Comment on paper arXiv: 17070526v1 "Electronic structure of FeSe monolayer superconductors: shallow bands and correlations" by Sadovskii group

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We comment two incorrect statements given in [1]. (A) - In order to show that the electron-phonon interaction (EPI) is very small and irrelevant for high $T_c$ superconductivity in 1UC FeSe/SrTiO$_3$ system, the authors of [1] use an EPI coupling constant ($\lambda_{Sad}$) which does not enter in any theory of superconductivity. So, their conclusion on the smallness of the EPI in 1UC FeSe/SrTiO$_3$ is incorrect. Accordingly, their coupling constant $\lambda_{Sad}$ has also nothing to do with the EPI coupling with the forward scattering peak (EPI-FSP), which is proposed recently in order to explain high $T_c$ in 1UC FeSe/SrTiO$_3$. (B) - In [1] it is claimed that the experimentally resolved ARPES replica bands can be explained by the LDA+DMFT method of Ref. [1]. We show that this statement is also incorrect, i.e. the LDA+DMFT method is unable to explain the replica bands.

I. INTRODUCTION

The recent discovery of high temperature superconductivity (SC) in the one unit-cell film of the iron-selenide FeSe grown on the SrTiO$_3$ substrate - called 1UC FeSe/SrTiO$_3$, with $T_c \sim 100$ K, as well as grown on the rutile TiO$_2$ (100) substrate with $T_c \sim 65$ K [2], has provoked an intensive debate on the origin of SC in this system. Additionally, ARPES spectra give strong evidence for the existence of replica bands with the same shape as the main electronic band responsible for SC. The replica bands are shifted by $\sim 100$ meV. In that respect in [3]-[4] is proposed that these experimental facts can be consistently explained by the theory of the electron-phonon interaction with the forward scattering peak - the EPI-FSP theory. The latter theory is proposed in [3], while its extreme case with the delta-like peak is elaborated in [6]. In [7] some important issues were elaborated and cleared up. Additionally, the range of microscopic parameters relevant for 1UC FeSe/SrTiO$_3$ is estimated. The basic assumption of the EPI-FSP theory is that the transverse oxygen optical phonon due to the TiO$_2$ layer with the frequency $\Omega_O \sim 90$ meV is the main pairing glue and that the corresponding EPI pairing potential is peaked at small transfer momenta $q \approx 0$, i.e. $g(q) = g_0 \exp(-q/q_c)$ with $q_c \ll k_F$. The important predictions of the EPI-FSP theory are: (A) the SC critical temperature $T_c$ and the gap $\Delta$ are linear functions on the pairing potential, i.e. $T_c \sim V_{FSP}/4$, $\Delta = 2T_c$, $V_{FSP} \sim (q_c/G)^2 (2g_0/\Omega_O)$, $G = \pi/a$ and $a$ is the lattice constant. In the derivation of these results it is assumed that $q_c v_F < \pi T_c \ll \Omega_O$. Note, that $T_c$ and $\Delta$ do not depend on the oxygen mass - since $V_{FSP}$ is mass independent in leading order; (B) in ARPES spectra there are sharp replica bands with the same shape as the main band and shifted by the multiple of energy $\Omega_O$. These results are contrary to the standard isotropic Eliashberg theory (ET) where $T_c$ is mass-dependent, i.e. $T_c^{ET} \sim M_O^{-1/2}$, and the replica bands would be drastically deformed. At the same time the low-energy ($\omega \ll \Omega_O$) slope of the self-energy $\Sigma(\omega)$ is mass-dependent in the EPI-FSP theory, while in the ET it is not, i.e. $\Sigma_{FSP}(\omega) \sim -\lambda_m \omega$ with $\lambda_m \sim M_O^{1/2}$. This means that the predictions of the EPI-FSP theory are very different from the ET theory.

Recently, intensive efforts were done in order to discredit and disregard the EPI mechanism of pairing and its origin of the replica bands in 1UC FeSe/SrTiO$_3$. These approaches are mainly based on the spin-fluctuations interaction described by the extended Hubbard or phenomenological Heisenberg models. For instance, the Sadovskii’s group [3] claims to have shown: (A) that the EPI coupling is extremely small and irrelevant for high $T_c$ and (B) - the replica bands are due to strong correlations in the LDA-DMFT approach. Let us show that both claims are incorrect.

(A) Role of EPI on $T_c$ - In order to show that the EPI is irrelevant in 1UC FeSe/SrTiO$_3$, i.e. that $T_c$ due to EPI-FSP is small, in [1] this problem is studied in the framework of the ET theory (with the band energy $\epsilon_p = \epsilon_p - \mu$ and with the Einstein phonon with the energy $\Omega_O$) by calculating a quite inappropriate coupling constant $\lambda_{Sad}$ ($N$ is the number of unit cells)

$$\lambda_{Sad} = \frac{2}{N \Omega_O} \sum_{p,q} g(q) | \delta(\xi_p) \delta(\xi_{p+q} - \Omega_O) | \sum_p \delta(\xi_p)$$

$$\lambda_{Sad} \sim \lambda_0 \frac{\Omega}{\pi \varepsilon_F} \sqrt{\frac{q_c v_F}{\Omega_O}} \exp(-\frac{2 \Omega_O}{q_c v_F}) \sim 10^{-9} \lambda_0$$

for experimental values ($\Omega_O/\pi \varepsilon_F \sim 1$ and $\Omega_O/q_c v_F \sim 10$). If this analysis were correct it would give an enormous small $T_c^{Sad} \sim \exp(-10^{9})$ K in the ET theory. However, the coupling $\lambda_{sad}$ never appears in any theory
of superconductivity! Namely, in the ET theory by assuming that the phonon line-width $\Gamma_0$ is much smaller than the phonon energy $\Omega_0$, i.e. $\Gamma_0 \ll \Omega_0$, the critical temperature $T_c$ is determined by the coupling constant $\lambda_{ET}$ defined by

$$\lambda_{ET} = \frac{2}{N\Omega_0} \sum_{p, q} [g(q)^2] (\xi_p^0)^2 (\xi_{p+q}^0) \sim \lambda_0 \frac{q_c}{4\pi k_F},$$

i.e.

$$\lambda_{ET} \gg \lambda_{Sad}!$$

It is clear that the Eliashberg coupling is much larger than the one introduced and calculated by Sadowskii’s group, i.e. $\lambda_{ET} \gg \lambda_{Sad}$. It is physically clear why $\lambda_{Sad}$ cannot be related to SC, since it describes real scattering of electrons on phonons where one optical phonon is emitted (or absorbed). This is seen in Eq. 1 where $\lambda_{Sad}$ contains two delta functions which describe conservation of energy in the scattering processes. On the other side the Eliashberg coupling $\lambda_{ET}$ describes virtual excitation and absorption of phonons by electrons, which are responsible for the mass renormalization and superconductivity. In conclusion, in [1] the EPI coupling constant is enormously underestimated by nine order of magnitude due to using quite inappropriate EPI coupling constant. We point out, that in spite of the fact that $\lambda_{ET} \gg \lambda_{Sad}$ the ET approach would still give rather small $T_c$, since for an optimistic estimation one has $\lambda_{ET} \sim 0.1$ and $T_{c,ET}$ is rather small, i.e. $(T_{c,Sad}) \ll (T_{c,ET}) \sim \Omega_0 \exp(-1/\lambda) < 0.01 K$. In that respect the recently proposed EPI-FSP mechanism of pairing in $UC FeSe/SrTiO_3$ [4, 7] is much more favorable due to its linear dependence of $T_c$ on the pairing potential, i.e. $T_{c,FSP} \sim (q_c/G)^2(2g_0/\Omega_0) = (q_c/G)^2 V_{FSP}^0$. It is matter of fine nature-tuning that in $UC FeSe/SrTiO_3$ the reasonable value for $(q_c/G) \sim 0.1 - 0.2$ is realized and for $V_{FSP}^0 \sim (0.5 - 1) eV$ one has $T_c \sim 100 K$ [4, 7]. In reality the EPI-FSP pairing mechanism acts not alone, since one should add a "residual" pairing which is responsible for SC in the single $FeSe$ plane but with the electron-like Fermi surface at the point $M$. This means that $T_{c,FSP} < T_c$, i.e. $T_{c,FSP} \ll T_c$. We stress again, that the the EPI-FSP theory is already partly confirmed by the perfect shape of the ARPES replica bands [3] and by the mass-dependent of their energy shift with respect to the main electronic band and by the linear dependence of $\Delta$ on the coupling strength [8]. Measurements of the oxygen mass-independence of $T_c$ and $\Delta$, as well as of the mass-dependence of the self-energy - predicted in [7], would be an important step in proving the relevance of the EPI-FSP pairing mechanism in $UC FeSe/SrTiO_3$.

The above discussion shows that the claims done in [1] - on the weakness of EPI in $UC FeSe/SrTiO_3$ are unfounded, since the analysis in [1] is based on an inappropriate coupling constant and on an inappropriate EPI theory. In that respect any eventual reply on our comment of the point (A) is superfluous.

**FIG. 1:** ARPES bands in $UC FeSe/SrTiO_3$ - from [3]. Left: The hole band $D$ and its replica $D'$ at the $\Gamma$ point; Middle: The electronic band $A$ and its replica $A'$ at the $M$ point, shifted by 100 meV at $T < T_c$; Right: The electronic band $A$ and its replica $A'$ at the $M$ point, shifted by 100 meV at $T > T_c$.

(B) **Sharp replica bands** - Important ARPES results related to the energy spectra of $UC FeSe/SrTiO_3$ are reported in [3] - see Fig.1: (i) two electronic (almost degenerate) bands are clearly resolved with the Fermi surfaces centered at the point $M$ - these bands are labelled by $A$ with the band bottom energy $\sim 60 eV$ from the Fermi surface; (ii) the existence of the replicated bands $A'$ with the same shape as $A$ but shifted downward by the energy $\sim 100 meV$ - this energy is of the order of the optical phonon energy $\Omega_0$; (iii) in the superconducting state both bands $A$ and $A'$ show typical superconducting behavior with banding away from the Fermi surface (at $k_F$) - see the backbending at $k_F$ in Fig.1(Middle); (iv) in [3] it is found the isotope effect in the energy shift ($\sim M_0^{-1/2}$) of the band $A'$ with respect to $A$.

However, in [1] it is claimed that the replica band $A'$ can be explained (even semi-quantitatively) exclusively in the LDA-DMFT approach, i.e. to be due to electronic correlations. They found that the electronic band $A$ is formed by the $Fe - 3d_{xy}, 3d_{yz}$ states while its bottom energy is $\sim 100 meV$, i.e. larger than the experimental value, while the band $A'$ is due to the $Fe - 3d_{xy}$ state. However, the band $A'$ does not have the shape and properties of the $A$ band - see Fig.2. Namely, the ARPES replica band $A'$ exists for $k < k_F$ and is reminescent of the vibron shake-offs in the photoemission of $H_2$ molecule [3, 4], while the LDA-DMFT (ARPES) band $A'$ goes up to the Fermi surface. In fact the band $A'$ from [1] is more reminescent of the second almost degenerate band around the point $M$, as reported in [3].

Moreover, the LDA-DMFT brings in unpleasant artefact since it predicts an hole-like Fermi surface near the $\Gamma$ point with the band-top at $\sim 50 meV$. Experimentally there is only a hole band $D$ at the $\Gamma$ point, which is approximately 40 meV below the Fermi surface and its replica band $D'$ shifted downward by the energy $\sim \Omega_0$. This means that the experimental results (i)-(iv) cannot
be explained by the LDA-DMFT approach.

In conclusion, the band spectra with their replica bands and high $T_c$ superconductivity in 1$\text{UC FeSe} - \text{SrTiO}_3$ cannot be explained by the LDA-DMFT approach proposed in [1]. Contrary to LDA-DMFT, the theory based on the electron-phonon interaction with the forward scattering peak (EPI-FSP) is able to explain some important experimental facts by including the isotope effect in the shift of the replica bands.

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