Superconductivity at low density near a ferroelectric quantum critical point: Doped SrTiO_{3}

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Superconductivity at low density near a ferroelectric quantum critical point: doped $SrTiO_3$

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Recent experiments on electron- or hole-doped $SrTiO_3$ have revealed a hitherto unknown form of superconductivity, where the Fermi energy of the paired electrons is much lower than the energies of the bosonic excitations thought to be responsible for the attractive interaction. We show that this situation requires a fresh look at the problem calling for (i) a systematic modeling of the dynamical screening of the Coulomb interaction by ionic and electronic charges, (ii) a transverse optical phonon mediated pair interaction and (iii) a determination of the energy range over which the pairing takes place. We argue that the latter is essentially given by the limiting energy beyond which quasiparticles cease to be well defined. The model allows to find the transition temperature as a function of both, the doping concentration and the dielectric properties of the host system, in good agreement with experimental data. The additional interaction mediated by the transverse optical soft phonon is shown to be essential in explaining the observed anomalous isotope effect. The model allows to capture the effect of the incipient (or real) ferroelectric phase in pure, or oxygen isotope substituted $SrTiO_3$.

I. INTRODUCTION

The question of the nature of the superonducting state in $SrTiO_3$ (STO) recently has been sharply brought into focus. There are at least two main issues driving the current debate about superconductivity in STO. One is the observation of the superonducting state at extremely low dopings, well below those of any other known superconductors. Recent observations of superconductivity in STO at such low doping levels[1,2] that the Fermi energy is much less than the relevant phonon energies are calling for a fresh look at the theory of superconductivity, even in a so-called weakly correlated material. Another issue that is clearly present is the interplay between superconductivity and the ferroelectric quantum critical point in STO. STO is a "quantum paraelectric" close to the quantum phase transition into the ferroelectric state[3], and may be tuned into the ordered phase, e.g. by isotope substitution of ^{16}O by ^{18}O[5] or by substituting Ca for Sr[6]. It becomes a metal by substituting, e.g. Sr with La, or Ti with Nb, or by removing O. These two questions: electron-electron interactions and the ferroelectric quantum critical point (QCP) are often intermingled in current discussions, yet they represent very different physics that might be connected at the end but does not have to be. Hence we start by discussing pairing due to dynamically screened electron-electron interaction, which is only weakly dependent on the proximate ferroelectric quantum criticality. It is, however, strongly modified by the large static dielectric constant. We thus will first focus on the role of screening and pairing at low doping levels in STO. Then we advocate the importance of an additional interaction sensitive to the ferroelectric fluctuations and giving rise to a strong isotope effect.

Superconductivity in STO metal at low temperatures has been observed long ago[4], the transition temperature as a function of doping peaking at a maximum of $T_c \approx 0.4$K at a carrier density of $n \approx 10^{20}\text{cm}^{-3}$[7–9]. According to the conventional view of superconductivity the main question is to identify the "glue" binding conduction electrons into a Cooper pair. An attractive interaction component may be obtained from suitable boson exchange processes: phonons, spin fluctuations, plasmons, etc. The remaining Coulomb repulsion is often neglected, on the grounds that it is substantially reduced in magnitude if downfolded into the low energy regime where the exchange bosons live. While this line of argumentation works reasonably well for superconductors with well separated energy scales, such that the Fermi energy $\epsilon_F >> \omega_{boson}$, a typical boson energy, it breaks down in case that the energy scales are no longer separated. It is then necessary to treat dynamical screening by ionic charges and by conduction electrons on the same footing. Early theories of superconductivity of STO , e.g. Koonce et al.[7] and Appel[10] , and even recent theories[11] did not address this problem properly and are therefore not suitable in the low doping domain $n < 10^{20}\text{cm}^{-3}$. A later theory by Takada[12] focusses on the interplay of ionic and electronic screening, starting from a pair interaction given by the screened Coulomb interaction (see below) and using the pairing theory in terms of the dynamical dielectric constant[13]. Takada uses additional approximations such as a plasmon pole approximation and a frequency cutoff of the order of the Fermi energy, without justification (for a discussion of the proper cut-off see below and Appendix A)), so that his results are questionable. A similar starting point has been chosen recently by Ruhman and Lee[14], who again use additional approximations (treatment of the Coulomb interaction at high frequency, and energy cut-off at the Fermi energy) without sufficient justification. The latter authors identify at least two problems with this more conventional approach: (i) by employing the Fermi energy as an energy cutoff the relevant interaction regime in energy space is found to shrink much too fast for decreasing density, leading to tiny transition temperatures; (ii) even at higher densities the T_c values come out too low, so that the authors propose that the extremely high dielectric constant found in

the undoped system is substantially reduced by doping, which helps to increase the screened Coulomb interaction and thus, T_c. Experimentally there is no indication that the very large dielectric constant is substantially reduced by doping at the low levels in question here. Both problems are resolved below by applying the proper cutoff and by taking into account an additional attractive pair interaction mediated by transverse optical (TO) phonons.

A careful treatment of the frequency cutoff ω_c is all-important in this problem, since here the cutoff frequency enters the result for the transition temperature in an essential way. We argue below that the processes limiting the pairing to a low energy regime in the case that the Fermi energy is less than the typical phonon energy are given by the self-energy entering the anomalous Green's function in the gap equation. While in our present solution of the gap equation we do not fully include the self-energy, we approximate its effect by introducing an energy cutoff at the energy beyond which quasiparticles are no longer well defined. In Appendix A we estimate this cutoff in three separate density regimes, with different dependencies on density in each regime. At the lowest densities electron-phonon interaction causes a vanishing of the cutoff with falling density n, $\omega_c \propto n^{1/3}$, while at the highest densities Fermi liquid theory provides $\omega_c \propto n^{2/3}$. The surprising result of the study of the quasiparticle relaxation rate (see Appendix A) is that at intermediate densities, where $\epsilon_F \ll \omega_{LO}$, the longitudinal optical phonon energy, the cutoff is found to have a reversed trend, $\omega_c \propto n^{-1/6}$, leading to a nonmonotonic dependence of $\omega_c(n)$.

In the conventional theory of superconductivity the small parameter ω_{phon}/ϵ_F allows to show that higher order correction terms (vertex corrections, crossed diagrams, etc) are small and may be safely neglected (Migdal's theorem). In the case of STO the presence of different small parameters again allows to neglect higher order corrections: the ratio of the transverse optical (TO, soft mode) and the longitudinal optical (LO) phonon frequencies squared, $(\omega_{TO}/\omega_{LO})^2$, which is of order 10^{-3} at wavevectors $q = \kappa$, the screening wave vector, and the weak coupling of electrons to TO phonons. The dimensionless Coulomb interaction, $N_F V_C$ is of order 10^{-2} in the relevant energy and wavevector domain, rather than of order unity as in conventional metals (here N_F is the density of states at the Fermi level). As a consequence vertex corrections are small, as estimated in Appendix C. Moreover, the nominally small density of carriers might suggest that the electron system is in the low density, strong interaction regime. The opposite is the case: the effective Bohr radius a_B^* is a factor of $\varepsilon_0(m/m_1) \approx 10^4$ larger than in usual metals, such that the parameter $r_s^* = (3n/4\pi)^{-1/3}/a_B^* \approx 0.01$, which puts the system into the effectively high density, weakly coupled regime. The additional interaction mediated by TO-phonon exchange is on one hand small due to the in general small coupling of transverse phonons to electronic quasiparticles, but is on the other hand boosted by the unusual screening properties arising with the soft TO-phonon mode, leading to large dynamical effective charges. Nonetheless, the vertex corrections induced by the TO-phonon mediated interaction are again small, as estimated in Appendix C.

The role of ferroelectric fluctuations is prominent in the observed gigantic isotope effect, occurring when the usual oxygen isotope O^{16} is replaced by the heavier O^{18}. In conventional BCS-theory this substitution should reduce the transition temperature T_c by a few percent. What is observed is, however, a drastic increase of T_c by as much as 50% for an O^{18} concentration of $x = 0.35$[19]. As mentioned above, the isotope substitution moves STO towards the ferroelectric phase, as signaled by the divergence of the paraelectric susceptibility and the concomitant vanishing of the TO-phonon soft mode frequency $\omega_{TO}(q = 0)$. The latter is expected to boost the contribution of the TO-phonon mediated pair interaction, as is indeed found (see below). The fundamental effect of the critical ferroelectric fluctuations on the superconductivity in STO has been proposed early on by[17,18]. These authors employed a model of quantum criticality featuring a soft mode, which may be identified as the TO phonon mode. In a phenomenological model they estimated the effect of a pairing interaction mediated by exchange of the soft mode on the transition temperature and found a significant effect, as found later in experiment[19].

What is the interaction between two conduction electrons in a metal, really? On the one hand it is given by the dynamically screened Coulomb interaction V_C, including any process contributing to the screening, phonons, plasmons, or any other coherent or incoherent type of excitation. This fully screened interaction between two charges in the solid has to be repulsive in the static limit, for reasons of stability. As will be shown below, in Matsubara frequency space the interaction is always positive, $V_C(\mathbf{q}, i\omega_n) > 0$, where $\mathbf{q}$,ω_n is the momentum and energy transferred in the interaction process. The second type of interaction is of exchange character, and is thought to provide the pairing "glue" for many unconventional superconductors such as the cuprates, the pnictides and the heavy fermion compounds, often by exchange of spin fluctuations. We will show below that in the present case of a soft transverse phonon mode, exchange of these excitations may make a substantial contribution to the pairing interaction.

II. PAIR INTERACTION.

The pair interaction thus consists of two parts

$$V_{pair}(\mathbf{q}, i\omega_n) = V_C(\mathbf{q}, i\omega_n) + V_{soft}(\mathbf{q}, i\omega_n) \qquad (1)$$

Here the dynamically screened Coulomb interaction is given by

$$V_C(\mathbf{q}, i\omega_n) = \frac{4\pi e^{*2}}{\varepsilon(\mathbf{q}, i\omega_n) q^2}, \qquad (2)$$

with the dielectric function capturing the screening by electronic and ionic charges

$$\varepsilon(\mathbf{q},i\omega_n)=[1+\frac{4\pi e^{*2}}{q^2}\chi_{el}(\mathbf{q},i\omega_n)]\frac{(i\omega_n)^2-\omega_{LO}^2(\mathbf{q},i\omega_n)}{(i\omega_n)^2-\omega_{TO}^2(\mathbf{q})}. \quad (3)$$

The dielectric function vanishes at $i\omega_n=\omega_{LO}(\mathbf{q},i\omega_n)$, defining the longitudinal optical phonon frequency, and diverges at the transverse optical phonon frequency, $i\omega_n=\omega_{TO}(\mathbf{q})$. The electronic screening effect is embodied in the irreducible electronic charge susceptibility χ_{el}. In the undoped limit $\chi_{el}\to 0$. The effect of higher lying excitations is lumped into the optical dielectric constant ε_∞, renormalizing the electron charge as $e^*=e/\sqrt{\varepsilon_\infty}$. We employ a single mode model, recognizing the fact that the TO-phonon mode becoming soft in the nearly ferroelectric $SrTiO_3$, and its longitudinal partner are the dominant modes . If necessary the model may be generalized to include further phonon modes. For simplicity we consider a fully isotropic model, approximating the ellipsoidal Fermi surfaces[20] by spheres. The phonon properties are actually very anisotropic (see Appendix B), but we will approximate the phonon dispersion by an angular average as well.

We may then parametrize the phonon frequencies as (for details see Appendix B)

$$\omega_{TO}^2(\mathbf{q})=\omega_D^2(\tau+\lambda q^2),$$
$$\omega_{LO}^2(\mathbf{q},i\omega_n)=\omega_{TO}^2(\mathbf{q})+\frac{4\pi\omega_D^2q^2}{q^2+4\pi e^{*2}\chi_{el}(\mathbf{q},i\omega_n)} \quad (4)$$

in the interval $0<q<q_c$. The parameter τ is closely related to the dielectric constants of the host, $\varepsilon_0=\varepsilon_\infty(1+4\pi/\tau)$. The static dielectric constant at $q=0$, is very large, $\varepsilon_0\approx 2\times 10^4$ at Kelvin temperatures[21] and the optical dielectric constant is $\varepsilon_\infty\approx 5.2$[22,23]. Substituting these values, we find $\tau\approx 3.27\times 10^{-3}$. We note that τ acts as a control parameter of the quantum phase transition to the ferroelectric phase, tending to zero at the transition, $\tau(x)=\tau(1-x/x_c)\to 0$ at $x=x_c$, where x is the concentration of O^{18} in the case of isotope substitution. The analysis of Raman scattering data [24] and of inelastic neutron scattering data[25], on the zone-center soft-mode transverse optical phonon allows to extract the following values of the above parameters: $\omega_{TO}(\mathbf{q}\to\mathbf{0})\approx 1.9$meV (22K in Kelvin units), which using τ gives a characteristic phonon energy $\omega_D\approx 33$meV (380K). The parameter λ averaged over the direction of $\mathbf{q}$ is found as $\lambda\approx 4.38\mathring{A}^2$ (see Appendix B).

With five atoms in the unit cell, $SrTiO_3$ has 15 phonon modes in total. The three acoustic modes are less relevant for the pairing and will be discarded. Of the remaining four triplets of optical phonon modes one is not infrared active, i.e. does not couple well to electrons, and may be omitted. The most relevant triplet consists of the two degenerate TO soft modes, which are surprisingly correlated with the highest lying longitudinal mode (usually called LO4)[26]. This is the set of phonon excitations which is well described by a phenomenological Ginzburg-Landau-Wilson model of the dynamic electric polarization of the system as shown in Appendix B. We neglect the remaining two triplets of modes. The experimental observation of a relatively strong e-ph coupling of the highest LO phonon mode[27,28] seen in tunneling experiments is compatible with our model, considering that real rather than virtual phonon excitations are involved.

We approximate χ_{el} by its non-interacting limit for an isotropic system, given by

$$\chi_{el}^{(0)}(\mathbf{q},i\omega_n)=2\int\frac{d^dk}{(2\pi)^d}\frac{n(\epsilon_{\mathbf{k}+\mathbf{q}})-n(\epsilon_{\mathbf{k}})}{i\omega_n-\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}}}, \quad (5)$$

where $\epsilon_{\mathbf{k}}=\frac{k^2}{2m_1}$, with $m_1\approx 1.8m$ a Fermi surface average of the effective mass of the lowest band (assuming $\epsilon_{\mathbf{k}}\ll W$, bandwidth) , and $n(\epsilon_{\mathbf{k}})=[1+e^{(\epsilon_{\mathbf{k}}-\mu)/T}]^{-1}$ is the Fermi function (we use units for which Planck's constant $\hbar$ and Boltzmann's constant k_B are equal to unity). The chemical potential μ at doping density n will be determined in the low temperature limit as $\mu=\epsilon_F=k_F^2/2m_1$, where $k_F=(3\pi^2n)^{1/3}$, considering that for the low doping levels in question here only states near the bottom of the lowest band are of interest. It will be seen later that the temparatures of interest satisfy $k_BT\ll\mu$. In case of several occupied electronic bands and effective mass renormalizations the expression for χ_{el} may be generalized correspondingly. The above assumes a rigid band model, i.e. the effect of doping is simply to populate the unoccupied conduction bands of $SrTiO_3$ (Ti derived $d-$bands).

The TO-phonon mediated interaction takes the form

$$V_{soft}(\mathbf{q},i\omega_n)=-2|M_{\mathbf{q}}^{TO}(\mathbf{k})|^2\frac{2\omega_{TO}(q)}{\omega_n^2+\omega_{TO}^2(q)} \quad (6)$$

and adds an attractive contribution to V_{pair} (the factor of 2 accounts for the two nearly degenerate soft TO modes). Here $M_{\mathbf{q}}^{TO}(\mathbf{k})$ is the electron-phonon coupling function, the transition amplitude for scattering of a conduction electron from momentum state $\mathbf{k}$ to state $\mathbf{k}+\mathbf{q}$ by emission of a TO phonon (we consider only the one mode going soft at the QCP; we also neglect umklapp processes). In deformation potential approximation it is given by

$$M_{\mathbf{q}}^{TO}(\mathbf{k})=-i\sqrt{\frac{\hbar N/V}{2m_{ion}\omega_{TO}}}\sum_\alpha\frac{(\mathbf{q}\cdot\mathbf{e}_{TO,\alpha})U_{\mathbf{q},\alpha}}{1+(\kappa/q_{typ})^2}B_{\mathbf{q}}(\mathbf{k}) \quad (7)$$

where m_{ion} is an effective ion mass, and $U_{\mathbf{q},\alpha}$ are the Fourier components of the Coulomb potential of ion α inside a unit cell, $U_{\mathbf{q},\alpha}=\int_{uc}d^3re^{i\mathbf{qr}}U_\alpha(\mathbf{r})$. The soft TO phonon mode is essentially a vibration of oxygen against the titanium ion. We therefore single out these two ions and assume the displacement vectors to be equal

and opposite, $\mathbf{e}_{TO,Ti} = -\mathbf{e}_{TO,O} = \mathbf{e}_{TO}$. This leads to a total deformation potential of $U_{\mathbf{q}} = U_{\mathbf{q},Ti} - U_{\mathbf{q},O} \approx \int_{uc} d^3r e^{i\mathbf{qr}} (\frac{e^{*2} Z^*_{Ti}}{|\mathbf{r}-\mathbf{R}_{Ti}|} - \frac{e^{*2} Z^*_O}{|\mathbf{r}-\mathbf{R}_O|})$. The effective charges Z^*_α have been determined from a first principles calculation[26] and are found to be unusually large in perovskite compounds such as $SrTiO_3$, $Z^*_{Ti} = 7.1$ and $Z^*_O = -5.7$. The reason is that the corresponding Ti-O ionic bond is on the verge of being covalent, leading to large charge transfers. We thus see that $U_{\mathbf{q}}$ comes out to be an order of magnitude larger than usual deformation potentials. We account for the effect of electron screening of the electron-ion potential by a factor $1/[1 + (\kappa/q_{typ})^2]$, with κ the screening wave number and $q_{typ} \approx 1/a$ a typical wave number inside the first Brillouin zone ($a \approx 3.9\mathring{A}$ is the lattice constant). This screening factor causes a suppression of V_{soft} with increasing electron density.

The momentum dependence of the matrix element of Bloch wave functions $u_{\mathbf{k}}(\mathbf{r})$ (of a single band, for simplicity), integrated over a unit cell of volume V_{uc}, $B_{\mathbf{q}}(\mathbf{k}) = V_{uc}^{-1} \int d^3r u^*_{\mathbf{k}+\mathbf{q}}(\mathbf{r}) u_{\mathbf{k}}(\mathbf{r})$ plays an important role here, as it describes the symmetry components of the coupling to the electron system. Separating out the average over the Brillouin zone we define the anisotropic part $\Delta B_{\mathbf{q}}(\mathbf{k})$ of $B_{\mathbf{q}}(\mathbf{k})$ as $\Delta B_{\mathbf{q}}(\mathbf{k}) = B_{\mathbf{q}}(\mathbf{k}) - \langle B_{\mathbf{q}}(\mathbf{k})\rangle_{av}$, where the average is over all $\mathbf{k}$ in the first Brillouin zone. The coupling provided by the averaged B is to density excitations of the electron system, which are strongly screened, as seen above. As a consequence, the frequncies of TO-phonon modes coupled to density excitations are shifted up to the LO-phonon frequencies and are no longer soft. In contrast, the anisotropic coupling mediated by $\Delta B_{\mathbf{q}}(\mathbf{k})$ does not couple the TO-phonon mode to density modes, leaving the phonon frequency unchanged, i.e. soft. A microscopic calculation of $\Delta B_{\mathbf{q}}(\mathbf{k})$ requires an electronic band structure calculation, which should take into account the substantial charge transfers in the unit cell. The latter may be expected to give a strong anisotropic component of $B_{\mathbf{q}}(\mathbf{k})$. We will assume $\Delta B_{\mathbf{q}}(\mathbf{k})$ of order unity in the following and approximate $(\Delta B_{\mathbf{q}}(\mathbf{k}))^2$ by its average.

A crucial factor in Eq.(7) is the inner product $(\mathbf{q} \cdot \mathbf{e}_{TO}(\mathbf{q}))$ of the wave vector and the polarization direction of the phonon mode. Along the principal directions $\mathbf{q}$ the polarization is perpendicular to the propagation direction and the inner product vanishes. In between these special directions $\mathbf{q}$ and $\mathbf{e}_{TO}(\mathbf{q})$ are not exactly orthogonal. The angular average of the e-ph coupling function is therefore nonzero, if small. In Appendix B the angular average $s = \langle(\widehat{\mathbf{q}}\cdot\mathbf{e}_{TO}(\mathbf{q}))^2\rangle$, where $\widehat{\mathbf{q}} = \mathbf{q}/|\mathbf{q}|$, is calculated as $s \approx 0.1$, independent of q. Some evidence for a coupling of electrons to the soft mode of $SrTiO_3$ has been found from transport experiments[29].

The dimensionless TO phonon mediated interaction is then given by

$$N_F V_{soft}(\mathbf{q}, i\omega_n) = -\eta \frac{k_F}{q_R} \frac{q^2}{q_R^2} \frac{\omega_D^2}{\omega_n^2 + \omega_T^2(q)} \qquad (8)$$

where

$$\eta = \frac{2s}{\pi^2} (q_R a)^3 (\frac{\overline{U}}{\omega_D})^2 \frac{m_1}{m_{ion}} \langle \Delta B^2_{\mathbf{q}}(\mathbf{k})\rangle_{av} \qquad (9)$$

Using the values $a = 3.9\mathring{A}$, $q_R \approx 0.124\mathring{A}^{-1}$, $\omega_D \approx 380$K , $\overline{U} \approx 35$eV, $m_{ion}/m_1 = 16320$ (taking the atomic mass of O^{16}), and $\langle \Delta B^2\rangle \approx 1$, we estimate $\eta \approx 0.1$. The above can provide only a rough estimate of the coupling strength η. A more accurate determination requires a microscopic calculation, which is beyond the scope of this work. We take a somewhat larger value, $\eta = 0.18$, in the numerical evaluation, giving rise to the observed magnitude of the isotope effect.

III. GAP EQUATION

Given the pair potential, the equation determining the gap function $\Delta(\mathbf{k}, i\omega_n)$ in the spin singlet channel is given by[30]

$$\Delta(\mathbf{k},i\omega_n) = -T \sum_{\omega_l} \sum_{\mathbf{p}\in BZ} V_{pair}(\mathbf{k}-\mathbf{p}, i\omega_n - i\omega_l) \quad (10)$$
$$\times \frac{\Delta(\mathbf{p},i\omega_l)}{[\omega_l - \Sigma(\mathbf{p},i\omega_l)]^2 + \xi^2_{\mathbf{p}} + |\Delta(\mathbf{p},i\omega_l)|^2},$$

where $\omega_l = (2l+1)\pi T$ is a fermionic Matsubara frequency, and $\xi_{\mathbf{p}} = \epsilon_{\mathbf{p}} - \mu$. Here $\Sigma(\mathbf{p}, i\omega_l)$ is the normal self-energy, which is negligible at low ω_l, but will provide a cut-off at $|\omega_l| = \omega_c$ as discussed below. The cutoff is determined by the condition $Im\Sigma(\mathbf{k}_F, \omega_c - i0) = \omega_c$; at frequencies $|\omega| > \omega_c$ quasiparticles are no longer well defined and the electron spectral function drops rapidly to zero with growing ω.

For small V_{soft}, $V_{pair}(\mathbf{q},i\omega_n)$ is a positive definite function (on the real frequency axis $ReV_C(\mathbf{q},\omega - i0)$ does have negative parts). The solutions $\Delta(\mathbf{k},i\omega_l)$ must therefore necessarily have negative components. This is well known from the examples of spin fluctuation mediated d-wave superconductivity, or of p-wave superfluidity of He^3, where the gap parameter has nodes on the Fermi surface. We see here that it may also hold for s-wave superconducting states. There the negative components must arise in the frequency dependence. A negative part of Δ at high frequency was actually calculated by Morel and Anderson[15], and even before by Bogoliubov[16]. To find such solutions requires to solve the gap equation as an integral equation in frequency. For larger V_{soft} (such as for $\eta = 0.18$, used below) the pair interaction has sufficiently attractive (negative) character that a solution without sign change in frequency becomes possible.

We restrict our considerations to the linear gap equation, which allows to determine the transition temperature. It is expected that the e-ph interaction gives rise to dominant s-wave pairing. Subdominant anisotropic pairing, induced by the lattice anisotropy and the general

momentum dependence of the pair interaction, will not be considered here.

A. Transition temperature

Assuming a momentum independent gap function, the transition temperature T_c follows from the linearized gap equation

$$\Delta(i\omega_n) = -T_c \sum_{\omega_l} K(\omega_n;\omega_l)\Delta(i\omega_l), \qquad (11)$$

The kernel of the gap equation may be expressed as

$$K(\omega_n;\omega_l) = \int_0^{q_c} \frac{dqq^2}{2\pi^2} V_{pair}(\mathbf{q}, i\omega_n - i\omega_l) F(q, i\omega_l),$$
$$F(q,i\omega_l) = \frac{1}{2}\int_{-1}^{1} \frac{d\cos\theta}{\omega_l^2 + (\xi_{\mathbf{k}_F} + \frac{q^2+2qk_F\cos\theta}{2m_1})^2}, \qquad (12)$$

taking proper account of the cut-off induced by the self-energy. At small ω_l the function $F(q,i\omega_l) \propto 1/\omega_l$, leading to the wellknown logarithmic divergence of the kernel of the gap equation. At large ω_l the self energy is dominant and $|\omega_l - \Sigma(\mathbf{p},i\omega_l)| \to \Sigma(\mathbf{p},i\omega_l) \propto (\omega_l)^\beta$, where $\beta = 2$ or 3, depending on density (see Appendix A), thus providing the frequency cutoff at ω_c. The momentum integral may be done numerically or even analytically, employing further approximations, with a cutoff q_c of the order of π/a, the extension of the first Brillouin zone. In view of the expected smallness of $T_c << \omega_{phon}$ the frequency summation extends over thousands of terms, allowing to replace the summation by an integral with a lower cutoff at the smallest fermionic frequency, $\omega_1 = \pi T$. It is useful to consider even- frequency and odd-frequency solutions separately, by introducing the corresponding kernels $K_{e,o}$. We define the eigenfunctions $\psi_\nu^{e,o}(\omega)$ and eigenvalues $\alpha_\nu^{e,o}(T_c)$ of the kernels $K_{e,o}$ on the imaginary frequency axis as

$$\alpha_n^{e,o}(T_c)\psi_n^{e,o}(\omega) = \int_{\pi T_c}^{\omega_c} \frac{d\omega'}{2\pi} K_{e,o}(\omega;\omega')\psi_n^{e,o}(\omega'),$$
$$K_{e,o}(\omega;\omega') = K(\omega;\omega') \pm K(\omega;-\omega') \qquad (13)$$

where the cutoff ω_c is found from an estimate of the imaginary part of $\Sigma(\omega + i0)$ presented in the Appendix. We adopt the interpolation expression

$$\omega_c = \frac{\omega_D}{(c_1(\frac{k_F}{q_R})^{-1/2} + c_2(\frac{k_F}{q_R})^2)^{-1} + c_3(\frac{k_F}{q_R})^{-1}} \qquad (14)$$

with parameters c_1, c_2, c_3 (and where we defined $q_R^2/2m = \omega_D$). As shown in Appendix A one may distinguish three density regimes with different dominant quasiparticle relaxation processes: (i) a high density Fermi liquid regime with $\omega_c \approx \epsilon_F$, (ii) an intermediate regime with dominant electron-electron scattering and anomalous density dependence $\omega_c \approx \omega_D(\frac{k_F}{q_R})^{-1/2}$, and (iii) a low density regime where electron-phonon scattering dominates, providing a cutoff $\omega_c \approx 30\omega_D(\frac{k_F}{q_R}) \gg \epsilon_F$. For typical parameter values ω_c is a nonmonotonic function of density, increasing at low density, passing through a maximum at around $n \approx 5\times 10^{17}\text{cm}^{-3}$ and through a minimum around $n \approx 2\times 10^{19}\text{cm}^{-3}$ and increasing for higher densities.

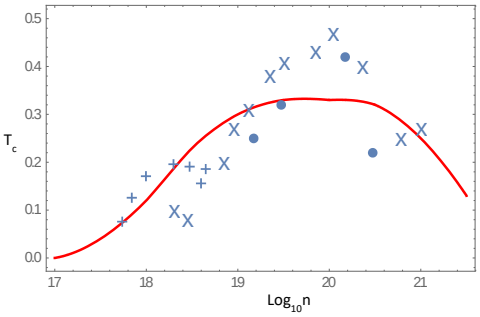

FIG. 1. Transition temperature Tc in Kelvin versus logarithm of electron density in cm^{-3}. Theory: solid line; Experiment: crosses (Schooley et al., 1964); filled circles: Nb-doped; + symbols: O-reduced (Lin et al., 2014)

The solution $\psi_\nu^{e,o}(\omega)$ with the highest transition temperature may be obtained by finding the largest negative eigenvalue

$$\max_{\{n\}}[-\alpha_n^{e,o}(T_c)] = -\alpha_{n_0}^{e,o}(T_c) = 1 \qquad (15)$$

and the gap function is given by $\Delta(i\omega) = \psi_{n_0}^{e,o}(\omega)$. It is found that the highest transition temperature appears in the even-frequency class for an eigenfunction $\psi^e(\omega)$ with a single zero on the positive semi-axis (small V_{soft}) or without zero (sufficiently strong, but still small V_{soft}).

In Fig. 1 we show the transition temperature T_c as a function of doping density n . For a reasonable choice of the parameters of the cutoff ω_c, $c_1 \approx 1.1$, $c_2 = 0.6$ and $c_3 \approx 0.036$, the T_c values compare well with the experimental data. For higher densities the higher electronic bands are successively populated (gaps to the second band 4meV and third band 30meV, and population of the second band starting at $n = 3\times 10^{18}\text{cm}^{-3}$). Their contribution is expected to increase T_c.

B. Isotope effect

As already mentioned, a further spectacular finding about the superconducting phase of doped $SrTiO_3$ is the observed isotope effect[19]. One finds that substitution of O^{16} by a concentration $x_c = 0.35$ of O^{18} enhances T_c

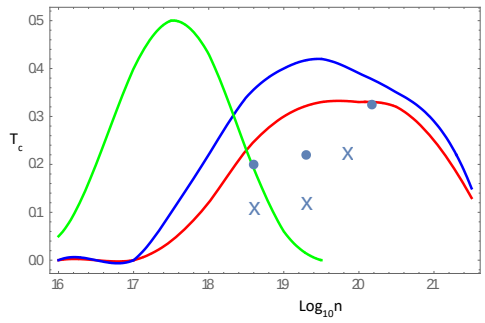

FIG. 2. Transition temperature Tc in Kelvin versus logarithm of electron density in cm^{-3}. Theory: solid red line, isotope concentration x=0; solid blue line, x=0.34; solid green line, only Coulomb interaction ($\eta = 0$) and x=0. Experiment: crosses, x=0; filled circles, x=0.34 (Stucky et al., 2016)).

by as much as 50%. In conventional superconductors substitution by a heavier isotope leads to a reduction of T_c by a few percent, as caused by a slight decrease of the prefactor in the BCS-expression for T_c. The isotope substitution moves the system closer to the ferroelectric quantum critical point (or even beyond it, into the ordered phase). This leads to a major change in the pair interaction, through its dependence on the TO-phonon frequency $\omega_{TO}(q = 0)$, which vanishes at the QCP. Correspondingly, the pair attraction is boosted by isotope substitution. We have calculated this effect by putting $\omega_{TO}(q = 0; x) = (1 - x/x_c)\omega_{TO}(q = 0; x = 0)$. As shown in Fig. 2 we find that for the parameter specifying the strength of V_{soft}, $\eta = 0.18$ and keeping the cut-off frequency ω_c as presented above, T_c is indeed increased by a factor ≈ 1.5 at densities $n \approx 10^{18}\mathrm{cm}^{-3}$, with somewhat smaller enhancement at higher densities. We point out that this approach is different from the proposals by Edge et.al,[17,18], where the ferroelectric soft mode was discussed without taking into account the Coulomb interactions. Also shown in Fig. 2 is the result obtained without the TO-phonon mediated interaction ($\eta = 0$). Surprisingly, the T_c curve is shifted to lower densities, but is not lower, but even somewhat higher than the result obtained with both interaction components ($\eta = 0.18$). This clearly shows that the two interaction components superpose in a more complex manner as one may have thought, owing to their very different frequency dependence.

IV. CONCLUSION.

Our results show that superconductivity in doped $SrTiO_3$ may be interpreted as induced by two relevant interaction components, the dynamically screened Coulomb interaction and an interaction mediated by transverse optical phonons. Both, screening by ionic charges, in particular through the optical phonon modes responsible for the incipient ferroelectric transition and screening by electronic charges is important. At higher densities electronic screening leads to a suppression of pairing. On the low density side it is found that the rapid decay of quasiparticles for energies beyond $\omega_c \propto n^{1/3}$, caused by e-ph scattering confines the domain of quasiparticle pairing to ever lower energies, as density decreases, again leading to a suppression of T_c. An all-important feature of our theory is the careful consideration of the relevant frequency domain. We find that the cutoff frequency at low density is much larger than the Fermi energy, and even varies with density in a nonmonotonic fashion. Previous studies on, e.g. plasmon exchange mediated superconductivity[31] have found a strong effect of higher order contributions, substantially reducing the tendency for superconductivity[32]. In the present case higher order corrections are small because both, the screened Coulomb interaction and the soft phonon induced interaction are weak. The observation of a large and unusual isotope effect may be explained easily within the present model: isotope substitution can move the system closer to the ferroelectric transition, and thereby softens the TO-phonon frequency. This leads to a substantial enhancement of the pairing interaction.

The inclusion of higher phonon modes is not expected to lead to major changes, as it will only affect the high frequency part of the pairing interaction. In contrast, taking into account the two higher electronic bands, which begin to be populated at higher dopings is expected to increase the pairing tendency sizeably.

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VI. APPENDICES

A. Electronic self-energy

The purpose of this Appendix is to show that the quasiparticle relaxation rate Γ exceeds the energy ω for $|\omega| > \omega_c$, signaling that quasiparticles are no longer well defined and that the electron spectral function falls off faster than ω^{-2}. Consequently the contribution of processes from the energy domain $|\omega| > \omega_c$ to the gap equation is strongly suppressed, even though the screened Coulomb interaction is perfectly finite for such energies.

1. Coulomb interaction

We first estimate the contribution to $\Gamma(\mathbf{k}_F,\omega) = Im\Sigma(\mathbf{k}_F,\omega - i0)$ from electron-electron interaction, Γ_{el}, as approximately given by

$$\Gamma_{el}(\mathbf{k}_F,\omega) = \pi \sum_{\mathbf{k}_2,\mathbf{k}_3} |V(|\mathbf{k}_F - \mathbf{k}_3|, \omega - \epsilon_{\mathbf{k}_3})|^2 \times (1-n_{\mathbf{k}_3})(1-n_{\mathbf{k}_4}) n_{\mathbf{k}_2} \delta_\epsilon \quad (16)$$

where $\mathbf{k}_4 = \mathbf{k}_F + \mathbf{k}_2 - \mathbf{k}_3$ and $\delta_\epsilon = \delta(\omega + \epsilon_{\mathbf{k}_2} - \epsilon_{\mathbf{k}_3} - \epsilon_{\mathbf{k}_4})$.

Let us first look at energy $\omega \approx \epsilon_F$, at the border of the Fermi liquid regime, when we have

$$\Gamma_{el}(\mathbf{k}_F,\epsilon_F) \approx \frac{\omega^2}{\epsilon_F} |N_0 V_C(|\mathbf{k}_F|, \epsilon_F)|^2 \quad (17)$$

In the limit of high densities, where $\epsilon_F \gtrsim \omega_{LO}(q=0)$ we have

$$N_0 V_C(|\mathbf{k}_F|, \epsilon_F) \approx \frac{\kappa^2}{k_F^2 + \kappa^2} \approx 1 \quad (18)$$

so that the cutoff frequency is given by $\omega_{c1} \approx \epsilon_F$.

At lower densities $\epsilon_F \ll \omega_{LO}(q=0)$ the screening provided by the ionic charges strongly weakens the Coulomb interaction. We have approximately

$$N_0 V_C(|\mathbf{k}_F|, \epsilon_F) \approx \frac{\kappa^2}{k_F^2 \frac{\omega_{LO,0}^2(q=0)}{\epsilon_F^2 + \omega_{TO}^2(q=0)} + \kappa^2} \approx \frac{\kappa^2}{k_F^2} \frac{\epsilon_F^2 + \omega_{TO}^2(q=0)}{\omega_{LO,0}^2(q=0)} \quad (19)$$

At a density of $n = 10^{18}\text{cm}^{-3}$, putting in numbers $k_F \approx 0.03\mathring{A}^{-1}$, $\kappa^2 \approx 0.012\mathring{A}^{-2}$ and $\omega_{TO}^2(q=0)/\omega_{LO,0}^2(q=0) \approx 10^{-3}$ it is apparent that $\gamma = |N_0 V_C(|\mathbf{k}_F|, \epsilon_F)|^2 \approx 10^{-4} \ll 1$. Therefore, the resulting cutoff frequency will be $\omega_c \gg \epsilon_F$.

For large $\omega \gg \epsilon_F$ energy conservation requires the qp energies $\epsilon_{3,4}$ to be large such that $n_{\mathbf{k}_3}, n_{\mathbf{k}_4} \ll 1$. The momentum integrations may be expressed in terms of integrations over the energies $\epsilon_{\mathbf{k}_2}, \epsilon_{\mathbf{k}_3}$ and over angles, in particular over $\cos\theta = (\mathbf{k}_F \cdot \mathbf{k}_3)/k_F k_3$

$$\Gamma_{el}(\mathbf{k}_F,\omega) \approx \pi \int_0^{k_F} \frac{dk_2 k_2^2}{2\pi^2} \int \frac{d\Omega_{\mathbf{k}_2}}{4\pi} \int_0^{\pi/a} \frac{dk_3 k_3^2}{2\pi^2} \times \int \frac{d\cos\theta d\phi}{4\pi} |V_C(|\mathbf{k}_F - \mathbf{k}_3|, \omega - \epsilon_3)|^2 \delta_\Gamma \quad (20)$$

Here $\delta_\Gamma = \delta_\Gamma(\omega + \epsilon_2 - \epsilon_3 - \epsilon_4)$ is a "delta function" of finite width Γ, allowing for the fact that Γ may be as large as the energy itself. The integral over $\cos\theta$ may be done with the help of the $\delta-$function, using $\epsilon_4 \approx v|\mathbf{k}_4| = v(\Delta\epsilon - 2k_F k_3 \cos\theta)^{1/2}$, for $\mathbf{k}_4$ inside the first Brillouin zone. We expect ϵ_4 to be large, beyond the regime where the quadratic dependence on $\mathbf{k}_4$ holds. We therefore use a rough approximation of the electronic energy dispersion for higher energies, replacing so to speak the $-\cos k$ - function of a tight-binding dispersion by a straight line. The result is

$$\Gamma_{el}(\mathbf{k}_F,\omega) \propto \int_0^{k_F} \frac{dk_2 k_2^2}{2\pi^2} \int_0^{\infty} \frac{dk_3 k_3^2}{2\pi^2} \times \frac{\omega}{k_F k_3 v^2} |V_C(|\mathbf{k}_3|, \omega - \epsilon_{\mathbf{k}_3})|^2 , \quad (21)$$

where we used $\epsilon_{\mathbf{k}_2} \ll \epsilon_{\mathbf{k}_3}$ and averaged over the remaining angles. What is the screened Coulomb interaction in the range $\omega_{TO}(q_{typ}), \epsilon_F \ll \omega \ll \omega_{LO}(q_{typ},\omega)$ and for typical values of momentum $q_{typ} \approx \omega/v$? Because of the large difference of the transverse and the longitudinal optical phonon frequencies in a polar material, there is a frequency regime where $V_C \propto \omega^2$, reflecting the huge difference in polarization at low and high frequencies. We may approximate the Coulomb potential by

$$V_C(q,\omega) = \frac{4\pi e^{*2}}{q^2 \frac{\omega^2 - \omega_{LO,0}^2(k_3)}{\omega^2 - \omega_{TO}^2(k_3)} + \kappa^2} \approx \frac{4\pi e^{*2}}{k_3^2 + \kappa_\omega^2} \frac{\omega^2}{\omega_D^2} \quad (22)$$

where $\kappa_\omega^2 = \kappa^2\omega^2/\omega_D^2$. Within the above approximations one finds

$$\Gamma_{el}(\mathbf{k}_F,\omega) \propto \frac{4k_F^2 e^{*4}}{\pi^2 v^2} \frac{\omega^5}{\omega_D^4} \int_{\kappa_\omega}^{\infty} dk_3 \frac{1}{k_3^3} \approx \omega \left(\frac{\omega}{\omega_{c2}}\right)^2 ,$$
$$\omega_{c2} \approx \pi\omega_D \frac{(mv^2)^{1/2}}{(e^{*2}q_R)^{1/2}} (q_R/k_F)^{1/2} \quad (23)$$

Using that $v \approx D/(\pi/a)$, $(\pi/a)^2/m \approx D$ and $e^{*2}/a \approx D$, where D is the half band width, it is seen that the ratio $(mv^2)^{1/2}/(e^{*2}/a)^{1/2} = O(1)$. The cutoff frequency is seen to decrease weakly with increasing k_F, in the intermediate density regime.

2. Electron-phonon scattering

At small densities the contribution from phonon scattering to Γ dominates. We consider scattering by acoustical phonons, approximating the dispersion by $\omega_{\mathbf{q}} = cq$ and taking into account that the polarization vector $\mathbf{e}_\lambda$ is parallel to $\mathbf{q}$ along the principal directions. The scattering rate may be estimated as

$$\Gamma_{ph}(\mathbf{k}_F,\omega) \approx \pi \sum_{\mathbf{q}} |M(\mathbf{q})|^2 (1-n_{\mathbf{k}+\mathbf{q}})\delta_\Gamma(\omega-\epsilon_{\mathbf{k}+\mathbf{q}}-\omega_{\mathbf{q}}), \tag{24}$$

We approximate the electronic dispersion by $\epsilon_{\mathbf{k}} \approx v(|\mathbf{k}|-k_F)$. Using $n_{\mathbf{k}+\mathbf{q}} = \Theta(\omega_{\mathbf{q}}-\omega)$ the angular integral yields

$$\Gamma_{ph}(\mathbf{k}_F,\omega) \approx \int \frac{dqq^2}{2\pi^2}\langle|M(\mathbf{q})|^2\rangle\Theta(\omega-\omega_q)\frac{\omega-\omega_q}{k_F q v^2} \times\Theta_\Gamma(2k_F q - |(\frac{\omega}{v})^2 - q^2|). \tag{25}$$

where $\Theta_\Gamma(x)$ is a step function of width Γ. Here the e-ph matrix element squared is approximated by

$$\langle|M(\mathbf{q})|^2\rangle \approx \frac{q^2}{\rho\omega_q}(\frac{4\pi e^{*2}}{a^3(q^2+\kappa^2)})^2, \tag{26}$$

where $\rho = m_{ion}a^{-3}$ is the ionic mass density and a is the lattice spacing. Here we are allowed to drop the ionic part of the screening, considering the fact that the relevant momentum transfer $q_{typ} \approx \omega_D/v$ and hence $\omega_{TO}(q_{typ}) \approx \omega_{LO}(q_{typ},\omega_D)$. We have $vq \gg \omega_{\mathbf{q}}$, so that we may drop $\omega_{\mathbf{q}}$ from the argument of the second step-function, also $k_F^2 \ll q^2$ may be neglected. The $q-$integral is then confined to a region of width $2k_F$ around $q_\omega = \omega/v$. As a result we get at $\omega < v\kappa$

$$\Gamma_{ph}(\mathbf{k}_F,\omega) \approx \omega^3 \frac{1}{\pi^2 m_{ion} c a}(\frac{4\pi e^{*2}}{a v^2\kappa^2})^2 = \omega(\frac{\omega}{\omega_{c3}})^2, \tag{27}$$

Estimating $v \approx \pi/(m_1 a)$, $c^2/v^2 \approx m_1/m_{ion}$, and using $4\pi e^{*2}/\kappa^2 = \pi^2/m_1 k_F$ one finds

$$\omega_{c3} \approx \omega_D(\frac{mv^2}{\pi^2\omega_D})^{1/2}(\frac{m_{ion}}{m_1})^{1/4}(\frac{k_F}{q_R}) \tag{28}$$

The two prefactors may be estimated as $(\frac{mv^2}{\omega_D})^{1/2} \approx 5$ and $(\frac{m_{ion}}{m_1})^{1/4} \approx 13$ (using the ionic mass of O^{16}), yielding an estimate of the parameter c_3 introduced in Eq.(14), $c_3 \approx 0.05$, which compares well with the value used in the numerical evaluation.

3. Cutoff energy

Combining the above results for the cutoff energies induced by Coulomb interaction at high and low densities, ω_{c1}, ω_{c2} and by the electron-phonon interaction, ω_{c3} into a single expression we may define

$$\omega_c = \frac{\omega_D}{(c_1(\frac{k_F}{q_R})^{-1/2} + c_2(\frac{k_F}{q_R})^2)^{-1} + c_3(\frac{k_F}{q_R})^{-1}} \tag{29}$$

For the values of the parameters c_1, c_2, c_3 used in the numerical evaluation, the cutoff energy is found to be a nonmonotonic function of k_F, which may be traced to $\omega_{c2} \propto k_F^{-1/2}$, decreasing with increasing density, mainly because $\Gamma \propto n/\kappa^4 \propto k_F$. This nonmonotonic behavior appears to be necessary for obtaining the observed T_c versus density values.

B. Phenomenological model of optical phonons of $SrTiO_3$

1. Optical phonons in a dynamical model of electric polarization

The soft mode properties of $SrTiO_3$ may be discussed in the framework of a Ginzburg-Landau-Wilson action for the electric polarization $\mathbf{P}(\mathbf{r},t)$, varying in space and imaginary time. The general form of the action (dropping nonlinear terms) is

$$S = \frac{1}{2}\int dt \int d\mathbf{r}[\frac{1}{\omega_D^2}(\frac{\partial\mathbf{P}}{\partial t})^2 + \tau\mathbf{P}^2 + \sum_{i,j,k,l}\lambda_{ijkl}\frac{\partial P_i}{\partial x_j}\frac{\partial P_k}{\partial x_l}]. \tag{30}$$

The fourth rank tensor λ_{ijkl} in a cubic lattice (we neglect the tetragonal distortion for simplicity) has three independent elements λ_j, $j = 1,2,3$

$$\lambda_{ijkl} = \lambda_1\delta_{ik}\delta_{kl}\delta_{ij} + \lambda_2\delta_{kl}\delta_{ij}(1-\delta_{ik}) + \lambda_3\delta_{ik}\delta_{jl}(1-\delta_{ij}). \tag{31}$$

Stability requires $\lambda_1 > \lambda_2 > 0$ and $\lambda_3 > 0$. The electric field $\mathbf{E}$ generated by $\mathbf{P}$ is obtained as

$$\mathbf{E}(\mathbf{r},t) = \frac{\delta S}{\delta\mathbf{P}(\mathbf{r},t)} = \chi\cdot\mathbf{P}, \tag{32}$$

where χ is the tensor of electric susceptibility, the elements of which are defined in Fourier space as

$$\chi_{ik}(\mathbf{q},i\omega_n) = (\frac{\omega_n^2}{\omega_D^2} + \tau)\delta_{ik} + q^2 A_{ik} \tag{33}$$

where we defined a tensor

$$A_{ik} = [\lambda_3(1-n_i^2) + \lambda_1 n_i^2]\delta_{ik} + \lambda_2 n_i n_k(1-\delta_{ik}) \tag{34}$$

and $\widehat{\mathbf{q}} = (n_1,n_2,n_3)$ is the unit vector in the direction of $\mathbf{q}$.

To determine the Fourier components of the potential $\varphi_{ion}(\mathbf{r},t)$ of a point charge screened by ionic charges we need to solve the equations

$$i\mathbf{q}\cdot(\mathbf{E}+4\pi\mathbf{P}) = 4\pi e$$
$$\mathbf{E} = -i\mathbf{q}\varphi_{ion} = \chi\cdot\mathbf{P}$$

with the result

$$\varphi_{ion}(\mathbf{q},i\omega_n) = \frac{4\pi e}{q^2+4\pi\mathbf{q}\cdot\chi^{-1}\cdot\mathbf{q}} = \frac{4\pi e}{\epsilon_{ion}(\mathbf{q},i\omega_n)q^2} \quad (35)$$

The projection of the inverse susceptibility along $\mathbf{q}$ is approximately given by

$$\mathbf{q}\cdot\chi^{-1}\cdot\mathbf{q} \approx \frac{q^2}{\frac{\omega_n^2}{\omega_D^2}+\tau+\lambda_1 q^2+2K(-\lambda_1+\lambda_3+\lambda_2)q^2} \quad (36)$$

where $K(\widehat{\mathbf{q}}) = n_x^2n_y^2+n_y^2n_z^2+n_z^2n_x^2$. Eq.(36) is exact for $\mathbf{q}$ along the axes, face diagonals or space diagonals. It follows that

$$\epsilon_{ion}(\mathbf{q},i\omega_n) \approx \epsilon_\infty\frac{\omega_n^2+\omega_{LO,0}^2(\mathbf{q})}{\omega_n^2+\omega_{TO}^2(\mathbf{q})} \quad (37)$$

where we defined the average frequencies of the soft TO phonon and the accompanying (bare) LO phonon by

$$\frac{\omega_{TO}^2(\mathbf{q})}{\omega_D^2} = \tau+\lambda_1 q^2+2K(-\lambda_1+\lambda_3+\lambda_2)q^2, \quad (38)$$
$$\omega_{LO,0}^2(\mathbf{q}) \approx \omega_{TO}^2(\mathbf{q})+4\pi\omega_D^2 \quad (39)$$

The exact TO phonon frequencies are obtained from the zeros of the eigenvalues of the tensor χ (see below).

2. Dielectric function of doped $SrTiO_3$

At finite doping the potential φ of a test charge is additionally screened by the conduction electron system

$$e\varphi(\mathbf{q},i\omega_n) = \frac{e\varphi_{ion}}{1+e\varphi_{ion}\chi_{el}} = \frac{4\pi e^2}{\epsilon(\mathbf{q},i\omega_n)q^2} \quad (40)$$

Here the dielectric function is given by

$$\epsilon(\mathbf{q},i\omega_n) = \epsilon_\infty[1+\frac{4\pi\mathbf{q}\cdot\chi(\mathbf{q},\omega_n)^{-1}\cdot\mathbf{q}}{q^2}+\frac{4\pi e^2}{\epsilon_\infty q^2}\chi_{el}(\mathbf{q},i\omega_n)] \quad (41)$$

where χ_{el} is the irreducible electric polarization of the conduction electrons. The potential of a fully screened test charge is equivalent to the screened Coulomb interaction $V_C(\mathbf{q},i\omega_n)$ between two conduction electrons, which may be reexpressed as

$$V_C(\mathbf{q},i\omega_n) = \frac{4\pi e^{*2}}{q^2+\kappa^2(\mathbf{q},i\omega_n)}\frac{\omega_n^2+\omega_{TO}^2(\mathbf{q})}{\omega_n^2+\omega_{LO}^2(\mathbf{q},i\omega_n)}, \quad (42)$$

where $\kappa^2(\mathbf{q},i\omega_n) = 4\pi e^{*2}\chi_{el}(\mathbf{q},i\omega_n)$ and $\omega_{LO}(\mathbf{q},i\omega_n)$ is the LO phonon frequency renormalized by electronic screening effects

$$\omega_{LO}^2(\mathbf{q},i\omega_n) = \omega_{TO}^2(\mathbf{q})+\frac{4\pi q^2}{q^2+\kappa^2(\mathbf{q},i\omega_n)}\omega_D^2. \quad (43)$$

To make contact with the usual representation of the phonon mediated interaction we note that V_C may be expressed as the sum of an electronically screened Coulomb interaction and a phonon induced interaction

$$V_C(\mathbf{q},i\omega_n) = \frac{4\pi e^{*2}}{q^2+\kappa^2(\mathbf{q},i\omega_n)} - \frac{4\pi e^{*2}q^2}{(q^2+\kappa^2(\mathbf{q},i\omega_n))^2}\frac{4\pi\omega_D^2}{\omega_n^2+\omega_{LO}^2(\mathbf{q},i\omega_n)}. \quad (44)$$

3. Transverse optical phonon eigenstates

We define the eigenstates of the tensor A_{jk} by

$$\sum_k A_{jk}e_k^{(m)} = a^{(m)}e_j^{(m)}. \quad (45)$$

The transverse optical phonon frequencies and polarization vectors are found as solutions of $\mathbf{E}(\mathbf{q},\omega_n) = \chi(\mathbf{q},\omega_n)\cdot\mathbf{P}(\mathbf{q},\omega_n) = 0$, at finite $\mathbf{P}$ and for transverse polarization. Consequently we are looking for eigenstates of the tensor χ with zero eigenvalue, such that

$$\frac{(i\omega_n)^2}{\omega_D^2} = \tau+q^2a^{(m)} \quad (46)$$

and eigenvectors $e_j^{(m)}$. We have calculated the eigenvalues and eigenstates of χ in their dependence on the direction $\widehat{\mathbf{q}}$, and hence the TO soft phonon frequency and eigenvector (identified as the lowest eigenvalue). For orientations $\widehat{\mathbf{q}} = (1,0,0)$ and $\widehat{\mathbf{e}}^{(1)} = (0,1,0)$ we find $a^{(1)} = \lambda_3$, which compared with INS data[25] yields a value $\lambda_3 \approx 2.0\mathring{A}^2$. For the only other experimental configuration of $\widehat{\mathbf{q}} = \frac{1}{\sqrt{2}}(1,1,0)$ and $\widehat{\mathbf{e}}^{(1)} = \frac{1}{\sqrt{2}}(1,-1,0)$ we get $a^{(1)} = \frac{1}{2}(\lambda_1-\lambda_2+\lambda_3)$, compared with the experimental value[25] $a^{(1)} \approx 4.5\mathring{A}^2$. Assuming a value of $\lambda_2 \approx 1.0\mathring{A}^2$ one then obtains $\lambda_1 \approx 8.0\mathring{A}^2$.

Using these values we have determined the eigenstates of the matrix A_{jk} numerically. The angular average of the scalar product of the unit vector along $\mathbf{q}$ and an eigenvector $\mathbf{e}^{(TO)}$ squared is found as

$$\langle(\widehat{\mathbf{q}}\cdot\mathbf{e}^{(TO)})^2\rangle \approx 0.1 \quad (47)$$

C. Vertex corrections

Here we provide a rough estimate of the vertex correction in first order of the interaction. It is given by

$$\Lambda(k,p) = \sum_q G(k-q)G(p-q)V(q) \tag{48}$$

where $G(k) = G(\mathbf{k}, i\omega_n) = (i\omega_n - \xi_{\mathbf{k}})^{-1}$, omitting the self-energy correction, and $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$. We first consider the screened Coulomb interaction, using the approximation

$$V_C(\mathbf{q}, i\omega_n) \approx \frac{4\pi e^{*2}}{q^2+\kappa_0^2}\frac{\omega_{TO}^2(\kappa_0)}{2\pi\omega_D^2}. \tag{49}$$

Here $\kappa_0^2 = \kappa^2(\mathbf{0},0) = 4\pi e^{*2} N_F$, which at a density of $n = 10^{18}\mathrm{cm}^{-3}$ amounts to $\kappa_0^2 \approx 0.026\mathring{A}^{-2}$. It follows that the frequency ratio is small, $\rho = \omega_{TO}^2(\kappa_0)/2\pi\omega_D^2 = (\tau + \lambda\kappa_0^2)/2\pi \approx 0.018$, so that the dimensionless interaction strength $N_F V_C \approx 10^{-2}$ in the relevant regime of momenta and frequencies. The vertex corrections are approximately given by (using $\xi_{\mathbf{q}} = v_F(q-k_F)$, where $v_F = k_F/m_1$ is the Fermi velocity, and neglecting k, p compared to q)

$$\Lambda_C(k,p) \approx N_F^{-1}\rho T\sum_{\omega_l}\int\frac{dqq^2}{2\pi^2}\frac{\kappa_0^2}{q^2+\kappa_0^2}\frac{1}{(i\omega_l - \xi_{\mathbf{q}})^2} \approx \rho \tag{50}$$

where the frequency summation has been done approximately as

$$T\sum_{\omega_l}\frac{1}{(i\omega_l-\epsilon_q)^2} \approx \{\int_{\pi T}^{\infty} + \int_{-\infty}^{-\pi T}\}\frac{d\omega}{2\pi}\frac{1}{(i\omega-\xi_{\mathbf{q}})^2} \approx \frac{T}{(\pi T)^2+\xi_{\mathbf{q}}^2} \tag{51}$$

and we used $T \ll \epsilon_F$ and $\kappa_0^2 + q^2 \approx \kappa_0^2$, since $q \approx k_F \ll \kappa_0$.

The TO-phonon mediated interaction gives rise to the following vertex correction

$$\Lambda_{soft}(k,p) \approx \frac{\eta}{N_F}\frac{k_F}{q_R}T\sum_{\omega_l}\int\frac{dqq^2}{2\pi^2}\frac{q^2}{q_R^2}\frac{\omega_D^2}{\omega_T^2(q)}\frac{1}{(i\omega_l-\xi_{\mathbf{q}})^2} \approx \frac{\eta}{N_F}\frac{k_F}{q_R}\int\frac{dqq^2}{2\pi^2}\frac{q^2}{q_R^2}\frac{\omega_D^2}{\omega_T^2(q)}\frac{T}{(\pi T)^2+\xi_{\mathbf{q}}^2} \tag{52}$$

where the frequency summation has been done as described above. The momentum integral is again dominated by the sharp peak at $\epsilon_q = 0$, i.e. at $q = k_F$, and may be approximately done as

$$\Lambda_{soft}(k,p) \approx \eta(\frac{k_F}{q_R})^3\frac{1}{\tau+\lambda k_F^2} \tag{53}$$

At a density of $n = 10^{18}\mathrm{cm}^{-3}$ we may estimate $k_F \approx 0.03\mathring{A}^{-1}$, therefore $\eta(k_F/q_R)^3 \approx 2\times10^{-3}$ (we recall $q_R \approx 0.124\mathring{A}^{-1}$). Taking $(\tau+\lambda k_F^2)^{-1} \approx 100$ we then find $\Lambda_{soft} \approx 0.2$.

These rough estimates demonstrates that vertex corrections are negligible on account of the unusually strong screening by ionic charges in this electrically highly polarizable material and due to the weak coupling of electrons to TO phonons.

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