Superconducting dome in the LaAlO$_3$/SrTiO$_3$ interfaces as a direct effect of the extended s-wave symmetry of the gap

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The two-dimensional electron gas (2DEG) at the LaAlO$_3$/SrTiO$_3$ interface exhibits gate tunable superconductivity with a domelike shape of $T_C$ as a function of electron concentration. Here, we propose that the experimentally observed behavior can be explained as a direct effect of the dominant extended s-wave symmetry of the superconducting gap. Our results quantitatively agree with the experimental data. Additionally, our calculations based on both the Hartee-Fock and the Gutzwiller approximations show that the influence of electronic correlations on the paired state in the considered system is not that crucial as commonly believed.

Introduction.

The two-dimensional electron gas (2DEG) at the interface between LaAlO$_3$ and SrTiO$_3$ (LAO/STO) has attracted growing interest as a fundamental system to study the interplay between superconductivity, spin-orbit interaction, and magnetism. It has been well established that LAO/STO exhibits gate tunable superconductivity with a dome-like shape of $T_C$ as a function of gate voltage. The origin of such behavior still remains unclear and is the subject of an ongoing debate, which mainly concentrates around the role of electronic correlations, multiband effects, and spin-orbit interaction.

According to the correlation effect scenario, the Coulomb repulsion between $d$ electrons from Ti atoms, leads to nonmonotonic population of the low energy $xy$ mobile band resulting in the dome-like shape of $T_C$ as the electron concentration increases. Within such approach the $xy$ band contributes significantly to the formation of the SC state and the maximal $T_C$ appears close to the Lifshitz transition (LT) when the change of electron concentration monotonicity takes place. Other reports suggest that the suppression of $T_C$ may appear above LT due to the strong pair-breaking effect if the interband interaction is repulsive. The negative influence of LT on the pairing in LAO/STO has been investigated experimentally in Refs. and. On the other hand, according to standard BCS theory an enhancement of $T_C$ should appear after new states are available for the Cooper pair formation. This discrepancy has not been completely resolved so far. Also, in contradiction to the mentioned proposal, some of the experimental analysis show that the upper $xz/yz$ bands play the major role in the formation of the paired state and superconductivity sets in close to the point when the multiband behavior appears (at the Lifshitz transition).

Finally, one should note that using magnetotransport measurements it has been established that the SOC energy follows the nonmonotonic dependence of $T_C$, what may indicate that SOC constitutes a significant factor, which tunes the pairing strength leading to the dome-like behavior of $T_C$. However, such effect is not seen in all the interface orientations and the interplay between superconductivity and SOC has not been recognised in detail so far. Therefore, it is not clear if the spin-orbit energy is in fact the primary cause of the characteristic shape of the phase diagram or a secondary effect.

In spite of several mentioned proposals aiming in explanation of the SC dome in LAO/STO, the satisfactory theoretical reconstruction of $T_C$ as a function of gate voltage has not been reached so far. Here, we show that the appearance of the superconducting dome as a function of gate voltage in the LAO/STO interfaces can be explained as a sole result of the extended s-wave superconducting gap symmetry appearing in the range of relatively low electron concentrations. As we show, the calculated phase diagram is in very good agreement with the available experimental data. To analyze the influence of the electronic correlations we carry out calculations with the inclusion of the Coulomb repulsion terms by using both Hartee-Fock and Gutzwiller approximation. We show that the correlation effects do not influence the physical picture of the paired state steaming out from our analysis.

Theory.

We consider the two-dimensional electronic gas at the LAO/STO interface with (100) orientation. The Hamiltonian of the system is given by

$$
\hat{H} = \hat{H}_{TBA} + \hat{H}_U + \hat{H}_{SC},
$$

where subsequent terms correspond to the kinetic energy, Coulomb repulsion, and the real-space pairing, respectively. The kinetic energy part of the Hamiltonian $\hat{H}_{TBA}$ is expressed with the use of the three-orbital tight binding approximation (cf. Supplemental Material)

$$
\hat{H}_{TBA} = \sum_{k\sigma} (\epsilon_k - \mu) \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} + \sum_{kk'\sigma} \epsilon_{kk'} \hat{c}_{k\sigma}^\dagger \hat{c}_{k'\sigma},
$$

where $\mu$ is the chemical potential, $\hat{c}_{k\sigma}^\dagger$ ($\hat{c}_{k\sigma}$) are the creation (annihilation) operators of electrons with momentum...
where \( k \), spin \( \sigma \), and orbital index \( l = xy, xz, yz \) corresponding to \( d_{xy}, d_{xz}, d_{yz} \) orbitals of the Ti atoms placed on a square lattice. The primed summation is restricted to \( l \neq l' \). The bare dispersion relations of the three unhybridized bands have the form

\[
\begin{align*}
\epsilon_{kl}^{xy} &= 4t_l - \Delta_E - 2t_l \cos k_x - 2t_l \cos k_y, \\
\epsilon_{kl}^{xz} &= 2t_l + 2t_h - 2t_l \cos k_x - 2t_h \cos k_y, \\
\epsilon_{kl}^{yz} &= 2t_l + 2t_h - 2t_h \cos k_x - 2t_l \cos k_y,
\end{align*}
\]

and the mixing between the \( xz \)- and \( yz \)-bands is the following

\[
\epsilon_{hk} = 2t_d \sin k_x \sin k_y, 
\]

where \( t_l = 8.75 \text{ meV}, t_h = 40 \text{ meV}, t_d = 40 \text{ meV}, \Delta_E = 47 \text{ meV} \). The resulting band structure of the model is presented in Fig. 1 and consists of the \( xy \)-band which is lower in energy at the \( \Gamma \) point than the two hybridized \( xz/yz \)-bands (cf. Supplemental Material).

The Coulomb interaction term \( \hat{H}_U \) has the form

\[
\hat{H}_U = U \sum_{il} \hat{n}_{il \uparrow} \hat{n}_{il \downarrow} + V \sum_{iil'} \hat{n}_{il \uparrow} \hat{n}_{il' \downarrow},
\]

where \( U \) and \( V \) are the intra- and inter-orbital Coulomb repulsion integrals. For simplicity we take \( U = V = 2 \text{ eV} \), which corresponds to the value calculated in Ref. [23].

In our model the superconducting state is introduced by a real-space intersite intraorbital pairing with the interorbital pair hopping

\[
\hat{H}_{SC} = -J \sum_{ijl} \hat{c}_{il \uparrow} \hat{c}_{jl \downarrow} \hat{c}_{il \downarrow} \hat{c}_{jl \uparrow} - J' \sum_{ijl'} \hat{c}_{il \uparrow} \hat{c}_{jl' \downarrow} \hat{c}_{il' \downarrow} \hat{c}_{jl \uparrow},
\]

for which the interorbital pair hopping energy, \( J' \), is one order of magnitude smaller than the intraorbital coupling constant, \( J \).

By applying the standard Hartree-Fock-BCS treatment of the pairing part and transformation to reciprocal space (cf. Supplemental Material) one can show that the resulting SC gaps in the three bands of the model take the following form

\[
\Delta_{k}^{xy} = 4\Delta_{k}^{s} \gamma_{k}^{s},
\]

\[
\Delta_{k}^{xz/yz} = 4\Delta_{k}^{s} \gamma_{k}^{s} \pm 4\Delta_{k}^{d} / \gamma_{k}^{d},
\]

where the \( xy \) and \( xz/yz \) superscripts correspond to the low-energy band and the two upper hybridized bands, respectively. In Eqs. \((7)\) and \((8)\) we have introduced the extended \emph{s-} and \emph{d-wave} pairing amplitudes \( \Delta_{k}^{s}, \Delta_{k}^{d} \) and \( \Delta_{k}^{d} \), as well as the corresponding \( k \)-dependent symmetry factors \( \gamma_{k}^{s} \) and \( \gamma_{k}^{d} \) of the form

\[
\gamma_{k}^{s} = (\cos k_x + \cos k_y)/2, \quad \gamma_{k}^{d} = (\cos k_x - \cos k_y)/2.
\]

The \( \alpha \) factor in Eq. \((8)\) results from the hybridization between the \( xz \) and \( yz \) bands and has the form

\[
\alpha_{k} = \frac{\epsilon_{k}^{xz} - \epsilon_{k}^{yz}}{\sqrt{(\epsilon_{k}^{xz} - \epsilon_{k}^{yz})^2 + 4\Delta_{k}^{s}^2}}.
\]

Note that in the bare (unhybridized) \( xz \) and \( yz \)-bands the four-fold rotational \( C_4 \) symmetry is broken, which leads to the appearance of both \emph{extended s-} and \emph{d-wave} pairing components of the gap. However, due to interband mixing the \( C_4 \) symmetry is restored both in the resulting \( xz/yz \)-hybridized bands and in the corresponding \( k \)-dependent gaps \( \Delta_{k}^{xz/yz} \). In the low energy \( xy \)-band the \( C_4 \) symmetry is conserved, and according to our calculations the \emph{extended s-wave} pairing wins over the \emph{d-wave} pairing for the electron concentration ranges realized in the LAO/STO interfaces.

The amplitudes appearing in Eqs. \((7)\) and \((8)\) are directly related to the intraorbital intersite real-space pairing expectation values

\[
\Delta_{k}^{s} \equiv \Delta_{k}^{s} \equiv \Delta_{k}^{s} = \Delta_{k}^{s} = \Delta_{k}^{s} = \Delta_{k}^{s}, \quad \Delta_{k}^{d} \equiv \Delta_{k}^{d} \equiv \Delta_{k}^{d} = \Delta_{k}^{d} = \Delta_{k}^{d} = \Delta_{k}^{d},
\]

where

\[
\Delta_{ij}^{s} = \frac{1}{4} \sum_{j(i)} \gamma_{ij}^{s} \Delta_{ij}, \quad \Delta_{ij}^{d} = \frac{1}{4} \sum_{j(i)} \gamma_{ij}^{d} \Delta_{ij}.
\]

Here the summations run over the four nearest-neighbor atomic sites of \( R_j \). These sums do not depend on the position of \( R_j \) since the system is homogeneous. The \emph{extended s-wave} and \emph{d-wave} real-space symmetry factors are \( \gamma_{ij}^{s} = 1 \) and \( \gamma_{ij}^{d} = 1 \) (\( \gamma_{ij}^{d} = -1 \)) for \( R_j = R_i \pm \hat{x} \) (\( R_j = R_i \pm \hat{y} \)). The \( \Delta_{ij} \) parameters correspond to the combination of the anomalous superconducting expectation values

\[
\Delta_{ij} = -J \langle \hat{c}_{il \uparrow} \hat{c}_{jl \downarrow} \rangle - J' \sum_{l(i \neq j)} \langle \hat{c}_{il' \uparrow} \hat{c}_{jl' \downarrow} \rangle.
\]

As one can see due to the pair-hopping terms there is a small contribution to the SC gap in a particular band.
which comes from the remaining bands (the second term above). Such mechanism connects all the gaps and guarantees the appearance of a single critical temperature.

The Coulomb interaction terms appearing in Eq. \( \text{Eq. 5} \) are treated with the use of Hartree-Fock (HF) approximation leading to an effective shift of the atomic energy (cf. Supplemental Material) which is dependant on the filling of particular bands. Due to the fact that such mean-field procedure neglects most of the electron correlations effects we also apply the statistically consistent Gutzwiller approximation (SGA)[27][28][29] for comparison. Within the SGA approach apart from the standard mean-field atomic energy shifts, the correlation induced renormalization of both electron hopping and pairing is taken into account (cf. Supplemental Material).

Results.-We start from the model with no Coulomb repulsion terms included \((U = V = 0)\) and analyze the superconducting properties of the 2DEG at the LAO/STO interface as a function of the chemical potential, \( \mu \), or equivalently the filling factor, \( n_{\text{tot}} = \sum_{i} n_{\text{sites}} / N \) (\( N \)-number of atomic sites). Note that, by increasing the gate voltage in experiments one adds electrons to the system what leads to increase of both \( \mu \) and \( n_{\text{tot}} \). The effect of the Coulomb repulsion is analyzed later on both by the use of HF and SGA approximations. In all the calculations the value of coupling constant has been set to \( J = 0.165 \) eV so as to reproduce the maximal critical temperature \( T_C \approx 0.35 \) K which is measured in experiments.

Results for \( T = 0 \) K presented in Fig. 2(a) show that the extended s-wave pairing amplitude in the two hybridized bands \( \Delta^*_{xz/yz} \) constitutes the dominant contribution to the superconducting phase and it reproduces the dome-like shape of the critical temperature as a function of gate voltage, reported in experiment[30][31][32] [cf. Fig. 2(b)]. Also, the gap amplitude in the low-energy band \( \Delta^d_{xy} \) follows the trend of the amplitudes in the two upper bands \( \Delta^*_{xz/yz} \). This results from the fact that in the former the density of states is too low for the pairing to appear naturally. Therefore, the gap in the \( xy \) band is induced by the pair hopping processes from the two upper bands with significantly higher DOS. Note, that the remaining \( \Delta^d_{xz/yz} \) gap amplitude has a negligible influence on the SC properties of the system being one
order of magnitude smaller than $\Delta_{x^2-y^2}$.

In Figs. 2(c) and (d) we present the results for $T > 0$ K, which show that indeed the dome like shape of $T_C$ as a function of the filling factor (and chemical potential) is reproduced in our model and matches very well the experimental data provided for comparison in Fig. 2(b). Here, we do not show the gap amplitude in the lower band, $\Delta_{xy}$, as it has virtually the same behavior as $\Delta_{x^2-y^2}$. However, the former is scaled down to approximately three times smaller values than the latter [cf. Fig. 2(a)].

The explanation for the obtained dome-like shape of $T_C$ within our approach is the following. As shown in Figs. 2(a), (c), and (d) the extended s-wave pairing amplitude dictates the changes of $T_C$, as the number of electrons increases. For such situation one can distinguish between two regions. The first one corresponds to very low electron concentrations when the Fermi surface is contained in the close proximity of the $\Gamma$ point in the center of the Brillouin zone [cf. Fig. 2(e)]. In this regime the extended s-wave symmetry factor $\gamma^e_k \approx 1$ at the Fermi surface and it does not tune the value of the gap significantly. As one can see in Fig. 2(c) for $\mu$ below the optimal value, the Fermi surface (blue line) is placed inside the closed isoline representing $\gamma^e_k = 0.9$. In this regime a standard behavior of rising $T_C$ with the chemical potential appears, similarly as in the conventional case of constant SC gap ($\Delta_k \equiv \Delta$) within the real-space pairing scenario. However, as $\mu$ increases the Fermi surface expands and moves closer to the nodal lines of the extended s-wave symmetry factor, where the gap closes [cf. Fig. 2(e)]. As one can see for $\mu$ above the optimal value, the Fermi surface (red line) reaches the isolines corresponding to $\gamma^e_k = 0.6$. At this point the suppression of the gap at the Fermi surface resulting from the extended s-wave symmetry becomes significant. In this regime superconductivity is gradually weakened as one adds electrons to the system. Between the two regions the optimal chemical potential is placed, for which the maximal $T_C$ appears.

In Fig. 2 we show how the electrons injected into the system are distributed between the $xy$ band (red line) and the two hybridized $xz/yz$ bands (black line). As one can see the Lifshitz transition corresponds to $\mu = 0$ when the two hybridized bands begin to be populated and the superconductivity sets in [cf. Fig. 2(a)]. This result is in agreement with the experimental data presented in Ref. 5, where the transition from the single to multiband behavior takes place in close proximity to the minimal critical electron concentration $n_{\text{min}}$ for the appearance of the paired state. Significantly increased contribution of the upper $d_{xz/yz}$ bands above $n_{\text{min}}$ also seems to be in agreement with the measurements of the SOC interaction presented in Ref. 22. It should be noted that in Fig. 2(f) both $n_{xy}$ and $n_{xz/yz}$ are monotonically increasing functions of the total electron concentration. As we show below the nonmonotonic behavior of $n_{xy}$, which is seen in experiment 23, can be reproduced only after the inclusion of the Coulomb repulsion terms.

Finally, in Fig. 3(a) we show the extended s-wave pairing amplitude $\Delta_{x^2-y^2}$ as a function of the filling factor for the case of nonzero Coulomb interaction integrals $U$ and $V$. As one can see, both HF and SGA methods lead to very similar results, which additionally are very close to those obtained earlier for the case of no Coulomb interaction ($U = V = 0$). Therefore, one can conclude that the interactions do not influence significantly the considered here paired state in the parameter regime significant for the LAO/STO interfaces. This result is consistent with the fact that the pairing has an intersite character, hence, it is not that much affected by the intrasite Coulomb repulsion terms. The interorbital Coulomb term makes the carrier density in the low-energy $xy$ band a nonmonotonic function of band filling in agreement with the experimental data presented in Ref. 19 (Fig. 3 in that paper). The influence of that mechanism on superconductivity, which was proposed in Ref. 41 does not play a role here because the pairing in our model originates mainly from the two upper $xz/yz$ bands.

One should also note that for relatively small number of electrons in the system, the number of multiple occupancies on a single atomic leading to interactions is very low. The regime analyzed here corresponds to $\lesssim 0.1$ electron per lattice site and is far from $n_{\text{tot}} \approx 1, 2, 3, \ldots$ for which the correlation effects are enhanced. In such case, the correlation induced renormalization taken into account within the SGA method is not significant making the HF and SGA results very close.

Summary—As we have shown the appearance of the superconducting dome in the LAO/STO interfaces can be explained as a sole result of the extended s-wave symmetry of the gap, which appears in the intersite real-space pairing scenario. The mechanism leading to the SC dome reconstruction is based on a simple fact that
the $k$-dependence of the gap leads to a significant suppression of the pairing, but only when the Fermi surface is placed relatively far from the $\Gamma$ point in the Brillouin zone. Such approach leads to very good agreement between the theoretical results and the available experimental data. To the best of our knowledge such high degree of reconstruction of the $T_C$ dome has not been obtained so far within any other theoretical proposal. It should be noted, that in our approach neither the spin-orbit coupling nor the electron correlation effects are responsible for the SC dome appearance. Calculations carried out with the inclusion of the Coulomb repulsion terms both by using HF and SGA methods has lead to very similar result as the one obtained for $U = V = 0$.

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