Disentangling Majorana fermions from conventional zero energy states in semiconductor quantum wires

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A proposed signature for the Majorana zero-energy quasiparticle predicted to occur in semiconductor nanowires proximity-coupled to an s-wave superconductor is the zero-bias conductance peak (ZBCP) for tunneling into the end of the wire. Recently, it has been shown that, in the presence of a smooth confining potential, nearly ZBCPs can occur even in the topologically trivial phase. Here we show that, for a smooth confinement, the emergence of the nearly ZBCP at Zeeman fields corresponding to the topologically trivial phase is necessarily accompanied by a gap closing signature in the end-of-wire local density of state (LDOS). A similar behavior is found for nearly ZBCPs that appear in the presence of strong disorder. Our results strengthen the identification of the ZBCP observed in the recent Delft measurements, which show no gap-closing signatures, with topological Majorana fermions localized at the ends of the wire.

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Introduction: Majorana fermions \cite{1} are zero energy quantum particles described by hermitian second quantized operators $\gamma^\dagger = \gamma$. The hermiticity of MF operators implies that they can be construed as particles which are their own anti-particles \cite{1,4}. MFs, first introduced in high energy physics as purely real solutions of the Dirac equation \cite{1}, have now been proposed to exist in low temperature systems in the context of fractional quantum Hall (FQH) effect \cite{2,4}, chiral p-wave superconductors/superfluids \cite{6}, heterostructures of topological insulators (TI) and superconductors \cite{7}, and cold fermion systems with artificially generated spin-orbit coupling and Zeeman field \cite{8, 9, 10}. More recently, it has been shown that a spin-orbit (SO) coupled semiconductor 2D thin film \cite{9, 10} or 1D nanowire \cite{10,12} with Zeeman spin splitting and proximity induced s-wave superconductivity can also be used to realize MFs as zero energy end states.

The 1D version of the semiconductor-superconductor heterostructure \cite{10,12} – the so-called semiconductor Majorana wire – is a direct physical realization of the so-called Kitaev model \cite{13} of topological superconductors (TS). For small Zeeman splitting $\Gamma$, the superconductor is in a conventional (proximity-induced) superconducting (SC) state with no MFs, while for $\Gamma$ larger than a critical value $\Gamma_c$, localized MFs exist at the wire ends where the superconducting pair potential vanishes. The semiconductor Majorana wire, which has recently received considerable experimental attention \cite{14, 17}, allows the detection of the zero-energy MF as a sharp zero bias peak in local charge tunneling measurements \cite{10, 18, 20} at experimentally realistic temperatures $T < E_{qp}$ \cite{10} where $E_{qp} \sim 1\, K$ is the quasiparticle gap in the semiconductor wire.

Despite their apparent conceptual simplicity, the zero bias conductance peak experiments do not constitute a sufficient proof of MFs at the ends of topological superconducting Majorana wires. This is because a non-quantized ($2e^2/h$) nearly zero bias peak, such as that observed in the recent experiments \cite{14, 15, 17, 22}, can in principle arise even without end state MFs provided the confinement potential at the wire end is smooth \cite{21}. A non-quantized near zero energy peak at the wire ends has also been shown to occur due to strong disorder, even when the nanowire is in the topologically trivial phase \cite{22}. A diagnostic signature is therefore needed to distinguish the ZBCP arising from MFs from these more conventional near ZBCPs that may appear even in the topologically trivial phase of the semiconductor wire. Here we show that, for smooth confinement at the ends of the wire, the emergence of the near ZBCPs is necessarily accompanied by a signature similar to a closing of the gap (henceforth, referred to as “gap closing signature” even though there is no corresponding quantum phase transition, as the system stays in the topologically trivial phase) in the end-of-wire local density of state (LDOS). In the absence of such a gap closing signature, a zero bias peak is unlikely to result from the soft confinement effect. We find similar results even when the ZBCP appears at the wire ends from strong disorder effects without MFs. These results strengthen the identification of the ZBCP observed in the recent Delft experiments (which find no signatures of gap closing before the emergence of the zero energy peak above a threshold Zeeman field) with topological Majorana fermions localized at ends of the wire.

We consider a rectangular SM nanowire with dimensions $L_x \gg L_y \sim L_z$ proximity coupled to an s-wave superconductor. For an infinite wire, $L_x \rightarrow \infty$, the effective BdG Hamiltonian has the form,

\begin{equation}
H_{nm}(k) = [\epsilon_{nm}(k) - \mu \delta_{nm}] \tau_z + \Gamma \delta_{nm} \sigma_x \tau_z + \alpha \delta_{nm} \sigma_y \tau_z - i \alpha y \delta_{nm} \sigma_x + \Delta_{nm} \sigma_y \tau_y, \tag{1}
\end{equation}

where $k = k_x$ is the wave number, $\sigma_i$ and $\tau_i$ are Pauli matrices associated with the spin-1/2 and
the particle-hole (p-h) degree of freedom, respectively, and we have used the basis \((u_\uparrow, u_\downarrow, v_\uparrow, v_\downarrow)\) for the p-h spinors. In Eq. 11, \(n = (n_y, n_z)\) and \(m = (m_y, m_z)\) label different confinement-induced sub-bands described by the transverse wave functions \(\phi_n(y) \propto \sin(n_y \pi y/L_y) \sin(n_z \pi z/L_z)\), \(\epsilon_{nm}\) describes the SM spectrum without SO coupling, \(\mu\) is the chemical potential, and \(\Gamma = g^\ast \mu_B B/2\) is the external Zeeman field along the \(x\)-direction. The Rashba spin-orbit coupling is \(\alpha = 0.2\) eV\(\AA\) and the effective parameters \(\epsilon_{nm}, q_{nm}, \Delta_{nm}\) are calculated numerically following the procedure described in Ref. [23].

With increasing \(\Gamma\), the SM wire evolves from a non-topological SC state with no MF to a topological SC state with MFs localized near the ends of the wire via a topological quantum phase transition (TQPT) at \(\Gamma = \Gamma_c\). For a single-band nanowire (in this paper by “band” we mean a pair of sub-bands which are degenerate at all \(k_x\)) in the absence of SO coupling and Zeeman field and the chemical potential \(\mu\) is measured relative to the energy of the top occupied band at \(k_x = 0\) and \(B = 0\) the required \(\Gamma\) for the TQPT is given by \(\Gamma = \Gamma_c = \sqrt{\Delta^2 + \mu^2}\) where \(\Delta\) is the proximity induced superconducting pair potential. In the high Zeeman field (\(\Gamma > \Gamma_c\)) side of the TQPT, the MF manifests itself as a sharp ZBCP when charge current is tunneled through the end of the wire [10].Such charge current is qualitatively related to the LDOS at the end of the Majorana wire which in experiments is separated from a normal current lead by a tunnel barrier [14]. The SC quasiparticle gap \(E_{qp}\) induced in the wire must vanish at the TQPT [3] [10] [23]. Such closing of the bulk gap will be visible in the total DOS for the semiconductor wire [24]. In the small Zeeman field side (\(\Gamma < \Gamma_c\)) of the TQPT the system is topologically trivial and there are no zero energy localized MF states at the wire ends. Consequently, in this regime of the phase diagram no end-of-wire ZBCP is expected from end-state MFs.

We consider a 1D nanowire system with four occupied bands (see Fig. 1). We consider two values of the chemical potential, one close to the minimum of the top band and another larger value that cuts both sub-bands of the top-most band. We couple the nanowire to a superconductor and for the confining potential at the wire-end we choose a soft potential. In Fig. 1(b) and 1(c) we show two model forms of the soft potential both of which qualitatively produce similar results. The only difference between the potentials in Fig. 1(b) and 1(c) is that, in case of the former, the nanowire wave-functions can better penetrate through the barrier and can hybridize with the states in the metallic lead. In Fig. 1(d) we show the calculated BdG wave-functions from the top band and one of the lower bands when the chemical potential cuts both sub-bands of the top band (i.e., the system is in the topologically trivial phase even for \(\Gamma \gg \Delta\)).

For \(B = 0\) the states from the lower bands are localized near the nanowire end and for a soft confinement they can penetrate deep inside the barrier potential. For the top band the BdG states can be both localized near the end and delocalized throughout the wire. These features of the BdG states from the various bands remain qualitatively the same even when the applied Zeeman field is increased beyond \(\Gamma \sim \Delta\).

It has been shown recently [21] that even in the topologically trivial phase of the nanowire (\(\Gamma \ll \mu\)) near-zero-energy localized end states are still possible provided the Zeeman field satisfies \(\Gamma \gg \Delta\) and the end-of-wire confinement potential is soft rather than a hard-wall potential. The physics behind these topologically trivial low energy states is as follows: The topological condition \(\Gamma > \Gamma_c = \sqrt{\mu^2 + \Delta^2}\) ensures (in the limit \(\Delta \to 0\)) that only one of the two spin-split sub-bands in the top-most
FIG. 2: (Color online) Dependence of the low-energy BdG eigenvalues on the slope of the the smooth confining potential for a system with $L_x \approx 3\mu m$, $\Delta \mu = 3.5$meV, $\Gamma = 0.65$meV, and $V(x)$ as shown in Fig. 1C. The slope of the confining potential is $\lambda = dV/dx$ and $\lambda_0 \approx 23$meV/µm. The approximately constant contribution from the top band (horizontal red line) corresponds to a state localized near the right end of the wire, which has a hard-wall confinement. The band of the nanowire is occupied.

Such an odd-number of occupied sub-bands is a necessary condition [13] for the emergence of MFs, arising from the top-most occupied band, at the wire ends. The condition $\Gamma \ll \mu$, on the other hand, corresponds to an even number of occupied sub-bands. In this case no MFs are possible because the individual zero energy solutions from the sub-bands are split in energy due to interband superconducting pairing (of order $\Delta$) as well as the confinement potential at the wire ends. In the limit $\Gamma \gg \Delta$ the effects of the interband pairings are suppressed. In this case a weakening of the confinement potential can result in the suppression of the splitting of the zero energy solutions of the uncoupled sub-bands and lead to conventional, topologically trivial, low energy end states at the wire-ends which can manifest as a ZBCP. The condition for such non-Majorana near-zero-energy end states in the semiconductor wire is therefore given by $\mu \gg \Gamma \gg \Delta$.

In Fig. 2 we show the dependence of the low-energy BdG eigenvalues on the slope of the the smooth confining potential for a system with $\mu \gg \Gamma \gg \Delta$. Interestingly, the energies of the BdG states from all the semiconductor bands become vanishingly small with decreasing slope of the barrier potential at the ends of the wire even in the topologically trivial phase with no MFs.

Recently we have shown that [24] for $\Gamma < \Gamma_c$ and $\mu > \mu_c \sim \Delta$ (note that the condition $\mu \gg \Gamma \gg \Delta$ falls in this range), the lowest energy BdG states associated with the top-most band are localized near the wire ends and contribute significantly to the end-of-wire LDOS. For a soft confinement potential the energies of these localized states gradually decrease with increasing $\Gamma$, and for $\Gamma \gg \Delta$ (still in the topologically trivial phase, $\Gamma < \Gamma_c$) they become nearly zero energy states. Interestingly, since in this evolution of the Zeeman field the states always remain localized at the wire ends and contribute significantly to the end-of-wire LDOS, the ZBCP arising from the near-zero-energy end states for $\Gamma \gg \Delta$ must necessarily be preceded by a strong dispersion of the LDOS with $\Gamma$ akin to a conventional gap-closing signature of a TQPT. In contrast, the lowest energy BdG states associated with the top band for $\mu < \mu_c \sim \Delta$ decay near the wire ends. Consequently their contribution to the end-of-wire LDOS is negligible and the end-of-wire LDOS does not reveal the bulk gap closing at a Majorana TQPT ($\Gamma = \Gamma_c$).

To illustrate the distinctions in LDOS between the cases $\mu \gg \Gamma \gg \Delta$ (suitable for producing a non-Majorana ZBCP with a soft confinement potential) and $\mu \ll \Delta$ (suitable for producing MFs with $\Gamma > \sqrt{\Delta^2 + \mu^2}$) we first show in Fig. 3 the dependence of the local density of states (LDOS) integrated over the applied magnetic field for a system with $d\mu = 3.5$meV (i.e., eight occupied sub-bands) and $V(x)$ as shown in Fig. 1C (top panel) and Fig. 1B (bottom). The energy of the states localized at the soft boundary decreases with $\Gamma$ and a zero-bias peak (ZBP) develops. Note that the closing of the gap is clearly visible, as the spatial dependence of the localized states does not change qualitatively with the magnetic field. For a finite confining barrier (see Fig. 1B), it is possible that the states corresponding to the low-energy bands penetrate though the barrier and hybridize with states from the leads, which results in a large broadening (see bottom panel).
FIG. 4: (Color online) LDOS integrated over the barrier region for a system with the chemical potential near the bottom of the forth band ($\Delta \mu = 0$ and smooth confinement corresponding to $V(x)$ shown in Fig. 1B. For $\Gamma > \Gamma_c \approx 0.3\text{meV}$ a ZBP corresponding to the Majorana bound states localized near the finite barrier is clearly visible. Notice the absence of any signature associated with the closing of the quasiparticle gap at the topological quantum phase transition ($\Gamma = \Gamma_c$). The smooth background inside the induced gap $\Delta_{\text{ind}} = 250\text{meV}$ is due to contributions from the low-energy states that penetrate though the barrier and hybridize with metallic states from the leads. Constant field cuts (shifted for clarity) are shown in the right panel.

To illustrate the behavior of the end-of-wire LDOS for a small chemical potential ($\mu < \mu_c \sim \Delta$) of the nanowire, in Fig. 4 we have plotted the LDOS integrated over the barrier region for a system with the chemical potential near the bottom of the fourth band. As discussed earlier, in this case the BdG states from the top band are delocalized in the nanowire and therefore do not contribute significantly to the LDOS. Consequently, the gap-closing signature of the TQPT is not visible in Fig. 4 with increasing $\Gamma$, even though for $\Gamma > \Gamma_c$ a ZBCP appears due to a end-localized MF state. Note also the smooth background inside the induced gap $\Delta_{\text{ind}} = 250\text{meV}$ which is due to contributions from the low-energy states that penetrate though the barrier and hybridize with metallic states from the leads. In Fig. 1 bottom panel we have shown that the BdG states from the lower bands typically have a considerable spectral weight beyond the quantum wire if the barrier potential at the wire-end is smooth. These states are then expected to hybridize with the metallic states in the lead. We have modeled such hybridization by introducing a damping proportional to the spectral weight of the states beyond the wire end. As shown in Fig. 4 the resultant LDOS then shows a considerable background within the induced gap at $\sim 250\text{meV}$ which is reminiscent of the data in Ref. [14]. Since the LDOS at the end of the wire is expected to be related to $dI/dV$, which is the experimentally measured differential tunneling conductance data, we expect that for $\mu < \mu_c \sim \Delta$ the bulk gap closing at the TQPT should not be seen in tunneling conductance measurements although the signature of the MFs would clearly show up in the zero-bias-conductance peak. This is consistent with the available experimental data [14]. Since the ZBCP arising from the non-Majorana end states (for a soft confinement potential) must necessarily be accompanied by a ‘gap-closing’ signature as a function of $\Gamma$, the experimental ZBCP [14], which is not preceded by such a closing of the gap with $\Gamma$, is unlikely to be due to this effect.

For zero bias peaks arising in the topologically trivial phase from strong disorder effects we find similar results. In Fig. 5 (top panel) we show the end-of-wire LDOS as function of the chemical potential for a disordered wire at constant Zeeman field. Near zero bias peaks appear for large values of $\mu$ corresponding to the topologically trivial phase ($\mu$ above $\sim 0.65$ meV). In the bottom panel of Fig. 5 we show the dispersion of the ZBCP with the Zeeman field for a constant value of $\mu$ in the topolog-
ically trivial phase, $\mu = 1\text{meV}$ . Note the appearance of a clear gap closing signature with the Zeeman field before the zero energy peak appears above a threshold magnetic field. The reason for the presence of this signature is that the states contributing significantly to the end-of-wire LDOS (and producing the near-zero energy peak above a certain value of $\Gamma$) are localized near the end of the wire and remain localized near the end even for small values of $\Gamma$ (in particular, for $\Gamma = 0$). With increasing Zeeman field their energies go down but their spectral weight contribution to the end-of-wire LDOS remains nearly the same. Without the clear gap closing signature as a function of $\Gamma$ that precedes the zero energy peak, a ZBCP is unlikely to be due to strong disorder effects.

In conclusion, we show that, for a smooth confinement potential at the ends of a semiconductor Majorana wire, the emergence of a ZBCP for Zeeman fields corresponding to the topologically trivial phase is necessarily accompanied by a gap closing signature in the end-of-wire local density of states. Such a gap closing signature as a function of the Zeeman field is also present when the ZBCP is due to strong disorder effects. In the absence of such a gap closing signature, the ZBCP observed in the recent experiments [14] is unlikely to be due to the conventional zero energy states [21, 22] in the topologically trivial phase with no Majorana fermions.

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