To Close or Not to Close: The Fate of the Superconducting Gap Across the Topological Quantum Phase Transition in Majorana-Carrying Semiconductor Nanowires

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To close or not to close: the fate of the superconducting gap across the topological quantum phase transition in Majorana-carrying semiconductor nanowires

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We investigate theoretically the low energy physics of semiconductor Majorana wires in the vicinity of a magnetic field-driven topological quantum phase transition (TQPT). The local density of states (LDOS) at the end of the wire, which is directly related to the differential conductance in the limit of point-contact tunneling, is calculated numerically. We find that the dependence of the end-of-wire LDOS on the magnetic field is non-universal and that the signatures associated with the closing of the superconducting gap at the Majorana TQPT are essentially invisible within a significant range of experimentally relevant parameters. Our results provide a possible explanation for the recent observation of the apparent non-closure of the gap at the Majorana TQPT in semiconductor nanowires.

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The recently reported observation [1] of a zero bias peak (ZBP) in conductance measurements on semiconductor (SM) nanowires coupled to superconductors (SCs) may represent the first experimental evidence of Majorana fermions (MFs), which are theoretically predicted to exist in topological superconductors [2]. Topological SC states capable of supporting MFs can be realized in SM wires with proximity-induced superconductivity by driving the system through a topological quantum phase transition (TQPT) using a suitably directed magnetic field [3–5]. At the TQPT, the SC gap necessarily vanishes [2–6]. The absence of any signature associated with the gap closure casts serious doubt on the Majorana fermion interpretation of the ZBP in the recent experiment [1].

In this paper, we offer a possible explanation for the observed non-closure of the gap. By solving numerically an effective tight-binding model for multiband nanowires with realistic parameters we show that, in the vicinity of the TQPT, the amplitude of the low-energy states near the ends of the wire may be orders of magnitude smaller than the amplitudes of the localized MFs. Consequently, the contributions of these states to the end-of-wire tunneling conductance and LDOS are essentially invisible, which results in an apparent non-closure of the gap in these quantities. By contrast, the closing of the gap mandated by the TQPT is clearly revealed by other quantities, such as the total density of states (DOS) and the LDOS near the middle of the wire. We also show that this non-closure of the gap is non-universal, being dependent on the behavior of certain low-energy wave functions, and we identify the parameter regimes in which signatures associated with the closing of the gap are present in the end-of-wire LDOS.

In Ref. [2] Sau et al. proposed that a spin-orbit (SO) coupled semiconductor (SM) thin film with Zeeman spin splitting and proximity induced s-wave superconductivity could be used to realize Majorana fermions. For small Zeeman splitting Γ, the semiconductor is in a conventional (proximity-induced) superconducting state with no MFs, while for Γ larger than a critical value Γ_c (corresponding to the TQPT where the SC gap vanishes), localized MFs [6–8] exist at defects of the SC order parameter. In subsequent works [3–5, 9–14] it was shown that in the 1D version of this system – the so-called 'semiconductor Majorana wire', a direct physical realization of the Kitaev model [8] – zero-energy MF states are trapped at the wire ends and protected from regular fermionic excitations by a large mini-gap [3] $\sim E_{qp} \sim 1$ K, where E_{qp} is the proximity-induced bulk SC quasiparticle gap. The semiconductor Majorana wire, which has recently received considerable experimental attention [1, 15–18], allows the detection of the zero-energy MF as a sharp zero bias peak in local charge tunneling measurements [3, 7, 19] at experimentally realistic temperatures $T < E_{qp}$ [3]. Here, we study the signatures of *nonzero* low-energy states in local end-of-wire measurements.

We consider a rectangular SM nanowire with dimensions $L_x \gg L_y \sim L_z$ proximity coupled to an s-wave superconductor. A realistic model of the nanowire that includes the effects induced by proximity to the SC is solved numerically for a set of effective parameters corresponding to InSb following the procedure described in Ref. [20] (see also the supplemental material for technical details). The wire has a cross section $L_y \times L_z \approx 45$ nm $\times$ 50 nm and is characterized by a Rashba spin-orbit coupling $\alpha = 0.2$ eVÅ. An external Zeeman field $\Gamma = g^* \mu_B B/2$, where B is the magnetic field and $g^* = 50$, is applied along the x-direction. We couple the wire to an s-wave SC with a bulk gap $\Delta_0 = 1.5$ meV. The proximity-induced effective pair potential in the SM is $\Delta = 0.25$ meV. With increasing Γ, the wire evolves from a non-topological SC state with no MF to a topological SC state with MFs localized near the ends via a TQPT at $\Gamma = \Gamma_c$. The SC quasiparticle gap induced in the wire *must* vanish at the TQPT [3, 6, 20]. Such closing of the bulk gap is clearly visible in the total DOS, as shown in the top panel of Fig. 1.

The main finding of this paper is that, despite the vanishing of the bulk SC gap at the TQPT, as mandated inflexibly by the

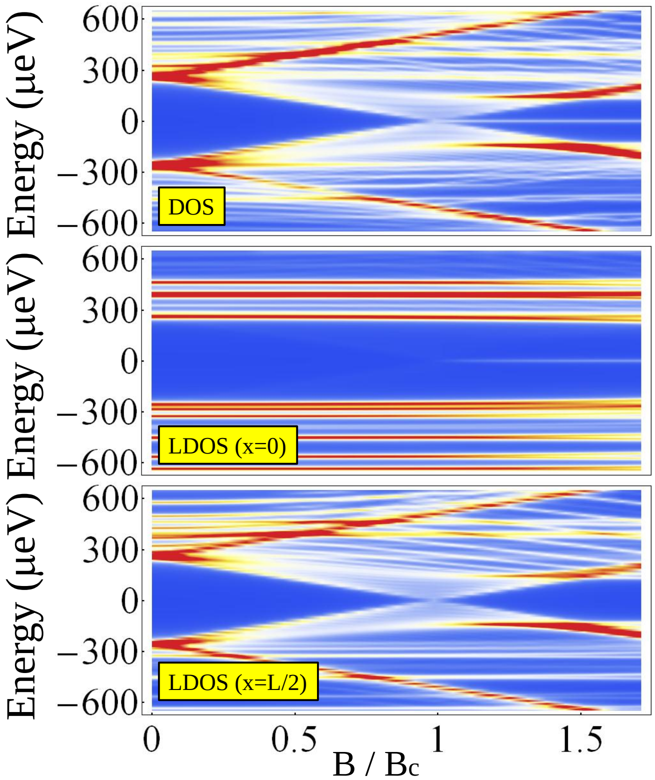

FIG. 1. (Color online) *Top*: Total DOS as a function of B for $\mu = \Delta/2$. The closing of the bulk gap is clearly visible at the TQPT, $B = B_c \approx 0.2$ T. *Middle*: LDOS at the end of the wire as a function of B. The strong features associated with $\Delta \sim 250$ μeV are only weakly dependent on B. For $B > B_c$ a peak associated with the Majorana bound state is present at zero energy. The LDOS shows no visible signature of the bulk gap closing at the TQPT. *Bottom*: LDOS at the middle of the wire. Note the closure of the gap at the TQPT and the absence of the zero-energy Majorana peak. Traces for selected values of B are provided in the supplemental material.

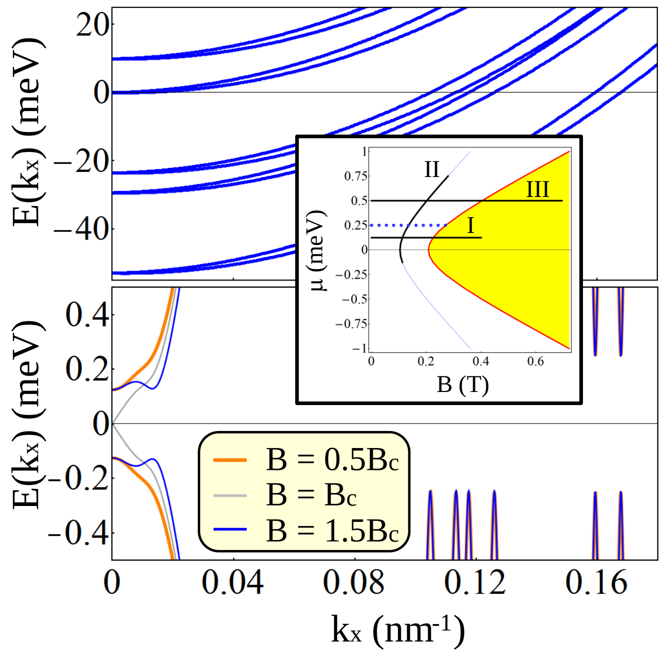

FIG. 2. (Color online) *Top*: Spectrum of an infinite non–superconducting wire. The lowest three bands (six sub–bands) cross the chemical potential at Fermi wave vectors $k_F^{n\pm} > 0.1\text{nm}^{-1}$, while the top occupied band has $k_F^{4\pm} \ll 0.1\text{nm}^{-1}$. The fifth band in unoccupied. *Bottom*: BdG spectrum for three different values of B. The induced SC pair potential is $\Delta = 0.25$ meV. The three lower–energy bands depend weakly on B and have nearly overlapping contributions characterized by six minima at energies ≈ 250 μeV. By contrast, the top occupied band is strongly B–dependent (three distinct curves at $k_x < 0.02\text{nm}^{-1}$) and is characterized by a gap that closes at the critical field $B_c \approx 0.2$ T. *Inset*: Relevant portion of the phase diagram showing the topological SC phase (yellow/light gray) and the topologically trivial phase (white). Fig. 1 corresponds to a cut with $\mu = \Delta/2$ (path I), Fig. 4 is for $\mu = 2\Delta$ (path III), while Fig. 5 corresponds to $B(\mu) = B_c(\mu)/2$ (path II).

theory [3, 6, 20], this gap closure may in fact *not* be visible in charge conductance experiments that aim to probe the end-state MFs. We show this by explicitly calculating the end-of-wire LDOS, which is qualitatively related to the charge current passed through the end of the nanowire coupled to a normal lead [1]. This relation becomes a close correspondence in the limit of point contact tunneling [21]. Since the LDOS can be related more directly to the physics at the microscopic level, we focus on this quantity to shed light on the recent experimental results. We consider a 1D nanowire system with four occupied bands, i.e., four pairs of spin sub-bands, (see Fig. 2, top panel) and a chemical potential close to the minimum of the top band. This is similar to the experimental situation in Ref. 1, where only a few sub-bands are thought to be occupied (results for the single-band case are provided in the supplementary section). Specifically, we have $\mu = \Delta/2$, where the chemical potential is measured relative to the energy of the top occupied band at $k_x = 0$ and $B = 0$. The results are shown in middle panel of Fig. 1. A zero-energy peak is clearly visible above the critical magnetic field B_c, as well as several strong features with energies $\geq \Delta = 250\mu$eV that depend weakly on B. Note that there is no visible signature associated with the closing of the gap at the TQPT. This type of behavior is very similar to the experimentally observed dependence of the end-of-wire differential conductance on the magnetic field [1]. By contrast, the LDOS calculated at the middle of the wire (Fig. 1, bottom) clearly shows the bulk gap closing but no Majorana fermion ZBP for $B > B_c$.

To understand the somewhat unexpected behavior of the LDOS in Fig. 1, we consider a nanowire with a chemical potential close to the bottom of the fourth band. This situation requires a low magnetic field to drive the system into the topological SC state, which is consistent with the experimental conditions [1]. The normal state spectrum of the SM wire (for $B = 0$) is shown in Fig. 2 (top panel). The Bogoliubov-de Gennes (BdG) spectra associated with the four occupied bands are shown in Fig. 2 (bottom panel) for different values of the magnetic field. From the weak dependence on B of the BdG minima associated with the three lower energy bands, it is clear that the prominent and weakly B-dependent finite energy features observed in the end-of-wire LDOS (Fig. 1, middle panel) are associated with these bands. By contrast, the contribution to the BdG spectra associated with the top band (or the 'Majorana band') depends strongly on B. Note that the gap in the top band has a minimum at $k_x = 0$ when $B \le B_c$, vanishes at $B_c \approx 0.2$ meV, then reopens for $B > B_c$. Thus, the low-energy physics in the vicinity of the TQPT and the gap closure at B_c is controlled by the Majorana band, while the bulk gaps at high Fermi momenta associated with the lower bands do not close at the TQPT and depend weakly on B.

Next, we consider a finite wire with $L_x = 4.5\mu$m and focus on the contributions to the LDOS coming from the BdG eigenstates associated with the lower bands. In general, the contribution to the LDOS at the end of the wire coming from a given state n depends on how fast the amplitude of the corresponding wave function $\Psi_n(x)$ increases as a function of x (note that all wave functions must vanish at the wire ends). For wires with confinement energy much larger than Δ, states near the Fermi-level that are associated with the lower-bands have a large kinetic energy $\mu_n^{\rm eff} \gg \Delta, \Gamma$ (see Fig. 2 upper panel), which is the difference between the chemical potential μ and the bottom of the band n. These lower-band states have large Fermi wave-vectors and, consequently, are characterized by amplitudes rapidly increasing away from the ends of the wire. We identify these states as responsible for the weakly magnetic field dependent feature at ≈ 250 μeV in Fig. 1. Note that the lowest energies of the lower-band states have values close to the edge of the bulk gap, which disperses weakly with B and does not close at the TQPT (Fig. 2, bottom panel).

By contrast, states associated with the Majorana band have long characteristic wave-lengths and, consequently, their contributions to the end-of-wire LDOS are strongly suppressed whenever these states are delocalized bulk states characterized by an envelope with a vanishing amplitude near the ends. In general, the lowest energy states associated with the Majorana band also contain a localized component characterized by an envelope that decays exponentially away from the ends of the wire. In the non-topological SC phase, we find that the lowest energy states are delocalized (i.e., have a negligible localized component) when the chemical potential is below a certain crossover value $\mu_c(\Gamma) \sim \mathcal{O}(\Delta)$ (blue dots in the inset of Fig. 2) and localized when $\mu > \mu_c$. This delocalized-localized crossover is relatively sharp, being characterized by an energy scale of order Δ. Also, we emphasize that there are multiple localized-delocalized crossovers characterized by values of the chemical potential $\mu_{c,n}$ slightly above the minimum of each band. The striking difference between the lowest energy states on the two sides of the crossover (for $n = 4$) is illustrated in Fig. 3 (red/dark gray lines). Note that in the topological SC phase ($B > B_c$) the lowest energy state is always a Majorana bound state (yellow/light gray lines in Fig. 3).

The localized/delocalized character of the low-energy states is directly reflected in the end-of-wire LDOS. If the system is in the delocalized regime, $\mu < \mu_c$, the signature of the low-energy states associated with the Majorana band in the LDOS is strongly suppressed. In particular, there is no visible signature of the gap closing at the TQPT. In this case, the dominant features originate from states in the lower bands, with energies

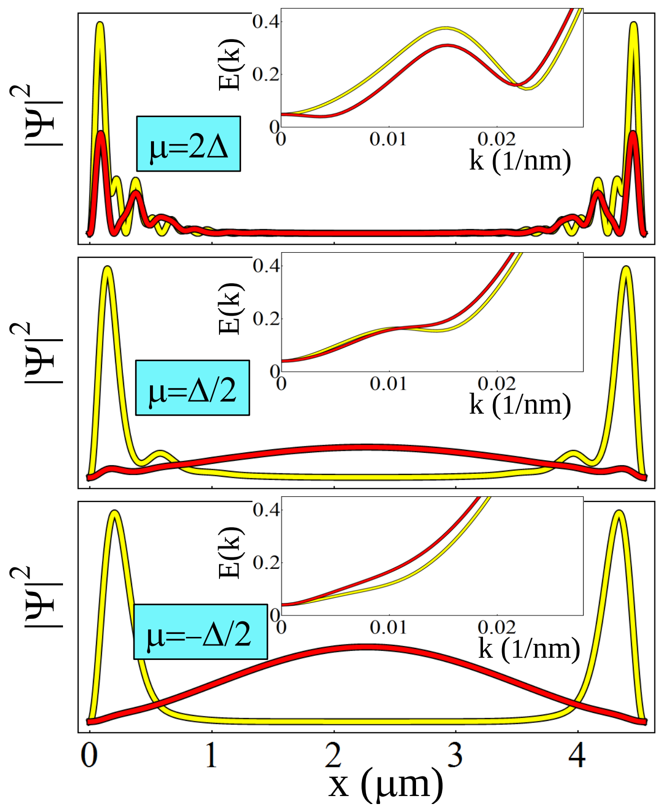

FIG. 3. (Color online) The lowest energy BdG states associated with the Majorana band near the TQPT for different values of μ. The red (dark gray) lines correspond to $B = 0.9B_c$, while the yellow (light gray) curves are for $B = 1.1B_c$. The insets show the BdG spectra for an infinite wire near $k_x = 0$. In the topological SC phase ($B > B_c$), the lowest-energy state is the MF state. In the non-topological SC phase ($B < B_c$), there is a crossover from the region with $\mu > \mu_c \approx \Delta$ characterized by localized lowest energy states (top panel) to the region with $\mu < \mu_c \approx \Delta$ where the states have mostly extended character (middle and bottom panels). The corresponding BdG spectra change from a structure with two minima ($\mu > \mu_c$) to a single minimum at $k_x = 0$ ($\mu < \mu_c$).

$\ge \Delta$ that depend weakly on the magnetic field. Note that for $\mu = 0$, which corresponds to the minimum of the critical Zeeman field $\Gamma_c(\mu) = \Delta$ (see the inset of Fig. 2) and is probably very similar to the experimental conditions [1], the system is in the delocalized region, hence no gap closure at the TQPT is visible in the end-of-wire LDOS. However, this behavior is not universal. Increasing the chemical potential above μ_c will move system into the a region characterized by localized lowest-energy states. Since the energy of the localized states is at the bulk gap edge, the LDOS will contain a feature associated with the gap edge that will depend strongly on the magnetic field and will reveal the gap closure at the TQPT. This situation is illustrated in Fig. 4. We therefore predict that measurements probing other regimes of nanowire parameters may very well observe gap closing signatures, along with the emergence of MFs, depending on the details of the system.

The qualitatively different behavior of the lowest energy BdG wave functions for $\mu < \mu_c \sim \Delta$ as compared to $\mu > \mu_c$

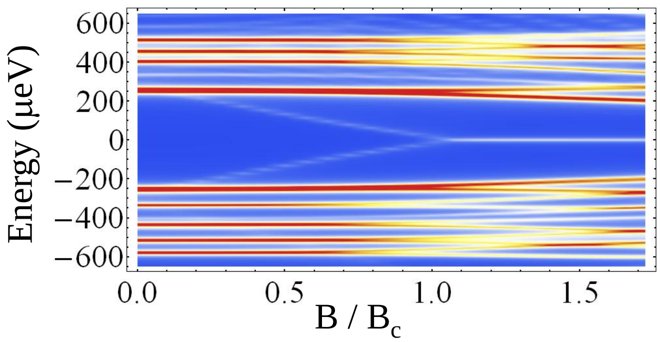

FIG. 4. (Color online) Dependence of the LDOS at the end of the wire on B for $\mu = 2\Delta$. The right panel shows traces (offset for clarity) calculated at different magnetic fields from 0 to 600mT in steps of 25mT. The gap-edge feature stemming from the localized end state clearly reveals the gap closing at the TQPT. For $B > B_c$ the finite energy states are de-localized and, consequently, there is no feature showing the re-opening of the gap.

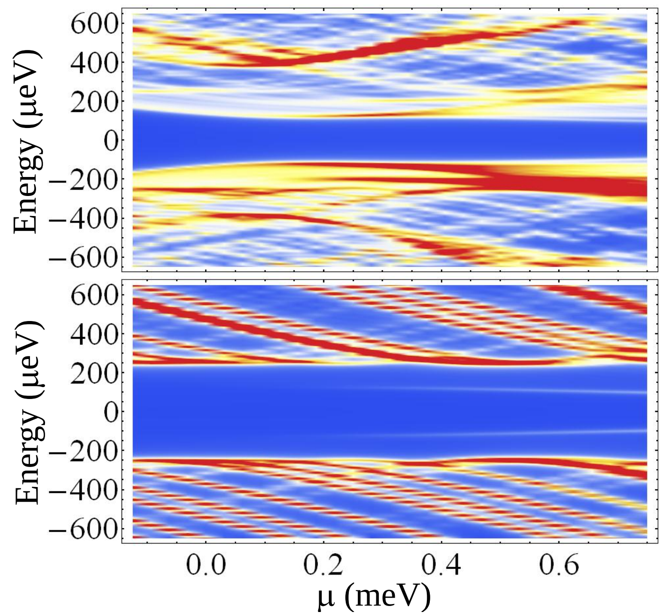

FIG. 5. (Color online) Total DOS (top) and LDOS at the end of the wire (bottom) as functions of μ. The dependence on the chemical potential is along path II (see inset of Fig. 2). The gap is smaller than the pair potential $\Delta = 250$ μeV, as shown by the DOS (top panel). In the LDOS, a feature associated with the gap edge becomes visible only in the localized region, $\mu > \mu_c \approx 250$ μeV (blue dots in the inset of Fig. 2).

can be correlated with the main features of the corresponding BdG spectra. As shown in the inset of Fig. 3 (top panel) the BdG spectrum for $\mu > \mu_c$ has two well defined minima at two non-zero values of k_x. This behavior is similar to that corresponding to the lower three bands (see Fig. 2, lower panel). By contrast, as shown in the insets of the middle and bottom panels in Fig. 3, the BdG spectra for $\mu < \mu_c$ have only a single minimum at $k_x = 0$. In the cross-over region, $\mu \sim \mu_c$, the lowest energy BdG state for the finite wire is a linear superposition of localized and extended states. Because of this clear pattern, we find that for $\mu \gtrsim \mu_c$ the end-of-wire LDOS generically reveal the dispersion of the bulk gap in the Majorana band via the localized end states at the gap edge, while for $\mu < \mu_c$ the end-of-wire LDOS does not disperse with B. This is further illustrated by the dependence of the LDOS on the chemical potential in Fig. 5. Note that the LDOS (bottom panel) shows features corresponding to the bulk gap edge only in the region $\mu > \mu_c$, while it shows no visible signatures associated with the gap edge for $\mu < \mu_c$. We emphasize that this behavior is dictated by the localization properties of the low-energy wave functions in various regions of the phase diagram. These properties are not expected to change qualitatively in the presence of a smooth confining potential [23], finite temperature [24], or weak disorder [25].

We establish that the LDOS in the semiconductor Majorana wire is a non-universal quantity sensitively dependent on the details of the system parameters and that it is entirely possible for the LDOS not to manifest any signature of the SC gap closing through the TQPT. When the chemical potential is in the vicinity of the minimum of an arbitrary band n, we identify a sharp localized-delocalized crossover characterized by a value of the chemical potential (relative to the bottom of band n) $\mu_c \sim \Delta$, where Δ is the proximity induced pair potential. For $B < B_c$ and $\mu > \mu_c$, the lowest energy BdG states associated with the top Majorana band are localized near the wire ends and contribute significantly to the end-of-wire LDOS. Since the energy of these localized states is close to the gap edge, the LDOS reveals the dispersion of the SC gap with B and the eventual closing at the TQPT. By contrast, for $\mu < \mu_c$ the lowest energy BdG states associated with the Majorana band decay near the wire ends. Consequently, their contribution to the end-of-wire LDOS is negligible and the LDOS does not reveal the bulk gap closing at the TQPT. This behavior is robust against disorder, if it is not too strong to destroy the topological phase. In the presence of a disorder potential, the low-energy extended states will become localized inside random segments of the wire, but, typically, will still decay near the ends (see the supplementary section for details). Also, finite temperature will generate broadening effects, but will not shift the spectral weight. Since the LDOS at the end of the wire is related to dI/dV, which is the experimentally measured quantity, we expect that for $\mu < \mu_c$ 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 as a zero-bias-conductance peak. This is consistent with recent experiments [1], which observe no feature associated with the bulk gap closing at $B = B_c$ and yet a ZBP for $B > B_c$. By contrast, charge conductance experiments in the regime $\mu > \mu_c$, or experiments that directly probe the bulk gap [22], should reveal the dispersion of the bulk SC gap and its eventual closing at $B = B_c$. Experiments probing the LDOS at the middle of the wire would reveal signatures of the bulk gap closing through the TQPT, but no Majorana ZBP.

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Note Added: After the original submission of this manuscript, a number of theoretical papers [26–34] appeared addressing various aspects of the experimental work on the possible observation of the Majorana zero mode in semiconductor–superconductor hybrid structures.

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