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Sr_2VO_3FeAs as compared to other iron-based superconductors

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One of the most popular scenarios for the superconductivity in Fe-based superconductors (FeBSCs) posits that the bosons responsible for electronic pairing are spin fluctuations with a wave vector spanning the hole Fermi surfaces (FSs) near Γ and the electron FSs near *M* points. So far, all FeBSCs, for which neutron data are available, do demonstrate such excitations, and the band-structure calculations so far were finding quasinested FSs in all FeBSC, providing for a peak in the spin susceptibility at the desired wave vectors. However, one of the new additions to the family Sr_2VO_3FeAs has been calculated to have a very complex FS with no visible quasinesting features. It was argued therefore that this material does not fall under the existing paradigm and calls for revisiting our current ideas about what is the likely cause of superconductivity in FeBSC. In this Rapid Communication, I show that the visible complexity of the FS is entirely due to the V-derived electronic states. Assuming that superconductivity in Sr_2VO_3FeAs, as in the other FeBSC, originates in the FeAs layers, and the superconducting electrons are sensitive to the susceptibility of the FeAs electronic subsystem, I recalculate the bare susceptibility, weighting the electronic states with their Fe character, and obtain a susceptibility that fully supports the existing quasinesting model. Besides, I find that the mean-field magnetic ground state is the checkerboard in the V sublattice and stripes in the Fe sublattice.

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The recently discovered Fe-based high-temperature superconductors (FeBSCs) represent a challenging case for the theory of superconductivity. They appear to be rather different from cuprates in terms of their electronic structure, magnetic order, correlation effects, and superconducting symmetry.[1] So far, the most popular suggestion for the pairing mechanism has been one that assigns the role of an intermediate boson to spin fluctuations with wave vectors close to $\mathbf{Q}=(\pi,\pi)$ (in the two-Fe Brillouin zone). There are two ways to generate such spin fluctuations: one assumes superexchange between the second neighbors in the Fe lattice and the other exploits the fact that the noninteracting spin susceptibility calculated using the one-electron band structure has a peak, or better to say, a broad maximum close to (π,π) (see review Ref. 1). A strong argument in favor of the latter scenario was the case of FeSe, where the parent magnetic compound FeTe shows an antiferromagnetic order at a different wave vector. both in the experiment and in the calculations, but the calculated spin susceptibility is still peaked $\mathbf{Q}=(\pi,\pi)$, and the experiment also observes spin fluctuations with the same wave vector. Also, the fact that FeBSC lack strong Coulomb correlations[2,3] speaks against the former alternative.

Recently, however, a different FeBSC, Sr_2VO_3FeAs, has been discovered,[4] which seemingly violates this so far meticulously observed rule. The calculated Fermi surface (FS) (Ref. 5) appears to be much more complex than in the other investigated FeBSC, and there is no visual indication of any quasinesting topology. Lee and Pickett[5] argued that Sr_2VO_3FeAs represents "a new paradigm for Fe-pnictide superconductors" and inferred that "there is no reason to expect an $s_\pm$ symmetry of superconducting order parameter (i.e., a different sign on the two FSs) in Sr_2VO_3FeAs."

I have repeated the calculations of Lee and Pickett and have obtained the FS that was similar to theirs[6] (Fig. 1). I have also verified that the bare susceptibility *without any account* for the *matrix elements*,

$$\chi_0(\mathbf{q}) = -\sum_{\mathbf{k}\alpha\beta} \frac{f(\varepsilon_{\mathbf{k}\alpha}) - f(\varepsilon_{\mathbf{k}+\mathbf{q},\beta})}{\varepsilon_{\mathbf{k}\alpha} - \varepsilon_{\mathbf{k}+\mathbf{q},\beta} + i\delta} \tag{1}$$

indeed does not have any peak at $\mathbf{Q}=(\pi,\pi)$ (Fig. 2). In fact, it has a peak at an entirely different wave vector $(\pi,0.4\pi)$, as anticipated by Lee and Pickett. However, this does not take into account the fact that the calculated Fermi surface is really a superposition of two FS systems: one originating from the FeAs planes, and the other from VO ones. While there is some hybridization between the two systems of bands (at least along the *XM* directions; see Ref. 5 for details), as well as a magnetic coupling and a magnetic moment on V, and maybe even Coulomb correlation effects on V site, electrons

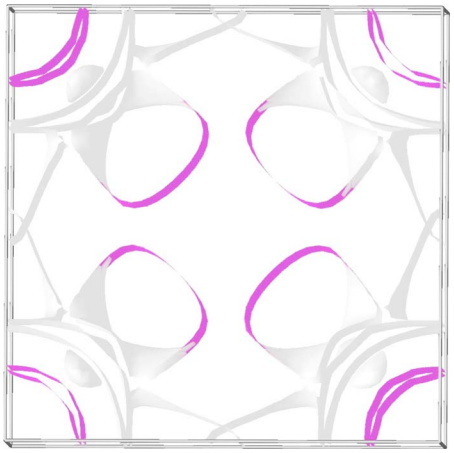

FIG. 1. (Color online) The Fermi surfaces of Sr_2VO_3FeAs. The Γ points are in the corners; the *M* point is in the center of the shown Brillouin zone. The colored (dark) portion are the parts with the predominantly Fe character. The rest is predominantly V.

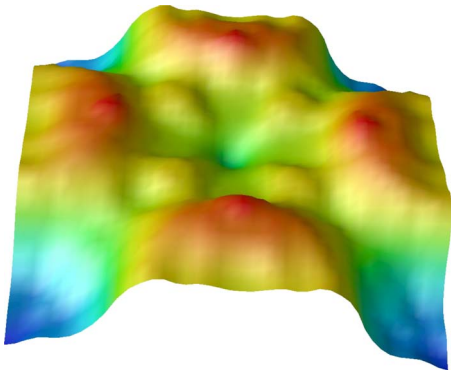

FIG. 2. (Color online) The bare susceptibility (the real part) calculated with a constant matrix element independently of the wave-function character. The band structure had been averaged over k_z before the integration. The corners of the plot correspond to $\mathbf{q}=(0,0)$, $(\pi,0)$, $(0,\pi)$, and (π,π). The vertical scale is in arbitrary units.

derived from the Fe *d* orbitals couple mostly with the spin fluctuations on the Fe sites. This is a simple consequence of the Hund's rule. With that in mind, I colored the parts of the Fermi surface in Fig. 1 that have predominantly Fe character.

Imagine now that the *unpainted* parts of the FS disappear. What remains after this mental *tour de force* closely resembles the familiar FSs of other FeBSC. Taking into account the above argument, regarding the special role of the Fe spin fluctuations, we can rewrite Eq. (1) as

$$\tilde{\chi}_0(\mathbf{q}) = -\sum_{\mathbf{k}\alpha\beta} \frac{f(\varepsilon_{\mathbf{k}\alpha}) - f(\varepsilon_{\mathbf{k}+\mathbf{q},\beta})}{\varepsilon_{\mathbf{k}\alpha} - \varepsilon_{\mathbf{k}+\mathbf{q},\beta} + i\delta} A_{\mathbf{k}\alpha} A_{\mathbf{k}+\mathbf{q},\beta}, \qquad (2)$$

where $A_{\mathbf{k}\alpha}$ is the relative weight of the Fe orbitals in the $|\mathbf{k}\alpha\rangle$ wave function. The result (Fig. 3), as expected, shows the same structure as for the other pnictides, especially for the real part of susceptibility, which is the one relevant for superconductivity.

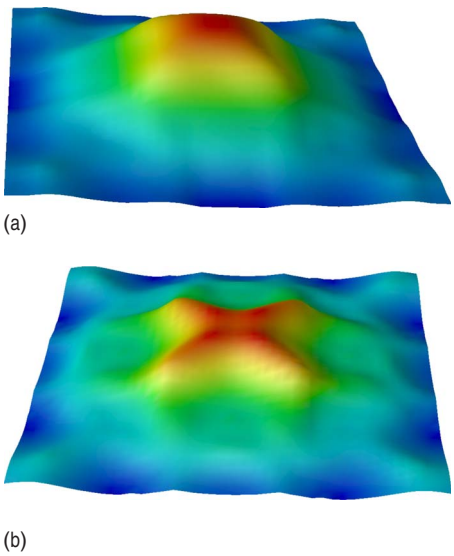

FIG. 3. (Color online) The bare susceptibility calculated, as in Fig. 2, but with matrix elements taken as the product of the Fe weights for the corresponding wave functions. The top panel shows the real part; the bottom one shows the imaginary part.

I conclude that, unfortunately, Sr_2VO_3FeAs, despite being an interesting and in many aspects unusual FeBSC, does not represent a new paradigm but rather falls into the same class as other pnictides. It is also worth noting that while it has been established both experimentally[2,3] and computationally[2,7] that the FeAs subsystem is only weakly correlated, this had not been obvious *a priori*, and it is not obvious for the V-O subsystem in Sr_2VO_3FeAs. Being essentially in a vanadium oxide layer (and vanadium oxide is strongly correlated in the bulk form), V in Sr_2VO_3FeAs may be subject to strong Hubbard correlations that would remove V states from the Fermi level.[8] Thus, strictly speaking, the conclusion above should be formulated as follows: *even if* Sr_2VO_3FeAs is a weakly correlated metal and the FS calculated within the density-functional theory (DFT) is realistic, the fact that the overall topology seems, on the first glance, to be different from other pnictides is misleading and the relevant spin-fluctuation spectrum is likely to be rather similar.

At the end, let me briefly touch upon a separate but equally (if not more) interesting issue of the magnetic ground state and magnetic properties of Sr_2VO_3FeAs within the DFT. It is well known[1] that DFT seriously overestimates the tendency to magnetism in FeBSCs, so that the calculated ground state appears strongly antiferromagnetic even in the materials that show no long-range magnetic order (phosphates, selenide). This is routinely ascribed to the mean-field character of DFT. However, it is of course interesting to see what is the (magnetic) ground state in the mean field even when in real life the ground state is paramagnetic. For all FeBSCs studied so far, the antiferromagnetic stripe magnetic structure is by far the lowest in energy (energy gain on the order of 200 meV per Fe compared to a nonmagnetic solution), while the ferromagnetic structure is barely stable if at all.

Most likely, the DFT ground state of FeBSCs is also antiferromagnetic in plane. However, even the nonmagnetic unit cell contains 16 atoms, which makes it extremely difficult to investigate the energy landscape for possible antiferromagnetic pattern. Thus, it makes sense to study possible ferro(ferri)magnetic solutions, in hope to extract at least some useful information. This approach was adapted in Ref. 9 (although these authors do not present any nonmagnetic calculations, actually relevant for superconductivity). They found a solution with a moment on V ($\sim 1.5\mu_B$) but not on Fe. Lee and Pickett found another ferrimagnetic solution, with opposite moments on V and Fe; the former being larger.[10] Using different starting configurations, I was able to converge to three different ground states within the same symmetry, as shown in Table I, as well as to two lower-symmetry states, as illustrated in Figs. 4(b)–4(d): interlayer antiferromagnetic V sublattice, where the V layers are ferromagnetic, and antiferromagnetically stacked, while Fe is nonmagnetic, and Fe-checkerboard, where Fe forms a Neel plane and V is nonmagnetic. After that, I have calculated two configurations in the double (four formula units) cell, which I feel are the most relevant because of the superexchange

TABLE I. Properties of some stable magnetic solutions in the generalized gradient approximation of the DFT. All energies are given with respect to the nonmagnetic state.

	M_{Fe} (μ_B)	M_V (μ_B)	ΔE (meV/Fe)
FM	2.0	1.4	−396
Half-FM	0.0	1.5	−381
FiM	2.1	−1.4	−387
V-AF	0.1	±1.4	−385
Fe-cb	±2.0	0.2	−219
V-cb	2.0	±1.2	−237
V-cb	0.1	±1.2	−232
V-cb + Fe-stripes	±2.2	±1.2	−409

interaction in the V layers: V-checkerboard with nonmagnetic Fe, and V-checkerboard combined with the stripe order in the Fe layers (Fig. 4).

A few observations are in place: (1) the state found in Ref. 9 is not the ground state even within that symmetry; (2) unlike all other FeBSCs, FeAs planes can support a very stable ferromagnetic state; (3) the interaction between V and Fe is ferromagnetic, that is, not of superexchange character; (4) the magnetic coupling between V and Fe is so weak that V does not induce any magnetization on Fe, unless one already starts with a magnetic Fe; (5) it is more important, from the total-energy point of view, to have a magnetic moment on V that on Fe (a bit surprising, given that V has a weaker Hund's rule coupling); (6) V sublattice itself has a net antiferromagnetic interaction: if Fe is not magnetic, V orders antiferromagnetically; (7) unless some more exotic ground state will be discovered, the total energy is minimized when V layers order in the Neel (checkerboard) fashion, while Fe orders the same way as in other pnictides, forming stripes; (8) most importantly, a number of very different magnetic states are nearly degenerate in energy. This last fact may be the key to the experimental fact that the actual material is paramagnetic despite the fact that on the mean-field level, it is more magnetic than other pnictides. This is an extremely intriguing situation and the magnetism

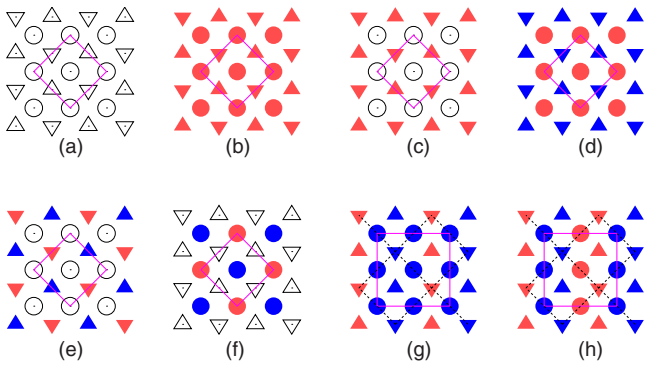

FIG. 4. (Color online). Magnetic configurations used in Table I. Hollow symbols indicate nonmagnetic atoms, blue (dark) spin-up moments, red (light) spin-down moments. Circles are Fe atoms, upward and downward pointing triangles are two V layers in the unit cell. The configurations are (a) NM: nonmagnetic, (b) FM: ferromagnetic, (c) half-FM, (d) FiM: ferrimagnetic (Fe and V spins are antiparallel), (e) V-AF: antiferromagnetically stacked FM V layers, nonmagnetic Fe, (f) Fe-cb: checkerboard Fe planes, weakly ferromagnetic V planes, (g) V-cb: checkerboard V planes, ferromagnetic Fe planes, (h) V-cb combined with Fe stripes. Minimal crystallographic unit cell is shown in each case, and in the last panel dashed lines connect V atoms in the same layer.

Sr_2VO_3FeAs deserves a more elaborated experimental and theoretical study that is beyond the scope of this Rapid Communication.

Note added in proof. Very recently, I became aware of another band structure calculation.[11] These authors have considered the "Shein-Ivanovskii" half-FM states and two antiferromagnetic states, with the checkerboard (Neel) and stripe ordering in the Fe sublattice, and unspecified, presumably ferromagnetic, ordering in the V subsystem. As is clear from the above, neither of these states represents an energy minimum even within the corresponding symmetry group. therefore these authors arrived at an incorrect conclusion that the lowest-energy magnetic state is characterized by Neel order in the Fe subsystem.

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