Supercurrent interference in HgTe Josephson junctions

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(Dated: November 15, 2022)

Wires made of topological insulators (TI) are a promising platform for searching for Majorana bound states. These states can be probed by analyzing the fractional ac Josephson effect in Josephson junctions with the TI wire as a weak link. An axial magnetic field can be used to tune the system from trivial to topologically nontrivial. Here we investigate the oscillations of the supercurrent in such wire Josephson junctions as a function of the axial magnetic field strength and different contact transparencies. Although the current flows on average parallel to the magnetic field we observe h/2e, h/4e- and even h/8e-periodic oscillations of the supercurrent in samples with lower contact transparencies. Corresponding tight-binding transport simulations using a Bogoliubov-de Gennes model Hamiltonian yield the supercurrent through the Josephson junctions, showing in particular the peculiar h/4e-periodic oscillations observed in experiments. A further semiclassical analysis based on Andreev-reflected trajectories connecting the two superconductors allows us to identify the physical origin of these oscillations. They can be related to flux-enclosing paths winding around the TI-nanowire, thereby highlighting the three-dimensional character of the junction geometry compared to common planar junctions.

I. INTRODUCTION

In wires made from a three-dimensional topological insulator (3DTI) the topological surface states form a two-dimensional conducting electron layer that envelopes the bulk. The energy spectrum of these wires features a gap at zero magnetic field which closes when an axial magnetic flux of φ0 = h/2e threads the wire cross section [1][2]. With closing of the gap, a non-degenerate perfectly transmitting mode appears, rendering the wire’s band structure topologically nontrivial. Whereas semiconductor wires with strong spin-orbit interaction are the so far prevailing material platform to search for Majorana bound states (C.29 and references therein), mesoscopic wires made of TI material are a promising alternative [10][16]. Recent experiments utilizing the fractional Josephson effect in HgTe-based Josephson junctions (JJ) indeed provided evidence that the 4π-periodic supercurrents observed for an axial magnetic flux > φ0/4 are of topological origin [17]. In these experiments two superconducting contacts are placed across a HgTe wire with the TI wire constituting the normal region forming a JJ.

So far, semiconductor wires with strong spin-orbit interaction have been the prevailing system class to search for topological superconductivity. The JJ built from such wire structures and their behavior in a magnetic field have been investigated, for instance, in Refs. [18][24]. Related work is also available on JJs made from Cd3As2 [24] or Bi2Se3 [26] wires and (Bi,Sb)2Te3 nanoribbons [27]. Here we investigate the evolution of supercurrent interference in HgTe wire-based JJs as a function of an axial magnetic field. The supercurrent flows between the two superconducting (sc) contacts along the TI and is driven by the difference φ of the superconducting phase between the two contacts. In the presence of an axial magnetic field the supercurrent amplitude oscillates as a result of interference between Andreev bound states acquiring different phases along their quasi-classical trajectory between the sc contacts [28]. In the case of a junction with the magnetic field perpendicular to the supercurrent, the supercurrent oscillations are described by Ic(φ) = Ic(0)[sin(πφ/φ0)/(πφ/φ0)], identical to the Fraunhofer pattern of a single slit experiment. Such a pattern is not expected for the TI-wire JJ mentioned above, since the current flows on average parallel to the magnetic field and the shortest ballistic trajectories should not pick up any phase from the magnetic flux. Remarkably, we find oscillations in the supercurrent which are h/2e, h/4e and even h/8e periodic, thus constituting a highly unusual interference pattern. Below we relate these findings, both experimentally and theoretically in a consistent way, to the three-dimensional JJ-geometry and the coupling of the superconducting contacts to the TI wire.

II. DEVICE PARAMETERS AND EXPERIMENTAL SETUP

We considered 9 devices (labeled A-J, ordered by descending JJ transparency D) made from wafers with an 80 nm thick, strained HgTe film, which is grown on CdTe by molecular beam epitaxy. A thin Cd0.7Hg0.3Te buffer
FIG. 1. **Sample layout, excess current, and critical current vs. magnetic field B.** a, Cartoon of the sample layout showing the HgTe wire and the two Nb contacts which form the Josephson junction. The topological surface states are shown in red. The magnetic field is oriented parallel to the axis of the wires. b, $I$–$V$ trace of nanowire G (black trace) for $B = 0$ at a temperature of 27 mK. For high bias voltages, the slope represents the normal-state resistance $R_N$, while for lower voltages Andreev reflections influence the trace resulting in an excess current $I_{exc} = 2\Delta/e$. The superconducting gap $\Delta$ can be extracted from the curve as the trace starts to deviate from the constant normal-state resistance (red curve) if $eV < 2\Delta \approx 1.8$ mV. With these values the parameter $Z \approx 0.98$ is estimated. Thus, the transparency is given by $D \approx 0.51$. c, Color map of the differential resistance $dV/dI$ of sample G as a function of the current $I$ and the magnetic flux $\phi/\phi_0$ ($\phi_0 = h/2e$). For sample G, $\phi/\phi_0$ corresponds to $B \approx 36$ mT. Superconducting regions are shown in blue. The critical current oscillates with a period $\phi_0/2$, while the side maxima at $\phi = \phi_0$ are most pronounced. d, Color map of the differential resistance $dV/dI$ of sample G up to higher values of the magnetic flux. For $\phi/\phi_0 > 3$, additional maxima appear resulting in a $\phi_0/4$ periodicity.

layer was introduced in between to improve the quality of the samples [29]. Finally, the wafers are capped by Cd$_{0.7}$Hg$_{0.3}$Te and CdTe. Fig. 1a sketches the wafer structure and the device. Typically, the Fermi level $\mu$ is located at the top of the valence band, and surface electrons as well as bulk holes co-exist. The electron density is of order $n_e \sim 10^{11}$ m$^{-2}$. Additionally, In-doping was added to the Cd$_{0.7}$Hg$_{0.3}$Te layers for specific wafers (sample D, G). This increases the electron density up to one order of magnitude, since the Fermi level $\mu$ is shifted to the conduction band. We fabricate the nanowires using electron beam lithography and wet-chemical etching [17, 30].

Due to the wet-chemical etching, the wires have a trapezoidal cross-section. In the following, we use the average width, which typically ranges between 500–700 nm. The wire perimeter is always shorter than the phase coherence length, which is of the order of several microns [30], and transport is thus coherent. The superconducting Nb contacts are placed on the surface of HgTe after removing the capping layers by wet-chemical etching. To enhance contact quality, we clean the HgTe surface by gentle in-situ Ar$^+$-sputtering and add a thin Ti layer ($\sim$ 3 nm), grown in-situ by thermal evaporation, below the Nb. As Nb tends to oxidize, we add a thin layer of Pt to protect the Nb. The distance between adjacent superconducting contacts is between 50 – 240 nm. The samples are cooled down in a dilution refrigerator with a base temperature of 27 mK. The $B$-field is aligned parallel to the wire’s axis so that the magnetic flux through the wire is $\phi = BA$, where $A$ is the cross-sectional area of the wire. The measurements are taken using standard dc techniques, while the dc lines are filtered by $\pi$-filters at room temperature and Ag-epoxy filters [31] as well as RC-filters in the mixing chamber. The differential resistance $dV/dI$ is measured by superimposing the dc bias with a small ac signal using lock-in amplifiers.

The transparency of the superconducting contacts is determined by voltage-biased measurements. An $I$–$V$
TABLE I. Sample transparencies and geometries. Junction width $w$, length $L$ and width $W_S$ of the deposited superconducting niobium fingers for samples A-J, ordered by sample transparency $D$.

<table>
<thead>
<tr>
<th>Sample</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
<th>H</th>
<th>J</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>0.70</td>
<td>0.66</td>
<td>0.64</td>
<td>0.63</td>
<td>0.62</td>
<td>0.57</td>
<td>0.51</td>
<td>0.49</td>
<td>0.43</td>
</tr>
<tr>
<td>$w$ [nm]</td>
<td>450</td>
<td>900</td>
<td>570</td>
<td>600</td>
<td>470</td>
<td>700</td>
<td>700</td>
<td>540</td>
<td>520</td>
</tr>
<tr>
<td>$L$ [nm]</td>
<td>50</td>
<td>160</td>
<td>100</td>
<td>180</td>
<td>65</td>
<td>70</td>
<td>110</td>
<td>40</td>
<td>240</td>
</tr>
<tr>
<td>$W_S$ [mm]</td>
<td>1.3</td>
<td>1.3</td>
<td>1.3</td>
<td>1.3</td>
<td>2.3</td>
<td>4.3</td>
<td>0.6</td>
<td>4.3</td>
<td>0.6</td>
</tr>
</tbody>
</table>

III. EXPERIMENTAL RESULTS

In a Josephson junction, a magnetic field parallel to the current direction is expected to act as a pair-breaker \[37,39\]. In this scenario, the critical current of the device decreases monotonously with increasing magnetic field strength. For some of our devices, however, we found a strong modulation of the critical current $I_C$ as a function of the axial magnetic field $B$. Fig. 1 presents a color map of the differential resistance $dV/dI$ for sample G as a function of current $I$ and magnetic flux $\phi$, threading the cross-sectional area of the nanowire. This device has a critical current $I_C \approx 600 \text{nA}$ and shows the most prominent oscillations of $I_C$. With the width of the wire $w \approx 700 \text{nm}$, one superconducting flux quantum $\phi_0 = h/2e$ corresponds to $B \approx 36 \text{mT}$. Blue regions in the color map illustrate superconducting states. The pattern displays maxima of $I_C$ for $\phi = n \cdot \phi_0/2$ with $n$ an integer, while $I_C$ is fully suppressed in between them. Furthermore, the maxima at multiples of $\phi_0$ are more pronounced than the $\phi_0/2$ maxima. Data of the same device up to higher fluxes is shown in Fig. 2. Here, additional maxima at $\phi = n \cdot \phi_0/4, n \in \mathbb{Z}$ appear. The $h/4e$ periodicity eventually changes to $h/8e$ at higher magnetic fields. The envelope of this pattern can be attributed to the expected pair-breaking mechanism. We note at this point that roughly $h/2e$ periodic oscillations were observed by Stamppfer et al. and ascribed to oscillations of the transmission due to the conventional Aharonov-Bohm effect \[24\]. Nonmonotonic behavior of $I_C(B)$ with multiple nodes and lobes but without clear periodicity were observed in semiconductor nanowire JJs in an axial field \[19,20\]. Only a fraction of the investigated junctions show an oscillatory interference pattern of the critical current as a function of the flux, while the critical current monotonously decreases with the magnetic field for other samples. Even the exact shape and periodicity of the pattern, if it exists, differs for various devices. Therefore, we will analyze the emergence of the $I_C(B)$-oscillations in the following for different experimental parameters like contact transparency and gate voltage.

A. Gated devices

Fig. 2 shows the data of sample J. This device has a critical current $I_C = 136 \text{nA}$ and an average transparency $D = 0.43$, while one flux quantum $\phi_0 = h/2e$ corresponds to $B \approx 50 \text{mT}$. For this sample we also observe $I_C(\phi)$-oscillations. However, only maxima at $\phi = n \cdot \phi_0$ are visible leading to a $h/2e$-periodicity. For more detailed studies, a top-gate was added to the junction. This allows to investigate the $I_C(\phi)$-oscillations as function of the gate voltage $V_G$. The structure of a gated device is sketched in Fig. 3. An insulator made of $\sim 30 \text{nm} \text{SiO}_2$, grown by PECVD, and $\sim 100 \text{nm} \text{Al}_2\text{O}_3$, grown by ALD, was deposited above the junction. The top-gate voltage $V_G$ is applied via a metallic Ti/Au-layer. Fig. 3 shows the critical current $I_C$ as a function of the top-gate voltage $V_G$. By tuning $V_G$ from $0 - 3 \text{V}$, $I_C$ increases by a factor $\sim 1.7$. Fig. 3 illustrates $dV/dI(\phi, I)$ of sample J for $V_G = 3 \text{V}$. Additional maxima appear at $\phi = (2n + 1) \cdot \phi_0/2$ in contrast to the data at $V_g = 0$. Hence, the $h/4e$-periodicity is recovered by increasing $V_G$. This observation emphasizes that the $h/2e$-oscillations are the dominating ones and are observable for any $V_G$. The maxima at $\phi = (2n + 1) \cdot \phi_0/2$ cannot be resolved for $V_g = 0$ due to the low $I_C$ at these positions. By increasing $V_G$, the number of contributing channels increases and the increased $I_C$ enables to resolve $I_C$ at $\phi = (2n + 1) \cdot \phi_0/2$. Compared to sample G, however, $I_C(\phi)$-oscillations with a period $h/8e$ are not observable, although the transparency of the devices are similar. Sample G was fabricated from a doped wafer. Its electron density, and thus the number of transport channels contributing to the signal, is much higher than in the undoped sample J, even when the latter is gated at high voltages. This suggests that for observing higher harmonics in the $I_C(\phi)$-oscillations a sufficiently large number of transport channels is necessary.

B. Influence of the transparency

In addition to differences in geometry, the transparency of the superconductor/nanowire interface is the
The critical current $I_C$ increases for higher gate voltages $V_G$. a, Sketch of the sample layout. An insulator and a metallic topgate is placed on top of the junction. b, The critical current $I_C$ is almost fully suppressed below $V_G = 0$. The critical current oscillates with a period of $\phi_0/2$. d, The corresponding color maps at $V_G = 3\, V$. Additional oscillations of $I_C$ appear recovering the $\phi_0/2$ periodicity.

For sample H, the observed periodicity is approximately 20 percent smaller than what one would expect from geometry. These deviations occur in samples with much wider superconducting contacts (see table I), suggesting that the larger contacts might affect the flux distribution in the junction.

Based on these experimental observations we conclude that the transparency $D$ is the most influential parameter that determines whether $I_C(B)$-oscillations occur or not. The oscillations appear preferentially for samples with low average transparency, while they are fully absent for high transparencies.

IV. THEORY

To proceed we summarize the desiderata and key aspects of the physical problem from a more theory-oriented point of view:

(i) there must be sufficiently many open surface channels between the two superconducting electrodes to ensure a fairly high $I_C$;
(ii) a number of open channels must be sensitive to the flux threading the nanowire cross-section, otherwise no $\phi$-periodicity would show up;
(iii) imperfect contacts, representing barriers for the transport electrons, suppress contributions from flux-insensitive channels relative to flux-sensitive ones.

Based on these premises we first define the model geometry, sketched in Fig. 3 and introduced in detail below. An assumption that will turn out to be critical is that the Nb fingers induce superconductivity only close to the contact regions (shaded green areas in Fig. 4), i.e. the nanowire
FIG. 3. Impact of sample transparency on $I_C(B)$-oscillations. Color maps of the differential resistance $dV/dI$ as a function of the current normalized $I/I_c$ and the magnetic flux $\phi/\phi_0$ for different samples. The color maps are ordered by decreasing transparency of the junctions, with the highest transparency shown in (a) to the lowest in (i). a, b, Samples A and B with high transparency ($D \approx 0.70$ and $D \approx 0.66$) show no oscillations as a function of the magnetic field. c, d, e, Intermediate transparencies in samples C, D, E ($D \approx 0.64, D \approx 0.63,$ and $D \approx 0.62,$ respectively): the shape of the critical current contour starts to deviate and first nodes and antinodes are observable. f, g, h, i, Samples F - J with the lowest transparencies ($D \approx 0.57$ to $D \approx 0.43$) show distinct oscillations as a function of applied magnetic field.

bottom surface remains normal conducting[40]. We will later demonstrate that modes formed by Andreev retroreflection (partially) winding around the circumference of the 3DTI nanowire pick up an Aharonov-Bohm phase and lead to the experimentally observed supercurrent oscillations. To reach our conclusions we combine semiclassical analytics with tight-binding numerical simulations. Semiclassics allow us to identify the fundamentals of the transport problems in terms of families of electronic paths which enclose (or do not enclose) a magnetic flux. This picture is validated by rigorous quantum transport simulations based on a tight-binding implementation of the corresponding Bogoliubov-de Gennes (BdG) Hamiltonian, see below. Our analysis shows that the relevant aspects of the problem are geometrical (non-planar surface conduction, winding vs. straight propagation, nanowire perimeter not fully superconducting), while the Dirac or trivial (quadratic) nature of the carri-
count for the fact that the supercurrent oscillations appear in the less transparent junctions; see Fig. 3. Indeed, the barriers turn out to be essential for the observation and understanding of the supercurrent oscillations with a flux-periodicity of $h/4e$. The reason for their presence lays in the fabrication process itself. Foremost, an incomplete removal of the capping layer induces a barrier at the interfaces between Nb and HgTe. These complex interface physics are simplified, but essentially captured, by the local delta barriers.

Starting from this geometrical model the JJ system is quantum mechanically described by the Bogoliubov-de Gennes Hamiltonian

$$H = \left( \frac{\hbar c \Delta e^{i\varphi}}{\hbar} \right),$$

where $\hbar$ and $\hbar c$ describe the electron and hole Hamiltonians and $\Delta$ and $\varphi$ denote the absolute value and phase of the pairing potential.

The topological surface states are described by the Dirac model Hamiltonian

$$h_{c/h} = \pm \hbar v_F \left[ \hat{k}_s \sigma_x + \left( \hat{k}_s \pm \frac{\varphi}{\phi_0 P} \right) \sigma_y \right] \mp \mu \pm U,$$

the upper (lower) sign denoting the electron (hole) Hamiltonian. Here, $z$ and $s$ are the coordinates along the wire axis and along the perimeter, and $\hat{k}_x$ and $\hat{k}_s$ the respective momentum operators. Furthermore, $\mu$ is the chemical potential and $U$ denotes the barriers at the NS-interfaces, see also below.

Only the nanowire surface in direct contact with the superconductor, shaded green in Fig. 3, is affected by the proximity effect. Its bottom surface, grey in Fig. 4, remains normal. Accordingly, the absolute value of the pairing potential is modelled as follows:

$$\Delta = \begin{cases} \Delta_0 & \text{for } 0 \leq s \leq C \text{ and } -W_S \leq z \leq 0, \\ \Delta_0 & \text{for } 0 \leq s \leq C \text{ and } L \leq z \leq L + W_S, \\ 0 & \text{otherwise}. \end{cases}$$

Furthermore, we assume that the thickness of the Nb contacts is much smaller than the London penetration depth of Nb such that no supercurrent develops around the perimeter and the magnetic field is not screened. Thus, the Hamiltonian (2) has to be defined in an gauge invariant way. To ensure this the superconducting phase $\varphi$ is defined only in the regions $W_S \leq z \leq 0$ and $L \leq z \leq L + W_S$, satisfies

$$\varphi = \begin{cases} -\frac{1}{2} \varphi_0 + 2\pi \frac{z}{P} & \text{for } -W_S \leq z \leq 0, \\ \frac{1}{2} \varphi_0 + 2\pi \frac{z}{\phi_0 P} & \text{for } L \leq z \leq L + W_S, \end{cases}$$

and the unitary transformation $V(\varphi)H(\varphi)V^\dagger(\varphi) = H(0)$ holds for

$$V(\varphi) = \exp \left( i\pi \frac{\varphi}{\phi_0 B} \tau_z \right).$$

FIG. 4. Geometry of the system used in the theoretical model. The upper panel shows a 3D sketch of the nanowire Josephson junction while the lower panel is a 2D sketch of the rolled out and periodically continued nanowire surface. Regions with induced superconductivity are shaded green, normal conducting regions gray. Superconductivity is not induced around the whole circumference, the bottom area is still considered as normal conducting. Additional barriers used in the model are marked as vertical orange lines in the lower panel. The different type of retro-reflecting paths arising from our semiclassical analysis, Sec. [IVB], are shown in red, purple and blue, respectively.

A. Geometry and Model

The upper panel of Figure 4 shows the model geometry of the 3D nanowire JJ and the lower panel its unrolled surface. In the figure, $w$ and $h$ denote the nanowire width and height, $L$ the junction length, and $W_S$ the width of the superconducting contacts. We also introduce the perimeter $P = 2w + 2h$ and the interfacial boundary $C = w + 2h$ which describes the length of the perimeter covered by the superconducting contacts.

In our model we include phenomenological delta-like barriers at the interfaces between normal and superconducting parts in the transverse direction only, i.e. along the perimeter, i.e.,

$$U(z, s) = U_0 \Theta(s) \Theta(w + 2h - s) \delta(z) + \delta(z - L).$$

The barriers are marked in orange in Fig. 4. They seem to play a secondary role.
The transformation also modifies the boundary condition of the wave function,
\[(V \Psi)(s + P) = \pm \exp \left( -i \pi \frac{\phi}{\phi_0} \tau_z \right) (V \Psi)(s),\] 
necessary for the calculation of the Andreev bound states.

Note that Eq. (3) for \( \varphi \) can also be derived using Ginzburg-Landau theory: The free energy density is proportional to the supercurrent \( J_s = -2(\epsilon s / m)(h \nabla \varphi + 2eA) \). Minimizing \( J_s \) leads to \( \nabla \varphi = -2eA / h \) [33,45].

### B. Semiclassical analysis

#### 1. Method

A semiclassical approach is justified in the limit \( k_F L \gg 1 \), which is fulfilled in our system, see Sec. [IV.D]. We thus follow the procedure from Ref. [28]. First we identify all classical self-retracing trajectories \( \Gamma \) that arise from pure retro-reflections at the left and right NS contacts. Such trajectories are thus composed of electron-like and hole-like path segments. Each trajectory \( \Gamma \) is then assigned a wave mode bound to a small tube of width \( \lambda_F = 2\pi / k_F \) and contributes a current of \( j(\Gamma) \) to the total current. The total current follows by integrating the contributions \( j(\Gamma) \) over all paths \( \Gamma \) at the Fermi surface. Choosing a cut \( z = z_{\text{cut}} \) through the normal part, the paths can be characterized by the \( s \) coordinate along this cut and the axial wave number \( k_s \) such that the integral reads [28]

\[ I = \frac{1}{2\pi} \int ds \int dk_s j(s, k_s) \]
\[ = \frac{k_F}{2\pi} \int ds \int d\theta \cos(\theta) j(s, \theta), \] (8)

with \( \theta \) the path angle with respect to the \( z \) direction.

The expression (8) contains a significant simplification: It does not account for specular normal reflection at the NS interfaces, which would modify the definition of the current in terms of paths. The inclusion of additional paths from such normal reflections substantially complicates the calculations of \( j(\Gamma) \) and \( I \) and requires the use of resummation techniques beyond the scope of this work. Moreover, we will establish \textit{a posteriori} via quantum mechanical simulations that only perfectly retro-reflected paths are particularly important. Note also that there is no bending of the paths due to the \( B \)-field, since the Lorentz force points perpendicular to the nanowire surface. Finally, for simplicity we stick to the short junction limit, \( L \ll \xi = \hbar v_F / \Delta_0 \), although we expect our findings to qualitatively hold for long junctions as well.

#### 2. Classification of the trajectories

The classical trajectories can be divided into different categories. First, we can assign a “crossing number” \( n \) to each path which counts the crossings through the non-proximitized bottom surface. Formally, one can define a line cut \( s = s_{\text{cut}} \) with \( C < s_{\text{cut}} < P \) and count the (directed) crossings through this cut. We emphasize that this integer \( n \) does not correspond to a proper winding number around the perimeter. It only counts the transverse crossings of the non-proximitized bottom surface.

Second, we can group the paths according to their start and end points, see Fig. [4]

1. **Type-1 paths** start and end on the \( z = 0 \) and \( z = L \) NS interfaces;

2. **Type-2 paths** are “mixed” paths, where start and end points are located on a \( z = \text{const} \) and a \( s = \text{const} \) interface;

3. **Type-3 paths** comprise paths with start and end points on the \( s = 0 \) and \( s = C \) interfaces.

Type-2 paths can be further subdivided into type-2L and type-2R paths, where type-2L paths start on the \( z = 0 \) interface and type-2R paths end on the \( z = L \) interface. It is important to notice that type-2 and type-3 paths only exist for \( n \neq 0 \), in other words there are only type-1 paths with \( n = 0 \).

For given initial coordinates \((s_0, z_0)\) and final coordinates \((s_1, z_1)\), the trajectories are parametrized as

\[ s(t) = s_0 + t \frac{k_s}{k_F} \quad \text{and} \quad z(t) = z_0 + t \frac{k_z}{k_F}, \] (9)

where the wave numbers satisfy

\[ \frac{k_z}{k_s} = \frac{z_1 - z_0}{s_1 - s_0} \quad \text{and} \quad k_z^2 + k_s^2 = k_F^2. \] (10)

#### 3. Current contributions

To calculate the current contribution \( j(\Gamma) \) for each classical trajectory \( \Gamma \), we employ the scattering matrix formalism introduced by Beenakker for 1D Josephson junctions [46]. In the short junction limit \( L \to 0 \), one gets for the energies of the the Andreev bound states (ABS) [46,47]

\[ E = \pm \Delta_0 \sqrt{1 - \tau \sin^2 \left( \frac{\phi}{\phi_0} - \gamma \right)} \] (11)

Here, the gauge-invariant phase difference \( \phi_0 - 2\gamma \) appears [43], where

\[ \gamma = \frac{e}{\hbar} \int_{\Gamma} ds \cdot A = n\pi \frac{\phi}{\phi_0}. \] (12)

is the Aharonov-Bohm (AB) phase of the classical trajectory. In Eq. (12) the parameter \( \tau \) depends on the transparency and is different for the different types of
paths. For zero temperature, the current contribution reads

$$j = \frac{e \Delta_0}{4\hbar} \frac{\tau \sin(\varphi_0 - 2\gamma)}{\sqrt{1 - \tau^2 \sin^2(\varphi_0/2 - \gamma)}},$$

(13)

approaching in the limit $\tau \to 1$

$$j = \frac{e \Delta_0}{2\hbar} \sin \left(\frac{1}{2} \varphi_0 - \gamma\right) \text{sgn} \left[\cos \left(\frac{1}{2} \varphi_0 - \gamma\right)\right],$$

(14)

where \(\text{sgn}\) is the sign function. For the different types of paths, one obtains different $\tau_m$, namely

$$\tau_1 = \frac{1}{\sin^2(\varphi_N) + X^2 \cos^2(\varphi_N)},$$

$$\tau_2 = \frac{1}{1 + Z^2(1 + Z^2)^{-1} \tan^2(\theta)},$$

and

$$\tau_3 = 1$$

(16)

with the dimensionless barrier strength $Z = U_0/\hbar v_F$.

The parameters $\varphi_N$ and $X$ are given by

$$\varphi_N = 2 \arctan \left(\frac{\cos(\theta) + Z \tan(\theta)}{\sin(\theta) - (1 + Z^2 + Z^2 \tan^2(\theta))^{1/2}}\right),$$

(17)

and

$$X = [1 + 2Z^2(1 + Z^2)^{-1} \tan^2(\theta)].$$

(18)

C. Numerical simulations

Besides the semiclassical approach we also employ numerical tight-binding simulations with the Python package Kwant. Using the finite difference method, the BdG Hamiltonian Eq. (2) and its components, consisting of nontrivial surface states with a linear dispersion Eq. (6), are evaluated on a discrete square grid with lattice constant $a$. Note that by putting the Dirac Hamiltonian on a lattice, the well known Fermion doubling problem arises. This issue can be circumvented by considering an additional Wilson mass term $H_W = E_W a/(4\hbar v_F)(k_x^2 + k_y^2)\sigma_z$ [49], which gaps out the artificial Dirac cones at the borders of the first Brillouin zone. This term is important to avoid non-physical inter-valley scattering introduced by the potential barriers $U(z,s)$, Eq. (1), in the JJ. Also, regarding these delta barriers, one has to appropriately scale the amplitude for the discrete representation. This is achieved by fixing $U_0 = U_0/a$.

Connecting the lattice sites with coordinates $(z,s = 0)$ and $(z,s = P)$ by a hopping with phase factor $\exp(i\pi \gamma)$ we introduce anti-periodic boundary conditions. Moreover, the flux through the wire cross section is accounted for by a Peierls substitution with the additional phase factor $\exp(2\pi a/\sigma z \phi)$. Finally, superconductivity is introduced as simple onsite s-wave pairing given by Eq. (4). For the numerics we assume semi-infinite leads, i.e. $W_s \to \infty$, because we directly attach translationally invariant superconducting leads to the normal JJ part to keep the numerical cost to a minimum. Additionally, we consider the local phase modulation of $\Delta$ introduced in Eq. (5).

To access the current-phase relation and incorporate all geometrical junction details we compute the supercurrent following Ref. [55]. Furthermore we exploit part of the code package provided in a repository of Ref. [19], and adapt it to our implemented tight-binding model. The core of the numerical method is the computation of the current-phase relation via Green’s functions. The supercurrent is given by

$$I_{LR}(\varphi_0, \phi) = 2 \frac{e k_B T}{\hbar} \sum_{n = 0}^{\infty} \sum_{i \in R} \sum_{j \in L} \text{Im} (H_{ij} G_{ij}^r(i\omega_n)) \sum_{i \in R} \sum_{j \in L}$$

(19)

where $\omega_n = \frac{k_B T}{\hbar}(2n + 1)\pi$ are fermionic Matsubara frequencies. The labels $i$ and $j$ run over lattice sites in two adjacent transversal lattice rows $R$ and $L$. In Eq. (19) the terms $H_{ij}$ and $G_{ij}$ denote the hopping matrix elements and the off-diagonal elements of Green’s function, respectively, connecting those sites. Furthermore, the phase difference $\varphi_0$ is incorporated into the hopping matrix elements as a phase factor. This is simply introduced by performing a gauge transformation that shifts the phase difference into a vector potential inside the JJ. For more details of the methodology we refer the reader to Refs. [19] [28]. For a fixed magnetic flux, the critical current is

$$I_c(\phi) = \max_{\varphi_0} |I_{LR}(\varphi_0, \phi)|,$$

(20)

i.e., the maximum of the corresponding current-phase relation.

D. Semiclassical and numerical results for the critical current

We are now in a position to combine semiclassics and quantum mechanical simulations to explain the central experimental findings for the critical current reported in Sec. III. For the realistic JJ setup discussed in Sec. IV A we choose the following parameters to model the SNS-junction geometry, see Fig. 3: $w = 300 \text{ nm}, h = 80 \text{ nm}, L = 100 \text{ nm}, W_S = 1000 \text{ nm}, \ h v_F = 330 \text{ meV nm}, \mu = 30 \text{ meV},$ and $\Delta_0 = 0.8 \text{ meV},$ in accordance with Refs. [17] [30] [56]. The corresponding Fermi wave number is $k_F \approx 0.09 \text{ nm}^{-1}$, i.e. the Fermi wavelength $\lambda_F \approx 70 \text{ nm},$ and $k_F L \approx 10$. Hence, the semiclassical limit ($k_F L \gg 1$) is well justified. Since the coherence length reads $\xi \approx 400 \text{ nm},$ working in the short junction limit is also justified. In the semiclassical calculations we include only paths with crossing numbers $n = 0, \pm 1,$ since their angle $\theta$ is small and maximizes the cos $\theta$ factor in
the integral $\int$. Paths with higher crossing number $|n|$ have lower weight, and indeed we checked that including them modifies our results only marginally. Furthermore, higher-crossing paths quickly approach the coherence length cutoff, i.e. phase coherence is lost before the electron crosses the junction. The value of $\mu$ is chosen to have a high number of open channels while still keeping the numerical simulations in an energetically converged regime.

Numerical and semiclassical results for the critical current are shown and compared to each other in Fig. 5. On the whole the numerics (left panel) and semiclassics (right panel) show qualitative agreement. It is convenient to start by looking at the numerics, which show peaks only at integer values of $\phi_0 = h/2e$ in the case of perfect interface transparency, i.e. without any barrier ($U_0 = 0$). We note that in high transparency samples no oscillation was measured at all. Our theory model predicts no oscillation for fully proximitized systems, which is indeed more likely when the NS junction is good. In a fully proximitized nanowire there is no phase variation around the perimeter, except in integer multiples of $2\pi$, describing a vortex. Without any kind of accounting for the vector potential in the superconducting phase, the gap and thereafter also the critical current will show just an exponential decay.

For increasing barrier strength $U_0$, the interfacial transparency $\tau_{1,2}$ decrease, leading to an overall reduction of the critical current. At the same time, with increasing $U_0$ new maxima emerge and grow at fluxes $\phi = h/4e = \phi_0/2$ and $3h/4e = 3\phi_0/2$, reaching a peak height of nearly one half the major peaks (for $U_0 = 600 \text{ meV nm}$).

The semiclassical results from the right panel of Fig. 5 show a corresponding trend: a decreasing critical current with increasing barrier height and the emergence of additional peaks at $\phi = h/4e$ and $3h/4e$. In the semiclassical calculation the dominant peaks arise mainly from the short lead-connecting trajectories marked as type-1 paths with crossing number $n = 1$ in Fig. 4. Upon increasing the barrier height contributions from such type-1 paths are suppressed relative to those from type-2 and type-3 paths with $n = \pm 1$, since the former involve two barrier reflections while the latter only one, or none at all. For instance, the current associated with type-3 paths is not influenced by the barrier at all. The growing relevance of paths with $n = \pm 1$ and no barrier reflection leads to the emergence of the peaks at $h/4e$ and to their increase relative to the peaks at $h/2e$.

To conclude the comparison, semiclassical and numerical results agree on the fundamental aspects: they both predict the emergence of peculiar $h/4e$ peaks for larger barrier strength $U_0$, the increase of their magnitude relative to the $h/2e$ peaks, and the broadening of all peaks with increasing $U_0$.

A few differences between them, however, remain: Numerics give a considerably smaller value of the current, and the peak current also decreases faster with increasing barrier strength $U_0$. With regard to this, first note that the actually induced "effective" gap of each of the ABSs as obtained in the numerical calculations is smaller than $\Delta_0$; see App. A for a detailed discussion. To fix this issue in the semiclassical calculation, one would need to introduce an effective gap $\Delta_{\text{eff}} < \Delta_0$ (possibly different for each mode). Second, as mentioned in Sec. IV B 1 the semiclassical method neglects contributions from paths with normal specular reflection. We expect the resulting effects to reduce the current further, as more normal electron reflection reduces the contribution of Andreev reflection. Furthermore, numerics is not limited to the short junction limit, and in fact fully captures effects of finite length and finite temperature. For shorter junctions the
difference between the semiclassical and numerical current magnitude is indeed smaller, an explicit hint that the short junction assumption of semiclassics loses accuracy for longer systems.

To conclude the theory discussion, the semiclassical approach is approximate but enables us to interpret the different peculiar peaks in terms of specific (quantized) relevant families of trajectories. The emergence of the additional peaks related to paths (partially) winding around the nanowire highlights the three-dimensional character of the SNS junction geometry, compared to common planar junctions.

V. COMPARISON OF EXPERIMENT AND THEORY

We finally compare the experimentally measured critical currents with the corresponding theoretically calculated results. Consider first samples with a high average transparency, which can also be modeled in the framework of the effective surface model. As mentioned in Sec. IV A a high quality NS interface should allow for superconducting pairing to be induced across the entire nanowire perimeter. This implies that no phase variation around the perimeter as given by Eq. 5 can develop, and the Andreev bound states states become similar to those of planar Josephson junctions. In such a scenario the magnetic field is simply destroying pair correlations, and the superconducting gap decreases monotonically with increasing field strength. As a consequence the critical current decays exponentially without any oscillation, as indeed measured in high-transparency samples.

On the contrary, flux periodic supercurrent oscillations are observed in samples with low average transparency. In Sec. IV A we argued that the junction transparency might be reduced due to an imperfect removal of a capping layer, which lowers the interface quality between the superconducting Nb and HgTe. The imperfect interface was modelled both semiclassically and numerically via barriers of varying strength, whose presence suppresses the large current contributions which have no or only a $\hbar/2e$ periodicity. Vice versa, the $\hbar/4e$-periodic current components are not affected and their signatures emerge, providing a clear explanation for the observed behaviour of low-transparency junctions.

Irrespective of the sample quality, all measurements show also a decrease of the current for increasing magnetic field. This is expected and attributed to the reduction of the induced superconducting gap by the magnetic field $\hbar/8e$ which weakens pairing correlations. One can phenomenologically account for this behavior by multiplying the theoretical data with an appropriate envelope function, mimicking the weakening of the BdG pairing amplitude $\Delta_0$ of Eq. (4). An example is shown in Fig. 6 where we assumed a simple exponential decay of the pairing potential with respect to the applied flux. The data was numerically computed with the same system parameters as for Fig. 5, except that the length was increased to $L = 200 \text{ nm}$ to better match the experimental dimensions. The blue curve is the raw simulation data, while the orange one is adjusted with the phenomenological flux-induced decay. The adjusted critical current exhibits all qualitative features of the experimental curve plotted in Fig. 3g. In particular the peak at $\phi/\phi_0 = 1$ is larger than the first half-integer one.

We further remark that also oscillations with a period of $\hbar/8e$ were observed in sample G. From the semiclassical model such a periodicity is to be expected if paths with crossing number $n = \pm 2$ contribute considerably to the current flow. This should be possible in the presence of a large overall number of conducting channels, with sufficiently many belonging to the $n = \pm 2$ family to make their signature visible – recall that such paths are identified by a large angle $\theta$, such that the weight of a single path in Eq. (5) is usually very low. This agrees with the observation that sample G has indeed the highest number of open transport channels. Our argument is also in line with the behavior from sample J: A gating potential of $V_G = 3 \text{ V}$ has to be applied to the junction, such that the $\hbar/4e$ periodic oscillations can be measured. The gating potential increases the Fermi energy, ergo the number of open transport channels. As a consequence the contribution of type-2 and type-3 paths grows and maxima at $\phi = (2n + 1) \cdot \phi_0/2$ appear.
VI. CONCLUSIONS

We realized Josephson junctions made of HgTe 3D topological insulator nanowires and demonstrated the fine sensitivity of surface supercurrents to a coaxial magnetic field. The field does not pierce the topologically protected surface states of the wires, yet Fraunhofer-like critical current patterns develop, notably with unusual non-integer flux periodicity in lower-quality samples. Our theoretical analysis shows that such peculiar magneto-transport properties are essentially resulting from a series of nontrivial geometrical constraints. First, contrary to standard Josephson junctions, propagating electronic modes form Andreev bound states uniquely on a non-planar surface enclosing the insulating HgTe bulk. Second, such states may have a purely longitudinal character – associated with semiclassical paths roughly parallel to the axial direction – or a partially transverse behavior – corresponding to paths winding fully or partially around the wire perimeter – and are differently affected by the quality of the NS contacts along different directions. Third, superconductivity is in general not induced across the entire nanowire perimeter, nor is the magnetic field screened by the Nb fingers, which are thinner than the London penetration depth. As a consequence the partially transverse Andreev bound states pick up an Aharonov-Bohm phase which is not necessarily integer, i.e. electrons are not limited to enclosing a fixed number of vortices. This yields the observed peculiar critical current oscillations.

On the other hand, while the existence of surface states is necessary, spin-momentum locking of topological Dirac states appears to play a minor role. We numerically found similar overall features for surface states obeying an effective Schrödinger equation.

For further studies it is certainly desirable and interesting also to measure the current-phase relation. Due to the Aharonov-Bohm phase, which is picked up by the Andreev bound states, related signatures could be observable in such measurements and serve as an additional check for the theoretical model.

ACKNOWLEDGMENTS

We thank Denis Kochan, Henry Legg and Philipp Rüßmann for useful discussions. This work was funded by the European Research Council under the European Union’s Horizon 2020 research and innovation program (Grant Agreement No. 787515, 253 ProMotion). We also acknowledge support by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) within Project-ID 314695032 – SFB 1277 (projects A07, A08, B08) and through the Elitenetzwerk Bayern Doktorandenkolleg “Topological Insulators”.

Appendix A: Numerical calculation of Andreev bound state spectra for partially covered nanowires

The difference in current magnitude of the semiclassical analytical approach and the numerical data can be partially explained by the difference in the spectra of the ABS. For the analytical approach the ABS spectrum for each mode is assumed to be given by the standard expression Eq. 11, where the amplitude factor is determined by a constant gap $\Delta_0$. However, in the numerical calculation, this is not the case. Due to the partial coverage of the nanowire circumference with the s-wave supercondct-
tor, each mode in the surface state spectrum experiences an effective induced gap. We can show this by numerically computing the ABS spectrum of such a system. The eigenenergies of this nanowire Josephson junction can be determined by diagonalization of a finite tight-binding system with long superconducting reservoirs. The advantage of this method is the natural incorporation of the complex geometry. The superconducting reservoirs are connected by a periodic boundary hopping, where the superconducting phase difference enters again in a longitudinal hopping in the center of the normal region. In Figs. 7 (a) and (b) the calculated ABS spectra are plotted for $U_0 = 0$ and $U_0 = 600 \text{ meV nm}$, respectively. For simplicity we neglect here the axial magnetic flux and choose $U_0 = 0$. In Fig. 7 (a) the calculated ABS spectra are plotted for $U_0 = 0$ and $U_0 = 600 \text{ meV nm}$, respectively. For simplicity we neglect here the axial magnetic flux and choose $U_0 = 0$. In Fig. 7 (b) the differently induced gaps for each mode are no longer degenerate. This indicates that each mode experiences a different effective pairing strength, depending on their angular momentum quantum number. Also, the values at $\varphi_0 = 0$ differ quite strongly from $\Delta_0$, which is used in the semiclassical analysis. Therefore, the difference in current magnitude between numerics and semiclassics can be partially explained by the simplified assumption of a constant superconducting gap in the ABS energies in the latter case. This holds also true for the case of a non-zero barrier, which is illustrated in Fig. 7 (b). The differently induced gaps for each mode are still present, only the spectra become gapped at a phase difference of $\varphi_0 = \pi$.

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Josephson to quantum dot regimes, [Nanotechnology 28, 085202 (2017)]


[36] We are aware that OBTK-theory fails for low junction transparencies, because it does not correctly take into account interferences from multiple reflections (see, e.g., [13-15] in the supplement to [17]).


[38] Heikilä, T. T., Wilhelm, F. K., and Schön, G., Non-equilibrium supercurrent through mesoscopic ferromagnetic weak links, [EPL 51, 434 (2000)]


[40] Except for the highest-quality samples, see the discussion in Sec. [29].


[47] T. M. Klapwijk, Proximity effect from an andreev perspective, [J. Supercond. 17, 593 (2004)]


[57] A microscopic description would require a self-consistent treatment of the superconductor in its electromagnetic environment, which is beyond the scope of the present work.