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Detecting perfect transmission in Josephson junctions on the surface of three dimensional topological insulators

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Abstract
We consider Josephson junctions on surfaces of three dimensional topological insulator nanowires. We find that in the presence of a parallel magnetic field, short junctions on nanowires show signatures of a perfectly transmitted mode capable of supporting Majorana fermions. Such signatures appear in the current-phase relation in the presence or absence of the fermion parity anomaly, and are most striking when considering the critical current as a function of flux \( \Phi \), which exhibits a peak at \( \Phi = \hbar/2e \). The peak sharpens in the presence of disorder at low but finite chemical potentials, and can be easily disentangled from weak-anti-localization effects. The peak also survives at small but finite temperatures, and represents a realistic and robust hallmark for perfect transmission and the emergence of Majorana physics inside the wire.

Keywords: topological insulators, transport in nanowires, Majorana fermions, Josephson junctions, topological superconductivity, perfect transmission
1. Introduction

Three dimensional topological insulators (3DTIs) are materials with a bulk energy gap, supporting surface states with a low energy description of a gapless Dirac fermion, similar to that of graphene [1–6]. Unlike graphene, a 3DTI surface state spectrum may host an odd number of Dirac cones, making it robust to time reversal symmetry conserving perturbations. While the Dirac spectrum has already been identified in experiments, transport signatures of the non-trivial topological properties of the surface state are more ambiguous [7]. A principal reason for this is the large contribution to transport coming from the bulk, which is not truly insulating [7]. It is therefore highly desirable to identify realistic experimental setups and observables that will provide unique signatures of the surface states, and help characterize them.

A topological insulator nanowire threaded by magnetic flux $\Phi = \Phi_0/2$, where $\Phi_0 = h/e$ is the magnetic flux quantum, is predicted to host a perfectly transmitted mode (PTM) [8–11]. This mode is a manifestation of the spin–momentum locking and a direct consequence of the cancellation between two phases: a $\pi$ Berry phase accumulated when an electron encircles the wire, and an Aharonov–Bohm phase due to the presence of flux. Transport measurements have already demonstrated the Aharonov–Bohm effect in nanowires threaded by flux [12–16]. When the PTM dominates transport (for example, at the Dirac point in a long wire), the wire is expected to show a universally quantized conductance of $e^2/h$ [17]. The formation of a PTM in the spectrum occurs since time reversal symmetry is restored at the surface for $\Phi = \Phi_0/2$, but with an odd number of modes (at zero flux the number of modes is even and there is no PTM). As long as time reversal symmetry remains intact, that mode is guaranteed to exist [7].

Transport in the presence of a superconductor (SC) offers a good way to disentangle the bulk and surface contributions, as well as contributions from modes within the surface. Suppression of bulk transport has been observed experimentally [18]. Once the contribution from the bulk is suppressed, Josephson junctions (JJs) can be used to form a discrete set of Andreev bound states on the surface, separated by an energy scale determined by the SC gap $\Delta$. A JJ with a superconducting phase difference of $\phi = \pi$ situated on the surface of a 3DTI is predicted to host a zero energy Majorana bound state [19–21]. Several recent theoretical works target effects associated with this Majorana bound state [22–24]. This zero energy mode is intimately related to the PTM of the normal region, as will become clear in our discussion of equation (2) below: it is only when the normal region has such a mode that the JJ can host a zero energy bound state. If the normal region between two SCs is further gapped (for example, by placing it adjacent to a ferromagnet or terminating the wire altogether), the Majorana modes remain confined at the edge of the SC region [25, 26]. Hence JJs on 3DTI nanowires also constitute a promising pathway for observing effects associated with Majorana fermions.

2. Setup and methods

In this paper, we propose using JJs to explore a surface state behavior unique to 3DTIs. We single out effects associated with the emergence of the PTM and, as a result, zero energy Majorana bound states. The current phase relation (CPR) in the presence of flux through the wire can be a $2\pi$ or a $4\pi$ periodic function, and we show that the $2\pi$ periodic structure displays a
characterizing discontinuity at $\Phi = \Phi_0/2$. Furthermore, the critical current as a function of flux should peak around $\Phi = \Phi_0/2$, obtaining a quantized value at zero temperature. Both features are shown to exist at a finite chemical potential and in the presence of disorder. In particular, the peak shows a remarkable behavior: its presence is unaffected by non-magnetic disorder and its features sharpen with increasing disorder strength. The observation of this critical current peak would provide clear evidence for the formation of the PTM in the junction and a Majorana bound state at a superconducting phase difference of $\pi$.

Consider a 3DTI nanowire placed on top of two superconducting leads as shown in figure 1. Define $y$ to be the circumferential coordinate of the wire $0 < y < W$ and $x$ to be the coordinate along the wire. The Hamiltonian for the surface state of the wire is $H = \frac{1}{2} \Psi^\dagger \mathcal{H} \Psi$, with

$$\mathcal{H} = \begin{pmatrix} h_0 & \Delta \\ \Delta^* & -T^{-1}h_0^* T \end{pmatrix},$$

$\Psi = \begin{pmatrix} \psi_i, \psi_i^\dagger, \psi_j, \psi_j^\dagger \end{pmatrix}$ a Nambu spinor, $\Delta = \Delta(x)$ the induced pair potential, $h_0 = -iv \left( \sigma \partial_x + \sigma \partial_y \right) + V(x, y)$ the two dimensional Dirac Hamiltonian for a particle with Fermi velocity $v$, in the presence of a disorder potential $V(x, y)$, and $T$ is the time reversal operator. For a clean wire, the quantized values of the transverse momenta $q_n$ are determined by the boundary conditions of the Dirac fermion wave functions. In the absence of a magnetic flux through the wire $q_n = 2\pi \left( n + 1/2 \right)/W$ with $n = 0, \pm 1, \ldots$, while in the presence of flux, the boundary conditions are shifted due to the Aharonov–Bohm effect, $q_n = 2\pi \left( n + 1/2 + \phi/\Phi_0 \right)/W$ [17]. When $\Phi = \Phi_0/2$, the set of momentum values contains a state with $q = 0$, and therefore the total number of modes is odd. The SC leads induce a superconducting gap $\Delta$ on the surface of the wire for $x < 0$ and $x > L$, forming a JJ of length $L$. In this paper we consider only short junctions, for which $L \ll \xi$, the SC coherence length. The long junction limit could be studied by generalizing the results of [27].

The transport properties of the wire can be accounted for within a scattering matrix formalism, reviewed in [28, 29] and applied in [30] for studying JJs on graphene. The critical current is obtained by solving the Dirac–Bogoliubov–de Gennes equation for the SC—normal surface state—SC junction with phase difference $\phi$. The energies of the Andreev bound states inside the junction are
\[ E_n = \Delta \sqrt{1 - \tau_n \sin^2(\phi/2)} \]  

(2)

where \( \tau_n \) is the normal state transmission probability for the \( n \)th mode, which in a clean wire is given by [30]

\[ \tau_n = \frac{k_n^2}{k_n^2 \cos^2(k_nL) + (\mu/\hbar)^2 \sin^2(k_nL)}. \]  

(3)

Here \( k_n = \sqrt{(\mu/\hbar)^2 - q_n^2} \) and \( \mu \) is the chemical potential. The Josephson current is given by

\[ I(\phi) = \frac{e}{\hbar} \sum_n \frac{\partial E_n(\phi)}{\partial \phi} = \frac{e\Delta}{4\hbar} \sum_n \frac{\tau_n \sin \phi}{\sqrt{1 - \tau_n \sin^2(\phi/2)}}. \]  

(4)

The transmission probabilities \( \tau_n \) are exponentially suppressed in \( L/W \) for the modes \( q_n \) that render \( k_n \) imaginary. Therefore, tuning the chemical potential (or the ratio \( L/W \)) allows selecting a small number of modes contributing to transport. The possibility of tuning the boundary conditions with the flux now proves to be crucial; when the flux amounts to half a flux quantum, the zero momentum state has perfect transmission, \( \tau = 1 \). The energy for that particular mode remains a function of \( \phi \)

\[ E(\phi) = \pm \Delta \cos(\phi/2), \]  

(5)

and is zero at \( \phi = \pi \) [21]. The two low energy branches in equation (5) represent the standard expression encountered when two Majorana modes hybridize and their energy is split around zero as \( \phi \) deviates from \( \pi \). Note that the fermion parity of the ground state changes as the branches cross. This is known as the parity anomaly [19, 20].

The current equation (4) still holds in the presence of disorder with the transmission coefficients \( \tau_n \) obtained numerically following [31]. The disorder potential is Gaussian correlated

\[ \langle V(r)V(r') \rangle = g \frac{(\hbar y)^2}{2\pi \xi_0^2} e^{-|r-r'|^2/2\xi_0^2}, \]  

(6)

\( \xi_0 \) is the disorder correlation length and \( g \) a dimensionless measure of the disorder strength. The transmission probabilities are all modified by disorder, apart from that of the PTM as time reversal symmetry binds its value to unity. Our data is obtained by averaging over \( 5 \times 10^2 \)–\( 10^4 \) disorder configurations.

3. Results

The PTM has a strong signature in transport. Let us start by considering the CPR \( I(\phi) \), shown in figure 2 for \( \Phi = 0 \) and \( \Phi = \Phi_0/2 \) at a fixed value of \( L/W = 4 \) for various values of \( \mu \). For \( \Phi = 0 \) the CPR is a \( 2\pi \) periodic function, with an exponentially vanishing amplitude at \( \mu = 0 \). As \( \mu \) is increased from zero, more modes acquire a finite transmission probability and the CPR oscillates with a growing amplitude. In contrast, when \( \Phi = \Phi_0/2 \), a finite amplitude is expected for any value of \( \mu \) due to the presence of a PTM. The two sets of curves, figures 2(b) and (c), are distinguished by the systems ability to maintain a fixed parity of the number of fermions at
\[ \phi = (2m + 1)\pi, \quad \text{where} \quad m \text{ is an integer} \ [19, 20]. \]

If the system follows the ground state regardless of its parity (figure 2(b)), the current has a period of 2\(\pi\), and the shape of the low energy band equation (5) forces the current to have a sharp discontinuity at \(\phi = (2m + 1)\pi\). If the fermion parity cannot change as the ground state parity is changing (figure 2(c)), the current contributed by the PTM has a \(\pi/4\) periodicity. In both cases, the contribution of higher energy modes has a period of 2\(\pi\), and the total current will be 2\(\pi\) periodic at large \(\mu\). Note that the system need not be at the Dirac point to have a \(\pi/4\) periodicity in the parity conserving case, or a sharp discontinuity in the case where there is no parity conservation. Both features extend to finite values of \(\mu\).

Given the importance of disorder in current experiments, we now test the robustness of these features. Disorder tends to localize modes that are not protected by time reversal symmetry and diminish their contribution to the supercurrent. Hence the effect of increasing the disorder strength at a fixed and finite value of \(\mu\) is to reduce the value of the unprotected transmission probabilities. Figure 2(d) presents the CPR at \(\Phi = \Phi_\text{D}/2\) for various values of the disorder strength \(g\). Indeed, the amplitude of the current is reduced with disorder until it becomes identical to that contributed by the PTM, and crucially the current discontinuity survives to finite \(g\).
As another hallmark of the PTM appearing at $\Phi = 20$, the most striking differences between the CPR at $\Phi = 0$ and $\Phi = 20$ appears in the critical current at the Dirac point. At $20$ it is finite, while it is exponentially small at $0$. This implies that the critical current as a function of $\Phi$ should peak while approaching $20$, as shown in figure 3. At low disorder, a broad distribution of current emerges, which narrows and converges with increasing disorder strength into a sharp peak of height $e\Delta/2h$ (at the Dirac point the sharp peak is instead broadened but still maintains an exponential form, see inset in figure 3). The right panel of figure 3 shows the critical current in the presence of strong disorder, $g = 2$, for various values of chemical potential. Note the weak anti-localization peaks emerging at $\Phi = 0, 20$ above $\xi_D/h\nu = 1$.

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Figure 3. (Left panel) Critical current as a function of flux at $\nu = 0.5$ for various values of disorder. The peak sharpens with increasing disorder. The inset shows the behavior at $\mu = 0$, where disorder broadens the peak. (Right panel) Critical current as a function of flux for strong disorder $g = 2$ and various values of chemical potential. Note the weak anti-localization peaks emerging at $\Phi = 0, 20$ above $\xi_D/h\nu = 1$.

Figure 4. The product $I_R\theta$ as a function of flux for $g = 2$ and various values of chemical potential. At large chemical potential the product becomes independent of flux.
critical current, appendix A contains a comparison between the right panel of figure 3 and the same data taken at a lower value of \( g \).

Note that the curves in both figures 3 as well as 4 where calculated using equation (4), which was derived for time reversal symmetric systems. While time reversal symmetry is present at zero flux, and is restored at the surface of the wire for \( \Phi = \phi_0/2 \), it is broken for any value of the flux in between. Therefore away from these values, equation (4) provides an approximated solution extrapolating the behavior of the critical current between the two time-reversal symmetric points. A careful study of matching the quantum mechanical wave functions at the interface between the normal and superconducting segments of the wire shows that there is no Andreev reflection at the interface until there is a twist forming in the order parameter, which should occur around \( \Phi = \phi_0/2 \), and until that happens, the conductance should remain exponentially small. Once a vortex forms within the SC part of the wire, the critical current will peak. The precise value of the flux in which the twist forms should be non-universal and depend on energetic considerations that are material dependent. For details on the behavior of Andreev reflection at the interface, see [32].

The appearance of a peak in the critical current and \( IR_N \) at \( \Phi = \phi_0/2 \) reflects the emergence of a PTM. The behavior at finite \( \mu \) and \( g \) can be understood as follows. According to equation (4), for a clean wire at \( \mu = 0 \), the critical current is expected to exhibit a sharp peak of height \( e\Delta/2\hbar \) that drops exponentially as \( \exp\left(-L\left|\Phi/\Phi_0 - 1/2\right|/W\right) \). At finite \( \mu \), the form of the current becomes slightly more involved as the transmission probabilities of the lowest lying modes increases away from \( \Phi = \phi_0/2 \), and thus \( e\Delta/2\hbar \) represents the lowest bound for the peak height and its tails may no longer drop to zero. At low chemical potential, disorder localizes all modes apart from the PTM at \( \Phi = \phi_0/2 \), recovering the sharp exponential peak. This implies that in the real experimental systems, the stark difference between the critical current at the two values of the flux will emerge already at finite chemical potential and will serve as an indication that the PTM dominates transport.

At large values of the chemical potential, the two peaks in \( I_c(\Phi) \) developing around \( \Phi = 0 \) and \( \Phi = \phi_0/2 \) are a direct result of time reversal symmetry recovered at the surface. This is manifested as an increase of the transmission probabilities \( \tau_n \) due to quantum interference of time reversed paths, i.e., weak anti-localization [33]. Evidently, weak anti-localization and the PTM peak can be disentangled by considering \( IR_N \). Hence, an appearance of a peak at \( \Phi = \phi_0/2 \) in \( IR_N \) is a genuine hallmark of the PTM.

4. Discussion and summary

The above calculations show that signatures of the PTM are found in the CPR, and the critical current and \( IR_N \) as a function of flux; we now comment on the effects of stray quasiparticles and finite temperatures. In practice, fermion parity is unlikely to be conserved, resulting in a supercurrent with a period of \( 2\pi \).\(^4\) Hence the discontinuity of the current at low chemical potentials for \( \Phi = \phi_0/2 \) is the most promising unconventional effect in the CPR. As the critical

\(^4\) In fact, even if the crossings at \( (2m + 1)\pi \) are protected, the \( 4\pi \) periodic CPR could be compromised by the low energy branches in equation (5) approaching \( \Delta \) at \( \phi = 2\pi m \), resulting in a decay from the upper to the lower branch. We thank Gil Refael for this observation.
current is unaffected by fermion parity, such considerations are irrelevant for observing the peak at $\Phi_0/2$. At small but finite temperatures, transitions between the two energy branches in equation (5) are expected to occur around $\phi = \pi$ [34]. Since the current contribution of the two branches is equal in amplitude but of opposite sign, such transitions will average the current to zero near $\phi = \pi$. This softens the current discontinuity and renders the critical current peak height temperature-dependent. Assuming temperature is much smaller than $\Delta$, the maximal current drops from $e\Delta/2\hbar$ at $\phi = \pi$ to $e\Delta\sqrt{1 - (T/\Delta)^2/2\hbar}$ slightly away from $\phi = \pi$.5

These predictions should be observable in experiments with currently available materials. To be in the short junction limit, $\xi$ should be larger than $L$. Experimental estimates suggest $\xi$ can reach several hundred nanometers [35], setting an upper bound for $L$. Ideally, the ratio $L/W \lesssim 1$, while $W$ is large enough to support reasonable flux values without destroying superconductivity. For a realistic value of $W = 400$ nm [36, 37], threading a flux of $\Phi_0/2$ through the cylinder requires a field strength of about $0.2T$. The disorder correlation length and the disorder strength are estimated to be $\xi_D \approx 10$ nm and $g = 0.5-1$ [38]. Hence, the crossover value of $\mu^\xi=\xi_D/\hbar\nu$ into the range where many modes acquire finite transmission corresponds to a density of $n \approx 8 \times 10^{10}$ cm$^{-2}$, which is close to densities obtained in gated TI structures [39]. Recent experiments have been carried out at temperatures $T \approx 30$ mK, while the gap size is estimated at about $\Delta = 1$ K, rendering corrections to the peak height small.

To further clarify the experimental value of the proposed system, we point out that the main mechanisms that hinder the identification of effects related to Majorana fermions in other systems do not affect the signatures discussed here. Prominent examples of other proposed signatures of Majoranas include the fractional Josephson effect and the zero-bias anomaly of SC-normal interfaces in helical wires [21, 34, 40–45]. The fractional Josephson effect is sensitive to quasi-particle poisoning interfering with the system’s ability to maintain a fixed fermion parity. The zero-bias anomaly, recently observed in one-dimensional conventional semiconductor nanowires [46, 47], could originate from non-topological sources such as disorder and geometrical effects [48–51]. In contrast, we show that in the present setup signatures of the non-chiral (extended) Majorana bound state exist in the CPR with and without parity conservation, while the appearance of a peak in the critical current is indifferent to quasi-particle poisoning. Furthermore, disorder strengthens rather than obscures the desired signature of the PTM. Recently, transport across a normal-superconducting (NS) interface in a 3DTI nanowire was discussed in [32]. There, it is argued that the formation of Majorana fermions at the interface in the presence of half a flux quantum through the wire (as well as a twist in the order parameter), will be evident from a quantized conductance of $2e^2/h$ as a function of chemical potential. An advantage to the JJ geometry studied here over the NS geometry is that while observing an NS conductance plateau requires efforts to keep the wire in the single mode regime, the peak in the critical current within the JJ should be visible also when several modes reside below the chemical potential.

Finally, we discuss another motivation for studying 3DTI nanowires. Recently, JJs on the surface of 3DTI thin films were studied experimentally [18, 35, 52–55]. Typical length scales for devices made out of thin films are tens of nanometers for $L$, and a few hundred nanometers

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5 A more precise estimate can obtained from [34] using the full functional form of the critical current. The actual power of $T/\Delta$ is slightly lower than 2 at small $T/\Delta$. 
to several microns for $W$. For such small values of $L/W$ we expect effects of the PTM to be overwhelmed by contributions of other modes. In appendix B we take the semiclassical approach for calculating the Fraunhofer diffraction pattern of the critical current in the presence of a perpendicular field, one of the most common measurements used to characterize JJs on thin films. We find that it is identical to the standard pattern, hence such wide junctions may not be an ideal arena to realize theoretical proposals targeting Majorana modes. Alternatively, suggestions for interferometric measurements in the presence of a perpendicular field were made [56, 57], however, those require elements currently not within experimental reach. In contrast, the nanowire geometry allows access to signatures of those low energy degrees of freedom while taking into consideration realistic conditions such as disorder, finite chemical potential, and temperature, using the combination of currently available components.

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Appendix A. Comparing the effect of weak and strong disorder on the critical current as a function of flux through the wire

It is shown in the main text that disorder in 3DTI nanowires has an effect on the critical current through a JJ as a function of flux. Due to the fragile nature of modes not protected by time reversal symmetry, disorder leads to their localization which sharpens the current features that result from the PTM. Hence we expect that for stronger disorder, it would be possible to

Figure A1. Critical current as a function of flux for weak disorder $g = 0.5$ (left panel) versus strong disorder $g = 2$ (right panel). Note the weak anti-localization peaks emerging at $\Phi = 0, \Phi/\Phi_0$ above $\mu_0/\hbar v = 1$ for strong disorder, while for week disorder those emerge already above $\mu_0/\hbar v = 0.2$. 
observe the exponential peak more clearly up to higher chemical potentials. This section compares the effects of weak versus strong disorder to validate our prediction.

Figure A1 contrasts the critical current for $g = 0.5$ and $g = 2$ (the right panel is identical to one appearing in figure 3 of the main text). Qualitatively the same effects emerge for both disorder strengths, although the sharp peak survives to lower values of the chemical potentials with stronger disorder. For $g = 0.5$, the exponential peak disappears at about $\mu_{\xi_0}/\hbar \sim 0.2$, while for $g = 2$ it survives up to $\mu_{\xi_0}/\hbar \sim 1$.

Appendix B. Fraunhofer diffraction pattern for wide JJs on 3D topological insulator films

One of the most common measurements done on planar JJs is that of the critical current as a function of flux through the junction. The critical current displays a diffraction pattern, which for standard junctions with uniform current injection between two S-wave SCs takes the ‘Fraunhofer’ form $I_c(\Phi)/I_c(0) = \left| \sin\left(\pi\Phi/\Phi_0\right) / (\pi\Phi/\Phi_0) \right|$ [58].

To consider the effect of a magnetic flux penetrating a wide JJ junction situated on a thin film of a 3DTI, we generalize equations (2) and (3) of the main text to include the effect of the flux via a semi-classical approach. The effect of the field on the modes in the normal part is neglected such that the current and the transmission probabilities remain the same, while the phase difference between the SC gets shifted and becomes $y$ dependent, $\phi \to \phi - 2\pi \frac{\Phi}{\Phi_0} \frac{y}{W}$, with $\Phi = BLW$ the total flux through the junction. Such an approximation is valid provided the length of the junction is much smaller than the magnetic length $\ell = \sqrt{\epsilon e B / \hbar}$. For current experimental systems and conditions $\mu \ell > 0.5 \text{ m}\mu$, while $L$ is of the order of tens of nanometers, hence the semiclassical approach is appropriate and should capture the physics those junctions display. The $y$ dependence of the superconducting order parameter translates into a $y$ dependent Josephson current, and the total current is obtained by integrating over that current across the junction.

For the case of a wide junction ($W \gg L$) the calculation becomes independent of the choice of boundary conditions determining the values of the momenta $q_n$. We would like to pause here and note the implications of that: in the nanowire geometry extensively discussed in the main text, the boundary conditions had a crucial role in transport, and their manipulation determined whether or not a PTM will be present. Here they play no role, explaining the insignificant role the PTM plays in transport within wide junctions. Here we choose $q_n = \pi/W\left(n + 1/2\right)$, $n = 0, 1, 2, \ldots$ corresponding to the so called infinite mass boundary condition [30]. The Fraunhofer interference pattern as a function of flux is presented in figure B1. In addition to it being identical to the standard pattern, it also appears not to depend on the chemical potential (patterns corresponding to different values of the chemical potential collapse when rescaled by $I_c(\Phi = 0)$).

Fraunhofer patterns in JJ on 3DTIs were measured by several groups [18, 35, 52]. Note that in some measurements already performed in 3DTI, deviations from the standard pattern were observed [18, 35]. For example, for some measurements the minima of the interference pattern do not approach zero [35], but in fact a finite current is measured. A possible explanation is that these residual currents might be flowing through the side surfaces of the thin film (see figure B1) or result from some other inhomogeneous current pattern. For these side
surfaces, the shift in the phase of the order parameter is constant (since the field is parallel to the surface), and hence these will not display an interference pattern, but rather contribute an amount of current which is periodic in $\phi$. Since that piece of the current will not show a diffraction pattern, it will contribute to lifting the nodes of the pattern coming from the top and bottom surfaces. This conjecture can be checked in experiment by tilting the field, thereby having the flux penetrating the side surfaces as well. Other reported deviations from the standard pattern include a periodicity that is different than a single flux quantum, as well as irregular spacings of the zeros of the diffraction pattern [18, 35]. While we find a pattern for which the minima appear at integer multiples of $\phi_0$, it is possible that different length scales in the system (such as the penetration depth for example) are field dependent. Such physics is beyond the scope of our calculations.

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