized in 5$d$ distorted perovskites with an half-filled $t_{2g}$ bands such as NaOsO$_3$, where the strong $p$−$d$ hybridization reduces the local moment, and spin-orbit coupling causes a large renormalization of the electronic mobility. This weakens the role of electronic correlations and drives the system towards an itinerant magnetic regime which enables spin-fluctuations.

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Metal-to-insulator transitions (MITs) are one of the most important phenomena in solid-state physics and their fundamental understanding represents an enduring challenge in solid state theory [1, 2]. Different mechanisms have been invoked to explain the formation of an insulating regime. Classical examples are realized in 3$d$ transition metal oxides (TMOs), where the nonconducting state is typically understood within the Mott-Hubbard model as arising from the competition between strong electron-electron interaction ($U$) and the electronic mobility, associated to the (non-interacting) bandwidth ($W$) [3-5]. When moving to the more spatially extended 4$d$ and 5$d$ orbitals the $W$ increases and the $U$ is expected to become smaller, leading to the tendency towards metallic as in the itinerant magnet SrRuO$_3$ [6]. In contrast to these theories, recent theory and experiment have revealed that in ‘heavy’ 5$d$ TMOs, the enhanced spin-orbit coupling (SOC) strength [7] can lead to the formation of a variety of novel types of quantum states including unexpected insulating regimes [8-11]. In the most representative example, Sr$_2$IrO$_4$, the concerted action of a strong SOC and a moderate $U$ leads to the opening of a small spectral gap [11, 12] denominated relativistic Mott gap. Other and more rare types of MITs have been recently proposed for magnetic relativistic osmium oxides based on the Slater mechanism [13-16], driven by antiferromagnetic (AFM) order, where the gap is opened by exchange interactions and not by electronic correlation, [17] or Lifshitz-like processes [18, 19], involving a rigid change of the Fermi surface topology [20].

In this work we show that in weakly correlated (small $U$) itinerant magnets the combined effect of longitudinal and rotational spin-fluctuations can cause a continuous MIT with Lifshitz characteristics, fundamentally different from relativistic Mott or purely Slater insulating states. The necessary conditions for the onset of this type of spin-driven Lifshitz MIT are the coexistence of a small $U$, a small local moment and an high degree of orbital hybridization. This places the system at the border of a magnetic and electronic instability where a Lifshitz MIT is possible. This situation can be realized in structurally-distorted, half-filled $t_{2g}$ (or close to half-filled) 5$d$ oxides such as NaOsO$_3$ and Cd$_2$Os$_2$O$_7$ or iridates. By taking NaOsO$_3$ as a prototypical example, we show that here the balance between $U$ and $W$ is controlled by the SOC: the SOC induces a surprisingly large reduction of electronic mobility which renormalizes the $U$ and pushes the system into a weakly correlated and magnetically itinerant regime subjected to spin fluctuations. We find that at high-temperature NaOsO$_3$ is a paramagnetic metal but as temperature decreases the changes of the amplitude and direction of the spins lead to the continuous vanishing of holes and electrons pockets in the Fermi surface (FS), that do not involve any substantial modification of the underlying band structure [20], consistent with a Lifshitz-type MIT.

Experimental observations indicate that NaOsO$_3$ undergoes a second-order MIT concomitant with the onset of an antiferromagnetic long-range ordering at a Néel temperature ($T_N$) of $\approx$ 410 K. This behavior is apparently adaptable to a Slater mechanism [13, 21]. However, the bad-metal behavior observed in a wide intermediate temperature region ($0.1 T_N < T < T_N$) [13], the Curie-Weiss behavior of the susceptibility above $T_N$, and the need of a sizable $U$ in Density Functional Theory (DFT) calculations to open the gap, is in conflict with an authentic Slater mechanism [21, 22].

The fundamental properties of NaOsO$_3$ have been clearly exposed by Jung et al. [21]. In particular, it
Spin-orbit induced renormalization. In the presence of a MIT in a TMO, the clarification of the role played by the electronic correlation $U$ is a central aspect for the theoretical understanding. We begin, hence, by studying the effects of $U$ and its interplay with the SOC for the case of our interest, NaOsO$_3$. All calculations were performed using the Vienna $ab$ initio simulation package (VASP) $^2$ using the DFT+$U$ method and including relativistic effects (see Supplement).

We start by computing the dependence of experimentally accessible observables on $U$. As usual, the value of the spectral gap $\Delta$ and the magnetic moment $\mu_{\text{Os}}$ are highly sensitive on the choice of $U$, as visualized in Figure 1(a). For $U=0$ the system is metallic, but for $U \geq 0.3$ eV NaOsO$_3$ exhibits a finite gap that increases linearly with $U$. The experimentally reported low-temperature optical gap, 0.1 eV $^{13}$ and the $\mu_{\text{Os}} \approx 1 \mu_B$ $^{13}$ clearly indicate that the optimal value of $U$ for NaOsO$_3$ should be chosen around 0.5 eV. At the same time, if we calculate $U$ entirely $ab$ initio within the constrained random phase approximation (cRPA) $^{27}$, neglecting all relativistic effects (SOC=0), we obtain $U^{\text{no SOC}}=1.58$ eV, a value similar to the one used in previous studies (i.e., $U=2$ eV $^{21}$. As we demonstrate here, the root of this apparent controversy lays in the surprising “competition” between SOC and electronic correlation.

We study the interplay between SOC and correlation by comparing our DFT+$U$ results with available infrared optical experiments. One rather general way $^{13, 30, 31}$ to estimate the degree of electronic correlation of a system is to evaluate the reduction of the electronic kinetic energy (mass renormalization) due to Coulomb repulsion. This can be quantified by the ratio $K_{\text{exp}}/K_{\text{DFT}}$ between the experimentally measured kinetic energy ($K_{\text{exp}}$), determined by integrating over frequency the Drude contribution in the optical conductivity $\sigma_D$ and the corresponding “non-correlated” kinetic energy $K_{\text{DFT}}$ obtained by DFT at $U=0$. Considering that $\sigma_D$ can be expressed in terms of the plasma frequency, $\omega_p$, via $\int d\omega \sigma_D(\omega) = \omega_p^2/8$, one can rewrite the kinetic energy ratio as:

$$\frac{K_{\text{exp}}}{K_{\text{DFT}}} = \frac{\omega_p^{\text{exp}}}{\omega_p^{\text{DFT}}}$$

Surprisingly, $K_{\text{exp}}/K_{\text{DFT}}$ in NaOsO$_3$ is dramatically dependent on the SOC strength as shown in Fig. 1(b). Without SOC, one should have classified the system as intermediate-strong correlated with $K_{\text{exp}}/K_{\text{DFT}} = 0.33$, which is close to Fe-pnictide superconductors. As SOC is considered in the DFT calculations, however, $K_{\text{DFT}}$ gets systematically reduced, as the estimated degree of correlation. For a full inclusion of SOC (SOC=1) we obtain $K_{\text{exp}}/K_{\text{DFT}} = 0.76$, a value similar to those of conventional metals like Cr. To our best knowledge, NaOsO$_3$ represents the first system where such a strong renormalization of the balance between SOC and correlations is reported.

Supporting evidence for the importance of SOC in NaOsO$_3$ is provided by the computed SOC energy, 0.4 eV/Os, and by comparing the electronic structure with and without SOC (Fig. 1(b)). The inclusion of SOC leads to a widening of the band width by about 0.3 eV, a linearization of the band near $\Gamma$ which yields the formation of a Dirac-like feature and, most importantly for the electron mobility, a band flattening near $E_F$ that increases the effective masses and therefore decreases $K_{\text{DFT}}$.

Therefore, by turning on the SOC the estimated degree of correlation moves gradually from the border to the Mott-physics to the one of conventional metallic systems. This significant relativistic renormalization clarifies the origin of the abovementioned inconsistencies on the value
First, we recall that the resistivity \( \rho \) of the continuous MIT at finite temperatures is determined by the SOC energy, which leads to a much better description of the bandgap (see arrow in Fig. 1(a)). This smaller value of \( \rho \) is also consistent with the \( U \) proposed for similar compounds like LiOsO\(_3\), \( U < 1 \) eV \[32\] and the itinerant magnet SrRuO\(_3\), \( U \approx 0.6 \) eV \[32\].

Importantly, the analogy with SrRuO\(_3\) is not limited to the low degree of correlation but also involves the magnetic itinerancy. Although NaOsO\(_3\) exhibits a high temperature insulating AFM ground phase, \( T_N = 410 \) K, the effective moment extracted from the the Curie-Weiss behavior of the high temperature susceptibility, \( 2.71 \mu_B \) \[13\], is much higher than the ground state magnetic moment measured by neutron diffraction, \( \approx 1 \mu_B \) \[14\], indicating a large Rhodes-Wohlfarth ratio and suggestive of an itinerant antiferromagnetic behavior \[32\]. This magnetic itinerancy would not be compatible with a large \( U \) and is essential to explain the MIT in NaOsO\(_3\), as discussed below.

**Spin fluctuations and Lifshitz MIT.** After clarifying the actual correlation degree in NaOsO\(_3\) and the crucial role played by SOC to determine it, we are ready to address the most intriguing feature of this compound – the origin of the continuous MIT at finite temperatures.

Our main results are summarized in Figs. 2 and 3. First, we recall that the resistivity \( \rho \) curve of NaOsO\(_3\) (Fig. 3(a)) shows two anomalies: one at \( T_N = 410 \) K, corresponding to a sudden increase of \( \rho \), and the second one around \( T_A = 30 \) K \( (T/T_N \approx 0.1) \) \[13\], characterized by a steeper increment. The region below \( T_A \) has a clear metallic behavior with a large and rapidly growing \( \rho \), whereas in the intermediate region, \( T_A < T < T_N \), \( \rho \) is always smaller then 1 \( \Omega \)cm and grows more slowly, with a bad-metal/pseudogap behavior. This hypothesis is supported by the experiments of Lo Vecchio et al. showing that the optical conductivity does neither vanish at \( T_N \) \[15\], nor shows a clear downturn at low frequencies in the intermediate temperature region. Such a peculiar temperature dependence of the conductivity is very unusual for TMOs \[15\], where – in the presence of a Mott-Hubbard MIT- the opposite trend can be observed \[35\].

Similar temperature dependence properties were reported, instead, for the narrow-gap semiconductor FeSi: at low temperature FeSi is a paramagnetic insulator but it develops a pseudogap associated with a bad-metal state as temperature increases \[36\]. This anomalous behavior is explained well by spin fluctuations in the context of the theory of itinerant magnetism elaborated by Moriya \[32\]. This similarity is of course very inspiring for the identification of the physical mechanisms at play in NaOsO\(_3\).

To substantiate this idea we explore the effect of transverse (rotational) and longitudinal spin fluctuations by means of non-collinear fixed spin moment calculations. As a first step, we have simulated the effect of rotational spin fluctuations in the high-temperature spin disordered configuration by performing non-collinear magnetic calculations on large supercells containing 32 Os sites starting from randomly rotated Os spin moments in a paramagnetic arrangement \( (i.e., \text{the total magnetic moment is zero}) \), by fixing the magnitude of the magnetic moments to the ground state value. The results are summarized in Fig. 2. The starting point is the density of states (DOS) of the reference collinear AFM insulating state at \( T = 0 \), Fig. 2(a). The paramagnetic DOS, Fig. 2(b), clearly shows that above \( T_N \) the system is an ordinary metal independently on the value of the local magnetic moment. By allowing a full relaxation of the moments the non-collinear paramagnetic state converges to a unrealis-

\[ T \]
FIG. 3. (color online). Temperature-dependent MIT. (a) Indirect band gap ($\Delta_i$) and direct pseudogap ($\Delta_d$) as a function of temperature compared with the experimental resistivity curve readapted from Ref. [13]. The two anomalies in the resistivity curves at $T_A$ and $T_N$ set the transition from an insulating (I) to a pseudogap (PS) state and from the PS to a purely metal (M) state, respectively. These two anomalies are correlated with the closing of the insulating ($\Delta_i$) and pseudo ($\Delta_d$) gaps (indicated by arrows). (b) Partial DOS (c) band structure and (d) FS for different temperatures ($T/T_N$) corresponding to different Os magnetic moment $\mu_{Os}$ (Eq. 2). (e) Schematic diagram of the MIT. I: AFM insulator; PS: AFM pseudogap state with longitudinal (and small rotational) spin fluctuation; M: magnetically itinerant metal.

By refining our analysis, and considering the corresponding evolution of the electronic bandstructure (Fig. 3(c)), we finally gain the complete description of the MIT in NaOsO$_4$. The bands changes almost rigidly with temperature and lead to a continuous change of the FS topology in terms of the appearance of progressively larger holes and electrons pockets (Fig. 3(d)): this represents a clear hallmark of a Lifshitz transition [19, 20].

Lifshitz transitions like the one described here are likely to be relevant for other magnetic materials laying at the border between a localized Mott picture and a metallic regime such as NiS [44], or 5$d$ TMOs with a close to half-filled $t_{2g}^3$ configuration like Cd$_2$Os$_2$O$_7$ [18, 19] and iridates. Nearly half-filling, in fact, appears to be the optimum balance between a localized (insulating) and delocalized (metallic) scenario: a reduced filling is generally associated to strong $U$ picture [18] (i.e. $d^1$ Ba$_2$NaOsO$_6$ and $d^2$ Ba$_2$CaOsO$_6$ are Mott-like insulator [23]), whereas larger occupation increases the degree of metallicity (i.e. $d^4$ BaOsO$_3$ and NaIrO$_3$ [42]); moreover, the nearly $L_{eff} = 0$ state reduces the SOC-induced splitting which weaken the tendency towards Mott-SOC states and is functional for a rigid-band Lifshitz MIT. Also, structural distortions in 5$d$ oxides are an impor-
tant factor for Lifshitz MIT as they enables the formation of small local moments that would be otherwise suppressed in undistorted and more strongly hybridized structures 21 42.

Conclusions. In summary, we have shown that the coexistence between weak electronic correlation and itinerant magnetism can lead to a spin-driven Lifshitz MIT, i.e., a magnetically induced continuous reconstruction of the Fermi surface. For NaOsO$_3$ we found that the MIT is prompted by transverse and longitudinal fluctuations of the itinerant Os moments, and is intimately bound to the SOC-driven renormalization of the electronic kinetic energy. Our study explains the three different regimes observed experimentally: (i) At low-$T$ NaOsO$_3$ is an AFM insulator; (ii) At $T = T_A$ it enters a bad metal regime due to longitudinal spin fluctuations; finally (iii) at $T = T_N$ rotational spin fluctuations closes the direct pseudogap and the system become a paramagnetic metal. Spin fluctuations and the tunability by doping and pressure of the Lifshitz FS reconstruction could give rise to novel magnetic, orbital and superconducting transitions, to be exploited for engeneering TMOs based heterostructures. Moreover, the surprising role played by the SOC in NaOsO$_3$, as well as its “competitive” action against correlations -highlighted here for the first time- could radically affect the theoretical description of the relativistic mechanisms controlling the electronic properties of many other oxides.

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Supplementary information: A new route to relativistic insulators: Lifshitz transition driven by spin fluctuations and spin-orbit renormalization in NaOsO$_3$

COMPUTATIONAL DETAILS

All calculations were performed using the Vienna \textit{ab initio} simulation package (VASP) \cite{Kresse1993, Kresse1996} using the DFT+$U$ method \cite{Dudarev1998} within the generalized gradient approximation and including spin-orbit interaction (with quantization axis along the (0, 0, 1) direction). The on-site Coulomb $U$ was computed fully \textit{ab initio} using the constrained random phase approximation (cRPA) \cite{Aryasetiawan2006}. For the cRPA calculations we used a maximally-localized Wannier functions basis including the $t_{2g}$ states that ensured an excellent match with the DFT band structure around the Fermi energy as shown in Fig. S1. We used $U = 0.4$ eV, slightly smaller than the value estimated by the cRPA, 0.68 eV (see main text). We adopted the generalized gradient approximation, $U=0.4$ eV, plane-wave cutoff of 400 eV and a $t_{2g}$ basis set for cRPA. The atomic position were fully relaxed at the experimental volume. A $10 \times 6 \times 10$ Monkhorst-Pack mesh was used (4\times3\times4 and 20\times20\times20 for non-collinear calculations and plasma frequency calculations, respectively). The lattice parameters were fixed to the experimental ones and internal positions of all atoms were fully relaxed. A $10 \times 6 \times 10$ Monkhorst-Pack mesh was used (reduced to 4\times3\times4 for non-collinear magnetic calculations in the large supercell containing 32 Os sites) with a plane-wave energy cutoff of 400 eV. In order to estimate the role of relativistic effects on the electron correlation (relativistic renormalization) we have followed the standard procedure described in Ref.\cite{Aryasetiawan2006} which involves the calculation of the plasma frequency in the paramagnetic phase using $U = 0$. For these calculations we increased the $k$-point grid up to 20\times20\times20 and very stringent energy convergence criteria ($10^{-8}$ eV).

To model the high-temperature paramagnetic phase we adopted a supercell containing 32 Os sites starting from randomly distributed magnetic moments within a non-collinear set-up resulting in a zero total magnetic moment \cite{Dudarev1998, Aryasetiawan2006}. The degree of disorder was verified by computing the spin-spin correlation function $S$: for the random system we have obtain $S=0.2$, to be compared with the ordered AFM system for which $S=1$.

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\begin{figure}[h]
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\includegraphics[width=0.8\textwidth]{fig_s1}
\caption{Superimposition of the DFT and $t_{2g}$ wannier-projected band structure.}
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