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Magnetic properties and electronic structure of $LaFeAsO_{0.85}F_{0.1}$

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The magnetic properties of the compound $LaFeAsO_{0.85}F_{0.1}$ were investigated by measurements of the dc magnetization for different values of the magnetic field $H = 0.02$, 1.0 and 2.0 T in the temperature range 4.2–300 K. Superconducting behavior was found below 26 K, whereas a distinct peculiarity in the low-field dependence of the magnetic susceptibility $\chi(T)$ was clearly observed at $T_M \simeq 135$ K, which resembles a weak ferromagnetic (FM) response with saturation magnetic moment of about 10^{-4} μ_B per formula unit at 50 K. The transition at T_M is presumably not governed by magnetic impurities but rather correlated with the antiferromagnetic (AFM) transition in undoped LaFeAsO at about the same temperature. We suggest that the observed magnetic properties of the $LaFeAsO_{0.85}F_{0.1}$ sample are due to an interplay of FM and AFM transitions, and are presumably related with an intrinsic feature of a small portion of the undoped LaFeAsO phase inherent in our sample. In order to shed light on the problem of magnetic instability of the LaFeAsO, *ab initio* DFT calculations of the electronic structure and paramagnetic susceptibility were performed within the local spin density approximation. It is shown that a V-shaped peculiarity in the density of electronic states close to the Fermi level can govern magnetic properties of LaFeAsO with fluorine doping and/or oxygen deficiency.

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I. INTRODUCTION

The recent report on superconductivity with $T_c \simeq 26$ K in $LaFeAsO_{1-x}F_x$ (Ref. 1) has opened a new class of the quarternary “1111” iron-based layered superconductors and stimulated intensive studies of their physical properties. A large increase of the superconducting transition temperature in $LaFeAsO_{1-x}F_x$ was later observed under high pressure (up to 43 K at $P \sim 4$ GPa (Ref. 2)) and with substitution of rare earths for La (the highest $T_c \simeq 55$ K was reported for $SmFeAsO_{1-x}F_x$ (Ref. 3)). Comprehensive reviews of experimental and theoretical reports on properties of the iron pnictide superconductors have been were recently published (see, e.g., Refs. 4–7).

The parent undoped compound LaFeAsO is not superconducting but shows a number of peculiarities of its physical properties (e.g., electrical resistivity, magnetic susceptibility, specific heat, and so on[1,8–10]), which are caused by a structural tetragonal-orthorhombic transition at 160 $T_S \approx 160$ K and antiferromagnetic (AFM) spin ordering at $T_N \approx 140$ K.[8,11–13] With electron or hole doping with F substitution at the O site[1,9,10,12–14] or with oxygen vacancies[15–17] both transformations are suppressed and superconductivity emerges, suggesting that there is a relation between the magnetic (and structural) properties and superconductivity. The electron–phonon interaction is estimated to be too small in pure and F-doped LaFeAsO to provide conventional superconductivity, and there is growing evidence that proximity to magnetic instability plays an essential role in the nature of superconductivity in these compounds.[4–7] It has been suggested that superconductivity is driven by spin-fluctuations due to strong AFM[18,19] or FM[20] instability in LaFeAsO and related compounds.

However, a nature of the complex interplay between magnetism and superconductivity in RFeAsO is still not well characterized and understood. Also, the recent experimental data on behavior of magnetic susceptibility of “1111” systems in the normal state are still incomplete and Contradictory.[9,12,20,21] Therefore further studies of the magnetic and superconducting properties and their evolution with doping, pressure, temperature, and on can help to elucidate a mechanism of the high-T_c superconductivity in the new class of Fe-based superconductors.

In this contribution we report experimental results on the magnetic susceptibility in the normal state for the superconductor $LaFeAsO_{0.85}F_{0.1}$, which is fluorine-doped but contains about 0.05 of the vacancies in the oxygen sublattice. The present experimental study is supplemented by *ab initio* DFT calculations of the electronic structure and magnetic susceptibility for a number of LaFeAsO based systems in the normal state within the local spin density approximation (LSDA). The aim of this investigation is to shed more light on the relation between the chemical composition, magnetic properties, and the interplay between superconductivity and magnetic instability in the “1111” systems.

II. EXPERIMENTAL DETAILS AND RESULTS

Polycrystalline sample of $LaFeAsO_{0.85}F_{0.1}$ was prepared using a two-step solid state reaction technique, similar to that

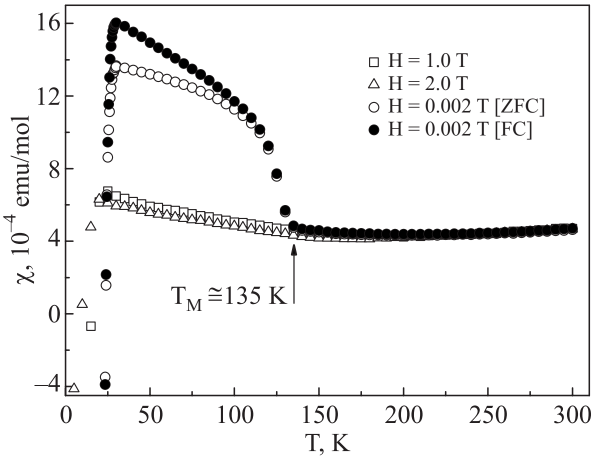

FIG. 1. Temperature dependences of the dc magnetic susceptibility of $LaFeAsO_{0.85}F_{0.1}$ in different magnetic fields: $H=2$ T (△); 1 T (□); 0.02 T (ZFC—○, FC—●).

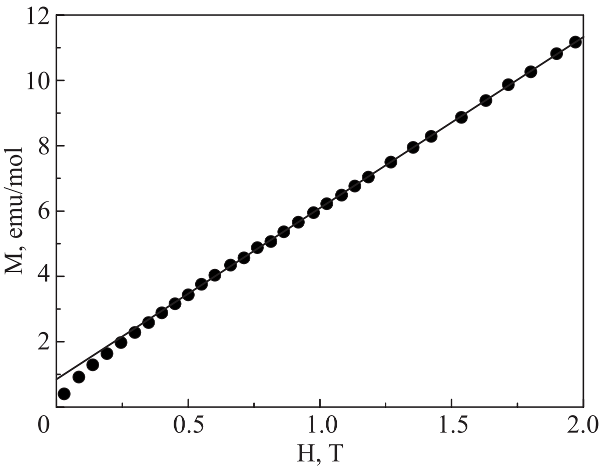

FIG. 2. Magnetization versus field for $LaFeAsO_{0.85}F_{0.1}$ at $T=50$ K.

described in Ref. 22. The crystal structure and the composition were investigated by powder x-ray diffraction and wavelength-dispersive x-ray spectroscopy. The basic phase content was determined to be about 97%.

Magnetic properties of $LaFeAsO_{0.85}F_{0.1}$ were studied by an in-house SQUID magnetometer in the temperature range 4.2–300 K. The sample with mass ~0.3 g was a 5 mm in diameter and 2.5 mm high cylinder. The temperature dependence of the magnetic susceptibility $\chi(T)$ was measured under cooling to helium temperature in zero magnetic field (ZFC) followed by slow heating at the rate of about 1.5 K/min in applied magnetic fields $H=0.02$, 1.0 and 2.0 T. The $\chi(T)$ dependence was also measured by cooling in the magnetic field $H=0.02$ T (FC). As can be seen in Fig. 1, the experimental sample shows a superconducting transition at temperature $T_c \simeq 26$ K, which is typical for fluorine-doped LaFeAsO systems.

For the normal state the $\chi(T)$ dependence measured in $H \geqslant 1$ T appears to be relatively flat and roughly described by the mean value $\chi_{av} \sim 5 \cdot 10^{-4}$ emu/mol. This value is comparable to the recently published data for the magnetic susceptibility of F-doped LaFeAsO at room temperature.[9,20] However, it should be noted that the temperature dependencies of χ for F-doped LaFeAsO are essentially different between the above two reports. The data obtained in Ref. 20 give χ increasing with decreasing temperature whereas those reported in Ref. 9 show χ gradually decreasing with decreasing temperature, as in the undoped LaFeAsO compound. The latter $\chi(T)$ behavior is consistent with the temperature dependence of the ^{75}As Knight shift in LaFeAsO:F,[23] whereas the former dependence (χ increasing with decreasing temperature[20]) is considered to be due to impurity phases which amount to a few wt.%.[12] An intermediate relatively flat $\chi(T)$ dependence is seen for our sample measured in high magnetic fields (see Fig. 1).

As is obvious from Fig. 1, the peculiar features of the low-field magnetic susceptibility of $LaFeAsO_{0.85}F_{0.1}$ is a clear cusp at $T \simeq 135$ K with a sharp rise of χ on cooling from $T_M \simeq 135$ K to $T_c \simeq 26$ K. On the basis of the magnetization data in Fig. 2 we can assume the emergence of a weak FM response at $T \leqslant T_M$. The corresponding saturation moment at $T=50$ K amounts to approximately 1 emu/mol or $\sim 1.5 \cdot 10^{-4}$ μ_B/f.u., about four orders of magnitude smaller than the magnetic moment at Fe sites for undoped LaFeAsO in the AFM state ($\sim 0.36\mu_B$ (Ref. 11)). A similar nonlinear behavior of $M(H)$ in the low-field region and the same order of the ferromagnetic moments were reported in Refs. 12 and 21, which that were considered to be caused by impurity phases. Typically, in F-doped LaFeAsO samples one can expect the formation of AFM iron-bearing secondary phases such as FeAs, FeF_2 (both with $T_N \leqslant 75$ K) and Fe_2As ($T_N \sim 350$ K).[12,21,24,25] Consequently, the observed FM transition at $T_M \simeq 135$ K is presumably not affected by the secondary magnetic phases mentioned above. On the other hand the FM transition evidently correlates with the point of the AFM transition in undoped LaFeAsO.[7,11]

III. COMPUTATIONAL DETAILS AND RESULTS

The undoped parent LaFeAsO compound as well as the $LaFeAsO_{1-x}F_x$ and $LaFeAsO_{1-y}$ systems possess tetragonal ZrCuSiAs-type crystal structure (space group $P4/nmm$).[1,2] With c/a ratio close to 2.16 the tetragonal structure of LaFeAsO exhibits strong two-dimensional features. The crystal lattice is composed of alternating La–O and Fe–As triple-layer slabs, which are stacked along the c axis. Each iron (oxygen) layer is sandwiched between two nearest-neighbor As (La) atomic layers, which form edge-shared tetrahedrons around the iron (oxygen) sites. The positions of As or La sheets are fixed by the internal parameters z_{As} and z_{La}, which define the inter-layer distances of Fe–As and La–O, respectively. It is suggested that there is partial ionic bonding between the Fe–As and La–O layers, which increases with fluorine doping.[4,6]

The previous *ab initio* calculations of the electronic structure of the “1111”-type iron-based oxypnictides were predominantly related to studies of the ground state AFM ordering in the undoped “1111” compounds (see Refs. 18, 19, and 26–28) and references cited there). In this paper detailed calculations of the electronic structure are performed for the paramagnetic phase of LaFeAsO based systems with the aim of studying the paramagnetic response in an external magnetic field and shedding more light on the nature of paramagnetism and the interplay between superconductivity and magnetic instability in "1111" systems.

In the present *ab initio* calculations of the electronic structure we employed a full-potential all-electron relativistic linear muffin-tin orbital method (FP-LMTO, code RSPt[29,30]). No shape approximations were imposed on the charge density or potential, which is especially important for the anisotropic layered crystal structures. The exchange-correlation potential was treated in the LSDA[31] and generalized gradient approximations (GGA, Ref. 32) of the density functional theory (DFT). The effect of the spin–orbit coupling, included in the Hamiltonian, appeared to be important for precise calculations of the atomic volume dependent density of states (DOS) at the Fermi level E_F. The FP-LMTO calculations were carried out for the LaFeAsO and LaFeAsO with oxygen replaced by virtual atoms with $Z=7.9$ and $Z=8.1$ in order to simulate doping.

The calculations were performed for a number of lattice parameters a close to the experimental values[1,5] with parameters c/a, z_{As} and z_{La} fixed to their experimental ambient-pressure values. The total energies E were calculated as a function of volume V and were fitted to Murnaghan's analytical parametrization for the equation of state.[29] Then the theoretical lattice spacings and the bulk moduli B were determined from calculated volume dependences of the total energy $E(V)$ with both the LSDA[31] and GGA[32] exchange-correlation potentials. The theoretical lattice parameter a appeared to be close to the experimental value[1,2,5] (about 1% smaller for the LSDA potential). The estimated bulk moduli of LaFeAsO, $B_{LSDA}\simeq 1.3$ Mbar and $B_{GGA}\simeq 1$ Mbar, are in agreement with the earlier reported theoretical value $B_{\mathrm{theor}}=0.98$ Mbar.[33]

According to our calculations, near the Fermi level E_F the electronic structure of LaFeAsO is governed by moderate hybridization of d (Fe) and p (As) states within the Fe–As layers. The Fe d states make the dominant contribution to the density of states (DOS) $N(E)$ extending between −2 eV and 2 eV around $E_F=0$, where the partial contributions of other states are substantially smaller. The p states of As are predominantly extended in the interstitial region, and there is no clear separation of the 3d states of Fe into the e_g and t_{2_g} manifolds in the crystal field of the As tetrahedron. In fact, theh pseudogap $\simeq 0.3$ eV above E_F corresponds to the occupation d^6 of Fe^{2+}. These basic computed features of the electronic structure and DOS(E) of LaFeAsO are in a qualitative agreement with results of previous calculations.[18,26,28]

As is seen in Fig. 3, in LaFeAsO the Fermi level E_F lies at the steep slope of $N(E)$, rapidly decreasing with energy. We found that E_F lies very close to the V-shaped local minimum of $N(E)$, which is also seen in Fig. 3. This V-shaped feature of DOS is related to a Fermi surface driven instability, reported in Refs. 18, 27, and 28, which forces the undoped LaFeAsO into the stripe AFM state.

The computed $N(E)$ for LaFeAsO with oxygen replaced by virtual atoms with $Z=7.9$ and $Z=8.1$ are also presented in Fig. 3. Within the virtual crystal approximation (VCA) a true atom in the phase is replaced by an "average" atom which is interpolated linearly in charge between the corresponding pure atoms. Hence, the VCA calculations have taken into account the hybridization and band-filling effects but neglected randomness and have not properly taken into account the effect of charge transfer. The chosen approximation has an advantage due to its simplicity and hence we can study small concentrations of F in the oxygen sublattice. The scattering effect of disorder is expected to be weak, since oxygen ions do not participate in the states at E_F. For all studied systems one can see a peculiar $N(E)$ behavior with the V-shaped feature at the Fermi level. Also, the evaluated volume derivatives of $N(E_F)$ were found to be positive ($d\ln N(E_F)/d\ln V\simeq 0.9$ for the undoped LaFeAsO), and this suggests the reduction of $N(E_F)$ with pressure for the $\mathrm{LaFeAsO}_{1-x}\mathrm{F}_x$ systems.

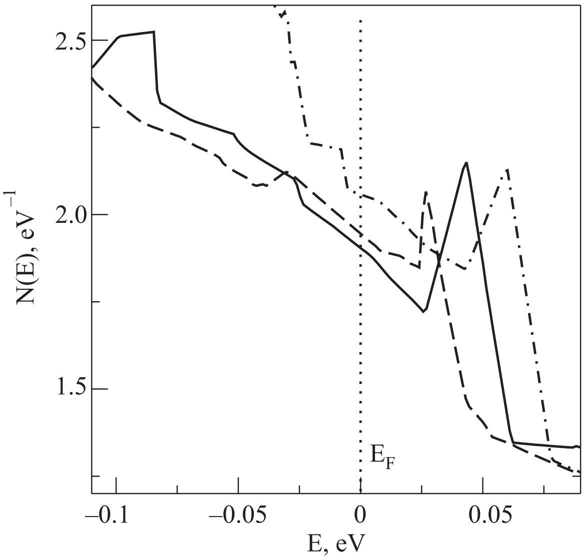

FIG. 3. LSDA density of states of paramagnetic LaFeAsO near E_F for the undoped compound (solid line) and for LaFeAsO with oxygen replaced by virtual atoms with $Z=7.9$ (dash-dot line) and $Z=8.1$ (dashed line). The calculations were performed with a fine energy mesh 0.001 eV. The Fermi level position (at 0 eV) is marked by a vertical line.

A. Calculated magnetic properties

The FP-LMTO-LSDA calculations of the field-induced spin and orbital (Van Vleck) magnetic moments were performed self-consistently within the procedure described in Ref. 30 by means of the Zeeman operator

$$H_Z=\mu_B H(2\hat{s}+\hat{l}), \tag{1}$$

which was incorporated in the original FP-LMTO Hamiltonian. Here H is the external magnetic field and $\hat{s}$ and $\hat{l}$ are the spin and orbital angular momentum operators, respectively. The field induced spin and orbital magnetic moments were calculated in external field 10 T and provided estimates of the related contributions to the magnetic susceptibility, χ_{spin} and χ_{orb}.

For the tetragonal crystal structure of LaFeAsO, the components of the paramagnetic contributions χ_{spin} and χ_{orb} were derived from the magnetic moments obtained in an external field applied parallel and perpendicular to the c axis. The evaluated magnetic anisotropy, which is determined by the orbital contribution, $\Delta\chi_{\mathrm{orb}}=\chi_{\mathrm{orb}\parallel}-\chi_{\mathrm{orb}\perp}$, was found to be negligible in comparison with the dominant spin χ_{spin} contribution. The orbital Van Vleck contribution χ_{orb} itself is at

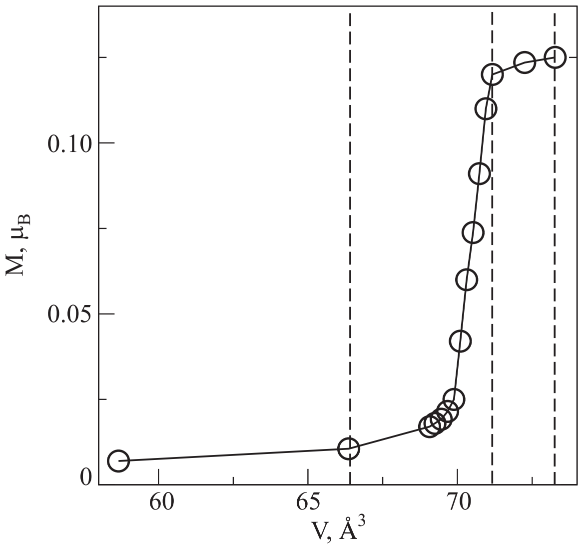

FIG. 4. Magnetic moment induced in the field $H=10$ T as a function of volume with lattice parameters c/a, z_{As}, and z_{La} fixed to their experimental ambient pressure values for undoped LaFeAsO. Dashed vertical lines denote the computed LSDA equilibrium volume, the experimental volume and the computed GGA equilibrium volume of LaFeAsO (from left to right).

least an order of magnitude smaller than the strongly enhanced spin susceptibility and comes almost exclusively from the *d* states of Fe. For the theoretical LSDA equilibrium volume the contributions χ_{spin} and χ_{orb} are found to be equal to $5.45\cdot 10^{-4}$ emu/mol and $0.46\cdot 10^{-4}$ emu/mol, respectively. The Langevin diamagnetism of filled shells, $\chi_{\mathrm{dia}}\simeq -0.54\cdot 10^{-4}$ emu/vol, was estimated according to Ref. 35 and assumed to be close to the free-ionic diamagnetic susceptibility.

Due to the close proximity of the induced spin-polarized state to the spontaneous magnetic ordering for the experimental lattice parameters, the computed total magnetic moment rises to $0.2\mu_B$, which in fact is close to the experimentally observed magnetic moment of $0.36\mu_B$ at an Fe site in the AFM state.[11] However, this is not an induced magnetization, since it turns out that an FM state with quite small moment is actually more stable than the paramagnetic solution. Actually, as seen in Fig. 4, the spontaneous spin polarization occurs in the field-induced calculations at lattice parameters above a_{LSDA}, whereas for $a\leqslant a_{LSDA}$ (approximately 2% lower than the experimental value), a paramagnetic response was obtained.

The enhanced Pauli spin contribution to the magnetic susceptibility was also calculated within the Stoner model:

$$\chi_{\mathrm{ston}}=S\chi_P\equiv\mu_B^2 N(E_F)[1-IN(E_F)]^{-1}, \tag{2}$$

where $\chi_P=\mu_B^2 N(E_F)$, S is the Stoner enhancement factor, and μ_B the Bohr magneton. The multi-band Stoner integral I, representing the exchange-correlation interactions for conduction electrons and appropriate for compounds, can be expressed in terms of the calculated parameters of the electronic structure:[34]

$$I=1/N(E_F)^2\sum_{qll'}N_{ql}(E_F)J_{qll'}N_{ql'}(E_F). \tag{3}$$

Here $N(E_F)$ and $N_{ql}(E_F)$ are the total density of electronic states and DOS at site q with angular momentum l projected on the Fermi level, respectively. The parameters of the exchange interaction $J_{qll'}$ are defined in terms of the intra-atomic exchange integrals:

$$J_{qll'}=\int g(\rho(r))\phi_{ql}(r)^2\phi_{ql'}(r)^2\mathrm{d}r, \tag{4}$$

and therefore depend upon the corresponding partial wave functions $\phi_l(r)$. Here $g(\rho(r))$ is a function of the electron density,[31] l and l' are the corresponding angular-momentum quantum numbers.

The computed value of the enhanced Pauli susceptibility $\chi_{\mathrm{ston}}\sim 5\cdot 10^{-4}$ emu/mol for $a_{LSDA}\leqslant a\leqslant a_{\mathrm{exp}}$) is close to the field-induced evaluated χ_{spin} for the same range of lattice parameters. The Stoner criterion is nearly fulfilled for LaFeAsO, and the computed susceptibility enhancement factor S appears to be about 8, which is comparable to the earlier estimation ($S\simeq 6$ (Ref. 26)). This means proximity to a quantum critical point in the pure LaFeAsO compound and a possibility of competition between FM and AFM spin fluctuations.

IV. DISCUSSION

To our best knowledge no clear anomalies were observed at $T\simeq 135$ K in $\chi(T)$ of the superconducting doped LaFeAsO$_{1-x}$F$_x$ systems, similar to that found in the present study (see Fig. 1). The disappearance of the static AFM order in the doped "1111" superconducting materials is widely reported,[4–7] and it is believed to be favorable for unconventional superconductivity.[18,19]

One may speculate that the experimental sample contains a fraction of the undoped (or weakly doped) parent phase, wherein a strong interplay of FM and different AFM spin fluctuations can take place. Firstly, the Fe–As–Fe positions angle is larger than 90° and provides a possibility of AFM superexchange interaction (see, e.g., Ref. 36) via the As p orbitals. Furthermore, a substantial direct Fe–Fe overlap in the Fe planes can yield an additional AFM exchange.[26] Finally, the computed band structure indicates a possibility of nesting-related AFM spin-density-wave type.[18,19,28]

The volume-dependent field-induced moments computed for $a\leqslant a_{LSDA}$ permit describing the experimental susceptibility of LaFeAsO in the paramagnetic region at temperatures above 140 K. The LaFeAsO compound is found to be on the verge of magnetic instability. The proximity to a quantum critical point is clearly seen in Fig. 4, and this results in strong FM spin fluctuations[26] and can provide weak FM ordering in the doped phase of the LaFeAsO$_{0.85}$F$_{0.1}$ sample. On the other hand it seems probable that the magnetization found at low temperatures is due to a weak ferromagnetism (or canted antiferromagnetism) of Dzyaloshinsky–Moriya (DM) type.[37,38] In this case the DM antisymmetric exchange interaction can provide incomplete cancellation of the magnetic moments at Fe sites for the AFM LaFeAsO phase. Also, the presence of defects in the iron sublattice, as well as crystal structure distortions, cannot be ruled out. Then the environments of the Fe sites are different, and this can be assumed to be another origin of the observed weak FM. It has been recently shown[39] that the combined effects of spin-orbit coupling, lattice distortion, and $p-d$ hybridization in tetrahedrally coordinated Fe in LaFeAsO can provide a highly anisotropic magnetic moment with an in-plane value of $0.25-0.35\mu_B$ per Fe with a small z projection $M_z \simeq 0.05\mu_B$. Curiously, the total moment of about $10^{-3}\mu_B$ was roughly estimated for the ground AFM state of LaFeAsO (Ref. 12) from the computed not fully equivalent densities of spin-up and spin-down electrons for a 16-atom supercell. However, this result could due to incomplete convergence of the DFT calculations of Ref. 12 for the AFM phase.

The present FP-LMTO calculations revealed a peculiar non-monotonic behavior of the density of states in the immediate vicinity of E_F. As seen in Fig. 3, for undoped LaFeAsO the V-shaped minimum of $N(E)$ is followed by a local maximum of DOS, about 0.05 eV above E_F. Our calculations for LaFeAsO with oxygen replaced by virtual atoms with $Z=7.9$ and $Z=8.1$ also showed similar behavior of $N(E)$ (see Fig. 3). Obviously, the VCA calculations are unable to reproduce the relative positions of E_F and the fine features of $N(E)$ with resolution better than 0.05 eV, which is basically the accuracy of LSDA calculations. However, one can expect that with the up-shifting of the Fermi level on F doping in $LaFeAsO_{1-x}F_x$, the density of states $N(E_F)$ slightly bounces up due to the local DOS maximum, but then eventually descends down with increased fluorine content x. Note, that the local DOS peak in Fig. 3 can be "smeared" substantially due to the scattering effect of disorder.

We presume that within the Stoner model (2) such $N(E_F,x)$, behavior can affect the spin paramagnetic susceptibility and can explain qualitatively the reported experimental dependence $\chi(T)$ and $\chi(x)$ in $LaFeAsO_{1-x}F_x$.[9,12,20,21] In particular, it has been shown in Ref. 12 that the paramagnetic susceptibility in the normal conducting state of $LaFeAsO_{1-x}F_x$ is enhanced with F-doping, showing a maximum around F content of 5%. Also, within the Stoner model (2) the observed weak behavior of $\chi(T)$ for $LaFeAsO_{0.85}F_{0.1}$ in the range 140–300 K (see Fig. 1) is qualitatively consistent with the calculated non-monotonic $N(E)$ dependence in Fig. 3, provided E_F is varied slightly in the range about 0.05 eV, which is well within the accuracy of *ab initio* calculations.

A detailed theoretical study of $\chi(T)$ and $\chi(T)$ in $LaFeAsO_{1-x}F_x$ merits a separate examination beyond the scope of this study. It would obviously require a more rigorous calculation of $N(E)$ in alloys, presumably employing the CPA (coherent potential approximation) method. Also, the thermal expansion and spin fluctuation effects have to be taken into account. Finally, according to the present calculations, the density of states $N(E_F)$ in $LaFeAsO_{1-x}F_x$ is found to be decreasing with pressure, as well as the enhanced Pauli susceptibility.

V. CONCLUSIONS

The magnetic susceptibility of the compound $LaFeAsO_{0.85}F_{0.1}$ was investigated in the temperature range 4.2–300 K, and the superconducting transition was detected at 26 K. A clear cusp at $T_M \simeq 135$ K was observed in the low-field dependence of the magnetic susceptibility $\chi(T)$ with a sharp rise of χ with further cooling to $T_c \simeq 26$ K. The obtained magnetization data $M(H)$ indicate the emergence of an FM phase at $T \leqslant T_M$.

Ab initio calculations of the electronic structure and paramagnetic contributions to susceptibility of the parent LaFeAsO compound have revealed that this system is in close proximity to the quantum critical point. It was shown that the paramagnetic susceptibility computed in an external magnetic field appears to be close to the experimental value. The Van Vleck contribution to χ comes mainly from d electrons of Fe and amounts up to 10% of the total susceptibility.

The V-shaped minimum and local maximum are revealed in the density of electronic states in the immediate vicinity of the Fermi level, which can govern magnetic properties of $LaFeAsO_{0.85}F_{0.1}$ with fluorine doping and/or oxygen deficiency. Our calculations for $LaFeAsO_{1-x}F_x$ indicate that the main role of pressure (and F-doping $x \gtrsim 0.1$) is to reduce the density of states at the Fermi level and to shift the "1111" system away from the FM instability. In general, the results reported results show that itinerant magnetism theory is relevant for describing the magnetic properties of the LaFeAsO based systems.

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