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Topological phase transitions in strongly correlated systems: application to $Co_3Sn_2S_2$

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Recently, the layered kagome lattice compound $Co_3Sn_2S_2$ has been a subject of numerous experimental and theoretical investigations. Its electronic structure contains Weyl points, Fermi arcs and nodal rings, which play an important role in the anomalous Hall effect. Single-crystal experimental data on the $Co_3In_xSn_{2-x}S_2$ kagome system [1] show that these systems have an almost two-dimensional itinerant magnetism and a chiral spin state; in addition, a strongly correlated state with a high electronic heat capacity is formed. The important role of correlations is confirmed by a considerable enhancement of γT-linear specific heat even in the ferromagnetic phase [1], especially at approaching the magnetic-nonmagnetic critical point somewhat below $x = 1$.

The ferromagnetism in $Co_3Sn_2S_2$ breaks time-reversal T-symmetry and is necessary for the existence of topological Weyl points. Above T_C, intrinsic magnetic field disappears, the Weyl points annihilate and the Dirac points acquire a gap. This restores T-symmetry and eliminates the topological behavior. A similar, but quantum transition occurs with disappearance of ferromagnetism in the $Co_3In_xSn_{2-x}S_2$ system at the hole doping [2]. The doping shifts the Weyl nodes away from the Fermi level. For small doping, the nodal rings are located around the Fermi energy, and for $x \sim 0.2$, the nodal lines surrounding the L point in the Brillouin zone cross the Fermi surfaces (Fig. 1). With further increasing x, the nodal lines are split into two rings as with the annihilation of Weyl points in the presence of the spin-orbit coupling. For $x > 0.6$, the nodal lines are located far from the Fermi level, resulting in the small Berry curvature on the whole Fermi surfaces [2]. At $x = 1$ the system becomes insulating; according to [1], this anomalous nonmetallic state may originate from the Fermi energy tuning through a Dirac point.

In the present work we treat the model picture of correlated half-metallic ferromagnetism in $Co_3Sn_2S_2$ and provide a description of these transitions within the topological classification [3].

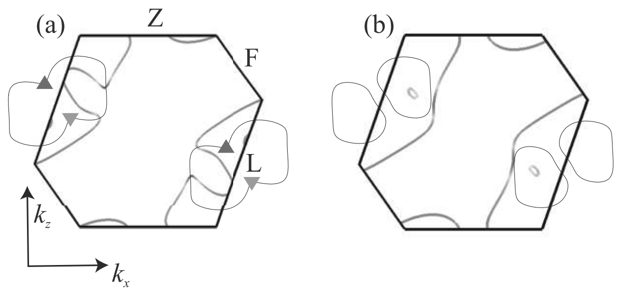

Fig. 1. (Color online) Schematic Fermi surfaces (solid green lines) for $Co_3Sn_2S_2$ in the $k_x - k_z$ plane at $k_y = 0$ according to [2]. The thin black solid line shows the nodal lines in the absence of spin-orbit coupling for (a) $x = 0.2$ and (b) $x = 0.4$. The upper and lower triangles on the nodal lines in (a) stand for the Weyl points with topological charges $+1$ and -1 in the presence of spin-orbit coupling

The half-metallic ferromagnetism of $Co_3Sn_2S_2$ occurs in the partially filled Co $3d_{x^2-y^2}$ band which crosses the Fermi level. The associated moment of $1\mu_B$ is spread over three Co atoms, in agreement with the $0.33\mu_B$ per Co magnetic moment from first-principle calculations and the experimental moment which is slightly less than $1\mu_B$/f.u. This enables one to formulate a local Hubbard model for the Co atom cluster [4].

According to [4], across the magnetic transition, $Co_3Sn_2S_2$ evolves from a Mott ferromagnet to a correlated metallic state. In fact, the "Mott ferromagnet" is a half-metallic ferromagnetic state, so that we have a partial Mott transition in the minority spin subband.

The picture of half-metallic ferromagnetism can be qualitatively described by the simplest narrow-band Hubbard model with large on-site repulsion U. In this model, doubly occupied states (doubles) are absent owing to the Hubbard splitting, but states with both spin projections are still present. Thus the situation is different from the Stoner model where spin splitting becomes infinitely large. The physics does not qualitatively change in the case of finite Hubbard U, since the dou-

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bles are automatically eliminated in the saturated half-metallic state [5]. We can use the slave fermion representation the Hubbard projection operators describing motion of holes in the correlated state on the background of magnetic moments. $X_i(0,\sigma) = |i0\rangle\langle i\sigma| = f_i^\dagger b_{i\sigma}$ where f_i are fermions and $b_{i\sigma}$ are Schwinger boson operators. In the saturated ferromagnetic state the $b_{i\uparrow}$ boson is condensed, and $b_{i\downarrow}$ becomes magnon annihilation operator. The spin-up (majority) states propagate freely on the background of strong ferromagnetic ordering and possess an exotic spectrum of chiral Weyl fermions in the internal magnetic field.

The spin down (minority) Green's function in the leading approximation is obtained as a convolution of the Green's functions for free fermions and bosons, so that

$$G_{\mathbf{k}\downarrow}(E) = \sum_{\mathbf{q}} \frac{N(\omega_{\mathbf{q}}) + f(t_{\mathbf{k+q}})}{E - t_{\mathbf{k-q}} + \omega_{\mathbf{q}}}, \qquad (1)$$

where $N(\omega)$ and $f(E)$ are the Bose and Fermi functions, $\omega_{\mathbf{q}}$ is the magnon spectrum, $t_{\mathbf{k}}$ the band energy. Similar results for a Hubbard ferromagnet were obtained earlier in the many-electron representation of X-operators [5], the analogy with Anderson's spinons being discussed. The Green's function (1) has a purely non-quasiparticle nature. The number of minority states is equal to the number of majority states n_0 owing to the sum rule

$$\sum_{\mathbf{k}} \langle X_{-\mathbf{k}}(0,\sigma) X_{\mathbf{k}}(\sigma,0)\rangle = \langle X_i(0,0)\rangle = n_0 \qquad (2)$$

for both projections σ, so that the current carriers (Hubbard's holes) are in a sense spinless.

The description of the transition to the half-metallic state can be described as a partial (orbital-selective) Mott transition in the minority spin subband. The Lifshitz transitions with vanishing quasiparticle poles can be viewed as quantum phase transitions with a change of the topology of Fermi surface, but without symmetry breaking. Indeed, the Fermi surface itself is the singularity in the Green's function, which is characterized by topological invariant N_1 and topologically protected: it is the vortex line in the frequency-momentum space [3]. In the gapped phase, usual Fermi surface does not exist, but its topology is preserved if we take into account the Luttinger contribution. Then the Luttinger theorem (the conservation of the volume enclosed by the Fermi surface) is still valid. Thus the Fermi surface becomes ghost (hidden) in the Mott phase for both spin projections and in our half-metallic situation for minority states, since the Fermi level lies in the corresponding gap.

On the contrary, the transition with disappearance of the Weyl points is essentially topological: topological invariants are changed. In the Weyl semimetal phase, the Weyl points have topological charges $N_3 = +1$ and -1 and annihilate in the critical Dirac semimetal. Further on, in the normal paramagnetic state the topology owing to the Berry curvature vanishes. Thus the conservation law for the topological charge [3] is fulfilled. In the insulator case, we have a transition from topological to normal insulator with restoring time-reversal symmetry. A still more complicated situation occurs in the case of Chern insulators with a change of the Chern number [6, 7].

In the half-metallic ferromagnetic state Hubbard correlations do not result in narrowing of bare bands for majority states, but in the paramagnetic state the situation changes: we come to the regime of narrow correlated bands for both spin projections. These may be characterized either by strongly renormalized quasiparticle residue, or even by a non-Fermi-liquid (e.g., marginal Fermi-liquid) behavior. Besides absence of T-breaking internal magnetic field in the paramagnetic phase, this can be important for vanishing of topological effects. Thus the topological properties and strong correlations in $Co_3Sn_2S_2$ are intricately linked, so that one cannot be adequately considered without the other [4].

According to [8], at finite temperatures the magnetic structure includes the out-of-plane ferromagnetism, in-plane antiferromagnetism, and hidden phases. The corresponding values of transition temperatures are $T_C = 182\,K$, $T_N = 177\,K$, and $T_{com} = 150\,K$. The corresponding first-order phase transition may again indicate strong half-metallic magnetism and be important for a combined description of the non-topological ferromagnetic and topological transitions.

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