Fluctuations superconductivity and giant negative magnetoresistance in a gate voltage tuned 2D electron liquid with strong spin-orbit impurity scattering

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We present a quantitative theory of the gate-voltage tuned superconductor-to-insulator transition (SIT) observed experimentally in the 2D electron liquid created in the (111) interface between crystalline SrTiO$_3$ and LaAlO$_3$. Considering two fundamental opposing effects of Cooper-pair fluctuations: the critical conductivity enhancement, known as para-conductivity, and its suppression associated with the loss of unpaired electrons due to Cooper-pairs formation, we employ the standard thermal fluctuations theory, modified to include quantum fluctuations within a novel phenomenological approach. Relying on the quantitative agreement found between our theory and a large body of experimental sheet-resistance data, we conclude that spin-orbit scatterings, via significant enhancement of the interaction between fluctuations, strongly enhance the sheet resistance peak at high fields, and reveal anomalous metallic behavior at low fields, due to mixing of relatively heavy electron bands with a light electron band near a Lifshitz point.

Recently, it has been shown [1] that the two-dimensional (2D) electron liquid formed at the (111) interface between the two insulators: SrTiO$_3$ and LaAlO$_3$, can be smoothly tuned by gate bias from the superconducting (SC) state deep into an insulating state with pronounced magnetoresistance (MR) peaks developed at low temperatures. Similar electrostatically tuned superconductor-to-insulator transition (SIT) was reported for the LaAlO$_3$/SrTiO$_3$ (001) interface [2], showing however [3], [4] no clear indication of MR peaks similar to those reported for the (111) interface. Earlier studies of the (111) interface have found coexistence of magnetism and 2D superconductivity [5], and a correlation between superconductivity and strong spin-orbit interaction [6]. The linear magnetic field dependence observed at low perpendicular fields and its hysteresis, have indicated the importance of flux-flow in the detected resistance. These effects persisted deep into the insulating state, revealing the importance of Cooper-pair fluctuations even when superconductivity is completely suppressed. The large smearing of the SC resistive transitions observed under parallel fields may also reflect strong SC fluctuations effect. The transition temperature, $T_c$, and the critical fields, $H_{\text{c,\parallel}}, H_{\text{c,\perp}}$ for both parallel and perpendicular fields, respectively, were found [6] to follow non-monotonic (dome-shaped) gate-voltage dependence of the spin-orbit interaction.

The phenomenon of SIT has been investigated for many years, notably in thin films of materials like bismuth [7], InO [8], MoGe [9], TiN [10], and cuprate superconductors [11]. Many intriguing phenomena have been associated with the observation of SIT. Noteworthy examples are: scaling behavior near a quantum critical point [11, 12, 13], large MR peaks [14, 15, 16] and thermally activated insulating behavior [17, 18, 19]. However, some of these effects have not been observed in all materials that exhibit a SIT, making the interpretation of the various SIT phenomena controversial, with no consensus as to their mechanism and expected behavior.

Here we present a scenario of SIT in a 2D electron system, based on the opposing effects generated by fluctuations in the SC order parameter: On the one hand, the singular enhancement of conductivity due to fluctuating Cooper pairs in approaching the critical magnetic field (paraconductivity), and on the other hand, the suppression of conductivity associated with the loss of unpaired electrons resulting from Cooper pairs formation. Specializing this scenario to the LaAlO$_3$/SrTiO$_3$ (111) interface, the strongly enhanced fluctuations effect is due to the remarkable combination of marginal superconductivity driven by spin-orbit scattering versus the pair-breaking of Zeeman spin-splitting effect embodied in a 2D electron system. Focusing on the parallel field orientation case enables us to investigate the essence of our model of SIT without interference from the complex vortex kinematics and flux lines pinning processes involved in the perpendicular field case. Furthermore, the striking observations of giant negative MR in both the (111) and the (001) LaAlO$_3$/SrTiO$_3$ interfaces, driven by spin-orbit coupling under parallel field, at temperatures above the SC transition [10, 17], are of special interest here: It has been associated [17] with spin-orbit induced band mixing between orbitals of different symmetries near a Lifshitz point in the d-electron interface band structure [18].

We test the validity of the above mentioned SIT scenario by performing calculations based on an effective mixed-bands DOS model, and comparing the results with the large body of experimental magnetic sheet resistance (MSR) data presented in Ref.[1]. The calculations were done within an extended version of the Fulde-Maki Aslamazov-Larkin theory of fluctuations in paramagnetically-limited superconductors [19, 20, 21], in which the time-dependent-Ginzburg-Landau (TDGL) equation describing free (Gaussian) fluctuations is modified by taking into account interactions between free fluctuations, self-consistently in the Hartree approx-
imation [22]. Very good quantitative agreement between theory and experiment has been achieved, confirming our SIT scenario. Dynamical quantum tunneling of Cooper-pair fluctuations through GL energy barriers is taken into account, on equal footing with thermal activation, within a phenomenological approach, preserving the level of agreement with the experiment in the low temperatures region. Our calculations also reveal how a Lifshitz transition in the d-electron interface band structure [23], [25] can drive large enhancements of the MSR peak observed at the end of the SIT path [1] upon gate-voltage variation. This feature is exploited to construct the mixed-band DOS function around the Lifshitz-point from the gate-voltage dependence MSR data.

We consider a planar, 2D SC electron system subject to strong spin-orbit impurity scattering [24], [25], with a characteristic relaxation time $\tau_{SO} = \hbar/\varepsilon_{SO}$, under a strong magnetic field $H$, applied parallel to the plane. Superconductivity in this system is governed both by the Zeeman spin splitting energy $\mu_B H$ and the spin-orbit scattering rate, $1/\tau_{SO}$ (see a detailed description in Supplemental Material [26] and in early papers dealing with similar 3D systems [27], [19], [28]). The underlying spin-orbit induced band mixing, which was evaluated microscopically for the (001) interface by several authors [18], [29], [17], [30], is taken into account here phenomenologically within a minimal model of 2D DOS function $N_{2D}(E)$ (see Fig.1). Consistently with this, we use in our transport calculations a 2D electron gas, in the dirty limit, confined within a thin rectangular film of thickness $d$. In deriving the corresponding self-consistent field (SCF) equation (see SM [26]), a key quantity is the Cooper-pair fluctuation propagator: $D(q; \varepsilon_H) = 1/N_{2D}(E_F) \Phi(x; \varepsilon_H)$, obtained from the well-known function of the dimensionless fluctuation kinetic energy variable $x = hDq^2/4\pi k_BT$ [19]:

$$\Phi(x; \varepsilon_H) = \varepsilon_H + a_+ [\psi(1/2 + f_- + x) - \psi(1/2 + f_-)] + a_- [\psi(1/2 + f_+ + x) - \psi(1/2 + f_+)] \quad (1)$$

and the Gaussian critical shift-parameter:

$$\varepsilon_H \equiv \ln \left( \frac{T}{T_c} \right) + a_+ \psi \left( \frac{1}{2} + f_- \right) + a_- \psi \left( \frac{1}{2} + f_+ \right) - \psi(1/2) \quad (2)$$

Here $T_c$ is the mean-field SC transition temperature at zero magnetic field, $\psi$ is the digamma function, $f_\pm = \delta H^2 + \beta \pm \sqrt{\beta^2 - \mu^2 H^2}$, $a_\pm = \left( 1 \pm \beta / \sqrt{\beta^2 - \mu^2 H^2} \right)/2$ are functions of the magnetic field $H$, with the basic parameters: $\beta \equiv \varepsilon_{SO}/4\pi k_BT$, $\mu \equiv \mu_B/2\pi k_BT$, $\delta \equiv D (de)^2/2\pi k_B T h$, where $\mu_B = e\hbar/2m_e$ is the Bohr magneton, $D \equiv \hbar E_F/m^* \varepsilon_{SO}$ the electron diffusion coefficient, $E_F$ the Fermi energy and $m^*$ is the band effective mass.

The values of the fluctuation wavenumber $q$ are bound by a cutoff $q_c$, which typically satisfies: $x_c \equiv hDq_c^2/4\pi k_BT < 1$, so that one may exploit the linear approximation: $\Phi(x; \varepsilon_H) \approx \varepsilon_H + \eta(H) x$. The Gaussian critical shift parameter $\varepsilon_H$ (Eq.2) should be corrected, due to interaction between fluctuations [21]. The correction can be evaluated analytically from the cubic term of the GL equation discussed above, and is given by (see SM [26]): $\alpha F(H) \eta(H) \int_0^{\eta(x)} dx / \Phi(x; \varepsilon_H)$, where:

$$\alpha \equiv 1/\hbar \pi^3 D N_{2D}(E_F) \quad (3)$$

The Hartree SCF approximation amounts to replacing $\varepsilon_H$, appearing in the the interaction correction, with the "dressed" critical shift-parameter $\tilde{\varepsilon}_H$, leading to the SCF equation:

$$\tilde{\varepsilon}_H \approx \varepsilon_H + \alpha F(H) \ln \left( 1 + \frac{\eta(H) x_c}{\tilde{\varepsilon}_H} \right) \quad (4)$$

where the logarithmic factor is obtained from the integral over $x$ by using the linear approximation of $\Phi(x; \tilde{\varepsilon}_H)$, and the field distribution function of the interaction $F(H)$, is given by the Matzubara sum [26]:

$$F(H) = \frac{1}{\eta(H)} \sum_{n=0}^{\infty} \frac{x_n \left( x_n^2 + \mu^2 H^2 \right)}{\left[ x_n - 2\beta + \mu^2 H^2 \right]^2} \quad (5)$$

where $x_n = n + 1/2 + 2\beta + \delta H^2$. Equation (4) has no solution with $\tilde{\varepsilon}_H \leq 0$ (see Ref.[31]), indicating the absence of a genuine SC phase transition due to the interaction between fluctuations. Indeed, as shown in Fig.(2), all solutions of the SCF equation [4] satisfy $\tilde{\varepsilon}_H > 0$, implying that the critical divergence of the free fluctuations propagator is strictly removed. This also eliminates the critical divergence from both the Aslamazov-Larkin (AL) and the suppressed normal-state conductivities (see below).

Quantum fluctuations at low temperatures—For temperatures above $T_c$, our calculated MSR accounts quantitatively well for the experimental MSR data reported in [1]. However, in the low temperatures regime well below $T_c$, large deviations between the calculated and measured MSR data were found (see SM [26]), with the
FIG. 2. The field distribution function \((1 + T_Q/T) F_U (H)\), calculated at \(T = 1\) mK for \(T_Q = 0\) and \(T_Q = 80\) mK. Inset: "Bare", \(\varepsilon_H\) (dashed line), and "dressed", \(\varepsilon_H\) (solid line), critical shift parameters, calculated at \(T = 1\) mK and \(T_Q = 80\) mK.

calculated MSR peak quickly narrowing upon decreasing temperature, as compared to the rather broad experimental MSR peak. This discrepancy is due to the fact that, at low temperatures \(\varepsilon_H\), determined by Eq. [4] is not significantly different from \(\varepsilon_H\) in the vicinity of the critical point \(\varepsilon_H = 0\). The reason, as illustrated by Fig. (2), is in the progressive narrowing of \(F (H)\) (Eq. [5]) upon decreasing temperature, having too small tail intensity in the vicinity of the free-fluctuations critical field.

We argue that the observed broadening at very low temperatures is due to quantum fluctuations effect similar to the quantum phase slips reported for SC nanowires [32, 33, 34, 35], a phenomenon which was also reported for ultrathin granular SC film [36, 37]. We invoke a phenomenological approach describing dynamical tunneling of Cooper-pairs through energy barriers, separating SC puddles [38], on equal footing with thermal activation across the same barriers. Thus, we introduce a unified quantum-thermal (QT) fluctuations partition function:

\[ Z_{\text{fluct}}^U = \prod_q \int D\Delta_q D\Delta^*_q e^{-\frac{1}{\hbar} \int \left[ \psi^*_q (x) \partial_q \psi^*_q (x) + \frac{\psi^*_q (x) \psi^*_q (x)}{x} \right] dx^2} |\Delta|^2 N_{2D} (E_F), \]

where \(1/\tau_U\) is the combined QT attempt rate, defined by: \(\hbar/\tau_U = k_B T + \hbar/\tau_Q\), with \(1/\tau_Q = k_B T_Q/\hbar\) the tunneling attempt rate \((\varepsilon_H, \eta_U (H)\) will be defined below). The corresponding Gaussian, unified QT-fluctuations propagator is given by: \(D_U (q; \varepsilon_H, \eta_U (H)\) = \(k_B (T + T_Q)/N_{2D} (E_F) \left( \varepsilon_H + \frac{\hbar Dq^2 \eta_U (H)}{4\pi k_B T} \right) \).

The inherent dynamics of the quantum tunneling of Cooper-pair fluctuations is introduced to the equilibrium Gorkov-GL functional-integral through imaginary time [39]. Consistency requires that the introduction of an excess quantum-tunneling "temperature", \(T_Q\), into the unified QT fluctuation propagator, should be complemented by introduction of a bosonic excitation Matzubara frequency-shift \(\Omega_m/2 = \pi k_B T_Q/\hbar\) into the definitions of the electron-pairing functions \(\varepsilon_U (H), \Omega_U (H)\), under summation over the fermionic Matzubara frequency \(\omega_n = (2n + 1) \pi k_B T/\hbar\). Thus, one evaluates these unified QT functions from the respective thermal functions: \(\tilde{F} (H), \tilde{\varepsilon}_U (H)\), by introducing the shift \(n \rightarrow n + T_Q/2T\) under the summations over \(n\) in Eq. [8] and by shifting the argument of the digamma function and its derivative, respectively, with the same additive constant \(T_Q/2T\) in Eqs. [9] and [10]. The corresponding unified Hartree SCF equation [11] reads:

\[ \varepsilon_U (H) = \varepsilon_U (H) + \alpha F_U (1 + T_Q/T) \ln \left( 1 + 2 \varepsilon_U (H)/\pi k_B T \right). \]

Fluctuation paraconductivity under a parallel magnetic field—In the calculation of the paraconductivity we adopt a modified version of the formalism developed by Fulde and Maki [19] for calculating the AL contribution [21]. Thus, the static AL sheet conductivity, calculated in the unified QT fluctuations approach (see SM [20]) is given by:

\[ \sigma_{AL} = \left( 1 + \frac{T_Q}{T} \right) \frac{1}{4} \left( \frac{G_0}{\pi} \right) \int_0 (\Phi_U (x; \varepsilon_H) )^2 dx \]

where \(G_0 = e^2/\pi \hbar\) is the conductance quantum, and \(\Phi_U (x; \varepsilon_H)\) is obtained from Eq. [11] by replacing \(\varepsilon_H\) with \(\varepsilon_H\), and by shifting the argument of all the digamma functions in Eq. [11] with the additive constant \(T_Q/2T\).

Cooper-pair fluctuations suppressed normal state conductivity—The idea, first exploited by Larkin and Varlamov [40] for the zero field case, is to replace the electron number density \(N_e\) in the simple Drude formula for the conductivity \(\sigma = N_e e^2 T/m^*\), with the number density of electrons occupying quasi-particle states minus the number density \(\Delta N_e\) of electrons paired into SC puddles. Since \(\Delta N_e = 2n_s\), where \(n_s\) is the number density of Cooper pairs in SC puddles, the corresponding correction to the Drude conductivity is given by: \(\delta \sigma_{DOS} = -2(n_s e^2/m^*) \tau_{SO}\). The subscript DOS indicates that this contribution to the conductivity is associated with the suppression of the normal electrons DOS by Cooper-pair fluctuations. The number density, \(n_s = (1/d) \int (|\psi (x)|^2) d^2 q / (2\pi)^2\), is obtained from the superfluid momentum distribution-function \(\langle |\psi (q)|^2 \rangle \approx 2E_F/\pi^2 k_B T \Phi(x; \varepsilon_H)\), so that:

\[ \delta \sigma_{DOS} \approx -4 \left( \frac{G_0}{\pi} \right) \int_0^{\pi} dx / \Phi(x; \varepsilon_H) \]

This result is, to a good approximation, equal to the DOS conductivity obtained in [40] by means of a microscopic (diagrammatic) approach in the dirty limit (see SM [20]). The unified QT fluctuations version of the DOS conductivity can be derived by introducing quantum fluctuations into the superfluid momentum distribution function as follows: \(2E_F/\pi^2 k_B T \Phi(x; \varepsilon_H) \rightarrow 2E_F/\pi^2 k_B (T + T_Q) \Phi_U(x; \varepsilon_H)\), resulting in the following expression:

\[ \delta \sigma_{DOS} \approx -4 \left( \frac{G_0}{\pi} \right) \int_0^{\pi} \frac{dx}{(1 + 2 \varepsilon_H/\pi k_B T)} \Phi_U(x; \varepsilon_H) \]
It is shown in SM (26) that both \( \sigma_{\text{AL}}^U \) and \( \delta \sigma_{\text{DOS}}^U \) have well defined quantum \((T \to 0)\) limit.

Combining all contributions to the sheet conductivity, Eqs. [6]-[7] including the normal-state conductivity \( \sigma_n \), we have:

\[
\sigma^U d = \sigma_n d + \sigma_{\text{AL}}^U d + \delta \sigma_{\text{DOS}}^U d \quad (8)
\]

Determination of the normal-state conductivity, \( \sigma_n \), can reflect on the strong negative MR reported in Ref. [16] for temperatures well above the SC transition. Thus, in our fitting procedure we assume a field-dependent normal state conductivity contribution \( \sigma_n (H,T) \), which produces negative MR similar to that observed in Ref. [16], by employing the quadratic function: \( \sigma_n (H,T) = \sigma_0 + \sigma_0 (H/H_n (T))^2 \), with two adjustable parameters \( \sigma_0, H_n (T) \), where the latter is temperature dependent. Employing an extensive fitting procedure, as described in detail in SM [26], the resulting calculated MSR, best fit to the experimental data sets [1], are shown in Fig. (3). Very good quantitative agreement between the calculated and measured data is seen for the entire data presented. The decreasing magnitudes of the normal-state MR curves, shown in Fig. (3), with increasing temperature are seen to be in qualitative agreement with the experimental negative MR data, presented in Ref. [16] for temperatures well above \( T_c \).

The best fitting carrier density \( n_{2D} (R_N) \) \( \sim 0.5 \times 10^{14} \text{cm}^{-2} \) and band effective mass, \( m^* \simeq 1.6m_e \), are found in good quantitative agreement with the carrier density and cyclotron mass, respectively, extracted from SdH oscillations measurements reported in Ref. [23]. Note that \( n_{2D} (R_N) \) extracted in our fitting is a small fraction of the measured inverse hall coefficient \( e/R_{HI} \equiv n_{2D}^{-1} (R_N) \) reported in Ref. [1] \( \sim 10^{14} \text{cm}^{-2} \). The situation is quite similar to that reported for the (001) LaAlO\(_3\)/SrTiO\(_3\) interface (see 41,42). The large difference between the carrier densities extracted from the two methods was attributed 43,44 to contributions to transport of at least two bands with different mobilities, a band contributing minority carriers with high mobility, dominating the SdH oscillations and superconductivity, and majority-carriers band with low mobility, which dominate the Hall resistance.

The key parameter in our theory is the fluctuations-interaction parameter \( \alpha (R_N) \), which depends on the normal-state sheet resistance parameter \( R_N \) 44, through \( N_{2D} (E_F) \) (see Eq.5). For the values of \( R_N \), presented in Fig.(3), \( \alpha (R_N) \) shows a moderate rise upon increasing \( R_N \) from 7.5kΩ to 10.5kΩ, and a significantly larger ascent upon increasing \( R_N \) from 10.5kΩ to 20.5kΩ (see Fig.1). This has two important consequences seen in Fig.(3) (see SM 25 Sec.VIII); a large enhancement of the MSR peak at high fields, and strong amplification of the quantum tunneling induced resistance at low fields, which characterizes anomalous metallic behavior 45. The corresponding negative normal state MR curves, shown in Fig.(3), are seen to exhibit similar enhancements upon increasing \( R_N \), indicating the sharing roles between Cooper-pair (bosonic) fluctuations and (fermionic) quasi-particles in driving the
system to insulator. The implication with regard to $N_{2D}(E_F)$ is that, since $N_{2D}(E_F) \propto 1/(R_N)$, its relatively large drop upon down-shifting the Fermi level from $E_F (R_N = 10.5k\Omega)$ to $E_F (R_N = 20.5k\Omega)$ reflects electron transfers between bands of considerable effective mass ratio \cite{23} (see Fig.1), which is, however, significantly smaller than that calculated for the (001) interface in Refs.\cite{15,17}.

Discussion:—The main new message of this letter to the current understanding of the various SIT phenomena is in proposing the concept of suppressed DOS by Cooper-pairs formation as a dominant origin of the insulator side of the SIT. The good quantitative agreement found between the calculated MSR and the extensive experimental data \cite{1}, supports this proposal. The presence of disorder-induced spatial inhomogeneity, in the form of SC islands, which has been extensively discussed in the SIT literature \cite{46,47,48,49}, is reflected in our approach by the Fourier transform to real space of the fluctuation propagator in the dirty limit $D(q;\tilde{\xi}_H)$, which reveals the underlying structure of mesoscopic SC puddles, whose average localization length is: $\xi_H = [(4\pi\hbar B T) \eta(H)/\bar{\varepsilon}_H]^{1/2}$ (see SM \cite{20} for details).

The emerging physical picture is as follows: Upon increasing the magnetic field towards the sheet-resistance peak region the 2D SC fluctuations system breaks into mesoscopic puddles of localized Cooper-pair fluctuations, which consume much of the unpaired mobile electrons contributing to the normal state conductivity. The localization arises from opening of an energy gap, $\varepsilon_H$, in the fluctuations spectrum and diminishing their effective stiffness coefficient, $\hbar D\eta(H)$, occurring upon increasing magnetic field. In parallel with this localization process upon increasing field, the AL conductivity decreases more sharply than the absolute value of the DOS conductivity, so that at the point of their crossing one observes the onset of the insulating state.

Dynamical quantum tunneling enhances localization and suppresses the density of SC puddles by enhancing the energy gap $\varepsilon_H$, so that in the low-fields region, where the AL conductivity is dominant, finite resistance is generated (even at zero temperature), leading to anomalous metallic behavior \cite{45}.

Notwithstanding the general nature of the proposed mechanism for SIT, the role played by spin-orbit scattering in this system is found quite unique: It strongly mixes relatively heavy electron bands with a lighter electron band and so sharply suppresses the effective DOS upon down shifting the chemical potential across a Lifshitz point. The latter effect is associated with strong enhancement of interaction between Cooper-pair fluctuations, which at low temperatures, significantly enhances the sheet resistance peak at high fields and strongly amplifies the low resistance in the low fields region \cite{45}.

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