Interface-mediated pairing in field effect devices

V. Körtig\textsuperscript{1}, Qingshan Yuan\textsuperscript{1,2,3}, P. J. Hirschfeld\textsuperscript{1,4}, T. Kopp\textsuperscript{1}, and J. Mannhart\textsuperscript{1}

\textsuperscript{1}Center for Electronic Correlations and Magnetism, EP6, Univ. Augsburg, Augsburg Germany
\textsuperscript{2}Texas Center for Superconductivity and Advanced Materials, Univ. of Houston, Houston, TX 77204 USA
\textsuperscript{3}Pohl Institute of Solid State Physics, Tongji University, Shanghai 200092, P.R. China
\textsuperscript{4}Department of Physics, University of Florida, PO Box 118440, Gainesville FL 32611 USA

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Shortly after the publication of the BCS theory of superconductivity, W. A. Little proposed a possible pairing mechanism for electrons in long organic molecules involving localized electronic excitations in the molecules’ side chains \[1\]. The suggested advantages of such an arrangement included the large characteristic energy of the couplings, which might lead to high temperature superconductivity (HTSC), and the separation of the excitations themselves from the screening effects of the electron gas. Such a pair mechanism has never been realized, presumably due to large fluctuation effects in quasi-1D systems. Later, Ginzburg \[2\] and Allender, Bray and Bardeen \[3\] proposed a similar excitonic 2D mechanism in superconductor-semiconductor sandwiches. The enormous body of early work on this problem has been reviewed in \[2\]. One problem with these schemes is clearly that the localized nature of the excitations implies that at most one or two atomic layers of the intercalating insulator can contribute to the pairing, meaning that the enhancement of pairing in the relatively thick nearby superconductor is negligible.

Here we propose that a similar scheme might work for an insulating layer in proximity with a superconducting layer of near-atomic thickness. Such systems can in principle be prepared in several ways, but the most promising is perhaps the field effect method pioneered in the early 90’s with the intent of increasing the carrier density and hence \(T_c\) in HTSC cuprate devices \[4,5,6,8,9\]. This work has shown incontrovertibly that \(T_c\) and other superconducting properties in metallic samples can be influenced by an applied gate voltage. While the experiments have most often been interpreted in terms of electronic structure variations near the interface, they are not understood in detail.

It is interesting to ask if new physics can result from field doping of insulators. In the most recent reports on field-doping of SrTiO\(_3\), Pallecchi et al. \[10\] and Ueno et al. \[11\] were able to achieve an areal carrier density of \(\sim 0.01–0.05\) per unit cell. It is difficult to achieve higher densities due to electrical breakdown in the insulating layer at high fields. But there seems to be no fundamental objection to even higher charge densities, since complex oxide dielectrics and ferroelectric oxides can achieve polarizations in the range of \(\sim 0.5\) \[12\]. In fact, very recently the first observation of field-induced superconductivity was reported for a device with a Nd\(_{1.2}\)Ba\(_{1.8}\)Cu\(_3\)O\(_7\) epitaxial film grown on SrTiO\(_3\) substrates \[12\].

Therefore one may legitimately ask the question what critical temperature can be achieved in a system where the pairing comes entirely from the excitations in the proximate insulating layer, and how \(T_c\) is likely to vary with field in this case. Alternatively, one can assume the existence of a 2D superconducting layer with pre-existing pair interaction and bare critical temperature \(T_c^0\), and ask by how much the presence of the insulating layer enhances \(T_c\). While in a strictly 2D system the \(T_c^0\)’s referred to cannot correspond to true long-range order, the creation of a field-tuned superconducting state with algebraic order at finite temperatures would be of considerable interest and applicability in small devices.

We begin by considering an insulating amorphous film \(L_1\) in proximity to a correlated insulator \(L_2\) (drain-source (DS) channel of a field effect device), similar to Ref. \[12\] with a small density of localized charge carriers. Applying an electric field as shown in Fig. \[1\] sweeps charge carriers to the interface with the film \(L_1\) where they accumulate \[13\]. The formation of the 2D band induced by an electric field has been studied by Poilblanc et al. \[13\]. We assume for the moment that in the absence of the film \(L_1\) there are no pairing interactions between the electrons in the material \(L_2\). Qualitatively, we expect the following picture to apply: virtual excitations in the dielectric \(L_1\) induce Cooper pairing in the adjacent layer \(L_2\). The critical temperature must increase initially with the field since carriers are being injected into the system. With increasing electric field the larger level splitting of the two level system leads to a suppression of the polarization fluctuations and the pair potential decreases. \(T_c\) is therefore expected to reach a maximum at a characteristic field strength; it is our objective to estimate the scale of possible \(T_c\)’s through this process, as well as the field strength required to attain it.
We now propose a crude but concrete framework within which one can calculate these effects. Roughly speaking, the dielectric can have two effects on $T_c$. First, it can reduce the Coulomb pseudopotential of electrons in the field-doped layer due to the large dielectric constant of the amorphous insulator $L1$. We are more concerned here with the second effect, namely an additional contribution to the residual pairing interaction at the interface due to virtual polarization of the dielectric itself.

I. MODEL

The Hamiltonian we consider describes a single layer $L2$ of electrons $c^\dagger_i$ hopping on a square lattice with lattice constant $a$, nearest neighbor hopping $t$, and a set of localized two-level systems in an adjacent layer $L1$ with ground state $s_i^\uparrow$ and excited state $p_i^\uparrow$ separated in energy by $\Delta_{sp}$, and their respective dipole moment is $ed_{sp}$ (Fig. 1). Note these states simply designate ground and excited states, which are coupled to the free electrons in the layer $L2$ by a contact interaction $V_{sp}$.

The Hamiltonian contains, according to our assumptions, the following elementary processes:

$$H_{tot} = H_t + H_{2l} + H_{ext} + H_{int} + H_\mu + H_{e-e}$$  \hspace{1cm} (2)

with

$$H_t = -t \sum_{<i,j>,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma}$$  \hspace{1cm} (3)

$$H_{2l} = \frac{1}{2} \Delta_{sp} \sum_i (p_i^\uparrow s_i - s_i^\uparrow p_i^\uparrow)$$  \hspace{1cm} (4)

$$H_{ext} = E_{sp} \sum_i (p_i^\uparrow s_i + s_i^\uparrow p_i^\uparrow)$$  \hspace{1cm} (5)

$$H_{int} = V_{sp} \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} (p_i^\uparrow s_i + s_i^\uparrow p_i^\uparrow)$$  \hspace{1cm} (6)

$$H_\mu = -\mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}$$  \hspace{1cm} (7)

$$H_{e-e} = U \sum_i c^\dagger_{i,\uparrow} c_{i,\downarrow} c^\dagger_{i,\downarrow} c_{i,\uparrow}$$  \hspace{1cm} (8)

Here $H_t$ describes a band of noninteracting $2D$ electrons on a square lattice, $H_{2l}$ the energies of the localized two level system, $H_{ext}$ the coupling of the electric field to these orbitals, $H_{int}$ the Coloumb interaction between electrons in the metallic layer and the two level system, and $H_\mu$ the chemical potential. The direct electron-electron interaction term $H_{e-e}$ is taken to be local and repulsive. Very similar models have been used recently to discuss dielectric properties of bulk cuprates [15], the competition between charge density wave and superconductivity in two dimensional electronic systems [16], and superconductor-ferroelectric multilayers [17]. The system is not exactly soluble, but will be treated under the assumption that the polarization through the charges in $L2$ is not large enough to drive the system into the ferroelectric state. We first diagonalize $H_{2l} + H_{ext}$, and then express the corresponding quasiparticle operators in a pseudospin representation where $S_i^z$ measures the occupation of the $2$-level system and $S_i^{\pm}$ induces transitions between the two eigenlevels. The occupation constraint on the two-level system is preserved by the usual spin algebra. The (exact) final form of the Hamiltonian is

$$H_{2l} + H_{ext} = -2 \sqrt{E_{sp}^2 + (\frac{1}{2} \Delta_{sp})^2} \sum_i S_i^z$$  \hspace{1cm} (9)

$$H_{int} = -V_z \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} S_i^z$$  \hspace{1cm} (10)

$$+ V_x \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} (S_i^+ + S_i^-)$$  \hspace{1cm} (11)

where

$$V_z = 2V_{sp} \frac{E_{sp}}{\sqrt{E_{sp}^2 + (\frac{1}{2} \Delta_{sp})^2}}$$

$$V_x = V_{sp} \frac{\frac{1}{2} \Delta_{sp}}{\sqrt{E_{sp}^2 + (\frac{1}{2} \Delta_{sp})^2}}$$

The system of interacting spins-1/2 and fermions may now be treated within linear spin wave theory, an ap-
proximation which is justified \textit{a posteriori} by the observation that the occupation of the higher-energy 2-level state is very small, due to the sufficiently large 2-level splitting [13]. Introducing the usual Holstein-Primakoff bosons [19], we make the approximate replacements $S_j^+ \rightarrow b_j$, $S_j^- \rightarrow b_j^\dagger$, $S_j^z \rightarrow \frac{1}{2} - b_j^\dagger b_j$ to find

$$H = -t \sum_{\langle i,j \rangle,\sigma} c_{i,\sigma}^\dagger c_j^\sigma - \mu_r \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} - E_{2l} \sum_i \left( \frac{1}{2} - b_i^\dagger b_i \right) + V_z \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} b_i^\dagger b_i + V_x \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} (b_i + b_i^\dagger) + H_e - \epsilon$$

and the chemical potential has been renormalized $\mu_r = \mu + V_z/2$.

We now declare that the Hamiltonian $H$ is as good a starting point as [3]–[3] provided $(b_i^\dagger b_i) \ll 1$. We therefore proceed to apply a Feynman variational procedure to the exact $H$, Eq. (12), after a unitary transformation, and attempt to extract the pairing mechanism. The dominant term for this mechanism is the term with $V_x$ which, as in the phonon-induced superconductivity, produces Cooper pairing in second order perturbation theory [1]. However, for the field strengths which we will consider, the term with $V_x$ is also negligible and it will alter pairing in one significant respect: since it modifies the 2-level splitting when a charge carrier occupies the site coupled to the considered 2-level system, it will either increase the pairing interaction (for reduced splitting, i.e., negative $V_x$) or decrease pairing (for enhanced splitting, i.e., positive $V_x$) — an observation which may be derived straightforwardly from a mean field decoupling. For the physical system that we consider, $E_{2p}$ and $V_{sp}$ always have the same sign, and consequently $V_z$ is positive [20]. All of the above considerations can also be derived in terms of states where charges in $L1$ are localized in states of definite position with respect to the interface, as depicted schematically in Fig. 1. In this representation, the $V_z$ interaction may be shown to correspond to the repulsion of the electron in layer $L2$ and the field-induced dipole in $L1$.

In order to incorporate this effect we will include below the thermal average $V_z \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} b_i^\dagger b_i = V_z n \sum_i b_i^\dagger b_i$ explicitly in the energy of the two-level system before handling the bosonic degrees of freedom. This is achieved by rewriting the fourth term of Eq. (12)

$$V_z \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} b_i^\dagger b_i = -NV_z n b_i + V_z n \sum_i b_i^\dagger b_i + V_z n \sum_i c_{i,\sigma}^\dagger c_{i,\sigma}$$

$$+ V_z \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} - n/2 \right] [b_i^\dagger b_i - n_b]$$

where $n_b = \langle b_i^\dagger b_i \rangle$ is the number of bosons (the relative number of inverted 2-level systems per site), $n = (1/N) \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma}$ is the charge carrier density in layer $L2$, and $N$ is the number of sites in $L2$. The second term on the right hand side accounts for a density-dependent renormalization of the two-level splitting:

$$E_{2l}^* = E_{2l} + n V_z$$

In a first step we apply a Lang-Firsov (LF) transformation of the Hamiltonian $H$ in order to identify the pairing interaction, and in a second step we control the decoupling of the interaction terms through Feynman’s variational principle which also fixes the parameters of the LF transformation.

The LF transformation of the Hamiltonian $\tilde{H} = U^\dagger H U$ is achieved by the following unitary operator $U$:

$$U = \exp \left[ -S_1(\theta) \right] \exp \left[ -S_2(\gamma) \right]$$

with

$$S_1(\theta) = -\frac{1}{2V_x} \theta \sum_i (b_i^\dagger - b_i)$$

$$S_2(\gamma) = \frac{V_z}{E_{2l}} \gamma \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} (b_i^\dagger - b_i)$$

The parameters $\theta$ and $\gamma$ will be fixed through the variation of the free energy. The standard form of the LF transformation for the Holstein model takes $\theta = 0$ and $\gamma = 1$. With a “zero-phonon” approximation the (phononic) Holstein model accounts for exact results in the adiabatic limit $E_{2l}/t \gg 1$. The variation of the parameters $\theta$ and $\gamma$ has been devised in order to reproduce the adiabatic limit of the Holstein model as well [21, 22, 23, 24]; the static case is realized with $\gamma \rightarrow 0$ and with a finite $\theta$ which signifies a displacement field. For the Holstein model, a second canonical transformation of Bogoliubov type $U_B = \exp \left[ -\alpha \sum_i (b_i^\dagger b_i + b_i b_i^\dagger) \right]$ is sometimes applied to allow for the anharmonicity of the lattice fluctuations. For our model, we have to suppress states with two bosons (corresponding to our initial constraint for the 2-level system), and subsequent variation of the free energy shows that in fact $\alpha = 0$. Also the “static displacement” should be suppressed since we do not intend to consider a finite static polarization. We verified from the minimization that indeed $\theta \simeq 0$ for the considered range of small to intermediate $V_{sp}/4t$. For
this reason, and to simplify the notation, we fix θ and α to zero.

With the LF transformation $U = \exp [-S_2(\gamma)]$ we obtain

$$
\tilde{H} = E_0 + H_{LF} + H_{Vz} + H_{Vs} + H_{Vs'}
$$  \hspace{1cm} (19)

where $E_0 = -\frac{1}{2}NE_{2l} - NV_zn_nb$, and

$$
H_{LF} = -t \sum_{<ij>,\sigma} c_i^{\dagger}c_j e^{\pm 2d\gamma}\sigma_{ij} (b_i^{\dagger}b_j - b_i^{\dagger}b_j) - V_{\text{eff}} \sum_i c_i^{\dagger}c_i c_i^{\dagger}c_i - \mu_{\text{LF}} \sum_{i,\sigma} c_i^{\dagger}c_i - E_{2l}^* \sum_i b_i^{\dagger}b_i
$$  \hspace{1cm} (20)

with

$$
H_{Vs} = (1 - \gamma) V_z \sum_{i,\sigma} c_i^{\dagger}c_i (b_i^{\dagger} + b_i)
$$  \hspace{1cm} (21)

$$
H_{Vs'} = V_z \sum_{i,\sigma} (c_i^{\dagger}c_i c_i^{\dagger}c_i - n/2) (b_i^{\dagger}b_i - n_b)
$$  \hspace{1cm} (22)

$$
H_{Vs} V_{Vs'} = -\gamma V_z V_{2l}^* \sum_{i,\sigma,\sigma'} (b_i^{\dagger}c_i^{\dagger}c_i^{\dagger}c_i^{\dagger}c_i^{\dagger}c_i^{\dagger} - b_i^{\dagger}b_i)
$$  \hspace{1cm} (23)

where the effective chemical potential is given by

$$
\mu_{\text{LF}} = \mu + V_z / 2 + \gamma(2 - \gamma) \frac{V_z^2}{E_{2l}^*} - (1 - n) V_z \left( \gamma \frac{V_z}{E_{2l}^*} \right)^2 - V_z n_b
$$  \hspace{1cm} (24)

The induced electronic interaction $V_{\text{eff}}$ is now

$$
V_{\text{eff}} = 2 \frac{V_z^2}{E_{2l}^*} \gamma \left[ (2 - \gamma) - \gamma (3 - n) \frac{V_z}{E_{2l}^*} \right] - U,
$$  \hspace{1cm} (25)

where we note that the Hubbard term $H_{c-c}$ has been unaffected by the above transformations of the electron-two level system coupling terms, due to the fact that it is simply a product of local densities. The local repulsion therefore merely diminishes the effective attraction by $U$.

If $\gamma = 1$, the first term within brackets in Eq. (25) coincides with the well-known result from the exact mapping of the Holstein model to the attractive Hubbard model in the high-frequency limit ($E_{2l}^* \rightarrow \infty$). The second term in the brackets $\propto V_z$ is always repulsive and suppresses $T_c$ for increasing field. The electric field dependence enters through $V_z, V_{2l}^*, E_{2l}^*$ and the implicit dependence of $\gamma$ on $E_{sp}$.

We have now achieved the desired result of expressing the Hamiltonian in terms of an effective BCS-like interaction between electrons, at the cost of introducing bosonic phase factors into the hopping matrix elements.

We begin by setting $U = 0$ and investigate the magnitude of the attractive interaction obtainable by polarizing the two level systems. In Fig. 2 we illustrate how $V_{\text{eff}}$ depends on applied electric field. The main point is physically obvious: if the electric field is sufficiently large, it polarizes the electric dipoles in $L1$ and suppresses the Little-type mechanism. We also note that if the bare excitation energy $\Delta_{sp}$ of the dipoles in the insulating layer is small, the intrinsically low-field pairing strength can be quite large, up to several electron volts. However $\Delta_{sp}$ should not be set to considerably smaller values than in Fig. 2 in order to guarantee the condition that the occupation of the excited state is negligible.

In the second step we introduce an exactly solvable test Hamiltonian $H_{\text{test}}$ and determine the fields in $H_{\text{test}}$ through a Bogoliubov inequality for the free energy $F$ of the model system [25]:

\begin{equation}
F \leq F_{\text{test}} + \langle \tilde{H} - H_{\text{test}} \rangle_{\text{test}}
\end{equation}

where $\langle \cdot \rangle_{\text{test}}$ signifies the thermodynamic average with the test Hamiltonian. We already anticipate the result of this variational scheme [26] and write

$$
H_{\text{test}} = E_{0,\text{test}} - t_{\text{eff}} \sum_{<ij>,\sigma} c_i^{\dagger}c_j + \mu_{\text{LF}} \sum_i c_i^{\dagger}c_i - \Delta \sum_i (c_i^{\dagger}c_i^{\dagger}c_i^{\dagger}c_i^{\dagger} + h.c.) + E_{2l}^* \sum_i b_i^{\dagger}b_i
$$  \hspace{1cm} (27)
with

\[ E_{0,\text{test}} = E_0 - \frac{N}{4} n^2 V_{\text{eff}} \]  

\[ t_{\text{eff}} = t \exp \left[ -\left( \frac{V_x}{E_{2l}} \gamma \right)^2 \coth \left( \frac{\beta E_{2l}}{2} \right) \right] \]

We have assumed s-wave pairing for simplicity. The associated gap equation then reads

\[ \Delta = V_{\text{eff}} \sum_k \frac{\Delta}{2E_k} \tanh \frac{E_k}{2T} \]  

and the Bogoliubov quasiparticle dispersion

\[ E_k = \sqrt{\xi_k^2 + \Delta^2} \]  

\[ \xi_k = \varepsilon_k - \mu_{\text{LF}} \]  

\[ \varepsilon_k = -2t_{\text{eff}} (\cos k_x + \cos k_y) \]

To understand qualitatively the physics of the correlations induced by interaction of the metallic layer with the 2-level systems in L1, we display in the left panel of Fig. 3 the magnitude of the renormalized hopping \( t_{\text{eff}} \). The band narrowing can be rather significant for small excitation energies \( \Delta_{sp} \) but for the parameters of greatest interest will turn out to be only a factor of 1–5.

The fields still depend on the parameter \( \gamma \); correspondingly the rhs of relation Eq. (20) has to be minimized with respect to \( \gamma \). For this purpose we need the explicit form of \( F_{\text{test}} \):

\[ F_{\text{test}} = E_{0,\text{test}} + \frac{1}{\beta} N \ln \left( 1 - e^{-\beta E_{2l}} \right) + F_{\text{BCS}} \]

with

\[ F_{\text{BCS}} = -\frac{2}{\beta} \sum_k \ln \left( 1 + e^{-\beta E_k} \right) \]

\[ -\sum_k \left( E_k - \xi_k + \Delta \langle c_{k,\uparrow}^\dagger c_{k,\downarrow} \rangle \right) \]

Since we have chosen \( E_{0,\text{test}} \) so as to guarantee the relation \( \langle \hat{H} - H_{\text{test}} \rangle_{\text{test}} = 0 \), the variation reduces to finding the optimal value of \( \gamma \) from the minimization of \( F_{\text{test}} \):

\[ \gamma = \frac{n(n + 2)}{n(n + 2) + n(n + 1)(2 - n)(V_x/E_{2l})^2 + \delta(\gamma)} \]  

where

\[ \delta(\gamma) = 2 \frac{\xi}{E_{2l}^2} \coth \left( \frac{\beta E_{2l}}{2} \right) \]

and

\[ \xi = \sum_k \frac{\varepsilon_k}{1 + e^{\beta \varepsilon_k}} \]

For the range of parameters considered in our evaluation the function \( \delta(\gamma) \) can be neglected with respect to the other terms in the denominator of Eq. (34). This allows us to calculate \( \gamma \) algebraically from Eq. (34). The validity of this approximation has been proved by iterating the implicit Eq. (34). Fig. 2 (right panel) displays the decrease of \( \gamma \) with increasing \( E_{sp} \) for various values of \( \Delta_{sp} \) at fixed \( V_{sp}/4t \).

Finally the assumption below Eq. (11) that the bosonic occupation number \( n_b \) is very small is in fact justified a posteriori for temperatures up to the transition temperature \( T_c \). In the considered parameter range of the two-level splitting \( \Delta_{sp} \) and of the applied gate field \( E_{sp} \), \( n_b \) is always smaller than \( 10^{-5} \). Typical field dependences of \( n_b \) are displayed in the right panel of Fig. 3.

FIG. 4: The derivative of the chemical potential with respect to particle density, \( \partial \mu/\partial n \), versus particle density \( n \) at the respective \( T_c \), calculated in Sec. II. All parameters are identical to those of Fig. 2. For a positive derivative, the normal and superconducting states are globally stable in the vicinity of the transition.

The effective model does not implement the long-range part of the Coulomb interaction. A model with purely local interactions, however, has a tendency towards phase...
In order to investigate if the transition from the normal to the superconducting state is a transition between global minima of the free energy, we evaluated the derivative of the chemical potential with respect to carrier density. In this work, we focus on the transition into the superconducting state and not on the evolution of the superconducting state at lower temperatures. Then it is sufficient to discuss the stability in the vicinity of $T_c$. Fig. 4 illustrates our conclusion that the derivative of the chemical potential with respect to particle density is always positive for $\Delta_{sp}/4t$ larger than approximately 1.4. Correspondingly, the transition into the superconducting state is not preempted by a competing transition into a phase separated state. At somewhat lower values of $\Delta_{sp}/4t$, the phase separation will probably be suppressed by the non-local part of the Coulomb interaction. As discussed in the following section, the relevant values of $\Delta_{sp}/4t$ for a sufficiently strong interface-mediated pairing appear in the regime where $\partial\mu/\partial n$ is positive.

II. RESULTS

In order to present the numerical results in the physically relevant range of control parameters, we have to relate microscopic quantities to laboratory parameters, such as the dielectric constant $\epsilon$ of the insulating layer, the dipole length $d_{sp}$ of the two-level systems, and the distance $r$ from the two-level systems to the sites of the conducting layer. Furthermore we have to establish a relation between the electric field energy $E_{sp}$ (see Eq. (1)) and the number of charge carriers in $L_2$. In our calculation we assume that the charge carrier density is a linear function of the electric field with a field independent capacitance $C$ of the dielectric $L_1$: $Q = CV$, where $V$ is the voltage drop across the dielectric and $Q$ is the total, accumulated charge at the interface in $L_2$. Then, the charge per square unit cell is

$$n = C \frac{E d}{e} \frac{a^2}{A}$$

(37)

where $a$ is the lattice constant, $A$ is the area of $L_2$ and $d$ its thickness (cf. Fig. 1). With $C = \epsilon_o \epsilon A/d$ and Eq. (1) we establish

$$n = c \frac{E_{sp}}{4t}$$

(38)

with

$$c = \epsilon_o \epsilon \frac{a^2}{e^2} \frac{4t}{d_{sp}}$$

(39)

The interaction energy between the dipoles next to the interface and the electric field of a charge carrier on the nearest site is

$$V_{sp} = \frac{1}{4\pi \epsilon_0} \frac{e^2 d_{sp}}{r^2}$$

(40)

We note that dynamical screening of the interaction $V_{sp}$ should be included in order to get more precise estimates. Although this will reduce somewhat the high values of $T_c$ in our evaluation, it will not alter the qualitative behavior of the $T_c$-dependence on the gate field (see below).

Finally, the excitation energy of the dipoles has to be identified. A generic dielectric is not composed of a single species of well-defined 2-level systems. Dipole excitations at various energies are always present. We now address excitations in three different energy ranges: for 10 eV (low atomic excitations with dipole length $d_{sp} \approx 1$ Å), in the 1 eV range (charge transfer excitations with $d_{sp} \approx 2$ Å), and in the meV range (ionic displacement in atomic clusters with $d_{sp} \approx 0.1$ Å).

A. Ionic displacement

In dielectrics a displacement of ions, well localized at atomic positions, usually accounts for the high dielectric constant. Such displacements in atomic clusters typically correspond to a dipole length of the order of $d_{sp} \approx 0.1$ Å and a small excitation energy. In this case, the excitation energy is related to $\epsilon$ and $d_{sp}$ through $\Delta_{sp} = 8\pi e^2 d_{sp}^2/(a^3 (\epsilon - 1))$. This relation follows directly from the polarization density $\langle P \rangle$ of the dielectric (with a cubic unit cell of volume $a^3$) in linear response: $\langle P \rangle = ed_{sp} \langle \delta_i p_i + p_i^t \delta_i^t \rangle/a^3 = (2e^2 d_{sp}^2/a^3 \Delta_{sp}) E$ where $\langle P \rangle = (\epsilon - 1)/4\pi \epsilon E$ holds. Ionic displacements may have energies of the order of 10 meV (for $\epsilon$ of the order of 20). However, the induced pair interaction is far too small (see Fig. 4) to find sizable transition temperatures. It is the repulsive term in $V_{eff}/4t$ of Eq. (25) which very effectively impedes a transition to the superconducting state for such small values of $\Delta_{sp}$.

B. Charge transfer excitations

In order to realize a sizable $T_c$ of the order of 100 K, excitations at intermediate energy and sufficiently large dipole length have to be available for polarization. Charge transfer excitations in the dielectrics are found at these energies — e.g. for the transition metal (TM) oxides at energies of the order of 1 eV, the charge transfer gap. Although these excitations of, for example, a TM-oxygen plaquette or octahedron become delocalized through hybridization, we assume that most states near the interface have been localized by disorder and local strain [27]. Furthermore localized bound states below the charge transfer gap are conceivable. It is not the focus of our present investigation to identify these local excitations for a specific material. We rather point out that such processes are possible and then evaluate $T_c$ as a function of their respective energy.

We intend to focus in this latter type of localized charge transfer excitations. For the evaluation we now
fix the following parameters: the bandwidth, the dipole length, and the lattice constant:

\[
\begin{align*}
4t &= 400 \text{ meV} \\
\delta_{sp} &= 2 \text{ Å} \\
a &= 4 \text{ Å}
\end{align*}
\]  

(41)

Here, we chose a bandwidth and lattice constant typical of the high-\(T_c\) cuprates and many other oxides, and we take a dipole length which corresponds to the interatomic oxygen-TM distance. For excitation energies \(\Delta_{sp}\) of more than 0.2 eV, the primary polarization processes are electronic in nature.

In Fig. 5 the transition temperature to the superconducting state is displayed as a function of the excitation energy. In the range of small, increasing values of \(\Delta_{sp}\), we observe a strong enhancement of \(T_c\), whereas the transition temperature decreases with excitation energies \(\Delta_{sp}/4t\) above \(\approx 2.5\). The latter observation is expected since the pairing interaction \(V_{\text{eff}}\) is inversely proportional to the excitation energy for large \(\Delta_{sp}\). For small \(\Delta_{sp}\), the repulsive term (second term in \(V_{\text{eff}}\), cf. Eq. (25)) dominates and suppresses the transition to the superconducting state for a finite value of \(\Delta_{sp}\). Note that the finite longitudinal pseudospin-charge \(V_z\) is decisive for the decay of \(T_c\) at small excitation energies, outside the regime where the Holstein model is appropriate.

For small increasing electric field, the transition temperature is raised due to the accumulation of charge in the metallic layer (cf. Fig. 7). The electric field strength is directly related to the band filling or induced areal charge density. Strong electric fields with sizable band filling lower the transition temperature as the repulsive term in \(V_{\text{eff}}\) is enhanced and, moreover, the effective level splitting is enlarged. In fact, as seen from the \(\Delta_{sp}/4t = 1.25\) curve in Fig. 7, there are two scales for the suppression of \(T_c\) at higher fields. The lower scale is set by the repulsive term in \(V_{\text{eff}}\) and is also responsible for the observed decay of \(T_c\) in the two further curves (with \(\Delta_{sp}/4t = 2.5 \text{ and } 3.75\)). In this regime, \(T_c\) is being suppressed primarily by the increasing repulsion \(V_z\) between the polarized dipoles and the 2D electrons, which scales with the applied field.
The larger scale, which is responsible for the slow decay at even higher fields, is set by $\Delta_{sp}/4t$, and corresponds to the eventual saturation of the dipole moment of the 2-level systems.

The nonmonotonic dependence on filling or electric field is reflected in the varying height of the three different curves in Fig. 6. However more striking is the small variation of the position of the maxima in Fig. 6 with filling (from 0.01 to 0.5). A value of $\Delta_{sp} \approx 1$ eV seems to be optimal for a bandwidth of $4t = 400$ meV. This optimal excitation energy in units of the band width is approximately

$$\Delta_{sp}^{opt}/4t \approx 2.5$$ (42)

$\Delta_{sp}^{opt}$ is weakly dependent on the parameters $V_{sp}$, $d_{sp}$ and $\epsilon$ which mostly influence the maximum value of $T_c$. For fixed charge density, dielectrics with larger $\epsilon$ display a higher transition temperature (for given $\Delta_{sp}$), see Fig. 5 as the electric field necessary to create the charge density is smaller, accounting for a larger $V_{eff}$.

An increasing dipole charge-carrier interaction $V_{sp}$ is not only responsible for an enhancement of $T_c$ but, for sufficiently large $V_{sp}$, also for a “retarded” initial increase of $T_c$ with electric field (see Fig. 9). Again, this observation may be traced back to the field and interaction dependence of the repulsive term in $V_{eff}$.

For direct comparison with experimental devices, we note that the gate voltage is related to the electric field energy plotted in the figures through $E_{sp}/4t = ed_{sp}V/d$ where $d$ is the thickness of the dielectric gate. As a concrete example for a dielectric gate layer, we take SrTiO$_3$. Breakdown fields of $4 \times 10^7$ V/m are reported for this material with a low-$T$ dielectric function of order 100 [28].

The maximum of the $T_c$ versus electric field energy curves occurs for $n = 0.2$ at about $2 \times 10^8$ V/m. Thus the required fields for the maximum $T_c$ are only about 5 times higher than those already realized in this system. Given that breakdown occurs due to “pinhole”-type defects in the films, it seems to us that the manufacture of samples with the required breakdown fields is challenging but far from impossible.

We conclude this subsection with a brief discussion of the consequences that a nonzero local interaction $U$ within the charge-carrier layer L2 has on the reduction of $T_c$ in a weak-coupling evaluation. As shown in Eq. (25), such a repulsive Hubbard-type interaction does not modify the field dependence of the effective interaction $V_{eff}$, but just adds a constant $-U$. For weak interaction $U/4t \lesssim 1$, the effective attraction $V_{eff}$ is reduced but not fully suppressed for small to intermediate fields (cf. Fig. 2) and corresponding filling. This observation is reflected in the field and filling dependence of $T_c$ (see Fig. 10): $T_c$ is reduced for small to intermediate fields and suppressed for strong field-induced doping. As a consequence of the field-dependent reduction of $T_c$, the maxima are shifted towards lower values of filling, from about $n = 0.2$ at $U = 0$ to $n = 0.1$ at $U/4t = 1$. The required fields for the maximum $T_c$ are reduced similarly.

C. Atomic excitations

At high energies, we encounter atomic excitations, such as the $2p$ to $3s$ transition of O$^{2-}$ states in the metal oxides. These states are treated in exactly the same way in the current theory, but are characterized by small dipole
FIG. 10: Charge transfer excitations: transition temperature $T_c/4t$ versus electric field energy $E_{sp}/4t$ and band filling $n$, lower axis and upper axis, respectively. A local electronic interaction $U$ (within layer 1.2) is included in a weak coupling evaluation. The dielectric constant $\varepsilon$ is 100 and $V_{sp}/4t = 1.89$ ($r/a = 1.5$).

FIG. 11: Atomic excitations ($d_{sp} = 1$ Å, $\Delta_{sp} = 10$ eV, $\epsilon = 100$): transition temperature $T_c/4t$ versus electric field energy $E_{sp}/4t$, parameterized by $r/a$: $V_{sp}/4t = 2.125$ (corresponds to $r/a = 1$), $V_{sp}/4t = 1.36$ ($r/a = 1.25$), $V_{sp}/4t = 0.94$ ($r/a = 1.5$).

lengths $d_{sp} \sim 1$ Å and large 2-level splittings $\Delta_{sp} \sim 10$ eV. Polarizing such dipoles is difficult and $T_c$'s are correspondingly small. Comparison of Fig. 10 for parameters consistent with atomic polarizations with Fig. 9 for charge transfer excitations makes the distinction of the two scenarios evident. In the atomic case, $T_c$ is so small that an observable effect may be found only for the smallest value of $r/a$. Moreover, the excitation energy is so high that a decrease of $T_c$ is not seen, even for the largest electric fields. Of course, when band filling is above half filling, the transition temperature will decrease with increasing field. However these field strengths are beyond electrical breakdown.

III. CONCLUSIONS

We have proposed that the field-induced 2DEG in a field effect device may become superconducting entirely due to pair interactions with a proximate insulating layer with high polarizability. In the general case, properties of a DS-channel embedded in an oxide field effect transistor will then be controlled not only by the electronic and structural properties of the DS-channel, as is usually assumed, but can furthermore be strongly influenced by the gate insulator or by other adjacent dielectric layers. The choice of the gate dielectric layer may then influence the device behavior of a field effect transistor far beyond controlling the maximum gate polarization and gate current.

For a concrete model of electrons in a 2D layer interacting with 2-level systems at the interface with the insulator, we calculated the superconducting critical temperature, which displays as a function of applied field a steep initial rise and subsequent decay. The rise is caused by the increasing density of charge carriers swept to the interface by the electric field and the decay is due to the interaction of the field-induced dipoles with the charge carriers. The optimal values of the field or gate voltage, as well as sample dimensions and dielectric properties, were discussed in some detail within the framework of this model.

The goal of these model calculations was to establish the plausibility of superconductivity in field-effect devices enhanced or induced by the presence of a polarizable interface, and to investigate the magnitude of the critical temperature and likely dependence on external field and materials properties. We recognize, however, that several potentially important aspects of the physics are not present in the model used. These include long-range Coulomb interactions, dynamics of the dielectric screening, and correlations in the 2DEG. We anticipate that the effects of long-range Coulomb interactions are less important in the present case than in 3D metallic superconductors due to the larger dielectric constants in the insulating material, but this must clearly be justified by a legitimate calculation of the true Coulomb pseudopotential entering the MacMillan formula. Screening of the bare electron-dipole interaction $V_{sp}$ must also be included; we expect, however, that the form of the dependence of $T_c$ on the electric field will not change significantly (see Fig. D). The inclusion of a repulsive local interaction $U$ does not qualitatively change this form either. However it reduces $T_c$ (by a factor of 2 for $U/4t = 0.8$) and it shifts the optimal value of the field-induced doping to lower levels (cf.
If the effective on-site Coulomb repulsion in the drain-source layer is much larger than we have considered, s-wave superconductivity will be completely suppressed. It is still tempting, however, to regard the starting Hamiltonian (3)–(7) as the hopping of correlated electrons (as in the $t-J$ model) where Coulomb interactions have already been accounted for. In this case, however, one must implicitly assume that doubly occupied sites have been already been accounted for. In this case, however, one must implicitly assume that doubly occupied sites have been projected out, so that non-retarded s-wave superconductivity is impossible. Modelling superconductivity within this framework in higher-angular momentum pair channels will require including interactions among the two-level systems at the interface, so as to produce a nonlocal pair potential. While we have not calculated these effects explicitly, as they are technically significantly more difficult, our expectation is that the creation and eventual suppression of the paired state by the electric field will be qualitatively similar to what we have calculated. This expectation is supported by the observation that an enhanced carrier density. Moreover, the buildup of a field-dependent repulsive interaction $V_Z$ has to take place due to the eventual saturation of the dipole moments with electric field, even when the two-level systems interact. Investigations along these lines are in progress.

In addition, our considerations can in principle be applied to other, more weakly correlated systems than the copper oxides. Our model may be used to treat situations in which the DS-channel contains an attractive s-wave interaction besides the interface-mediated pairing. In this case we expect a qualitatively similar behavior with a nonmonotonic $T_c$.

According to our calculations, devices with thickness of the insulating layer of order 1000 Å subjected to voltages of order $\sim 20$V could display superconductivity, if an optimal material can be found with a sufficiently large low frequency dielectric constant of order 30-100 and strong quasilocalized electronic modes of energy $\Delta_{sp}/4t \sim 2.5$ [29]. With a 20 V gate field and a typical 18 nF capacitance of a 0.03 cm$^2$ gate dielectric (1000 Å), this would correspond to a surface charge density of roughly $12 \mu C/cm^2$. It is now routine to fabricate epitaxial high $\text{c}$ oxide dielectries, such as SrTiO$_3$ with polarizations in the range of 10-40 $\mu C/cm^2$. Interface-mediated 2D superconductivity therefore seems to us to be plausibly within reach if good interfaces can be manufactured.

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In fact, the virtual exchange of delocalized excitons has been investigated in the previous literature, for example in Refs. [1, 3]. The delocalization is not adverse to the formation of the superconducting state.

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We note that the mechanism we discuss here may also be effective in optimized semiconducting field effect heterostructures, provided the charge carrier density \( n \) in the interfacial layer can be made of the order of 0.1.