Topological superconductivity and Majorana bound states at the LaAlO$_3$/SrTiO$_3$ interface

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received 27 September 2014; accepted in final form 29 November 2014
published online 22 December 2014

PACS 03.65.Vf – Quantum mechanics: Phases: geometric; dynamic or topological
PACS 74.20.Rp – Superconductivity: Pairing symmetries (other than s-wave)
PACS 74.62.Dh – Effects of crystal defects, doping and substitution

Abstract – The interface between two band insulators LaAlO$_3$ and SrTiO$_3$ exhibits low-temperature superconductivity coexisting with an in-plane ferromagnetic order. We show that topological superconductivity hosting Majorana bound states can be induced at the interface by applying a magnetic field perpendicular to the interface. We find that the dephasing effect of the in-plane magnetization on the topological superconducting state can be overcome by tuning a gate voltage. We analyze the vortex-core excitations showing the zero-energy Majorana bound states and the effect of non-magnetic disorder on them. Finally, we propose an experimental geometry where such topological excitations can be realized.

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Introduction. – Majorana fermion, which often arises as a quasi-particle excitation in condensed-matter systems, is being studied intensively due to its indispensable utility in defect-free topological quantum computation [1]. The Majorana bound state (MBS) naturally exists in spin-triplet chiral p-wave superconductivity in superfluid He$_3$ (A-phase) [2] and Sr$_2$RuO$_4$ [3] and in the fractional quantum Hall state at $5/2$ filling [4]. Also, there have been several proposals of experimentally feasible systems that host MBS such as quantum wire coupled to s-wave superconductor [5], semiconductor-superconductor heterostructure [6,7], proximity-induced superconductor at the surface of topological insulator [8], 2DEG at semiconducting quantum well [9], and the more promising Al-InSb nanowire topological superconductor [10]. Also there is a trend to realize topological orders in fermionic s-wave superfluids of ultracold atoms in optical lattices [11]. However, due to the lack of convincing experimental evidence so far, Majorana fermion still remains as elusive and its search, therefore, should expand onto uncharted routes, new systems and novel experimental designs.

The two-dimensional electron liquid (2DEL) at the LaAlO$_3$/SrTiO$_3$ interface is formed as a result of an intrinsic electronic transfer mechanism known as the polar catastrophe in which half an electronic charge is transferred from the top of the polar LaAlO$_3$ to the terminating TiO$_2$ layer on the non-polar SrTiO$_3$ side to avoid a charge discontinuity at the interface [12,13]. The 2DEL becomes superconducting below 200 mK [14,15] along with large magnetic moment ($\sim$0.3–0.4 $\mu_B$) aligned parallelly to the interface plane [16–18]. Suggestions for the mechanism responsible for the novel ferromagnetism include a RKKY interaction [19], a double-exchange process [20] and oxygen vacancies [21] developed at the interface during the deposition process. On the other hand, there are proposals for phonon-mediated electron pairing [19,20,22] as well as unconventional superconductivity [23–25]. Another important feature of the interface is the Rashba spin-orbit interaction (SOI) which arises because of the broken mirror symmetry along the direction perpendicular to the interface. A back-gate voltage can tune both the electron concentration and the Rashba SOI and therefore can drive a superconductor-insulator transition [26,27] making the system a potential candidate for novel electronic devices [28].

Here we show that a magnetic field, applied perpendicular to the interface plane, can induce topological superconductivity that harbours gapless edge states and MBS at the core of a vortex. The intrinsic in-plane magnetization favours a finite momentum pairing and, therefore, weakens the topological superconducting phase. We show that by tuning the Rashba SOI (i.e. the back-gate voltage) the topological superconducting phase can be stabilized against the deterrent effect of the in-plane
magnetization. We study the in-gap excitations and find that the zero-energy MBS located at the vortex core is accompanied by low-energy particle-hole symmetric in-gap states of electronic origin. We study the effect of non-magnetic disorder on the low-energy excitations and observe that the MBS vanishes with moderate disorder. We propose an experimental set-up where the existence of MBS can be tested experimentally and discuss about some future directions.

The large Rashba spin-orbit interaction (RSOI), arising from the broken inversion symmetry along the $z$-direction, converts the $s$-wave superconductivity into an effective $p_x \pm ip_y$ one. The in-plane magnetization $h_x$ introduces asymmetry in the two-sheeted Fermi surface leading to finite-momentum pairing of electrons [29]. The main idea to get a topological superconductivity in a two-dimensional $s$-wave superconductor with RSOI [30] is to apply a large perpendicular Zeeman field $h_z$ to essentially remove one of the helicities of the RSOI-induced $p_x \pm ip_y$ states. One has to circumvent the deterrent effect of the in-plane magnetization to stabilize topological superconductivity in this system.

In the present work, we predict that regardless of the asymmetry around the $\Gamma$-point in the Fermi surface, the single-species $p_x + ip_y$ superconductivity still harbour s a single MBS at the core of a vortex. We show that the tunable RSOI competes with the in-plane magnetization and restores the topological phase. However, we find that the excitation at the vortex core is highly sensitive to non-magnetic disorder; even a moderate disorder can destroy the MBS as the magnetization breaks time-reversal symmetry explicitly. As the interface in LAO/STO possesses intrinsic disorders like oxygen vacancies, developed during the deposition process, it is indeed quite challenging to detect a Majorana fermion here. Some remedies and possible experimental requirements for realizing the MBS in this system are discussed.

Model for interface 2DEL. – The electrons in the 2DEL occupy the three $t_{2g}$-bands ($v_{ix}$, $d_{xy}$, $d_{yz}$ and $d_{xz}$) of Ti atoms in the terminating TiO$_2$ plane giving rise to a quarter-filled ground state. Excess electrons supplied by the Oxygen vacancies or the back-gating accumulate on the the next TiO$_2$ layer below the interface. Electrons in the $d_{xy}$ band are mostly localized at the interface sites due to Coulomb correlation. The electrons in the itinerant bands, in the TiO$_2$ layer just below the interface couple to the localized moments via ferromagnetic exchange leading to an in-plane spin-ordering of the interface electrons. The temperature variation of the gap is found to be BCS-like, $2\Delta_0/k_BT_{gap} \approx 3.4$, where $\Delta_0$ is the pairing-gap amplitude at $T = 0$, $k_B$ is the Boltzmann constant and $T_{gap}$ is the gap-closing temperature [31] (the transition to the superconducting state is of BKT type [26]); it is therefore generally assumed that the itinerant electrons at the interface undergo conventional $s$-wave pairing, although there are suggestions of unconventional pairing as well [23–25]. The simple model describing the interface electrons, at the mean-field level, is

$$H = \sum_{k,\sigma} (\epsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma,\sigma'} |g_k \cdot \sigma| \sigma \cdot c_{k\sigma'}^\dagger c_{k\sigma'} + \sum_{k,\sigma,\sigma'} |h_x \sigma_x| \sigma \cdot c_{k\sigma'}^\dagger c_{k\sigma'} + \sum_{k} (\Delta c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \text{h.c.})$$

(1)

where $\epsilon_k = -2t(\cos k_x + \cos k_y)$ is the energy band dispersion with the hopping amplitude $t$ and chemical potential $\mu$, $g_k = (\sin k_y, -\sin k_x)$ describes the RSOI of strength $\alpha$ and $\Delta = -\langle c_k (c_{-k}) \rangle$ is the pairing gap and $\sigma = [\sigma_x, \sigma_y, \sigma_z]$ are the Pauli matrices.

Inducing topological superconductivity. – The RSOI breaks the spin degeneracy of the original bands and creates two new electronic bands while the in-plane magnetization $h_x$ shifts the Berry curvature from the $\Gamma$-point to the $P$-point ($0, -h_z/\alpha$), thus making it energetically favorable for the electrons to pair up at finite center-of-mass momentum proportional to $h_x$. In the diagonal basis of the Rashba Hamiltonian, one essentially obtains $p_x \pm ip_y$ pairing symmetry of the superconductivity [29]. When an external Zeeman field, perpendicular to the interface 2DEL, $H_Z = -h_z \sum_k [\sigma \cdot c_{k\uparrow} c_{-k\downarrow} - c_{k\downarrow}^\dagger c_{-k\uparrow}^\dagger]$ is applied, a gap is opened at the point $P$. The pairing amplitudes in the newly created bands, $\epsilon_k(k) = \epsilon_k \pm \xi$ are given by

$$\Delta_{\pm} = -\frac{\alpha}{2\xi} \Delta (\sin k_y \pm i \sin k_x): \text{intraband $p$-wave,}$$

$$\Delta_{+-} = \frac{h_z}{\xi} \Delta: \text{interband $s$-wave,}$$

where $\xi = (\alpha^2 |g_k|^2 + h^2 - 2ah_x \sin k_y)^{1/2}$, $h^2 = h_x^2 + h_y^2$ and $\epsilon_k = \epsilon_k - \mu$. As shown in fig. 1, when $h_z$ increases beyond a critical field $h_z^{\text{c}}$, there is only one Fermi surface (i.e., one of the two helicities $p_x \pm ip_y$ is removed) and the superconductivity is transformed into a topological superconductivity.

The effective Hamiltonian $\mathcal{H}_{\text{eff}} = \mathcal{H} + H_Z$ of the system can be written in the usual Nambu basis $\Psi(k) = [c_{k\uparrow}, c_{k\downarrow}, c_{-k\downarrow}^\dagger, c_{-k\uparrow}^\dagger]$ as

$$\mathcal{H}_0(k)\Delta_{\sigma}^{-\sigma} \Psi(k) = E_{\pm}(k)\Psi(k)$$

(2)

where $\mathcal{H}_0(k) = \epsilon_k + \alpha g_k \cdot \sigma - h_x \sigma_z - h_y \sigma_x$ and we obtain the bulk spectrum $E_{\pm}^0(k) = (\epsilon_k^2 + \Delta^2 + \xi^2) \pm \zeta$ where $\zeta = |\Delta^2 h_x^2 + \epsilon_k^2 \xi^2|^{1/2}$. The transition to the topological state occurs only when the gap of the bulk spectrum closes i.e., when $\zeta = \epsilon_k^2 + \Delta^2 + \xi^2$. This is satisfied (with $\Delta \neq 0$) when either $\xi^2 = h_x^2 + h_y^2$ or $\epsilon_k^2 + \Delta^2 = h_z^2$ which essentially reduces to the familiar relation $h_z = \sqrt{\Delta^2 + \mu^2}$ [9] when $h_x = 0$. As $h_z$ increases beyond this transition point, a topologically protected excitation gap $E_y$ (given by the minimum of $E_{\pm}(k)$), proportional to the Rashba coupling.
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Vortex core excitations. The induced topological superconductivity exhibits edge states and zero-energy MBS at the core of a vortex [32]. Since Majorana fermions are essentially half an ordinary fermion, they always come in pairs, generally located in different vortex cores. A system having only one vortex, hosts the second Majorana fermion at the boundary. The topological property of the gapless excitation at the boundary is connected to the bulk topological state as a consequence of the "bulk-boundary correspondence". In the following we study the vortex core states by solving the following effective BdG Hamiltonian in real space:

\[ \mathbf{H} = -t' \sum_{(ij),\sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} - \sum_{i,\sigma,\sigma'} (\mathbf{h} \cdot \mathbf{\sigma})_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}^\dagger - \frac{\alpha}{2} \sum_{(ij),\sigma,\sigma'} (\sigma_{\sigma\sigma'} \times \mathbf{d}_{ij})_z c_{i\sigma}^\dagger c_{j\sigma\sigma'}^\dagger + \sum_i (\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow} + \text{h.c.}), \]

where \( t' \) is the hopping amplitude of electrons on a square lattice, \( \mathbf{h} = (h_x,0,h_z) \), \( \mathbf{d}_{ij} \) is the unit vector between sites \( i \) and \( j \), and \( \Delta_i = -U(c_{i\uparrow}c_{i\downarrow}) \) is the onsite pairing amplitude with \( U \), the attractive pair potential. The Hamiltonian (3) is diagonalized via a spin-generalized Bogoliubov-Valatin transformation \( \hat{\mathbf{c}}_{i\sigma}(r_i) = \sum_{i,\sigma} u_{i\sigma\sigma'}(r_i) c_{i\sigma'} + v_{i\sigma\sigma'}(r_i) c_{i\sigma'}^\dagger \) and the quasi-particle amplitudes \( u_{i\sigma}(r_i) \) and \( v_{i\sigma}(r_i) \) are determined by solving the BdG equations: \( \hat{\mathbf{H}} \phi_{\sigma}(r_i) = \epsilon_{\sigma} \phi_{\sigma}(r_i) \), where \( \phi_{\sigma} = [u_{\sigma\uparrow}(r_i), u_{\sigma\downarrow}(r_i), v_{\sigma\uparrow}(r_i), v_{\sigma\downarrow}(r_i)] \). To model a vortex, we use open boundary conditions and solve self-consistently the BdG equations by taking an initial ansatz for the gap as \( \Delta_j = \Delta_0 r_j e^{i\phi_j} \sqrt{1 + 2r_j^2} \), where \((r_j,\phi_j)\) are the polar coordinates of site \( j \) with respect to the core at the center of the 2D plane, \( \Delta_0 \) and \( r_c \) are, respectively, the depth and size of the vortex core. The results, presented here, are for a 40 x 40 system with vortex-size \( r_c = 1 \). For the rest of the paper, we set \( \mu = 0, t' = 1 \) and \( U = 4.0 \), unless explicitly specified. In fig. 3(a), we plot the local density of states (LDOS) at the vortex core, given by \( \rho_N(r) = \frac{1}{N} \sum_{\sigma,\sigma'} ||u_{\sigma\sigma'}(r)||^2 [\delta(\epsilon - \epsilon_{\sigma}) + [v_{\sigma\sigma'}(r)]^2 \delta(\epsilon + \epsilon_{\sigma})] \) for various in-plane fields \( h_z \), \( N \) being the total number of lattice sites. Evidently, the zero-bias Majorana mode is accompanied by other low-energy vortex bound states which generally appear at a vortex core in conventional superconductors and are known as the Caroli-de Gennes Matrion states [33]. These states exist in both the normal and topological superconducting phase. With increasing \( h_z \), the fermionic states move away and mix with the bulk bands and the MBS vanishes suddenly as \( h_z \) reaches the critical value for the transition to the trivial superconducting state. The Majorana excitation at the vortex core is shown in fig. 3(b). As shown in fig. 3(c), the bulk band gap reduces slowly with increasing \( \alpha \) and the low-energy fermionic excitations merge with the MBS. Remarkably, similar features of the LDOS, for various gate voltages, have been seen in the tunneling spectra obtained...
superconductivity with a Majorana BS (the red lines at zero energy fermionic states for $U = 1$ and $h_z = 0.4$), showing the vortex-core state on the 2D plane for $h_y = 0.2$, $h_z = 1.0$ and $\alpha = 1.0$ for a $25 \times 25$ system. (c) LDOS for various $\alpha$ with constant $h_y = 0.2$ and $h_z = 1.0$. (d), (e): quasi-particle spectra as a function of $h_z$ ($\alpha = 0.2$, $h_y = 0.1$ and $U = 1$) and $\alpha$ ($h_z = 0.6$, $h_z = 0.2$ and $U = 1$) delineating three regions: (I) normal superconductivity, (II) normal superconductivity with magnetized vortex and (III) topological superconductivity with a Majorana BS (the red lines at zero bias).

![Fig. 3](image)

Fig. 3: (Color online) (a) The LDOS at the vortex core for in-plane fields $h_y$ showing the MBS at zero energy and the low-energy fermionic states for $\alpha = 1.0$ and $h_y = 1.0$. (b) Plot of the density of zero energy quasi-particles, $|u_{\sigma r}(r_z)|^2 + |v_{\sigma r}(r_z)|^2$, showing the vortex-core state on the 2D plane for $h_y = 0.2$, $h_z = 1.0$ and $\alpha = 1.0$ for a $25 \times 25$ system. (c) LDOS for various $\alpha$ with constant $h_y = 0.2$ and $h_z = 1.0$. (d), (e): quasi-particle spectra as a function of $h_z$ ($\alpha = 0.2$, $h_y = 0.1$ and $U = 1$) and $\alpha$ ($h_z = 0.6$, $h_z = 0.2$ and $U = 1$) delineating three regions: (I) normal superconductivity, (II) normal superconductivity with magnetized vortex and (III) topological superconductivity with a Majorana BS (the red lines at zero bias).

![Fig. 4](image)

Fig. 4: (Color online) Plot of the density of states as a function of the disorder strength $W$, revealing the behaviour of the low-energy excitations inside the bulk superconducting gap with (a) $h_y = 0.5$, $h_z = 0.4$, (b) $h_y = 0.5$, $h_z = 1.0$, (c) $h_y = 1.0$, $h_z = 0.4$ and (d) $h_y = 1.0$, $h_z = 1.0$. Other parameters are the same as in fig. 3.

**Influence of disorder.** – The topological excitations are, however, quite fragile against the imperfections of the host system. The LaAlO$_3$/SrTiO$_3$ interface contains intrinsic disorder such as oxygen vacancies, known to have significant effects on the interface electrons [21,36]. It is, therefore, imperative to study the robustness of the MBS against non-magnetic disorder, introduced through an on-site random potential $V_d$ in the Hamiltonian (3) by $\mathcal{H}_{\text{dis}} = V_d \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma}$, where $V_d \in [-W, W]$ uniformly. In fig. 4, we plot the density of states $\rho(\epsilon) = \frac{1}{N} \sum_{n,\sigma,\epsilon} |[u_{\sigma r}(r_z)]^2 \delta(\epsilon - \epsilon_n) + |v_{\sigma r}(r_z)]^2 \delta(\epsilon + \epsilon_n)|$ for disorder realizations of various disorder strengths $W$. The MBS is quickly destroyed as disorder increases and other in-gap excitations appear within the bulk gap due to the defects. The MBS is, in fact, not expected to be robust against perturbations like disorder in this system since the time-reversal symmetry is already broken explicitly [37].

As shown in fig. 4, the vulnerability of the zero-energy MBS is worse in the presence of larger magnetic fields. In other words, the MBS survives against larger strength of disorder when $h_y$ is smaller (provided, $h_z$ should always be greater than the critical value $h_{zc}$ to ensure a topological regime). In the present system, the degree of vulnerability is severe due to the in-plane magnetization which, in reality, weakens the topological state. Hence the low-energy excitations are destroyed even when there is a finite superconducting gap. In fig. 4, we show a situation where disorder of random strength (up to $W$) is present at all sites. We also consider a diluted situation by putting disorder at some random sites. Figure 5(a) describes how the low-energy in-gap excitations are affected as the disorder concentration ($N_d$) is varied. We find that the results are not different qualitatively from...
Minor obstacles towards a realization of the topological state is known to be a gross overestimation, a rescaling of the gap from the nearby excitations. Though the mean-field gap is sufficient to identify the zero-bias peak of the Majorana BS in the tunneling experiments is about 2 μV, gives a value of the resolution limit about 13 μV, close to the experimental values (∼9.5 μV) observed [34]. It is worth mentioning that the usual temperature range, in which the thermal fluctuation is small for the detection of the MBS, is less than 100 mK [7,10] which is far below the Curie temperature (200 mK) of this interface superconductivity.

Recently, it has been shown that superconductivity is possible in quasi-1D structures, grown at the LaAlO$_3$/SrTiO$_3$ interface [41,42] and may support Majorana zero modes at the ends of such quantum wires [43]. These are the steps towards developing qubits, using this interface, which is to be used as the building blocks of a topological quantum simulator.

**Conclusion.** In summary, we have shown that topological superconductivity hosting Majorana fermions can be realized in the two-dimensional metallic interface of LaAlO$_3$ and SrTiO$_3$ under the right conditions. The phase diagrams show that an additional Zeeman field with large RSOI is required to achieve a stable topological superconductivity. However, non-magnetic disorder such as oxygen vacancies are detrimental to the topological excitations. An experimental design likely to produce conditions conducive to observing Majorana excitations is proposed.

The authors thank C. Richter for sending his unpublished data and pointing out their similarity to fig. 3 above. NM thanks J. MANNHART for useful discussions and acknowledges MHRD, India for support.

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