Topologically trivial zero bias conductance peak in semiconductor Majorana wires from boundary effects

Dibyendu Roy$^1$, Nilanjan Bondyopadhaya$^2$ and Sumanta Tewari$^3$

$^1$ Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
$^2$ Integrated Science Education and Research Centre, Visva-Bharati University, Santiniketan, WB 731235, India and
$^3$ Department of Physics and Astronomy, Clemson University, Clemson, SC 29634, USA

We show that a topologically trivial zero bias conductance peak is produced in semiconductor-superconductor hybrid structures due to a suppressed superconducting pair potential and/or an excess Zeeman field at the ends of the heterostructure, both of which can occur in experiments. The zero bias peak (ZBP) (a) appears above a threshold parallel bulk Zeeman field, (b) is stable for a range of bulk field before splitting, (c) disappears with rotation of the bulk Zeeman field, and, (d) is robust to weak disorder fluctuations. The topologically trivial ZBPs are also expected to produce splitting oscillations with the applied field similar to those from Majorana fermions. Because of such strong similarity with the phenomenology expected from Majorana fermions we find that the only unambiguous way to distinguish these trivial ZBPs (of height $4e^2/h$) from those arising from Majorana fermions (of height $2e^2/h$) is by comparing the (zero temperature) peak height and/or through an interference experiment.

The search for zero-energy Majorana fermions in recent theoretical and experimental studies. A practical route to engineer such a system in the laboratory has been suggested in Refs. 9–12, following earlier similar proposals in topological insulators and cold fermion systems. The proposed system consists of a spin-orbit coupled semiconductor thin film or nanowire proximity coupled to a s-wave superconductor and in the presence of a suitably directed Zeeman spin splitting. The applied Zeeman field drives the engineered hybrid nanowire (semiconductor Majorana wire) through a topological quantum phase transition (TQPT) to a topologically nontrivial superconducting phase with localized zero energy Majorana bound states (MBSs) when the Zeeman splitting $\Gamma$ exceeds a critical value $\Gamma_c$. The Majorana wire is in a topologically trivial superconducting phase with no defect-localized MBS when the Zeeman splitting satisfies $\Gamma < \Gamma_c$. The zero energy MBS localized at the ends of the nanowire (for $\Gamma > \Gamma_c$) has been proposed to be observable by a zero bias conductance peak in charge current through the ends of the semiconductor wire. Here we show that such a charge current zero bias peak (ZBP) can exist even in the topologically trivial phase ($\Gamma < \Gamma_c$) due to excess Zeeman field and/or suppressed superconducting pair potential at the wire ends, both of which can occur in experiments. Our calculations establish that a (non-quantized) ZBP from tunneling into the ends of a spin-orbit coupled wire is unable to produce an unambiguous signature of MBS, even after taking into account all the proposed experimental checks for Majorana fermions that have appeared in recent theoretical and experimental works.

The critical Zeeman field $\Gamma_c (= \sqrt{\Delta^2 + \mu^2})$ in the quasi-1D heterostructure depends on the value of the superconducting pair potential $\Delta$ proximity induced in the semiconductor and the chemical potential $\mu$ of the semiconductor measured from the top-most occupied confinement energy band (by “band”, we mean a pair of spin-split sub–bands, the band themselves being separated by the energy gaps due to lateral confinement). The value of $\Gamma_c$ (for $\Delta \rightarrow 0$) corresponds to the value above which ($\Gamma > \mu$) an odd number of confinement induced sub–bands are occupied in the semiconductor. For an even number of sub-band occupancy the system is in the topologically trivial phase with no MBS localized at the ends of the nanowire.

The typical experimental nanowires, however, are more likely to have an even number of sub-band occupancy than odd. This is because the confinement energy gap $E_c$ is typically much larger than the Zeeman energy gap $\Gamma$, and, consequently, the chemical potential is expected to lie in the confinement gap between two pairs of spin–split sub–bands rather than in the Zeeman gap between two sub–bands in the same band. By a simple estimate (within the non-interacting electron model), assuming that the 1D density of states $\propto 1/\sqrt{E}$, the ratio of the number of samples with an even sub-band occupancy to that with an odd sub-band occupancy is $\sim \sqrt{E_c}/\Gamma \sim 6$. Here we have used typical values for $E_c \sim 6 – 7$ meV and the applied $\Gamma \sim \Delta \sim 150 – 200 \mu$eV from Ref. 25. It follows that, unless $\mu$ can be tuned by an externally applied gate potential (which is hard because of the strong coupling to a superconductor) the chemical potential in the experimental nanowires may cross both sub–bands of the top occupied band and the system may be topologically trivial. Here we show that, even in this case, a robust but topologically trivial ZBP can still appear in tunneling experiments due to excess local Zeeman field and/or suppressed superconducting pair potential at the wire ends. The excess Zeeman field at the wire ends can be due to the Meissner effect (the edge magnetic field larger than that in the bulk), or due to the presence of a magnetic impurity at the nanowire-lead interface, and
the suppressed $\Delta$ at the ends of the wire can be a consequence of the (spatially varying) proximity effect near the boundary of the bulk superconductor. Thus, both effects, capable of producing a ZBP even in the topologically trivial phase, can occur in the experimental systems.

About the origin of the topologically trivial peaks in our work we speculate on the following scenario: As discussed in Ref. \[30\] the zero energy bound states from the two different sub-bands (in the top occupied band) at the same end of the nanowire could contribute to a total ZBP height of $4e^2/h$ provided their coupling and the resultant energy splitting could be suppressed. Ref. \[30\] proposed that a large uniform bulk Zeeman field, coupled with a smooth barrier potential at the lead-nanowire interface, can suppress the inter-sub-band s-wave pairing \[31\], resulting in a near-zero-energy peak even in the topologically trivial phase. We speculate that the coupling between the two local zero energy states can be suppressed even when a perturbation is applied only near the heterostructure ends because the zero energy states from the (uncoupled) sub-bands are localized there within a length scale $\sim \xi$, the coherence length. The local excess Zeeman field and/or suppressed pair potential at the nanowire ends can however be a natural consequence of the experimental geometry and thus present an alternative explanation of the (quantized) ZBPs seen in the recent experiments on semiconductor-superconductor heterostructures \[25\] \[27\].

The trivial ZBP appears in our calculations entirely in the topologically trivial phase, that is, with only an even number of confinement induced sub-bands occupied. According to the scenario presented above, even though the ZBP (of height $4e^2/h$) can be viewed as the result of resonant local Andreev reflection from two (or an even number of) weakly coupled MBSs, it is important to mention that no TQPT is necessary for the near-zero-energy states to appear. In other words, an even number of Majorana fermions, even if they are only weakly coupled, can be thought of as a conventional Dirac fermion, and do not have non-Abelian statistics. It is in this sense that we call the ZBPs observed with local perturbations in our work topologically trivial ZBPs.

We consider a one-dimensional multichannel Rashba spin-orbit coupled semiconducting nanowire (for example, InSb) oriented along the x-direction, and in proximity to a s-wave superconductor (for example, NbTiN). The full hybrid structure is modeled by a discrete $N \times 2$ square-lattice tight-binding model \[32\] \[33\]

\[
H_{NW} = H_{KE} + H_{SO} + H_{Z} + H_{SC},
\]

\[
H_{KE} = \sum_{r,d,\alpha} -t(c_{r+d,\alpha}^{\dagger}c_{r,\alpha} + H.c.) + \mu(c_{r,\alpha}^{\dagger}c_{r,\alpha} - \frac{1}{2}),
\]

\[
H_{SO} = \sum_{r,d,\alpha,\beta} -i\alpha_{R}c_{r+d,\alpha}^{\dagger}\sigma_{\alpha,\beta} \times \hat{d} c_{r,\beta} + H.c.,
\]

\[
H_{Z} = \sum_{r,\alpha,\beta} c_{r,\alpha}^{\dagger}(B \sigma)_{\alpha,\beta} c_{r,\beta}, H_{SC} = \sum_{r} -\Delta c_{r,\uparrow}^{\dagger}c_{r,\downarrow}^{\dagger} + H.c.,
\]

where $r \in \{l,m\}$ denotes lattice sites with the index $l$ along the length, $l = 1,2..,N$, and the index $m$ along the width of the nanowire, $m = 1,2..,W$. \([W\text{ counts the number of tight-binding chains}]\) $d \in \{\epsilon_x, \epsilon_y\}$ is a unit vector connecting nearest-neighbor sites, $(\alpha, \beta) \in \{\uparrow, \downarrow\}$ are spin indices, and $\sigma$ is spin-1/2 Pauli matrix vector. Here $c_{r,\alpha}^{\dagger}$ is a creation operator of an electron with spin $\alpha$ at lattice site $r$ of the nanowire. The hopping strength $t$ of the electrons is related to the band mass $m^* = h^2/(2a^2)$ where $a$ denotes lattice spacing in the tight-binding model. The applied magnetic field $B \in \{B_x, B_y, B_z\}$ opens a Zeeman splitting $\Gamma = (\gamma \mu B/2)B$ in the sub-bands, and $\Delta$ is the proximity induced superconducting pair potential in the semiconductor. In the following we assume $\gamma \mu B/2 = 1$ and identify $\Gamma$ with $B$ in the reduced units. In recent experiments \[25\] \[27\] $B$ along the wire axis ($x$-axis) is increased to observe a ZBP, and then $B$ is tilted from the wire axis to remove the ZBP, both observations consistent with the Majorana origin of the ZBP at the wire ends \[10\]. In Eq. (1) $\mu = 2(\mu - t)$ and an energy shift $-\mu/2$ has been added for the local Majorana transformation used in our transport calculations. We couple the semiconductor-superconductor hybrid structure in Eq. (1) to two metallic leads at the two ends. The metallic leads are modeled by free electron tight binding chains. Each first $\{1,m\}$ and last sites $\{N,m\}$ with $m = 1,2..,W$ of all the transverse tight-binding chains of the semiconductor nanowire are coupled to a semi-infinite free-electron tight binding chain which forms the metallic leads. All the tight binding chains in the left lead are kept at chemical potential $\mu_L$ and temperature $T_L$, and those in the right lead are at chemical potential $\mu_R$ and temperature $T_R$. The Hamiltonian $H_{\alpha}^p (p = L, R)$ below describe the metallic lead Hamiltonians and $H_{\alpha}^p$ the corresponding tunnel couplings between the leads and the nanowire,

\[
H_{M}^p = -\gamma_p \sum_{\alpha,m=1}^{W} \infty \sum_{k=1}^{\infty} (c_{m,k,\alpha}^{\dagger}c_{m,k+1,\alpha}^{\dagger} + c_{m,k+1,\alpha}c_{m,k,\alpha}),
\]

\[
H_{L}^p = -\gamma_p \sum_{\alpha,m=1}^{W} (c_{m,1,\alpha}^{\dagger}c_{m,\beta,\alpha} + c_{m,\beta,\alpha}^{\dagger}c_{m,1,\alpha}),
\]

where $l_L = 1$ and $l_R = N$. Here $c_{m,k,\alpha}^{\dagger}$ is an electron creation operator on the $\alpha$th lead. The strength of tunnel coupling between the normal leads and the nanowire is $\gamma_p$. It controls the width and the height of the ZBP. Here we apply the quantum Langevin equations and Green’s function (LEGF) approach \[34\] \[38\] to calculate the current-voltage (I-V) characteristics and the corresponding differential conductance $dI/dV$ across the multichannel spin-orbit coupled semiconductor nanowires. To mimic the recent experimental conditions \[25\], we set $\mu_R = 0$ and drive $\mu_L$ from $-eV$ to $eV$. We fix the temperature of the two leads to be the same, $T_L = T_R = 0$.

An applied magnetic field along $x$ splits the two sub-bands of a single tight binding chain, and the MBSs appear when only one sub-band is occupied, i.e., the chemical potential lies in the gap between the two split sub-
find that a ZBP appears in the differential conductance of transverse chains of the semiconductor nanowire. We have confirmed that the results in this paper are robust to variations in the values of these parameters in physical units these parameters for a 2 µm long wire correspond to a Rashba spin-orbit coupling (in the continuum model) \( \alpha = \alpha_R a = 0.1 \) eVÅ, pair potential \( \Delta = 0.3 \) meV and Zeeman splitting \( \Gamma = 0.4 \) meV. We have confirmed that the results in this paper are robust to variations in the values of these parameters in particular to the Rashba spin-orbit coupling parameter \( \alpha \) (Fig. 2). In all the figures we quote the parameters in units of \( t = 1 \).

Now we turn on a local perturbation to the magnetic field at the first sites \( \{1,m\} \) \( (m = 1,2..W) \) of all the transverse chains of the semiconducting nanowire. We find that a ZBP appears in the differential conductance of the nanowire even in the topologically trivial phase (even number of occupied sub-bands for \( \Delta \to 0 \)) when the magnitude of \( B_z \) locally at \( \{1,m\} \) is larger than that in the bulk (Fig. 2a). The ZBP also appears in the topologically trivial phase when there is a local \( B_z \) field at the first sites (in addition to bulk \( B_z \)) of the same order of \( B_z \) (Fig. 2b). Note that a local \( B_z \) field is equivalent to a local shift of the chemical potential of the electrons with one spin with respect to the other. A topologically trivial ZBP appears also for a local suppression in the superconducting pair potential \( \Delta \) at the first sites of the transverse chains (Fig. 2d). The heights of the trivial ZBPs are of the order \( 4e^2/h \) (Fig. 2), which is double the height produced by the MBSs (Fig. 1).

Applying the local perturbation at multiple boundary sites on all the chains (Fig. 2b) we find that the topologically trivial ZBP appears in a larger range of the local perturbations than when the perturbation is applied at a single boundary site (as in Fig. 2b, 2d). This is also more natural experimentally since the excess Zeeman field and/or the suppressed pair potential at the wire ends are expected to gradually shift to the bulk values in the interior of the nanowire. In Fig. 2b we show that the trivial ZBPs due to a fixed set of local perturbations in the Zeeman field (applied at the two end sites)

FIG. 1. Zero-temperature differential conductance \( dI/dV \) vs. the applied voltage \( V \) for different numbers of transverse chains \( W \) for \( \mu = 0 \). Everywhere \( B_x = 0.8, B_y = B_z = 0 \) and \( |\Delta| = 0.6 \), so \( B_x > B_{z,c} = |\Delta| \). Number of chains \( W \) in the panels is as follows: (a) \( W = 1 \), (b) \( W = 2 \), (c) \( W = 3 \), and (d) \( W = 4 \). Since \( \mu = 0 \) in Eq. (1) (with periodic boundary conditions) corresponds to an equal number of sub-bands below and above \( E = \mu \), only \( W = 1,3 \) has a ZBP for \( B_x > B_{z,c} = |\Delta| \). For \( W = 2,4 \), \( B_x > |\Delta| \) produces no ZBP because only an even number of sub-bands are occupied.

FIG. 2. Emergence of ZBP in the topologically trivial superconducting phase (even band occupancy) due to excess Zeeman field and/or reduced pair potential at the wire ends. In all the panels, \( W = 2, \Delta = 0.6, \) and \( \mu = 0 \). In panels (a,b,d) \( \alpha_R = 0.2, B_z = 0.8 \). Note that for these values of \( B_x \) and \( \Delta \) there is no ZBP for \( W = 2 \) (even band occupancy) in the absence of a local perturbation (Fig. 1). The local end perturbations producing the topologically trivial ZBPs are as follows: (a) \( \delta B_z \{1,m\} = 0.45 \), (b) \( \delta \mu \{1,m\} = 1 \), \( \delta \mu \{1,m\} = 0.2 \), and (d) \( \delta \Delta \{1,m\} = -0.35 \), where \( m = 1,2 \). In panel (c) we show, for illustrative purposes, the emergence of the trivial ZBP even for a larger value of the spin-orbit coupling, \( \alpha_R = 0.5 \) and \( B_x = 1 \). For local end perturbations we have used, \( \delta B_z \{1,m\} = 0.7 \), \( \delta B_z \{2,m\} = 0.5 \), that is, the end perturbation is applied on two sites and gradually peters towards the bulk.
FIG. 3. Dependence of the topologically trivial ZBP on the uniform Zeeman field \( B_z \) for a fixed perturbation at two end sites on all chains (\( \delta B_x \{1, m\} = 0.32 \) and \( \delta B_z \{2, m\} = 0.2 \)). All panels have \( W = 2 \) (two transverse chains) and \( \Delta = 0.6 \). The ZBP is split in panel (a) (\( B_z = 0.7 \)), is fully developed in panel (b) (\( B_z = 0.8 \)), and stays in panel (c) (\( B_z = 1.0 \)), before splitting again with larger \( B_z \) (not shown). Panel (d) (\( B_x = 0.4, B_y = 0.4 \)) shows the disappearance of the ZBP with rotation of the uniform field in the plane formed by the wire and the effective spin-orbit coupling ((\( x - y \) plane)).

FIG. 4. Robustness of the topologically trivial ZBP to moderate disorder fluctuations and the role of barrier potential (tunnel coupling with the metallic lead). In all panels \( W = 2, B_z = 0.8, \) and \( \mu \{1, m\} = 1, \mu \{1, m\} = 0.2 \). Randomness in \( \mu \) is chosen from a uniform distribution between 0 and 0.1. \( \gamma' = 0.2 \) and (b) clean wire (\( \mu = 0 \)), but a stronger coupling with the lead, \( \gamma' = 0.3 (p = L, R) \). These figures should be compared with that in Fig. 3.

appear only above a threshold uniform Zeeman field in the bulk. The threshold bulk Zeeman field itself depends on the value of the local perturbations in the magnetic field or the pairing potential. For example, we find that the threshold field required for the emergence of the ZBP decreases with a larger value of the local perturbation. In Fig. 3 we show that the ZBP is robust to a further increase in the bulk field, before splitting into two peaks above a higher threshold (not shown). This sort of dependence of the topologically trivial ZBP on the uniform bulk field is consistent with the recent experiments [25–27]. The splitting of the trivial ZBP with increasing magnetic field can arise from two mechanisms. First, due to the overlap between the nearly zero energy states from the two ends of the nanowire, and second due to the local overlap between the zero energy states at the same end of the nanowire. In Fig. 3, we show that the trivial ZBP disappears as the bulk Zeeman field is rotated by \( \pi/4 \) from the axis of the wire in the plane formed by the wire axis and the direction of the effective spin-orbit field (the \( (x - y) \) plane). This behavior is also fully consistent with the recent experiments [25, 27], which is taken as an argument in favor of the Majorana origin of the ZBP [10].
can produce stable ZBPs above a threshold uniform bulk Zeeman field, even when the system is topologically trivial (sub-band occupancy even). The trivial ZBPs, since they arise from conventional BdG states, are expected to show splitting oscillations with the bulk field \cite{29} similar to the Majorana fermions. Given such strong similarities with the ZBPs observable from the MBSs, the only unambiguous way to distinguish the trivial ZBPs found here (of height $4e^2/h$) from those arising from Majorana fermions (of height $2e^2/h$) is by comparing the (zero temperature) peak height and/or by an interference experiment \cite{41}.

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