Majorana bound states and non-local spin correlations
in a quantum wire on an unconventional superconductor

Sho Nakosai,1 Jan Carl Budich,2 Yukio Tanaka,3 Björn Trauzettel,4 and Naoto Nagaosa1,5,6

1Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan
2Department of Physics, Stockholm University, SE-106 91 Stockholm, Sweden
3Department of Applied Physics, Nagoya University, Aichi 464-8603, Japan
4Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany
5Correlated Electron Research Group (CERG), RIKEN Advanced Science Institute (ASI), Wako 351-0198, Japan
6Cross-Correlated Materials Research Group (CMRG), RIKEN Advanced Science Institute (ASI), Wako 351-0198, Japan

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We study theoretically the proximity effect of a one-dimensional metallic quantum wire (in the absence of spin-orbit interaction) lying on top of an unconventional superconductor. Three different material classes are considered as a substrate: (i) a chiral superconductor in class D with broken time-reversal symmetry; a class DIII superconductor (ii) with and (iii) without a nontrivial $Z_2$ number. Interestingly, we find degenerate zero energy Majorana bound states at both ends of the wire for all three cases. They are unstable against spin-orbit interaction in case (i) while they are topologically protected by time-reversal symmetry in cases (ii) and (iii). Remarkably, we show that non-local spin correlations between the two ends of the wire can be simply controlled by a gate potential in our setup.

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Introduction.— Proximity effects of superconductors and normal metals as well as semiconductors have been a subject of continued interest due to the rich physical phenomena of these hybrid systems. Especially, the topological nature of the superconducting proximity effect is an issue of current research activities [1–4] stimulated by the possible occurrence of Majorana fermions in solid state systems [5–11]. For example, the interface between an s-wave superconductor and the surface state of a three-dimensional topological insulator (TI) is predicted to offer a platform to realize Majorana fermions [1]. The underlying idea here is holographic principle that entails the reduction of electronic degrees of freedom, i.e., electron fractionalization, at the surface of a topologically non-trivial bulk state. Furthermore, the proximity effect of a TI to unconventional superconductors has also been studied theoretically [12]. Another (highly interesting) proposal is to use semiconductors with Rashba spin-orbit interaction in combination with s-wave superconductors for this purpose. In the presence of a sufficiently strong magnetic field, an inverted gap opens at the $\Gamma$-point in this system and topological superconductivity as well as Majorana fermions may appear when the Fermi energy lies inside the gap [13–16]. A recent experiment observed the zero-bias conductance peak at the edge of an InSb quantum wire (QW) coupled to an s-wave superconducting substrate, which might be the first experimental observation of a Majorana fermion [17]. It has also been shown theoretically that a one-dimensional Rashba quantum wire coupled to a d-wave superconductor hosts doubly degenerate Majorana bound states (MBSs) at the edge [18]. Besides these distinct works, there are various other research activities on the basis of QWs (for example Refs. [16, 19–25]). In all the cases listed above, spin-orbit interaction and/or the Zeeman energy in the QW is essential. Therefore, an open question is if zero energy Majorana bound states are also realizable in a one-dimensional system in the absence of these interactions, which opens new opportunities as we will show below.

In this paper, we investigate electronic states caused by the proximity effect between a metallic QW and a two-dimensional (2D) unconventional superconductor to search for zero energy MBSs at the ends of the QW. We discover that the resulting MBSs are doubly degenerate, i.e., characterized by a spin degree of freedom. This leads to nonlocal spin-correlations between the two ends of the QW which can be manipulated by all-electric means. For a substrate in symmetry class D [26], i.e., in the absence of time reversal symmetry (TRS) the degenerate end states can be gapped out by switching on TRS preserving local imperfections that couple opposite spin. This is reflected in the fact these systems are characterized by a trivial $Z_2$ topological invariant. In contrast, for a TRS preserving substrate in symmetry class DIII, we find helical MBS pairs that are topologically protected by TRS.

Model.— Our setup is shown schematically in Fig. 1 and the model Hamiltonian given by

$$H_{SC} = \int d^2k \Psi_k^\dagger \left( \frac{k_x^2 + k_y^2}{2m_s} + \mu_s \right) \Psi_k,$$

$$\Psi_k = (a^\dagger \downarrow k, a^\dagger \uparrow -k, a \downarrow -k, a \uparrow k),$$

$$H_{wire} = \int dk \Psi_{\sigma k}^\dagger \left( \frac{k_x^2}{2m_s} - \mu \right) \Psi_{\sigma k},$$

$$H_t = c \int dx \left( \psi_{\sigma}^\dagger \sigma (x,0) \psi_{\sigma} + h.c. \right),$$
where $H_{\text{wire}}$ describes the QW put along $x$-direction on the surface of the superconductor described by $H_{\text{SC}}$ which infinitely spreads in the $xy$-plane. These two are connected by a tunneling Hamiltonian $H_t$ with the spin-independent constant matrix element $c$. We consider the following three cases for the order parameter matrix $\Delta$: (i) $\Delta = i\sigma_y \Delta \sigma_z (k_x + i k_y)$ for the chiral superconductor of class D with the topological invariant $Z = 1$, and (ii) $\Delta = i\sigma_y \Delta k \cdot \sigma$ for the time reversal symmetric class DIII superconductor with the topological invariant $Z_2 = 1$. Here, the $\sigma$ denotes Pauli matrices in spin space. As the third case (iii), we consider a system where two layers of a 2D superconductor of case (ii) are coupled to each other by an interlayer transfer integral, which is a topologically trivial case with $Z_2 = 0$. The model (i) is relevant to Sr$_2$RuO$_4$ where the chiral $p + ip$ superconductivity with broken time-reversal symmetry is believed to be realized [27]. The model (ii) is the 2D analogue of the He B phase, and is continuously connected to the helical non-centrosymmetric topological superconductor with Rashba spin-orbit interaction [28–30]. We present the calculational steps and results mainly for case (i) below, but it is straightforward to apply them to the other two cases (ii) and (iii). Our main purpose is to investigate the electronic states in the one-dimensional superconductivity formed in this way and to discuss its topological nature as well as resulting Majorana bound states.

Effective Green’s function.— First, we derive the effective Green’s function of the QW by integrating over the superconductor

$$G_{\text{eff}}^{-1}(i\omega_n, k_x) = i\omega_n - H_{\text{wire}}(k_x) \tau_z - c^2 I(i\omega, k_x),$$

$$I(i\omega_n, k_x) = \int dk_y \frac{i\omega_n + H_{\text{SC}}(k_x, k_y)}{(i\omega_n)^2 - H_{\text{SC}}^2(k_x, k_y)},$$

where $\tau$ denotes Pauli matrices in the Nambu space. As long as there is neither spin-orbit interaction in the wire nor spin-dependent tunneling between the wire and the superconductor, the induced superconducting order parameter is also spin-triplet and can be decoupled into two sectors $\sigma = \pm 1$. The integration can be analytically performed and we obtain

$$G_{\text{eff}}^{-1}(i\omega_n, k_x) = i\omega_n(1 - 2c^2 I_1) - h(k_x) \cdot \tau,$$

$$h(k_x) = (2c^2 \Delta k_x I_1 \sigma_x, 0, \xi k + 2c^2 \xi_{kz}^\text{SC} I_1 + 2c^2 I_2),$$

$$I_1 = \frac{m_s [\lambda^+_1 \arctan(\kappa/\lambda^+_1) - \lambda^-_1 \arctan(\kappa/\lambda^-_1)]}{2\pi \sqrt{\xi_{kz}^2 \Delta^2 - 2m_s \xi_{kz}^\text{SC}}} - \omega_n^2,$$

$$I_2 = \lambda^-_1 \arctan(\kappa/\lambda^-_1) - \lambda^+_1 \arctan(\kappa/\lambda^+_1),$$

where $\lambda$ is a momentum cut-off and $\lambda_{\pm} = (k_x^2 + 2m_s^2 \Delta^2 - 2m_s \mu_s \pm 2m_s \sqrt{m_s^2 \Delta^2 - 2m_s \xi_{kz}^\text{SC} - \omega_n^2})^{1/2}$, $\xi_{kz} = k_x^2/2m_s + \mu_s \xi_{kz}^\text{SC}$ likewise. In the following, we look at the $\sigma_x = 1$ sector, which is equivalent to a spinless $p$-wave superconductor. From Eq. (8), we can then calculate the spectral function $A(\omega, k_x)$ of the electron as

$$A(\omega, k_x) = -\frac{1}{2\pi} \Im \left[ \text{Tr} [\tau_z G_{\text{eff}}^R(\omega, k_x)] \right],$$

where $G_{\text{eff}}^R(\omega, k_x)$ is the retarded Green’s function obtained from $G_{\text{eff}}(i\omega_n, k_x)$ via the analytic continuation $i\omega_n \rightarrow \omega + i\delta$, where $\delta$ is an infinitesimally small positive number. In Fig. 2, we plot Eq. (11) with $m = m_s = 1.0, \mu_s = 1.0, \Delta =}$
we calculate the energy spectrum in the system with

\[ H_{\text{eff}}(k_x) = -\tau \cdot \mathbf{k} \]

and (b) correspond to the cases where the band of the QW is

\[ \text{in the 2D SC that will be further discussed below.} \]

\[ \text{Figures 2(a)} \]

![schematic structure of the spectrum. The red lines represent]

\[ \text{the topological phase transition as a function of the chemi-} \]

\[ \text{cal potential in the QW. In the strong coupling regime, where} \]

\[ \mu < \mu^* \text{, there are no states in the induced superconducting} \]

\[ \text{gap, while in the weak coupling regime, where} \]

\[ \mu > \mu^* \text{ there are zero energy states. It can be checked that four-fold degen-} \]

\[ \text{erate zero energy states are formed, two at each end.} \]

\[ \text{Fig. 3(b) shows the probability distributions of one of them.} \]

\[ \text{Red solid circles represent the weight in the QW, and we can see} \]

\[ \text{the state is localized at the ends of the wire.} \]

\[ \text{In sharp contrast to the Kitaev model, we have two spin sectors in the QW} \]

\[ \text{which are degenerate. This fact attaches a spin degree of freedom to} \]

\[ \text{the MBSs. However, in the presence of spin-orbit interaction,} \]

\[ \text{which mixes the} \]

\[ \text{cases, and we have found that the doubly degenerate zero en-} \]

\[ \text{ergy Majorana bound states appear when the chemical poten-} \]

\[ \text{tial} \]

\[ \mu \text{ of the QW is positive and large enough for the topologi-} \]

\[ \text{cal phase transition to occur.} \]

\[ \text{In cases (ii) and (iii), the spin degenerate pair of MBS stems from a non-trivial} \]

\[ \text{Z}_2 \text{ invariant for the composite system in symmetry class DIII. Therefore,} \]

\[ \text{these end states are topologically protected by TRS and cannot} \]

\[ \text{be gapped out by switching on spin-orbit interaction as long} \]

\[ \text{as the bulk gap is maintained.} \]

\[ \text{This is an essential difference to case (i) where the conservation of} \]

\[ \sigma_x = \pm 1 \text{ was needed in addition to the generic symmetries of the model to obtain} \]

\[ \text{zero energy MBSs, while TRS protects the doubly degenerate} \]

\[ \text{MBSs in cases (ii) and (iii).} \]

\[ \text{This is particularly remarkable for case (iii) where the substrate 2D superconductor} \]

\[ \text{is originally} \]

\[ \text{in a topologically trivial phase.} \]

\[ \text{Local and non-local fermions.— There have been many theo-} \]

\[ \text{retical proposals to use chiral MBSs for topological quantu-} \]

\[ \text{m computing [34–36]. Chiral MBSs are difficult to de-} \]

\[ \text{tect and to manipulate because they only couple in a lim-} \]

\[ \text{ited way to their environment.} \]

\[ \text{This is different in our pro-} \]

\[ \text{posal. On the one hand, the doubly degenerate MBSs dis-} \]

\[ \text{cussed above are more susceptible regarding their coupling to} \]

\[ \text{the environment. On the other hand, they can show novel re-} \]

\[ \text{sponses through a strong coupling between the fermion parity} \]

\[ \text{and the spin degree of freedom.} \]

\[ \text{The idea behind is schemati-} \]

\[ \text{cally shown in Fig. 4.} \]

\[ \text{The solid lines represent Kitaev chains} \]

\[ \text{with MBSs indicated by red circles.} \]

\[ \text{Let us elaborate a bit more on the two kinds of fermions that} \]

\[ \text{can be formed by our} \]

\[ \text{MBSs. Since Majorana fermions are real, normal fermions} \]

\[ \text{are formed from pairs of them. We can construct two kinds} \]

\[ \text{of normal (complex) fermions, non-local spin polarized ones} \]

\[ \psi_1 = 1/2(\gamma_{11} + i\gamma_{12}) \text{ and} \]

\[ \psi_2 = 1/2(\gamma_{11} - i\gamma_{12}) \].

\[ \text{The local pseudo spin operators are defined as} \]

\[ s_{12} = 1/2 \times \gamma_{12} \sigma_{\alpha \beta} \gamma_{21, \alpha \beta} \].

\[ \text{It is known that Majorana fermions have only Ising-type spin due to their anticommutation relation} \]

\[ \{\gamma_i, \gamma_j\} = 2\delta_{ij}, \text{ then,} \]

\[ s_x = s_z = 0 \text{ and} \]

\[ s_y = 1/2 - \psi^\dagger \psi \].

\[ \text{from the above definition.} \]

\[ \text{We would like to emphasize that} \]

\[ \text{these local variables are specific to the paired Majorana states.} \]
There will be various interesting physics as a consequence of the synthesis of the local and the non-local nature. Here, as an example, we focus on spin-spin correlation of two Ising spins formed at the ends. In preparation for that, we first review some aspects of the fermion parity. When we have two Majorana operators, $\gamma$ and $\gamma'$, there exist two orthogonal states $|0\rangle$ and $|1\rangle$, which satisfy $-i\gamma \gamma' |0\rangle = |0\rangle$ and $-i\gamma \gamma' |1\rangle = -|1\rangle$, respectively. The former has an even fermion parity and the latter odd. They can be rewritten by normal fermion operators defined as $\psi = 1/2 (\gamma + i\gamma')$ where $\psi^\dagger \psi |0\rangle = 0$ and $\psi^\dagger \psi |1\rangle = |1\rangle$. Note that if the wire is connected to ground by a capacitor, one can modify the fermion number via charging energy $U(n) = Q^2/(2C) - V(t)Q = (Q - Q_0)^2/(2C) + \text{const.}$ where $Q = ne$ is the charge, $V(t)$ is the gate voltage, and $Q_0 = CV(t)$. The importance of charging energy in the context of topological superconductors was first discussed in Ref. [37], where electron teleportation (mediated by the non-locality of the MBSSs) has been proposed. We now apply this idea to our model. Our Hilbert space is 4-dimensional and there are two kinds of bases one can construct, i.e., from $\psi_1$, $\psi_2$, or from $\psi_1^\dagger$ and $\psi_2^\dagger$. Namely, one can define $\psi_1^\dagger \psi_1 |1\rangle_1 = |1\rangle_1$, etc., and $|0\rangle_1$, $|1\rangle_1$, ... are local basis states while $|0\rangle_1^\dagger$, $|1\rangle_1^\dagger$, ... are non-local basis states. The relation between these two kinds of basis states is given by

$$
\left(\begin{array}{c} |0\rangle_1 \langle 0|_1 \\ |0\rangle_1 \langle 1|_1 \\ |1\rangle_1 \langle 0|_1 \\ |1\rangle_1 \langle 1|_1 \end{array}\right) = \frac{1}{\sqrt{2}} \left(\begin{array}{cccc} 0 & -i & 1 & 0 \\ 1 & 0 & 0 & i \\ 1 & 0 & -i & 0 \\ 0 & i & 1 & 0 \end{array}\right) \left(\begin{array}{c} |0\rangle_1^\dagger \langle 0|_1^\dagger \\ |0\rangle_1^\dagger \langle 1|_1 \\ |1\rangle_1^\dagger \langle 0|_1^\dagger \\ |1\rangle_1^\dagger \langle 1|_1^\dagger \end{array}\right).$$

(12)

In our system, the total number of fermions can be controlled by the gate voltage $V(t)$. We consider $s_{1y}$ correlation in the odd and even fermion number space, respectively. The density matrices are $\rho_{\text{odd}} = \frac{1}{2} (|1\rangle_1^\dagger |0\rangle_1^\dagger |0\rangle_1 |0\rangle_1 + |0\rangle_1^\dagger |1\rangle_1 |1\rangle_1 |1\rangle_1)$ and $\rho_{\text{even}} = \frac{1}{2} (|0\rangle_1^\dagger |0\rangle_1^\dagger |1\rangle_1 |1\rangle_1^\dagger + |1\rangle_1^\dagger |0\rangle_1^\dagger |1\rangle_1 |0\rangle_1^\dagger)$. Then we obtain

$$-\langle s_{1y}s_{2y}\rangle_{\text{odd}} = \langle s_{1y}s_{2y}\rangle_{\text{even}} = \frac{1}{4}.$$  

(13)

where $\langle \ldots \rangle_{\text{odd/even}}$ represents the statistical average with the density matrices $\rho_{\text{odd}}$ and $\rho_{\text{even}}$, respectively. These results show that by modulating charging energy we can control spin-spin correlation, which is independent of the distance between the two spins because they are connected through the superconducting wire in between. This effect is a consequence of both, the local and the non-local degrees of freedom of the system. One can also manipulate the two Ising spins by modulating the gate voltage as a function of time as $V(t) = V_0 + \delta V(t)$. The equations of motion of $s_{1y}$ and $s_{2y}$ by the driving force $\delta V(t)(i\gamma_1 \gamma_2 \gamma_1 \gamma_2 + i\gamma_1 \gamma_2 \gamma_1 \gamma_2)$ yield

$$\frac{d}{dt}(s_{1y} + s_{2y}) = 0$$

(14)

$$\frac{d^2}{dt^2}(s_{1y} - s_{2y}) = -4 \left(\frac{2e\delta V_0}{\hbar}\right)^2 (s_{1y} - s_{2y})$$

(15)

for a constant $\delta V_0$ during some time period $T$. By tuning $T$ to satisfy $4e\delta V_0 T/\hbar = \pi$ one can reverse the pseudospins $s_y$ components when they are anti-parallel while they remain unchanged when they are parallel.

Conclusion.– In this paper, we have studied theoretically the proximity effect of a one-dimensional metallic quantum wire without spin-orbit interaction on the substrate of an unconventional superconductor. We have considered three different cases for the substrate: (i) a chiral superconductor; (ii)
a class DIII superconductor with a non-trivial $\mathbb{Z}_2$ number, and (iii) a class DIII superconductor with a trivial $\mathbb{Z}_2$ number. Interestingly, we have found degenerate zero energy Majorana bound states at both ends of the quantum wire for all three cases. We have shown that these degenerate Majorana bound states for cases (ii) and (iii) can be nicely used for a combined spin/parity qubit. Furthermore, we have demonstrated that the resulting non-local spin correlations between the two ends of the wire can be controlled by the gate voltage potential acting on the wire. One of the candidate systems for the case (ii) substrate are thin films of $\text{Sr}_2\text{RuO}_4$ [38] or bi-layer Rashba system [30], where the class DIII superconducting state might be realized, and for the case (iii) super lattice structure of $\text{CeCoIn}_5$ [39].

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