The electron–phonon interaction with forward scattering peak is dominant in high \( T_c \) superconductors of FeSe films on SrTiO\(_3\) (TiO\(_2\))

M L Kulić and O V Dolgov

1 Institute for Theoretical Physics, Goethe-University D-60438 Frankfurt am Main, Germany
2 Institute of Physics, Pregrevica 118, 11080 Belgrade (Zemun), Serbia
3 Max-Planck-Institut für Festkörperphysik, D-70569 Stuttgart, Germany
4 P. N. Lebedev Physical Institute, RAS, Moscow, Russia

E-mail: kuli@th.physik.uni-frankfurt.de and o.dolgov@fkf.mpg.de

Keywords: forward scattering, FeSe, electron–phonon interaction

Abstract

The theory of the electron–phonon interaction (EPI) with strong forward scattering peak (FSP) in an extreme delta-peaks limit (Kulić and Zeyher 1994 Phys. Rev. B 49 4395; Kulić 2000 Phys. Rep. 38 1–264; Kulić and Dolgov 2005 Phys. Status Solidi b 242 151; Danylenko et al 1999 Eur. Phys. J. B 9 201) is recently applied in (Lee et al 2014 Nature 515 245; Rademaker et al 2016 New J. Phys. 18 022001; Wang et al 2016 Supercond. Sci. Technol. 29 054009) for the explanation of high \( T_c \) (~100 K) in a monolayer FeSe grown on SrTiO\(_3\) (Lee et al 2014 Nature 515 245) and TiO\(_2\) (Rebec et al 2016 arXiv:1606.09358v1) substrates. The EPI is due to a long-range dipolar electric field created by high-energy oxygen vibrations (\( \Omega \sim 90 \text{ meV} \)) at the interface (Lee et al 2014 Nature 515 245; Rademaker et al 2016 New J. Phys. 18 022001; Wang et al 2016 Supercond. Sci. Technol. 29 054009). In leading order (with respect to \( T_{c0}/\Omega \)) the mean-field critical temperature \( T_{c0} = \langle V_{\text{epi}}(q) \rangle_q/4 \sim (aq)^2 V_{\text{epi}}(0) \) and the gap \( \Delta_0 = 2T_{c0} \) are due to an interplay between the maximal EPI pairing potential \( V_{\text{epi}}(0) \) and the FSP-width \( q_c \). For \( T_{c0} \sim 100 \text{ K} \) one has \( \Delta_0 \sim 16 \text{ meV} \) in a satisfactory agreement with ARPES experiments. In leading order \( T_{c0} \) is mass-independent and a very small oxygen isotope effect is expected in next to leading order. In clean systems \( T_{c0} \) for s-wave and d-wave pairing is degenerate but both are affected by non-magnetic impurities, which are pair-breaking in the s-channel and pair-weakening in the d-channel. The self-energy and replica bands at \( T=0 \) and at the Fermi surface are calculated and compared with experimental results at \( T > 0 \) (Rademaker et al 2016 New J. Phys. 18 022001; Wang et al 2016 Supercond. Sci. Technol. 29 054009). The EPI coupling constant \( \lambda_m = \langle V_{\text{epi}}(q) \rangle_q/2\Omega \) is mass-dependent \((M^4/2)\) and at \( \omega (\ll \Omega) \) makes the slope of the self-energy \( \Sigma(k, \omega) \sim -\lambda_m \omega \) and the replica intensities \( A_i (\sim \lambda_m) \) mass-dependent. This result, overlooked in the literature, is contrary to the prediction of the standard Migdal–Eliashberg theory for EPI. The small oxygen isotope effect in \( T_{c0} \) and pronounced isotope effect in \( T_{c0} \) and pronounced isotope effect in \( \Sigma(k, \omega) \) and ARPES spectra \( A_i \) of the replica bands in FeSe films on SrTiO\(_3\) and TiO\(_2\) is a smoking-gun experiment for validity of the EPI–FSP theory to these systems. The EPI–FSP theory predicts a large number of low-laying pairing states, thus causing internal pair fluctuations. The latter reduce \( T_{c0} \), additionally, by creating a pseudogap state for \( T_c < T < T_{c0} \). Possibilities to increase \( T_{c0} \), by designing novel structures are discussed in the framework of the EPI–FSP theory.

1. Introduction

The scientific race in reaching high temperature superconductivity (HTSC) started by the famous Ginzburg’s proposal of an excitonic mechanism of pairing in metallic–semiconducting sandwich-structures [7]. In such a system an electron from the metal tunnels into the semiconducting material and virtually excites high-energy exciton, which is absorbed by another electron, thus making an effective attractive interaction and Cooper pairing.
However, this beautiful idea has not been realized experimentally until now. In that sense Ginzburg founded a theoretical group of experts, who studied at that time almost all imaginable pairing mechanisms. In this group an important role has played the Ginzburg’s collaborator Maksimov, who was an ‘inventor enemy’ of almost all other mechanisms of pairing in HTSC except of the electron–phonon one—see the arguments in [8]. It seems that the recent discovery of superconductivity in a Fe-based material made of one monolayer film of the iron-selenide FeSe grown on the SrTiO3 substrate—further called 1ML FeSe/SrTiO3, with the critical temperature \( T_c \approx (50–100) \) K [9], as well as grown on the rutile TiO2 (100) substrate with \( T_c \approx 65 \) K [6]—further called 1ML FeSe/TiO2, in some sense reconciles the credence of these two outstanding physicists. Namely, HTSC is realized in a sandwich-structure but the pairing is due to an high-energy (\(~90–100\) meV) oxygen optical phonon. This (experimental) discovery will certainly revive discussions on the role of the electron–phonon interaction (EPI) in HTSC cuprates and in bulk materials of the Fe-pnictides (with the basic unit Fe–As) and Fe-chalcogenides (with the basic unit Fe-Se or Te, S). As a digression, we point out that after the discovery of high \( T_c \) in Fe-pnictides a non-phononic pairing mechanism was proposed immediately, which is based on: (i) nesting properties of the electron- and hole-Fermi surfaces and (ii) an enhanced (due to (i)) spin exchange interaction (SFI) between electrons and holes [10]. This mechanism is called the nesting SFI pairing. However, the discovery of alkaline iron selenides \( K_xFe_{2–y}Se_y \) with \( T_c \sim 30 \) K, and intercalated compounds \( L_i(xC_{x}H_{y}N_{z})Fe_{2–y}Se_y \), \( Li_2(NH_2)(NH_3)_{1–x}FeSe_x \), which contain only electron-like Fermi surfaces, rules out the nesting pairing mechanism as a common pairing mechanism in Fe-based superconductors. In order to overcome this inadequacy of the SFI nesting mechanism a pure phenomenological ‘strong coupling’ SFI pairing is proposed in the framework of the so called \( j_1 = j_2 \) Heisenberg-like Hamiltonian, which is able to describe s-wave superconductivity, too. However, this approach is questionable, since the LDA calculations cannot be mapped onto a Heisenberg model and it is necessary to introduce further terms in form of a biquadratic exchange [10]. It is interesting, that immediately after the discovery of high \( T_c \) in pnictides the electron–phonon pairing mechanism was rather uncritically discarded. This attitude was exclusively based on the LDA band structure calculations of the electron–phonon coupling constant [11], which in this approach turns out to be rather small \( \lambda < 0.2 \), thus giving \( T_c < 1 \) K.

In the past there were only few publications trying to argue that, the EPI pairing mechanism is an important (pairing) ingredient in the Fe-based superconductors [12–15]. One of the theoretical arguments for it, may be illustrated in the case of 2-band superconductivity. In the weak-coupling limit \( T_c \) is given by

\[
T_c = 1.2 \omega_c \exp \left\{-1/\lambda_{\text{max}} \right\}, \quad \lambda_{\text{max}} = (\lambda_{11} + \lambda_{22} + \sqrt{(\lambda_{11} - \lambda_{22})^2 + 4\lambda_{12}\lambda_{21}}) / 2.
\]

In the nesting SFI pairing mechanism one assumes a dominance of the repulsive inter-band pairing \((\lambda_{12}, \lambda_{21} < 0)\), i.e.

\[
|\lambda_{12}, \lambda_{21}| \gg |\lambda_{11}, \lambda_{22}|.
\]

Since the intra-band pairing depends on \( \lambda_{ii} = \lambda_{\text{int}}^i - \mu_{\text{F}}^i \) where \( \lambda_{\text{int}}^i \) is the intra-band EPI coupling constant and \( \mu_{\text{F}}^i > 0 \) is a screened intra-band Coulomb repulsion, then in order to maximize \( T_c \) the intra-band EPI\( \lambda_{\text{int}}^i \) should at least compensate negative effects of \( \mu_{\text{F}}^i \) (on \( T_c \)), i.e. \( \lambda_{\text{int}}^i \geq \mu_{\text{F}}^i \). Since in a narrow band one expects rather large screened Coulomb repulsion \( \mu_{\text{F}}^i (\sim 0.2) \) then the intra-band EPI coupling should be also appreciable. Moreover, from the experimental side the Raman measurements in Fe-pnictides [16] give strong evidence for a large phonon line-width of some \( A_{1g} \) modes (where \( A_s \) vibrations along the c-axis dominate). They are almost 10 times larger than the LDA band structure calculations predict. In [13] a model was proposed where the high electronic polarizability of \( As (\alpha_{As^2–} \sim 12 \) Å) ions screens the Hubbard repulsion and gives rise to a strong EPI with \( A_{1g} \) (mainly As) modes. An appreciable ESI isotope effect in \( T_{c0} \) was proposed in [13], where the stable \(^{75}\)As should be replaced by an unstable, for instance \(^{73}\)As—with the life-time of 80 days, quite enough for performing relevant experiments. The situation is similar in Fe-Se compounds, where an appreciable EPI is expected, since \(^{78}\)Se is also highly polarizable \((\alpha_{Se^2–} \sim 7, 5 \) Å) and can be replaced by a long-living \(^{80}\)Se isotope—the half-time 120 days. Unfortunately these experiments were never performed.

We end up this digression by paying attention to some known facts, that the LDA band structure calculations are unreliable in treating, most high \( T_c \), superconductors, since as a rule LDA underestimates non-local exchange-correlation effects and overestimates charge screening effects—both effects contribute significantly to the EPI coupling constant. As a result, LDA strongly underestimates the EPI coupling in a number of superconductors, especially in those near a metal–isolator transition. The classical examples for this claim are: (i) the (BaK) BiO\(_3\) superconductor with \( T_c > 30 \) K which is K-doped from the parent isolating compound BaKBO\(_3\). Here, LDA predicts \( \lambda < 0.3 \) and \( T_c \sim 1 \) K, while the theories with an appropriate non-local exchange-correlation potential [17] predict \( \lambda_{\text{epi}} \approx 1 \) and \( T_c \sim 31 \) K; (ii) the HTSC, for instance YBaCuO\(_3\) with \( T_c \sim 100 \) K, whose parent compound YBaCuO\(_3\) is the Mott-insulator and cannot be described by LDA [2, 18].

After this digression we consider the main subject of the paper—the role of the EPI with FSP in pairing mechanism of the 1ML FeSe/SrTiO\(_3\) and 1ML FeSe/TiO\(_2\) superconductors with high critical temperatures \( T_c \sim (50–100) \) K. In that respect, numerous experiments on 1ML FeSe/SrTiO\(_3\) and 1ML FeSe/TiO\(_2\), combined with the fact that the FeSe film on the graphene substrate has rather small \( T_c \approx 8 \) K (like in the bulk FeSe), give strong evidence that interface effects, due to SrTiO\(_3\) (and TiO\(_2\)), are most probably responsible for high \( T_c \).
turns out, that the most important results in 1 ML FeSe/SrTiO$_3$ (and 1 ML FeSe/TiO$_2$) — related to the existence of quasi-particle replica bands and which are identical to the main quasiparticle band [4, 6, 19], can be coherently described by the EPI–FSP theory. This approach was proposed in seminal papers [4, 5]. The beauty of these papers lies in the fact that they have recognized sharp replica bands in the ARPES spectra and related them to a sharp FSP in the EPI. (This is a very good example for a constructive cooperation of experimentalists and theorists.) Let us mention, that the EPI–FSP theory was first studied in a connection with HTSC cuprates [1], while the extreme case of the EPI–FSP pairing mechanism with delta-peak is elaborated in [3] — see a review in [2]. Physically, this (exotic) interaction means that in some specific materials, for instance, in cuprates and in 1 ML FeSe/SrTiO$_3$, electron pairs exchange virtual phonons with small momentum transfer $q < q_k$ only. As a result, the effective pairing potential becomes long-ranged in real space [2]. It turns out, that this kind of pairing can in some cases give rise to a higher $T_c$ than in the standard (Migdal–Eliashberg) BCS-like theory. Namely, in the EPI–FSP pairing mechanism one has $T_c^{\mathrm{FSP}} = (V_{\text{epi}}(q))_q / 4 \sim \lambda^{\text{FSP}}(E_F) / N$ [3] — see below, instead of the BCS dependence $T_c^{\text{BCS}} = \Omega e^{-1/\lambda^{\text{BCS}}}$. Here, $\lambda^{\text{FSP}}$ and $\lambda^{\text{BCS}}$ are the corresponding mass-independent EPI coupling constants, where $\Omega$ — is the phonon energy, $N(E_F)$ — the electronic density of states (per spin) at the Fermi surface. So, even for small $\lambda^{\text{FSP}} \ll \lambda^{\text{BCS}}$ the case $T_c^{\text{FSP}} > T_c^{\text{BCS}}$ can in principle realized. We inform the reader in advance, that the in the case of a non-singular FSP what happens in 1 ML FeSe/SrTiO$_3$ (and 1 ML FeSe/TiO$_2$) — see below, where the EPI-coupling $g_{\text{epi}}(q)$ is finite at $q = 0$ — non-singular coupling, the EPI–FSP theory predicts also that $T_c^{\mathrm{FSP}} \sim (q_k / k)^d V_{\text{epi}}(0)$, where $d = 1, 2, 3$ is the dimensionality of the system, which means for $q_k \ll k$ high $T_c$ is hardly possible in 3D systems. However, the detrimental effect of the phase-volume factor $(q_k / k)^d$ on $T_c^{\text{FSP}}$ can be compensated by its linear dependence on the pairing potential $V_{\text{epi}}(0)$. In some favorable materials this competition may lead even to an increase of $T_c$. Note, that $T_c^{\text{FSP}} \approx (q_k / k)^d$ holds only for the non-singular EPI coupling, while for the singular one with $q \sim k_0 \sim 0$ — const—studied in [3], one has in the next to leading order $T_c^{\text{FSP}}(q_0) \approx T_c(0) \sim \alpha / (1 - \lambda(0))$ and $T_c^{\text{FSP}}(q_0) \sim \alpha^{-1/2}$, where $\alpha$ is the slope of $q_0(q_0)$. Furthermore, since $T_c^{\text{FSP}}(q_0) \sim \alpha^{-1/2}$, it is due to the interplay of the phase volume $(q \sim k_0)$ effects and the analytical behavior of the long-range EPI forces. We stress that properties of superconductors with the EPI–FSP mechanism of pairing are in many respects very different from the standard (BCS-like) superconductors, and it is completely justified to speak about exotic superconductors. For instance, the EPI–FSP theory [2, 3] predicts, that in superconductors with the EPI–FSP pairing the isotope effect should be small in leading order, i.e. $\alpha \ll 1/2$ [2, 3] — see discussion in the following. This result is contrary to the case of the isotropic EPI theory in standard metallic superconductors, where $\alpha$ is maximal, $\alpha = 1/2$ (for $\mu^\ast = 0$). We point out, that the EPI–FSP pairing mechanism in strongly correlated systems is rather strange in comparison with the corresponding one in standard metals with good electronic screening, where the large transfer momenta dominate and the pairing interaction is, therefore, short-range. As a result, an important consequence of the EPI–FSP pairing mechanism in case of HTSC-cuprates is that $T_c$ in the $d$-wave channel is of the same order as in the $s$-wave one. Since the residual repulsion is larger in the $s$- than in the $d$-channel ($\mu^\ast < \mu^0$) this result opens a door for $d$-wave pairing in HTSC-cuprates, in spite of the fact of the EPI dominance [1, 2].

In the following, we study the superconductivity in 1 ML FeSe/SrTiO$_3$ (and 1 ML FeSe/TiO$_2$ [6]) in the framework of a semi-microscopic model of EPI first proposed in seminal papers [4, 5]. Namely, due to oxygen vacancies: (i) an electronic doping of the FeSe monolayer is realized, which gives rise to electronic-like bands centered at the $M$-points in the Brillouin zone, while the top of the hole-bands are at around 60 meV below the electronic-like Fermi surface; (ii) the formed charge in the interface orders dipoles in the nearby TiO$_2$ layer; (iii) the free charges in SrTiO$_3$ screen the dipolar field in the bulk, thus leaving the TiO$_2$ dipolar layer near the interface as an important source for the EPI. The oxygen ions in the TiO$_2$ dipolar layer vibrate with a high-energy $\Omega \approx 90$ meV, thus making a long-range dipolar electric field acting on metallic electrons in the FeSe monolayer. This gives rise to a long-ranged EPI [4, 5], which in the momentum space gives a FSP — the EPI–FSP pairing mechanism.

In this paper we make some analytical calculations in the framework of the EPI–FSP theory with a very narrow $\delta$-peak, with the width $q_k \ll k_0$, where $k_0$ is the Fermi momentum [3]. Here, we enumerate the obtained results, only: (1) in leading order the critical temperature is linearly dependent on the pairing potential $V_{\text{epi}}(q)$, i.e. $T_c \approx (V_{\text{epi}}(q))_q / 4$. In order to obtain $T_c \sim 100$ K we set a range of semi-microscopic parameters (existence of $\delta$-peak, $q_k = 0$, $V_{\text{epi}}(q_k)$, $\Omega$ — see below) entering $(V_{\text{epi}}(q))_q$. Furthermore, since $(V_{\text{epi}}(q))_q$ is independent of the oxygen (O) mass, then $T_c$ is mass-independent in leading order with respect to $\Omega$. This means, that in 1 ML FeSe/SrTiO$_3$ (and 1 ML FeSe/TiO$_2$) one expects very small O—isootope effect ($\alpha_{0\Omega} \ll 1/2$). Note, in [5] a large $\alpha_{0\Omega} = 1/2$ is predicted; (2) the self-energy $\Sigma(k, \omega)$ at $T = 0$ is calculated analytically which gives: (i) the positions and spectral weights of the replica and quasiparticle bands at $T = 0$ — all these quantities are mass-dependent; (ii) the slope of the quasiparticle self-energy for $\omega \ll \Omega$ is mass-dependent, since $\sim \lambda_m \sim M_{0\Omega}^2$; (3) in the
EPI–FSP model (without other interactions) the critical temperature for s-wave and d-wave pairing is degenerate, i.e. $T_{\text{c}0}^{(s)} = T_{\text{c}0}^{(d)}$. The presence of non-magnetic impurities (with the impurity concentration $n_i$ and the parameter $\Gamma = \pi n_i N(E_f) u^2$) lifts this degeneracy. It is shown, that even the s-wave pairing (in the EPI–FSP pairing mechanism) is sensitive to non-magnetic impurities, which are pair–weakening for it, i.e. $T_{\text{c}0}^{(s)}$ decreases for large $\Gamma$, but never vanishes. It is also shown, that for the d-wave pairing $T_{\text{c}0}^{(d)}$ strongly depends on impurities, which are pair–breaking. The curiosity is that in the presence of non-magnetic impurities $T_{\text{c}0}^{(d)}$ in the EPI–FSP pairing mechanism is more robust than the corresponding one in the BCS model; (4) the long-range EPI–FSP pairing potential in real space makes a short-range potential in the momentum space. The latter gives rise to numerous low-laying excitation energies (above the ground-state) of pairs, thus leading to strong internal pair fluctuations which reduce $T_{\text{c}0}$. At $T_c < T < T_{\text{c}0}$ a pseudogap behavior is expected.

The structure of the paper is following: in section 2 we calculate the EPI–FSP pairing potential as a function of semi–microscopic parameters in the model of a dipolar layer TiO$_2$, with vibrations of the oxygen ions [4, 5]. In section 3 the self–energy effects, such as the replica bands and their intensities at $T = 0$, are studied. The critical temperature $T_{\text{c}0}$ is calculated in section 4 in terms of the semi–microscopic parameters $(\varepsilon_1^{\text{eff}}, \varepsilon_\perp^{\text{eff}}, q_{\text{eff}}, h_0, n_d)$. The range of of these parameters, for which one has $T_{\text{c}0} \approx 100 K$, is estimated, too. In section 5 effects of nonmagnetic impurities on $T_{\text{c}0}$ are studied, while effects of internal fluctuations of Cooper pairs are briefly discussed in section 6. Summary of results are presented in section 7.

2. EPI–FSP potential due to O–vibrations in the TiO$_2$ layer

It is important to point out that in 1ML FeSe/SrTiO$_3$, with 1–monolayer of FeSe grown on the SrTiO$_3$ substrate —mainly on the (0, 0, 1) plane, the Fermi surface in the FeSe monolayer is electron–like and centered at four M–points in the Brillouin zone—see more in [6, 20]. The absence of the (nested) hole–bands on the Fermi surface rules out all SFI nesting theories of pairing. Even the pairing between an electron– and incipient hole-band [21] is ineffective, since: (1) in the FeSe monolayer the top of the hole band lies below the Fermi level around 60–80 meV; (2) because of (1) the SFI coupling constant is (much) smaller than in the nesting case. This brings into play the interface interaction effects. The existence of the sharp replica bands in the ARPES spectra at energies of the order of optical phonons with $\Omega \sim 90 \text{ meV}$, implies inevitably that the dominant interaction in 1ML FeSe/SrTiO$_3$ (and also in 1ML FeSe/TiO$_2$ [6]) is due to EPI with strong FSP [4, 5]. The physical mechanism for EPI–FSP is material dependent and the basic physical quantities such as the width of the FSP, phonon energies and the bare EPI coupling constant can vary significantly from material to material. For instance, in HTSC–cuprates the effective EPI–FSP potential $V_{\text{epi}}(q)$ is strongly renormalized by strong correlations, which is a synonym for large repulsion of two electrons on the Cu ions—the doubly occupancy is forbidden. In that case the approximate $q$–dependence of $V_{\text{epi}}(q)$ is given by $V_{\text{epi}}(q) \approx (1 + (q/q_0)^2)^{-2} V_{\text{e},\text{epi}}(q)$, $q_0 \sim \delta/a$, where $V_{\text{e},\text{epi}}(q)$ is the bare (without strong correlations) coupling constant, $\delta (\ll 1)$ is the hole concentration and $a$ is the Cu–O distance [1, 2]. The prefactor is a vertex correction due to strong correlations and it means a new kind of (anti)screening in strongly correlated materials.

The interface in 1ML FeSe/SrTiO$_3$ can be considered as a highly anisotropic material with parallel and perpendicular (to the FeSe plane) dielectric constants $\varepsilon_1^{\text{eff}} \gg \varepsilon_\perp^{\text{eff}}$. It is assumed [4, 5] that the oxygen ions in the TiO$_2$ dipolar layer—placed at height $(-h_0)$ from the FeSe plane, vibrate and make oscillating dipolar moments $\tilde{\beta}_\text{p} = q_{\text{eff}}(x, y, -h_0)$ perpendicular to the FeSe $(x, y)$ plane—see figure 1. It gives rise to a dipolar electric potential $\Phi_{\text{dip}}(x, y, -h_0)$ acting on electrons in the FeSe $(x, y)$ plane. Here, $q_{\text{eff}}$ is an effective charge per dipole and $\delta h$ is the polar (dominantly oxygen) displacement along the z-axis [4]. Due to some confusion in the literature on the precise form of $\Phi_{\text{dip}}$ [4] we recalculate it here, in order to know its explicit dependence on the semi–microscopic parameters $\varepsilon_1^{\text{eff}}, \varepsilon_\perp^{\text{eff}}, q_{\text{eff}}, h_0, n_d$. An elementary electrodynamics approach [22] gives for the dipolar potential

$$\Phi_{\text{dip}}(x, y, \delta h) = \frac{\varepsilon_1^{\text{eff}}}{\varepsilon_\perp^{\text{eff}} h_0} \int \frac{dx'dy'd\delta h}{\left[h_0^2 + (x - x')^2 + (y - y')^2\right]^{3/2}} \left(\frac{\varepsilon_1^{\text{eff}}}{\varepsilon_\perp^{\text{eff}}} h_0\right)^2,$$

where $n_d$ is the number of the oscillating Ti–O dipoles per unit FeSe surface. The coefficient in front of the integral is different from that in [4]—where it is $\varepsilon_1^{\text{eff}} / (\varepsilon_\perp^{\text{eff}})^{3/2}(q_{\text{eff}} h_0)$ and with missed dipole density $n_d$. This coefficient does not fulfill the condition $\Phi \sim \varepsilon_1^{\text{eff}}$ in the isotropic case, while equation (1) does. By introducing $g_{\text{epi}}(q) = e^{\Phi}(q)$ the EPI Hamiltonian $H_{\text{epi}} = \sum_q e^{\Phi}(q) \hat{\rho}(q)$ is rewritten in the form $H_{\text{epi}} = \sum_k g_{\text{epi}}(q) \hat{c}_k \hat{c}_k^\dagger$, where $\hat{c}_k^\dagger \hat{c}_k^\dagger = \hat{b}^\dagger \hat{b}^\dagger$ are boson and fermion creation operators, respectively. The Fourier transformed potential $g_{\text{epi}}(q)$ is given by

$$g_{\text{epi}}(q) = \frac{\varepsilon_0 / \sqrt{N}}{e^{\Phi(q)}},$$
used in this study is the surface of the FeSe unit cell and the interface in the model with one TiO₂ dipolar layer at the end of the SrTiO₃ substrate. The anisotropy of the effective dielectric constant $\varepsilon_{\text{eff}}$ is shown. The similar schema holds also for the 1ML FeSe/TiO₂ structure.

\[
g_{\text{epi}}(q) = \frac{2\pi n_{\text{q}} e_{\text{eff}}}{\varepsilon_{\text{eff}}^{\parallel}} \sqrt{\frac{h}{M\Omega N}} e^{-q/\lambda_{m}},
\]

$g_{\text{0}} = (2\pi n_{\text{q}} e_{\text{eff}}^{\parallel} / \varepsilon_{\text{eff}}^{\parallel})(h / M\Omega)^{1/2}$, $e$ is the electronic charge. Here, the screening momentum $q_{s} = (\varepsilon_{\text{eff}}^{\parallel} / \varepsilon_{\text{eff}}^{\perp})^{1/2} h_{0}^{-1}$ characterizes the range of the EPI potential, i.e. for $q_{s} < k_{F}$ ($k_{F}$ is the Fermi momentum) the EPI is sharply peaked at $q = 0$—the FSP (FSP), and the potential in real space is long-ranged, while for $q_{s} \sim k_{F}$ it is short-ranged, like in the standard EPI theory. Since we are interested in the dependence on the effective parameters $\varepsilon_{\text{eff}}^{\parallel}$, $\varepsilon_{\text{eff}}^{\perp}$, $q_{\text{eff}}$, $h_{0}$, then an explicit dependence of the potential is important. We shall see below, that in order that this approach is applicable to 1ML FeSe/SrTiO₃ (and 1ML FeSe/TiO₂) $\varepsilon_{\text{eff}}^{\parallel}$, $\varepsilon_{\text{eff}}^{\perp}$ must be very different from the bulk values of $\varepsilon$ in the bulk SrTiO₃—where $\varepsilon \sim 500-10^{3}$, or in the rutile TiO₂ structure where $\varepsilon \sim 260$ [6].

3. Self-energy effects and ARPES replica bands

The general self-energy $\Sigma_{\text{epi}}(k_{\parallel}, \omega)$ at $T = 0$ in the extreme FSP–peak limit with the width $q_{s} \ll k_{F}$ is given by (see appendix)

\[
\Sigma_{\text{epi}}(k_{\parallel}, \omega) \approx -\lambda_{m} \frac{\omega}{1 - (\omega / \Omega)^{2}}
\]

where $\lambda_{m} = \langle V_{\text{epi}}(q) \rangle_{0} / 2\Omega$ is the mass-dependent coupling constant. Here, the average EPI potential is given by $\langle V_{\text{epi}}(q) \rangle_{0} = N_{k}(2\pi)^{-2} \int d^{3}q_{\text{epi}}(q, 0) \approx (1/4\pi)(\varepsilon_{\text{eff}}^{\parallel})^{2} V_{\text{epi}}^{0}$, where $s_{\text{c}} = 2\pi^{2}$ is the surface of the FeSe unit cell and $a$ is the Fe–Fe distance, and the bare pairing EPI potential is $V_{\text{epi}}^{0} = 2g_{\text{eff}}^{2} / \Omega$. The coupling constant $\lambda_{m}$ corresponds to $\lambda_{\text{m}}$ used in [5], where the self-energy effects are studied at $T > 0$. It is important to point out that $\lambda_{m}$ is (oxygen) mass-dependent, contrary to [5]. Since $\langle V_{\text{epi}}(q) \rangle_{0}$ is mass-independent then $\lambda_{m} \sim \lambda_{\text{m}} \sim \Omega^{-1} \sim M^{1/2}$. In the following we discuss the case when $k = k_{\parallel}$, i.e. $\xi(k) = 0$. For $\omega \ll \Omega$ one has $\Sigma_{\text{epi}}(k, \omega) = -\lambda_{m} \omega$ which means that the slope of $\Sigma_{\text{epi}}(k, \omega)$ is mass-dependent. The latter property can be measured by ARPES and thus the EPI–FSP theory can be tested. Note, that in the EPI–FSP theory the critical temperature $T_{c0} = \langle \langle V_{\text{epi}}(q) \rangle_{0} / 4 \rangle$—see details below, is mass-independent. Both these results are opposite to the standard Migdal–Eliashberg theory, where the self-energy slope is mass-independent and $T_{c0}$ is mass-dependent.

The quasiparticle and replica bands at $T = 0$ are obtained from $\omega - \Sigma_{\text{epi}}(\omega) = 0$. In the following we make calculations at $T = 0$ and at the Fermi surface $\xi(k_{0}) = 0$. The solutions are: (1) $\omega_{1} = 0$—the quasiparticle band; (2) $\omega_{2} = -\Omega \sqrt{1 + \lambda_{m}}$ is the ARPES replica band; (3) the inverse ARPES replica band $\omega_{3} = \Omega \sqrt{1 + \lambda_{m}}$. The single-particle spectral function is $A(k_{\parallel}, \omega, T = 0) = \sum_{\omega_{i}=1}^{2} (A_{i} / \pi) \delta(\omega - \omega_{i})$, where $A_{i} / \pi$ are the spectral weights. For the quasiparticle band $\omega_{1}$ one obtains $A_{1} = (1 + \lambda_{m})^{-1}$, while for the replica bands at $\omega_{2}$ and $\omega_{3}$ one has $A_{2} = A_{3} = (\lambda_{m} / 2)(1 + \lambda_{m})^{-1}$. The ratio of the intensities at $T = 0$ of the $\omega_{2}$ replica band and quasiparticle band $\omega_{1}$ is given by...
It is necessary to mention that at finite $T$ ($T > 0$) this ratio is changed as found in [5]. In that case $\lambda_m^{\text{eff}}(\mathbf{k}, \mathbf{q}, \omega)$ gives the quasiparticle and replica band $\omega_T^{(2)} = \Omega(1 + 4\lambda_m^{T})/2$ and $\omega_0^{(2)} = -\Omega(1 + \sqrt{4\lambda_m^{T}})/2$ and $(A_2/A_1)_{\mathbf{k}} = \lambda_m^{T}$. This intriguing difference of the $T = 0$ and $T = 0$ results for $(A_2/A_1)$ in the EPI-FSP theory. $(A_2/A_1)_{\mathbf{k}} = 2(A_2/A_1)_{\mathbf{k}}$ is due to the sharpness of the Fermi function $n_p(\xi_k, q)$ entering in $\Sigma_{\mathbf{q}}(\mathbf{k}, \omega)$—see equation (22) in appendix (see footnote 5).

We stress that the ARPES measurements of $A_2/A_1$ in 1ML FeSe/SrTiO$_3$ were done at finite temperatures ($T = 0$) and in the $k = 0$ point with $\xi(k = 0) \sim -50$ meV which gives $(A_2/A_1)_{\mathbf{k}} \approx 0.15$--0.2 [4, 19]. According to the theory and experiments in [4, 5] one obtains $\lambda_m^{\text{ARPES}} \approx 0.15$--0.2. Below we show, that $\lambda_m$ can be also extracted from the formula equation (6) for $\Theta = 100 K$, which gives $\lambda_m^{\text{ARPES}} \approx 0.18$. The latter value is in a good agreement with $\lambda_m^{\text{ARPES}}$ from ARPES (see footnote 5). If we put this value in equation (4) one obtains that at $T = 0$ and at $k = k_F$ one has $(A_2/A_1) \sim 0.1$. From this analysis we conclude that the ARPES measurements at $k_F$ and $T = 0$ should give the similar ratio as at $k = 0$. The calculated ARPES spectra at $T = 0$ K and at $k = k_F$ give $\Delta_{\omega} = |\omega_2 - \omega_1| = \Omega\sqrt{1 + \lambda_m}$, while the experimental value is $\Delta_{\omega} \approx 100$ meV. For $\lambda_m^{\text{ARPES}} \approx 0.2$ it gives, that the optical phonon energy is of the order of $\Omega \approx 90$ meV.

4. The superconducting critical temperature $T_{c0}$ and gap $\Delta_0$

In the weak coupling limit ($\lambda_m \ll 1$) of the Eliashberg equations with $q_k, v_F < \pi T_{c0}$ ($v_F$ is the Fermi velocity) the linearized gap equation near $T_{c0}$ is given by

$$\Delta(k, \omega_0) = T_{c0} \sum_{\mathbf{q}} \frac{V_{\text{epi}}(\mathbf{q}) \omega_0 - \omega_m}{\omega_0^2 + \xi^2(k + \mathbf{q})},$$

where $\omega_m = T_{c0}(\Delta + \sum_{\mathbf{q}} V_{\text{epi}}(\mathbf{q}) \omega_0) = T_{c0} \sum_{\mathbf{q}} \omega_0^2/(\Omega^2 + \Omega^2 + \Omega^2). \Omega_{\mathbf{q}} = \pi T_{c0} \cdot n. \text{ For } \Omega^2 \gg (\pi T_{c0})^2 \text{ one has } V_{\text{epi}}(\mathbf{q}) \omega_m \approx 2\xi^2(\omega_0)/\Omega. \text{ In the strong FSP limit when } q = v^2/2 \ll (\pi T_{c0})^2 \text{ the highest value of } \Delta(k, \omega_0) \text{ is reached at } k = k_F, (\xi(k_F) = 0 \text{ in equation (5)}). \text{ The solution } \Delta(k, \omega_0) \text{ is searched in the standard square-well approximation } \Delta(k_F, \omega_m) \approx \Delta_0 = \text{ const.} \text{ In leading order with respect to } (T_{c0}/\Omega) \ll 1 \text{ one obtains } T_{c0} \simeq (0.1 v_F)^2. \text{ For } \Omega^2 \gg (\pi T_{c0})^2 \text{ this gives } T_{c0} = (V_{\text{epi}}(\mathbf{q}))_{\mathbf{q}}/(\pi^2) \approx (1/16\pi)\text{(air)}^2(2g_0^2/\Omega). \text{ where } \text{a is the Fe–Fe distance. Note, that } T_{c0} \text{ is mass-independent (a0 = 0), while } \Omega = 1/2 \text{ is found in [5]. The small isotope-effect can be also a smoking-gun experiment for the EPI–FSP pairing mechanism in 1ML FeSe/SrTiO}_3 \text{ (and 1ML FeSe/TiO}_3). \text{ From equation (16) in the appendix it is straightforward to obtain the energy gap } \Delta_0 = 2T_{c0}. \text{ Note, that 1ML FeSe/SrTiO}_3 \text{ and 1ML FeSe/TiO}_3 \text{ is a 2D system and } T_{c0} \sim q^d, \text{ while in the d-dimensional space one has } T_{c0} \sim q^d. \text{ This means, that the EPI–FSP mechanism of superconductivity is more favorable in low-dimensional systems (d = 1, 2) than in the 3D one. Since high Tc cuprates are also quasi-2D systems, where strong correlations make a long-ranged EPI, one can see that the EPI–FSP mechanism of pairing may be also operative in cuprates [2, 3]. Note, that in estimating some semi-microscopic parameters we shall use as an etalon-value $T_{c0} \approx 100 K$, while in real systems $T_{c0} \approx (60–80)K < T_{c0}$, is realized. However, $T_{c0}$ is the mean-field value obtained in the Migdal–Eliashberg theory, while in 2D systems it is significantly reduced by phase fluctuations—to the Berezinskii–Kosterlitz–Thouless value. There is an additional reduction of $T_{c0}$ (which might be also appreciable) in the EPI–FSP systems, which is due to internal pair-fluctuations—see discussion below.)

One can estimate the coupling constant $\lambda_m = (V_{\text{epi}}(\mathbf{q}))_{\mathbf{q}}/2\Omega$ in 1ML FeSe/SrTiO$_3$ from the value of $T_{c0}$. Then for the etalon-value $T_{c0} \sim 100 K$ one has $V_{\text{epi}}(\mathbf{q})_{\mathbf{q}} \approx 33 meV$ and $\lambda_m^{T_{c0}} \approx 0.18. \text{ Since } \lambda_m^{\text{ARPES}} \approx \lambda_m^{\text{ARPES}}$, the consistency of the theory is satisfactory. Note, if one includes the wave-function renormalization effects (contained in $Z(\omega_n > 1)$ then in the case $T_{c0}/\Omega << 1$ and for the square-well solution for $\Delta(k_F, \omega_m)$, $T_{c0}$ is lowered to $T_{c0}^\text{low} = T_{c0}/Z^2(0)$, where $Z(0) \approx 1 + \lambda_m^{T_{c0}}$. This means, that the nonlinear corrections (with respect to $\lambda_m^{T_{c0}}$ in $T_{c0}$ and $\Delta_0$ [5, 23]) should be inevitably renormalized by the $Z$-renormalization.

Let us estimate the parameters $(\xi k_F, k_F, h_0)$ which enter in $T_{c0}$. In order to reach $T_{c0} \sim 100 K$ and $(V_{\text{epi}}(\mathbf{q}))_{\mathbf{q}} = 4T_{c0} \sim 400 K \approx 33 meV$ then for $a_{\text{eff}} \approx 0.2$ and $\Omega \approx 90 meV$ one obtains $g_0 \approx 0.7 eV$. Having in mind that $g_0 = (2\pi n \alpha^2 a_{\text{eff}}/\xi k_F^2)(h/M\Omega)^{1/2}$ and that the zero-motion oxygen amplitude is $(h/M\Omega)^{1/2} \approx 0.05 \AA$ and by assuming that $\alpha \approx 0.05 \AA$, $\xi \approx 3 \AA$, $a_{\text{eff}} \approx 2 eV$, $\epsilon \approx 0.05$ then in

$^5$ It turns out that in the first arXiv version of our paper we overlooked the fact that in [4, 5] they study the problem at finite temperature $T = 0$ while our study is limited to $T = 0$. This means that both, the $T = 0$ and $T = 0$ results are correct.
order to obtain \( g_0 \approx 0.7 \text{ eV} \) the value of \( \varepsilon_{\text{eff}} \) must be small, i.e. \( \varepsilon_{\text{eff}} \approx 1 \). Since \( a_q = (a/h_0) \sqrt{\varepsilon_{\text{eff}}} \approx 0.2 \) and for \( (a/h_0) \approx 1 \) it follows \( \varepsilon_{\text{eff}} \approx 30 \). Note, that in SrTiO\(_3\) the bulk \( \varepsilon \) is large, \( \varepsilon \approx 500-10^4 \). So, if \( T_{\text{c}} \) in 1ML FeSe/SrTiO\(_3\) is due solely to the EPI–FSP mechanism, then in the model where the oxygen vibrations in the single dipolar monolayer TiO\(_3\) are responsible for the pairing potential the effective dielectric constants \( \varepsilon_{\text{eff}} \) are very different from the bulk values in SrTiO\(_3\) (in 1ML FeSe/SrTiO\(_3\) one has \( \varepsilon \ll 260 \) \cite{6}). This is physically plausible since for the nearest (to the FeSe monolayer) TiO\(_3\) dipolar monolayer there is almost nothing to screen in the direction perpendicular to FeSe, thus making \( \varepsilon_{\text{eff}} \ll \varepsilon_{\text{bulk}} \). Note, that for the parameters assumed in this analysis and for \( T_{\text{c}} \approx 100 \text{ K} \) one obtains rather large bare pairing potential \( V_{\text{epi}}^0 \approx 10 \text{ eV} \). This means that in absence of the FSP in EPI and for the density of states of the order \( N(E_F) \sim 0.5\text{ eV}^{-1} \) (typical for the Fe-based superconductors) the bare coupling constant \( \lambda_{\text{epi}}^0 = N(E_F) V_{\text{epi}}^0 \) would be large, \( \lambda_{\text{epi}}^0 \sim 5 \). We stress that the above theory is also applicable to recently discovered 1ML FeSe/TiO\(_2\) \cite{6}. To conclude, the high \( T_{\text{c}} \) in 1ML FeSe/SrTiO\(_3\) (and 1ML FeSe/TiO\(_2\)) is obtained on the expense of the large maximal EPI coupling \( V_{\text{epi}}^0 \) which compensates smallness of the (detrimental) phase-volume factor \((a_q)^3\).

5. Effects of impurities on \( T_{\text{c}} \)

In clean systems with the EPI–FSP mechanism of superconductivity \( T_{\text{c}} \) is degenerate—it is equal in \( s \)- and \( d \)-channels. In the following we show, that the \( s \)-wave superconductivity is also affected by isotropic non-magnetic impurities, i.e. \( T_{\text{c}} \) is reduced and the Anderson theorem is violated. This may have serious repercussions on the \( s \)-wave superconductivity in 1ML FeSe/SrTiO\(_3\) and 1ML FeSe/TiO\(_2\)) where \( T_{\text{c}} \) may depend on chemistry. Then by using equation (19) from appendix one obtains \( T_{\text{c}}^{(s)} \)

\[
\frac{T_{\text{c}}^{(s)}}{T_{\text{c}}} = \frac{4}{\pi^2} \left[ \psi\left(1 + \frac{\rho}{2}\right) - \psi\left(\frac{1}{2}\right) \right],
\]

where \( \rho = \Gamma/\pi T_{\text{c}} \), \( \Gamma = \pi n_i N(E_F) u^2 \), \( n_i \) is the impurity concentration and \( u \) is the impurity potential. Let us consider some limiting cases: (1) for \( \Gamma << \pi T_{\text{c}} \) one has \( T_{\text{c}}^{(s)} \approx T_{\text{c}} [1 - \Gamma^2/(\pi^2 T_{\text{c}})] \); (2) for \( \Gamma > \pi T_{\text{c}} \) one has \( T_{\text{c}}^{(s)} \approx (\Gamma/2) \exp(-\pi/4 T_{\text{c}}) \), i.e. \( T_{\text{c}}^{(s)} \) never vanishes. This means that in the EPI–FSP systems the non-magnetic impurity scattering is pair-\textit{weakening} for the \( s \)-wave superconductivity.

In case of \( d \)-wave superconductivity the solution of equation (20) in limiting cases is: (1) \( T_{\text{c}}^{(d)} \approx T_{\text{c}} [1 - 2 \Gamma/(\pi T_{\text{c}})] \) for \( \Gamma \ll \pi T_{\text{c}} \). We point out that the slope \( -dT_{\text{c}}^{(d)}/d(\Gamma) = 2/\pi \) is smaller than the slope for the standard \( d \)-wave pairing, where \( -dT_{\text{c}}/d(\Gamma) = 4/\pi \). (2) For \( \Gamma > \pi T_{\text{c}} \) \( T_{\text{c}}^{(d)} \approx 0 \), i.e. the effect of non-magnetic impurities is pair-\textit{breaking}. Note, that \( \Gamma_{\text{c}}(\text{FSP}) > \Gamma_{\text{c}}(\text{pair}) \approx (2/\pi) T_{\text{c}} \). These two results mean, that in the presence of non-magnetic impurities the \( d \)-wave superconductivity, which is due to the EPI–FSP pairing, is more robust than in the case of the standard \( d \)-wave pairing. We stress, that the \( T_{\text{c}} \) dependence on non-magnetic impurities might be an important test for the EPI–FSP pairing in 1ML FeSe/SrTiO\(_3\) (and 1ML FeSe/TiO\(_2\)).

Finally, it is worth of mentioning, that the real isotope effect in \( T_{\text{c}} \) of 1ML FeSe/SrTiO\(_3\) (and 1ML FeSe/TiO\(_2\)) might depend on the type of non-magnetic impurities. If their potential is also long-ranged—for instance, due to oxygen defects in the TiO\(_3\) dipole layer, then there is a FSP in the scattering potential, i.e. \( u_{\text{imp}}(q) \approx u_{\text{dip}}(q) \). Then, such impurities affect in the same way \( s \)- and \( d \)-wave pairing and they are pair weakening, as shown in [3]. Namely, one has (a) \( T_{\text{c}}^{(s,d)} \approx T_{\text{c}} \approx \Gamma_{\text{c}} \approx (\pi/4 T_{\text{c}}) \), (b) \( T_{\text{c}}^{(s,d)} \approx 0.88 \pi \Gamma_{\text{c}} \approx \Gamma_{\text{c}} \approx (\pi/4 T_{\text{c}}) \), (c) \( T_{\text{c}}^{(s,d)} \approx 0.88 \pi \Gamma_{\text{c}} \approx \Gamma_{\text{c}} \approx (\pi/4 T_{\text{c}}) \). There are two important results: (1) There is a nonanalicity of \( \Gamma_{\text{c}} \approx (\pi T_{\text{c}}) \); (2) there is a full isotope effect in the ‘dirty’ limit \( \Gamma_{\text{c}} \approx \pi T_{\text{c}} \), i.e. \( \alpha_{\text{c}} \approx 1/2 \), since \( T_{\text{c}}^{(s,d)} \approx \Omega \approx M^{-1/2} \). We stress, that if the full isotope effect would be realized experimentally in 1ML FeSe/SrTiO\(_3\) (and 1ML FeSe/TiO\(_2\)), then this does not automatically exclude the FSP–EPI mechanism of pairing, since it may be due to impurity effects. In that case the nonanalicity of \( \Gamma_{\text{c}} \approx \pi T_{\text{c}} \) might be a smoking-gun effect.

6. Internal pair fluctuations reduce \( T_{\text{c}} \)

The EPI–FSP theory, which predicts a long-range force between paired electrons, opens a possibility for a pseudogap behavior in 1ML FeSe/SrTiO\(_3\) (and 1ML FeSe/TiO\(_2\)). As we have discussed above, the EPI–FSP theory predicts a non-BCS dependence of the critical temperature \( T_{\text{c}} \), i.e. \( T_{\text{c}} \approx \langle V_{\text{epi}}(q) \rangle/4 \). However, this mean-field (MFA) value is inevitably reduced by the phase and internal Cooper pair fluctuations—which are characteristic for systems with long-range attractive forces. Namely, in MFA the order parameter \( \Delta(\mathbf{x}) = \langle V(\mathbf{x}) \rangle \psi(\mathbf{x}) \psi(\mathbf{x}) \rangle \) depends on the relative (internal) coordinate \( \mathbf{r} = \mathbf{x} - \mathbf{x}' \) and on the center of mass \( \mathbf{R} = (\mathbf{x} + \mathbf{x}')/2 \), i.e. \( \Delta(\mathbf{x}, \mathbf{x}') = \Delta(\mathbf{r}, \mathbf{R}) \). In usual superconductors with short-range pairing potential one has \( V_{\text{epi}}(\mathbf{x} - \mathbf{x}') \approx V_{\text{epi}}(\mathbf{x} - \mathbf{x}) \) and \( \Delta(R, R') = \Delta(\mathbf{R}) \). Therefore only the spatial (R-dependent)
fluctuations of the order parameter are important. In case of a long-range pairing potential there are additional pair-fluctuations due to the dependence of $\Delta (r, R)$ on internal degrees of freedom (on $r$). The interesting problem of the internal fluctuations in systems with long-range attractive forces in 3D systems was studied in [24]. We sketch it briefly, because it shows, that standard and EPI–FSP superconductors belong to different universality classes. The best way to see importance of the internal pair-fluctuations is to rewrite the pairing Hamiltonian in terms of the pseudospin operators (in this approximation first done by P. Anderson the single particle excitations are not included)

$$\hat{H} = \sum_{k_0} 2\hat{c}_{k_0}^{\dagger} \hat{c}_{k_0} - \left(\frac{1}{2}\right) \sum_{k'k} V_{kk'} \left(\hat{c}_{k'}^{\dagger} \hat{S}_{kk'}^{x} + \hat{S}_{kk'}^{x} \hat{c}_{k'}\right),$$

where $\hat{S}_{kk'}^{x} = \left(\hat{c}_{k'}^{\dagger} \hat{c}_{k} - \hat{c}_{k'}^{\dagger} \hat{c}_{k}\right)/2$ [24]. This is a Heisenberg-like Hamiltonian in the momentum space. In case of the s-wave superconductivity with short-range forces $V_{\alpha\alpha}(x-x') \approx V_0 \delta(x-x')$ one has $V_{kk'} = \text{const}$ and the pairing potential is long-ranged in the momentum space. In that case it is justified to use the mean-field approximation $\hat{H} \to \hat{H}_{\text{MF}} = -\sum_k \hat{h}_k \hat{S}_{kk}^{x}$ with the mean-field $\hat{h}_k = -2\hat{c}_k^{\dagger} + \sum_k \hat{V}_{kk'} \hat{c}_{k'}^{\dagger}$, where the excitation spectrum (with respect to the ground state) in this system has a gap, i.e. $E(k) = 2\sqrt{\hat{c}_k^2 + \Delta_k^2}$ where the gap $\Delta_k$ is the mean-field order parameter defined by $\Delta_k = \sum_{k'} V_{kk'} \hat{S}_{kk'}^{x}$. However, in case of the EPI–FSP pairing mechanism the pairing potential is long-ranged in real space and short-ranged in the momentum space. For instance, in 1ML FeSe/SrTiO$_3$ (and 1ML FeSe/TiO$_2$) one has $V_{kk'} = V_0 \exp\left(-\left|\vec{k} - \vec{k}'/q_0\right|^2/\kappa_2^2\right)$ with $q_0 \ll \kappa_2$ and the excitation spectrum is boson-like $0 < E(k) < 2\sqrt{\hat{c}_k^2 + \Delta_k^2}$ (like magnons in the Heisenberg model) with large number of low-laying excitations (around the ground state). This means, that there are many low-laying pairing states above the ground-state in which pairs are sitting. The internal fluctuations effect reduces $T_{c0}$ to $T_c$. For instance, in 3D systems with $q_0 \zeta_0 \ll 1$ [24] one has $T_c \approx (q_0 \zeta_0) T_{c0} \ll T_{c0}$, where the coherence length $\zeta_0 = v_F/n \Delta_0$ and $\Delta_0 = 2T_{c0}$. It is expected, that in the region $T_c < T < T_{c0}$ the pseudogap (PG) phase is realized. However, in 2D systems, like 1ML FeSe/SrTiO$_3$ (and 1ML FeSe/TiO$_2$), there are additional phase fluctuations reducing $T_c$ further to the Berezinskii–Kosterlitz–Thouless value. We stress, that recent measurements of $T_c$ in 1ML FeSe/SrTiO$_3$ by the Meissner effect and resistivity ($\rho(T)$) give that $T_c^{\text{FSP}} < T_c^{\text{BM}}$ what may be partly due to these internal fluctuations of Cooper pairs. It would be interesting to study theoretically these two kind of fluctuations in 2D systems, such as 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$.

7. Summary and discussion

In the paper we study the superconductivity in the 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$ sandwich-structure, which contains one metallic FeSe monolayer grown on the substrate SrTiO$_3$, or rutile TiO$_2$ [200]. It turns out that in such a structure the Fermi surface is electron-like and the bands are pockets around the $M$-point in the Brillouin zone. The bottom of the electron-like bands is around (50–60) meV below the Fermi surface at $E_F$. The top of the hole-like band at the point $\Gamma$ lies 60–80 meV below $E_F$ which means that pairing mechanisms based on the electron–hole nesting are ruled out. This holds also for the pairing with hole-incipient bands (very interesting proposal) [10]. The superconductivity in 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$ is realized in the FeSe monolayer with $T_c \sim (60–100)$ K. The decisive fact for making a theory is that the ARPES spectra show sharp replica bands around 100 meV below the quasiparticle band, what is approximately the energy of the oxygen optical phonon $\Omega \approx 90$ meV. The analysis of the superconductivity is based on the semi-microscopic model—first proposed in [4, 5], where it is assumed that a TiO$_2$ dipolar layer is formed just near the interface. In that model the oxygen vibrations create a dipolar electric potential, which acts on electrons in the FeSe monolayer, thus making the EPI interaction long-ranged. In the momentum space a forward scattering peak (FSP) appears, i.e. EPI is peaked at small transfer momenta $q < q_c \ll \kappa_2$ with the non-singular EPI coupling $g_{\text{epi}}(q) = g_{\text{epi}} \exp(-q/\kappa_2)$. The EPI–FSP theory is formulated first in [1] for strongly correlated systems, while its extreme case with delta-peak is elaborated in [3]—see also [2]. This limiting (delta-peak) case makes not only analytical calculations easier, but it makes also a good fit to the experimental results [4, 5]. In the following, we summarize the main obtained results of the EPI–FSP theory and its relation to the 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$ sandwich-structures.

(1) The mean-field critical temperature $T_{c0}$ in s-wave and d-wave pairing channels is degenerate and given by $T_{c0} = \langle V_{\text{epi}}(q) \rangle_4 / 4 \approx (1/16\pi) (\mu_q^2 q^2 / \Omega)$. The first glance this linear dependence of $T_{c0}$ on $V_{\text{epi}}^{(0)}$ seems to be favorable for reaching high $T_{c0}$—note in the BCS theory $T_{c0}$ is exponentially dependent on $V_{\text{epi}}^{(0)}$ and very small for small $N(E_F) V_{\text{epi}}^{(0)}$. However, for non-singular $g_{\text{epi}}(q)$ when $g_{\text{epi}}(q = 0)$ is finite, $T_{c0}$ is limited by the smallness of the phase-volume effect, which is in 2D systems (such as 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$) proportional to $(aq_c)^2 \ll 1$. In that sense some optimistic claims that the EPI–FSP mechanism leads inevitably to higher $T_{c0}$—
than the one in the standard Migdal–Eliashberg theory, are not well founded for non-singular EPI potentials. This holds especially for 3D systems, where $T_{\text{c}0} \sim (aq_c)^2$ and $T_{\text{c}0}^{(\text{bd})} \ll T_{\text{c}0}^{(\text{epi})}$ for the same value of $V_{\text{epi}}^0$. However, higher $T_{\text{c}0}$ (with respect to to the BCS case) can be reached by fine tuning of $aq_c$ and $V_{\text{epi}}^0$. This is probably realized in HTSC cuprates and with certainty in 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$. The weak-coupling theory predicts the superconducting gap to be $\Delta_0 = 2T_{\text{c}0}$ and for $T_{\text{c}0} \approx 100$ K one has $\Delta_0 \approx 16$ meV, which fits well the ARPES experimental values [4, 6]. Note, in order to reach $T_{\text{c}0} = 100$ K for $aq_c \approx 0.2$ a very large maximal EPI coupling $V_{\text{epi}}^0 \approx 10$ eV is necessary. For $(E_p)_{\text{epi}} \sim 0.5$ (eV)$^{-1}$ the maximal coupling constant would be rather large, i.e. $\lambda_{\text{epi}}^0 = (N(E_p) V_{\text{epi}}^0)^{-1} \approx 5$. Note, that $V_{\text{epi}}^0$ is almost as large as in the metallic hydrogen under high pressure $p \sim 20$ Mbar, where $T_{\text{c}0} \approx 600$ K with large EPI coupling constant $\lambda_{\text{epi}}^0 \approx 6$—this important prediction is given in [25]. In real 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$ materials the contribution of another pairing mechanism, which exists in the FeSe film in absence of the substrate and is pronounced in the $s$-wave channel with $T_{\text{c}0} \approx 8$ K, triggers the whole pairing to be $s$-wave. The latter only moderately lowers the contribution of the EPI–FSP pairing mechanism. The existence of the sharp replica bands in 1ML FeSe/SrTiO$_3$ and 1UCFeSe/TiO$_2$ and large value of $V_{\text{epi}}^0$ imply inevitably that the EPI–FSP pairing mechanism is a serious candidate to explain superconductivity in these materials. We stress, that in 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$ high $T_{\text{c}0}$ is obtained on the expense of the large maximal EPI coupling $V_{\text{epi}}^0$, which compensates the small (detrimental) phase volume factor. Other possibilities to increase $T_{\text{c}0}$ is to search for exotic systems with singular EPI potential, (with $aq_c^2 V_{\text{epi}}^0 \to \infty$), which might be illusory.

(2)—The semi–microscopic model proposed in [4, 5] and refined partly in this paper, contains phenomenological parameters, such as $n_d$—the number of dipoles per unit cell, $q_{\text{eff}}$—an effective dipole charge, $\varepsilon_{\text{eff}}$, $\varepsilon_{\text{eff}}$—effective parallel and perpendicular dielectric constants in SrTiO$_3$ (and TiO$_2$) near the interface, respectively. For $T_{\text{c}0} \approx 100$ K and by assuming $aq_c \approx 0.2$, $q_{\text{eff}} \approx 2e$, $n_d \sim 2$ unit-cell makes $\varepsilon_{\text{eff}} \sim 30$, $\varepsilon_{\text{eff}} \sim 1$. These values, which are physically plausible, are very far from $\varepsilon$ in the bulk SrTiO$_3$, where $\varepsilon \sim 500–10^4$ (and $\varepsilon \ll 260$ in the rutile TiO$_2$). We point out that our estimation of these parameters is based on an effective microscopic model where the bulk SrTiO$_3$ is truncated by a monolayer (1ML) made of TiO$_2$ [4]. In reality it may happen that the bulk SrTiO$_3$ is truncated by two monolayers (2ML) of TiO$_2$, as it is claimed to be seen in the synchrotron x-ray diffraction [26]. This finding is confirmed by the LDA calculations in [26], which show that for the 2ML TiO$_2$ structure: (i) electrons are much easier transferred to the FeSe metallic monolayer and (ii) the top of the hole band is shifted far below the electronic Fermi surface than in the 1ML model. If the 2ML of TiO$_2$ is realized it could be even more favorable for the EPI–FSP pairing, since some parameters can be changed in a favorable way. For instance, the effective charge could be increased, i.e. $q_{\text{eff}}^{(2\text{ML})} > q_{\text{eff}}^{(1\text{ML})}$ and since $T_{\text{c}0} \sim q_{\text{eff}}^2$ the 2ML model may give rise to higher critical temperature.

(3)—The isotope effect in $T_{\text{c}0}$ should be small ($\alpha_{\text{O}} \ll 1/2$) since in leading order one has $T_{\text{c}0} \sim V_{\text{epi}}^0$ and $\alpha_{\text{O}} = 0$, where $V_{\text{epi}}^0$ is mass-independent. This is contrary to [5] where $\alpha_{\text{O}} = 1/2$. The next leading order gives $\alpha_{\text{O}} \sim (T_{\text{c}0}/\Omega) < 0.09$. We stress that the small isotope-effect maybe a smoke-gun experiment for the EPI–FSP pairing mechanism.

(4)—In the EPI–FSP pairing theory the non-magnetic impurities affect both $s$-wave and $d$-wave pairing. In the case of $s$-wave they are pair-breaking, while for $d$-wave are pair-weakening. However, for non-magnetic impurities with a FSP in the scattering potential the full isotope effect $\alpha_{\text{O}} = 1/2$ is restored in the ‘dirty’ limit ($\Gamma_F \gg \pi T_c$), since $T_{\text{c}0}^{(\text{bd})} \sim \Omega \sim M^{-1/2}$. In that case, the nonanaliciy of $T_{\text{c}0}^{(\text{bd})}$ with respect to the impurity concentration $n_i$ might solve the question—what kind of pairing is realized in 1ML FeSe/SrTiO$_3$ and 1UCFeSe/TiO$_2$—the EPI–FSP or the standard EPI.

(5)—In the case of the EPI–FSP pairing the superconducting order parameter depends strongly on the internal pair coordinate and of center of mass, i.e. $\Delta = \Delta(r, R)$. The internal pair fluctuations reduce additionally the mean-field critical temperature so that in the interval $T_c < T < T_{\text{c}0}$ a pseudogap behavior is expected.

(6)—The EPI self-energy in the normal state at $T = 0$ and $\xi(k) = 0$ is given by $\Sigma_{\text{epi}}(k, \omega) = -\lambda_{\text{m}} \omega / (1 - (\omega/\Omega)^2)$, where $\lambda_{\text{m}} = (V_{\text{epi}}(k) q_l^2 / 2 \Omega)$, which for $G^{-1}(k, \omega) = 0$ gives the dispersion energy of the quasiparticle band $\omega_1 = 0$ and the replica bands $\omega_2$ and $\omega_3$. The ratio of the ARPES intensities of the replica band $\omega_2$ and the quasiparticle band $\omega_1$ at $T = 0$ and at the Fermi surface ($k = k_F$) is given by $R(T = 0, k_F) = (A_2 / A_1)$ $\approx \lambda_{\text{m}} / 2$. This means, that for $\lambda_{\text{m}} \approx 0.2$ the experimental value of $R(T = 0, k_F)$ should be $(A_2 / A_1) \approx 0.1$. This ratio is slightly smaller than the experimental value $R(T = 0, k = 0) \sim 0.15–0.2$ measured in [4, 19].

(7)—Since the coupling constant $\lambda_{\text{m}}$ is mass-dependent, $\lambda_{\text{m}} \sim M^{1/2}$ then the isotope effect in various quantities, in 1ML FeSe/SrTiO$_3$ and 1ML FeSe/TiO$_2$ systems, may be a smoke-gun experiment in favor of the EPI–FSP theory. To remind the reader: (i) $T_{\text{c}0}$ is almost mass-independent; (ii) the self-energy slope at $\omega \ll \Omega$ is mass-dependent, $(-d\Sigma/d\omega) \sim M^{1/2}$; (iii) the ARPES ratio $R$ of the replica band intensities is mass-dependent,
Concerning the role of EPI in explaining superconductivity in 1ML FeSe/SrTiO$_3$ there were other interesting theoretical proposals. In [27] the EPI is due to an interaction with longitudinal optical phonons and since $\Omega > \omega_i$ the problem is studied in the anti-adiabatic limit, where $T_c$ is also weakly dependent on the oxygen mass. In [28] the substrate gives rise to an antiferromagnetic structure in FeSe, which opens new channels in the EPI coupling in the FeSe monolayer, thus giving rise for high $T_c$. In [29] the intrinsic pairing mechanism is assumed to be due to $J_2$-type spin fluctuations, or antiferro orbital fluctuation, or nematic fluctuations. The extrinsic pairing is assumed to be due to interface effects and the EPI–FSP interaction. The problem is studied by the sign-free Monte-Carlo simulations and it is found that EPI–FSP is an important ingredient for high $T_c$ superconductivity in this system.

Finally, we would like to comment some possibilities for designing new and complex structures based on 1ML FeSe/SrTiO$_3$ (or 1ML FeSe/TiO$_2$) as a basic unit. The first nontrivial one is when a double-sandwich structure with two interfaces is formed, i.e. SrTiO$_3$/1ML FeSe/SrTiO$_3$ (or TiO$_2$/1ML FeSe/TiO$_2$). Naively thinking, in the framework of the EPI–FSP pairing mechanism one expects, in an 'ideal' case, doubling of $T_{co}$ since phonons at two interfaces are independent. However, this would only happen when the electron-like bands on the Fermi surface due to the two substrates were similar and if the condition $q_{\perp} \cdot \vec{v}_F < \pi T_{co}$ is kept in order to deal with a sharp FSP. However, many complications in the process of growing, such structures may drastically change properties, leading even to a reduction of $T_{co}$. It needs very delicate technology to control the concentration of oxygen vacancies and appropriate charge transfer at both interfaces. However, eventual solutions of these problems might give impetus for superconductors with exotic properties. For instance, having in mind the above exposed results on effects of non-magnetic impurities on $T_{co}$, then by controlling and manipulating their presence at both interfaces one can design superconducting materials with wishful properties.

Acknowledgments

The authors are thankful to Radoš Gajić for useful discussions, comments and advises related to the experimental situation in the field. We highly appreciate fruitful discussions with Steve Johnston and Yan Wang on ARPES of the replica bands at finite temperature, and on the microscopic parameters of the theory. The authors are thankful to Michael V Sadovskii for discussions on various theoretical aspects of the Fe-based superconductivity.

Appendix

A.1. Migdal–Eliashberg equations in superconductors

We study superconductivity with the EPI–FSP mechanism of pairing by including effects of non-magnetic impurities, too. The full set of Migdal–Eliashberg equations is given for that case. The normal and anomalous Green’s functions are $G_n(k, \omega_n) = -[i\omega_n Z_n(k) + \xi_n(k)]/D_n(k)$, $G_{epi}(k, \omega_n) = -Z_{epi}(k)\Delta_n(k)/D_{epi}(k)$, respectively, where $D_n(k) = [\omega_n Z_n(k)]^2 + [Z_n(k)\Delta_n(k)]^2$ ($\omega_n = \pi T (2n + 1)$). Here, $Z_n(k)$ is the wave-function renormalization defined by $i\omega_n (1 - Z_n(k)) = (\Sigma(k, \omega_n) - \Sigma(k, -\omega_n))/2$, where the self-energy $\Sigma(k, \omega_n) = \Sigma_{epi}(k, \omega_n) + \Sigma_{imp}(k, \omega_n)$ describes the EPI and impurity scattering, respectively. The energy renormalization is $\xi_n(k) = \xi(k) + \chi_n(k)$, with $\chi_n(k) = (\Sigma(k, \omega_n) - \Sigma(k, -\omega_n))/2$ and $\Delta_n(k)$ is the superconducting order parameter

$$Z_n(k) = 1 + \frac{T}{\omega_n} \sum_{k', n'} V_{eff} (n - n', k - k') \frac{Z_{epi}(k')}{D_{epi}(k')},$$

$$\xi_n(k) = \xi(k) - \frac{T}{\omega_n} \sum_{k', n'} V_{eff} (n - n', k - k') \frac{\xi_{epi}(k')}{D_{epi}(k')},$$

$$Z_n(k) \Delta_n(k) = \frac{T}{\omega_n} \sum_{k', n'} V_{eff} (n - n', k - k') \frac{Z_{epi}(k') \Delta_{epi}(k')}{D_{epi}(k')},$$

where $V_{eff} (n - n', k - k') = V_{epi} (n - n', k - k') + V_{imp} (n - n', k - k')$, $V_{epi} (n - n', k - k') = -\xi_{epi}(k - k') D_{ph}(k - k', \omega_n - \omega_{n'})$, and $V_{imp} (n - n', k - k') = \delta_{n n'} n_i u^2 (k - k')/T$. Here, the phonon Green’s function in the Einstein model with the single frequency $\Omega$ is given by $D_{ph}(k - k', \omega_n - \omega_{n'}) = -2\Omega/(\Omega^2 + (\omega_n - \omega_{n'})^2)$, while the impurity scattering is described in the Born-approximation. Here, $n_i$ is the impurity concentration and $u(k - k')$ is the impurity potential. To these three equations one should add the

\[ R \sim M^{1/2}. \] Note, the properties (i)–(iii) are just opposite to the corresponding ones in the BCS- and Migdal–Eliashberg-theory for the standard EPI mechanism of pairing.
equation for the chemical potential $\mu$, i.e. $N = \sum_i \rho_i(\omega_n; \mu) = \text{const}$. However, in the following we study only problems where a (small) change of $\mu$ due to EPI and impurity scattering does not change the physics of the problem. For instance, we do not study problems such as BCS–BEC transition, where the equation for $\mu$ plays an important role, etc.

Note, that in the case of systems with very large Fermi energy $E_F$ and with an isotropic EPI ($Z_{\nu}(k) \equiv Z_{\nu}$, $\xi_{\nu}(k) \to 0$) one integrates over the energy $\xi_{\nu}$ by introducing the density of states at the Fermi surface $N(0)$, i.e. $\sum_{k'}(...) \to N(0) \int_{-\infty}^{\infty} (...) \mathrm{d} \xi$. This leads to standard Migdal–Eliashberg equations

$$Z_n = 1 + \frac{\pi T}{\omega_n} \sum_{n'} \frac{N(0) \langle V_{\nu}(n - n', q) \rangle \omega_n \omega_{n'} Z_{\nu}^{\text{eff}}}{\sqrt{(\omega_n \omega_{n'})^2 + \Delta_0^2}},$$

$$Z_n \Delta_n = \pi T \sum_{n'} \frac{N(0) \langle V_{\nu}(n - n', q) \rangle \omega_{n'} Z_{\nu}^{\text{eff}}}{\sqrt{(\omega_n \omega_{n'})^2 + \Delta_0^2}}.$$  \hspace{1cm} (12)

(13)

In the case of strongly momentum-dependent EPI–FSP, where $V_{\nu}(n - n', q)$ is finite for $|q| < \tilde{q}_c \ll q_0$, the Migdal–Eliashberg equations are given by

$$Z_n(\xi) = 1 + \frac{T}{\omega_n} \sum_m \langle V_{\nu}(n - m, q) \rangle \frac{\omega_m Z_m(\xi)}{D_m(\xi)},$$

$$\xi_n(\xi) = \xi(\tilde{k}) - T \sum_m \langle V_{\nu}(n - m, q) \rangle \frac{Z_m(\xi)}{D_m(\xi)},$$

$$Z_n(\xi) \Delta_n(\xi) = T \sum_m \langle V_{\nu}(n - m, q) \rangle \frac{Z_m(\xi) \Delta_m(\xi)}{D_m(\xi)}.$$  \hspace{1cm} (14)

(15)

(16)

A.2. Effects of non-magnetic impurities on $T_{\text{co}}$ in the EPI–FSP theory

In this paper we study the superconductivity which is due to EPI–FSP of the Einstein phonon with $\Omega \gg (2\pi T_{\text{co}})^2$. In that case $\langle V_{\nu}(n - m, q) \rangle \approx \langle V_{\nu}(0, q) \rangle / \Omega$ and the contribution to $Z_n(\xi)$ is $\sim \lambda_m = \langle V_{\nu}(0, q) \rangle / \Omega$. Since in the weak coupling limit one has $\lambda_m \ll 1$, then we neglect this contribution. Also the non-Migdal corrections can be neglected in this case—see [5]. The effects of non-magnetic impurities on $T_{\text{co}}$ is studied in the standard model with weakly momentum dependent impurity potential $u(k - k') \approx \text{const}$. In that case $Z_n(\xi)$ contains the impurity term only. After the integration of the impurity part over the energy $\xi_{\nu}$ in equations (9)–(11)—see [30], and for $\xi = 0$ (since in that case $\Delta_n(\xi = 0)$ is maximal) one obtains

$$Z_n = 1 + \frac{\Gamma}{\omega_n},$$

$$Z_n \Delta_n = T \sum_m \langle V_{\nu}(n - m, q) \rangle \frac{Z_m(\xi)}{D_m(0)} + \frac{\Gamma}{\omega_n} \Delta_n.$$  \hspace{1cm} (17)

(18)

Note, the the second term on the right side cancels the same term on the left side. In the square-well approximation $\Delta_n(\xi) \approx \Delta$ one obtains an equation for impurity dependence of $T_{\text{c}}^{(d)}(\Gamma)$ for the s-wave superconductor

$$1 = T_{\text{c}}^{(d)}(\xi) \sum_m \frac{1}{\omega_m^2 Z_m^2}.$$  \hspace{1cm} (19)

We point out, that in the case of the d-wave superconductivity $\Delta = \Delta(\varphi)$ is angle dependent on the Fermi surface and changes sign. In that case the last term in equation (18) for $\Delta$ should be replaced by $\langle \Delta(\varphi) = 0 \rangle$ giving equation for $T_{\text{c}}^{(d)}$

$$1 = T_{\text{c}}^{(d)}(\xi) \sum_m \frac{1}{\omega_m^2 Z_m^2}.$$  \hspace{1cm} (20)

Note, $Z_n$ versus $Z_n^2$ renormalization for the s-wave and d-wave superconductivity, respectively.

A.3. EPI–FSP self-energy in the normal state

We shall calculate the self-energy at $T = 0$. The leading order self-energy (on the Matsubara axis) in the Migdal–Eliashberg theory of EPI is given by

$$\Sigma_{\nu}(k, \omega_n) = -T \sum_{q, \Omega_m} \frac{1}{\omega_n^2} \langle 0 \right| G_{\text{ph}}(q, \Omega_m) G(k + q, \omega_n - \Omega_m),$$

where $\omega_n = \pi T (2n + 1)$ and $\Omega_m = 2\pi m T$, $D_{\text{ph}}(q, \Omega_m) = -2\Omega / (\Omega^2 + \Omega_m^2)$, $G(k, \omega_n) = 1 / (\omega_n - \xi_k)$. In the following we assume that $\Omega \gg T$ and neglect the bosonic distribution function $n_B(\Omega) \approx 0$. By defining

$$\Sigma_{\nu}(k, \omega_n) = -T \sum_{q, \Omega_m} \frac{1}{\omega_n^2} \langle 0 \right| G_{\text{ph}}(q, \Omega_m) G(k + q, \omega_n - \Omega_m),$$
\[ V_{epi}(q, 0) = 2g_{epi}^2(q) / \Omega \] and after summation over \( \Omega_m \) in equation (21) one obtains (note that 
\[ V_{epi}(q, 0) = V_{epi}(-q, 0) \]
\[ \Sigma_{epi}(k, \omega_n) = \frac{\Omega}{2} \sum_q V_{epi}(q, 0) \times \left[ \frac{n_F(\xi_{k+q})}{i\omega_n - \xi_{k+q} + \Omega} + \frac{1 - n_F(\xi_{k+q})}{i\omega_n - \xi_{k+q} - \Omega} \right]. \tag{22} \]

Let us calculate \( \Sigma_{epi} \) at \( k_0 \) and at \( T = 0 \). Since \( V_{epi} = g_{epi} \cos \theta \) and by taking into account that \( n_F(\xi_{k+q}) = 1 \) for \( \cos \theta < 0 \), \( n_F(\xi_{k+q}) = 0 \) for \( \cos \theta > 0 \) one obtains for \( g_{epi} \ll \Omega \)
\[ \Sigma_{epi}(k, \omega_n) = -\lambda_m \frac{i\omega_n}{1 - i\omega_n / \Omega}^2, \tag{23} \]
where \( \lambda_m = \langle V_{epi}(q) \rangle / 2\Omega \) and \( \langle V_{epi}(q) \rangle_q = N_S(-2\pi)^{-2} \int d^2q V_{epi}(q, 0) \), \( S \) is the surface of the FeSe unit cell. Note, that \( V_{epi}(q, 0) = 2g_{epi}^2(q) / \Omega \) and \( g_{epi}(q) = (g_0 / \sqrt{N}) e^{-(q/a)} \) so that \( N \) disappears from \( \lambda_m = \langle V_{epi}(q) \rangle_q / 2\Omega(1) \). After the analytical continuation \( \omega_n \rightarrow \omega + i\delta \) one obtains \( \Sigma_{epi}(k, \omega) \) in equation (3).

**References**

[1] Kulić M L and Zeyer R 1994 Phys. Rev. B 49 4395

Zeyer R and Kulić M L 1996 Phys. Rev. B 53 285

[2] Kulić M L 2000 Phys. Rep. 31 1–264

Kulić M L and Dolgov O V 2005 Phys. Status Solidi b 242 151

[3] Danylenko O V, Dolgov O V, Kulić M L and Oudovenko V 1999 Eur. Phys. J. B 9 201

[4] Lee J et al 2014 Nature 515 245

[5] Rademaker L, Wang Y, Berlijn T and Johnston T 2016 New J. Phys. 18 022001

Wang Y, Nakatoukas K, Rademaker L, Berlijn T and Johnston S 2016 Supercond. Sci. Technol. 29 054009

[6] Rebec S N, Jia T, Zhang C, Hashimoto M, Lu H D, Moore R G and Shen Z X 2016 arXiv:1606.09358v1

[7] Ginzburg V L 1968 Usp. Fiz. Nauk 95 91

Ginzburg V L 1970 Usp. Fiz. Nauk 101 185

Ginzburg V L 1976 Usp. Fiz. Nauk 118 316

[8] Dolgov O V, Kirzhnits D A and Maksimov E G 1981 Rev. Mod. Phys. 53 81

Dolgov O V, Kirzhnits D A and Maksimov E G 1987 Dielectric function and superconductivity Superconductivity, Superdiamagnetism and Superfluidity ed V L Ginzburg (Moscow: MIR Publication) ch 2

[9] Wang Q Y et al 2012 Chin. Phys. Lett. 29 037402

[10] Hirschfeld P J, Korshunov M M and Mazin I I 2011 Rep. Prog. Phys. 74 124508

Hirschfeld P J 2016 C. R. Phys. 17 197

[11] Boeri L, Dolgov O V and Golubov A A 2008 Phys. Rev. Lett. 101 026403

Kulić M L, Drechsler S L and Dolgov O V 2009 Eur. Phys. Lett. 85 47008

[12] Kulić M L and Haghhiard A A 2009 Eur. Phys. Lett. 87 17007

[13] Kulić M L Ginzburg Conf. on Physics (Moscov, 28 May–2 June 2012) (http://gc.lpi.ru/proceedings/kulic.pdf)

[14] Aperis A, Kotetes P, Varellogiannis G and Oppeneer P M 2011 Phys. Rev. B 83 092505

[15] Rahlenbeck M, Sun S L, Sun D L, Lin C T, Keimer B and Ulrich C 2009 Phys. Rev. B 80 064509

[16] Yin Z P, Kutepov A and Kotliar G 2001 Phys. Rev. X3 021011

[17] Maksimov E G, Kulić M L and Dolgov O V 2010 Adv. Cond. Mat. Phys. 2010 423725

[18] Peng R et al 2014 Nan. Commun. 2014 911

[19] Sadowski M V 2016 arXiv:1605.04426v2

Sadowski M V, Kuchinski E Z and Nekrasov I A 2010 J. Magn. Magn. Mater. 324 3481

Nekrasov I A and Sadowski M V 2014 Pisma v ZhETF 99 687

[20] Linscheid A, Majit S, Wang Y, Johnston S and Hirschfeld P J 2016 Phys. Rev. Lett. 117077003

Chen X, Majit S, Linscheid A and Hirschfeld P J 2015 Phys. Rev. B 92 224514

[21] Landau L D and Lifshitz E M 1989 Electrodynamics of Continuous Media (Oxford: Pergamon)

Murta B and Garcia-Garcia A M 2016 Phys. Rev. B 94 184508

[22] Yang K and Sondhi S L 2000 Phys. Rev. B 62 7778

[23] Maksimov E G and Savrasov D Y 2011 Solid State Commun. 119 569

[24] Zou K et al 2016 Phys. Rev. B 93 180506(R)

[25] Gor’kov L P 2016 Phys. Rev. B 93 060507

Gor’kov L P 2016 Phys. Rev. B 93 054517

[26] Coh S, Cohen M L and Louie S G 2015 New J. Phys. 17073027

[27] Li Z X, Fa W, Hong Y and Dung-Hai L 2016 Sci. Bull. 61 925

[28] Allen P B and Mitrović B 1982 Theory of Superconducting Tc (Solid State Physics vol 37) ed H Ehrenreich et al (New York: Academic) p 1