

Fractional Spin and Josephson Effect in Time-Reversal-Invariant Topological Superconductors

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Time-reversal-invariant topological superconducting (TRITOPS) wires are known to host a fractional spin $\hbar/4$ at their ends. We investigate how this fractional spin affects the Josephson current in a TRITOPS-quantum dot-TRITOPS Josephson junction, describing the wire in a model that can be tuned between a topological and a nontopological phase. We compute the equilibrium Josephson current of the full model by continuous-time Monte Carlo simulations and interpret the results within an effective low-energy theory. We show that in the topological phase, the 0-to- π transition is quenched via formation of a spin singlet from the quantum-dot spin and the fractional spins associated with the two adjacent topological superconductors.

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Introduction.—The interplay of many-body interactions in quantum dots and superconductivity has been the focus of interest for some time [1–6]. While electrons are paired in superconductors, the charging energy effectively suppresses pairing in quantum dots (QD). A prominent consequence of this competition is the transition between 0 and π junction behavior of the Josephson current in devices where a QD connects between ordinary (nontopological) singlet-superconducting wires (S-QD-S junction) [7–10]. As a result of numerous studies [11–19], this phenomenon is now well understood for conventional superconductors. Essentially, S-QD-S junctions exhibit π -junction behavior when the QD hosts an effective spin-1/2 degree of freedom.

Here, we address the 0-to- π transition for Josephson junctions in which a quantum dot connects between time-reversal-invariant topological superconductors (TRITOPS). Unlike their time-reversal-breaking cousins [20–23], TRITOPS preserve time-reversal symmetry and can coexist with an unpolarized quantum-dot spin. It is thus an interesting question whether π -junction behavior can be observed in TRITOPS-QD-TRITOPS junctions. Such junctions differ from conventional S-QD-S junctions in several ways. First, the Majorana-Kramers pairs present in the topological phase allow for the coherent transfer of single electrons, while the Josephson current of a conventional junction is carried by Cooper pairs. Even more intriguing, TRITOPS host a fractional $\hbar/4$ spin at their ends. Thus, a TRITOPS-QD-TRITOPS junction allows one to study the hybridization of fractional and ordinary spins. We show that the 0- π transition constitutes a signature that distinguishes between the topological and the nontopological phase, and trace the quenching of the transition for TRITOPS to the formation of a spin singlet from the

quantum-dot spin and the fractional spins of the adjacent TRITOPS.

In the wake of proposals to engineer time-reversal-breaking topological phases and corresponding experiments, there has also been substantial interest in time-reversal-invariant topological superconductors [24–37]. TRITOPS are characterized by Kramers pairs of Majorana end states and localized fractional spins [28]. Time reversal protects the pair of Majorana states from hybridizing, which therefore generically remain at zero energy. Similarly, the fractional spin is topologically protected and cannot be determined from a local measurement without breaking time reversal. Several routes have been proposed to engineer TRITOPS although their experimental realization is more demanding than that of time-reversal-breaking topological superconductors [36].

Conventional Josephson junctions assume their minimal energy at zero phase difference and their maximal energy at a phase difference of π (0-junction behavior). This behavior is reversed in π junctions, which assume their minimal energy at a phase difference of π [1,2]. In S-QD-S junctions, π -junction behavior occurs when the quantum dot forming the junction is singly occupied and acts effectively as a magnetic impurity. When the QD is weakly coupled to the superconductors, tunneling of Cooper pairs between the conventional superconductors relies on a fourth-order cotunneling process [1,10]. This process includes a π phase shift that originates from the Fermi statistics of electrons and becomes manifest in the π -junction behavior. As a consequence, the current-phase relation of the junction phase shifts by π when the occupation of the quantum dot is tuned from even to odd. When the quantum dot is strongly coupled to the superconductors, the impurity spin can be screened, turning

a doublet into a singlet ground state and resulting in 0-junction behavior. Depending on the parameter regime, this transition can be described as a result of Kondo correlations or a zero-energy crossing of a Yu-Shiba-Rusinov state [19].

Model.—Our considerations are based on a time-reversal-invariant superconductor with Hamiltonian [27],

$$H_\alpha = \sum_{j=1}^N \sum_{\sigma} (-tc_{\alpha,j+1,\sigma}^\dagger c_{\alpha,j,\sigma} + i\lambda_\sigma c_{\alpha,j+1,\sigma}^\dagger c_{\alpha,j,\sigma} + \Delta_\sigma e^{i\phi_\alpha} c_{\alpha,j+1,\sigma}^\dagger c_{\alpha,j,\bar{\sigma}} + \text{H.c.} - \mu n_{\alpha,j,\sigma}), \quad (1)$$

where $\lambda_{\uparrow,\downarrow} = \pm\lambda$, $\Delta_{\uparrow,\downarrow} = \pm\Delta$, and $\bar{\uparrow} = \downarrow, \bar{\downarrow} = \uparrow$. Moreover, t is the hopping parameter, μ is the chemical potential, and λ and Δ are the strengths of Rashba spin-orbit coupling and extended s -wave pairing, respectively. The index $\alpha = L, R$ labels the left and right superconductors of the junction with order parameter phases ϕ_α . The phase difference $\phi = \phi_L - \phi_R = 2\pi\Phi/\Phi_0$ can be tuned by including the junction in a superconducting loop and threading the loop by a magnetic flux Φ . ($\Phi_0 = h/2e$ denotes the superconducting flux quantum.) The entire TRITOPS-QD-TRITOPS Josephson junction is then described by the Hamiltonian

$$H = \sum_{\alpha=L,R} H_\alpha + H_c + H_d. \quad (2)$$

Here,

$$H_d = \varepsilon_d \sum_{\sigma} n_{d,\sigma} + U n_{d\uparrow} n_{d\downarrow} \quad (3)$$

describes the quantum dot with gate-tunable level energy ε_d , spin-resolved level occupation $n_{d,\sigma}$, and charging energy U , and

$$H_c = -t' \sum_{\sigma} [(c_{L,N,\sigma}^\dagger + c_{R,1,\sigma}^\dagger) d_\sigma + \text{H.c.}] \quad (4)$$

accounts for the hybridization between quantum dot and superconductors.

The Hamiltonian H_α supports topological and nontopological phases. The topological phase occurs when $|\mu| < 2\lambda$ and is characterized by Kramers pairs of Majorana end states. For each lead, the corresponding Majorana operators can be combined into conventional fermionic operators

$$\Gamma_{L/R} = \int dx \varphi_{L/R}(x) [\psi_\uparrow(x) \mp i\psi_\downarrow^\dagger(x)], \quad (5)$$

where $\varphi_{L/R}(x)$ denotes the Majorana wave functions of the left (L) and right (R) superconducting lead and $\psi_\sigma(x)$ denotes the electron field operator for spin σ (see Supplemental Material, Sec. II [38]). While the Majorana

operators mix the two spin components, the operators $\Gamma_{L/R}$ remove a spin of $\hbar/2$ from one end of the wire. Thus, $\Gamma_{L/R}$ and $\Gamma_{L/R}^\dagger$ toggle the system between ground states with fractional spins of $\pm\hbar/4$ localized at the ends of the wire [28].

Numerical results.—The Josephson current can be computed from the Green function expression

$$I = \frac{2t'^2}{\beta} \sum_{\sigma} \sum_n \text{Im}[g_{L,\alpha,\sigma}^{(12)}(i\omega_n) G_{d,\sigma}^{(21)}(i\omega_n)]. \quad (6)$$

The derivation is included in Ref. [38] (see Sec. I). The Green functions correspond to the Matsubara components of frequency $\omega_n = (2n+1)\pi/\beta$ (β is the inverse temperature) of the imaginary-time Green functions $g_{l\alpha,\sigma}^{(12)}(\tau) = -\langle T_\tau [\hat{c}_{\alpha,1,\sigma}^\dagger(\tau) \hat{c}_{\alpha,1,\bar{\sigma}}(0)] \rangle_0$ and $G_{d,\sigma}^{(21)}(\tau) = -\langle T_\tau [\hat{d}_\sigma(\tau) \hat{d}_\sigma(0)] \rangle$, where $\langle \dots \rangle$ ($\langle \dots \rangle_0$) denotes the ensemble average over the states of H_α (H). The first Green function can be obtained exactly.

First consider a junction with a noninteracting quantum dot. For $U = 0$, the Green function $G_{d,\sigma}(i\omega_n)$ and thus the Josephson current can also be evaluated analytically. Moreover, our model can be written in Nambu representation with a Bogoliubov–de Gennes (BdG) Hamiltonian $\hat{\mathcal{H}}_{\text{BdG}} = \hat{\mathcal{H}}_0 \tau_z + \hat{\Delta} \tau_x$, where $\hat{\mathcal{H}}_0$ results from the normal parts of the Hamiltonian H while $\hat{\Delta}$ originates from the pairing contributions. The Pauli matrices τ_i (with $i = x, y, z$) operate in particle-hole space. Diagonalizing the BdG Hamiltonian, the Josephson current can be obtained from $I = (2e/\hbar) \partial E_0(\phi) / \partial \phi$, where $E_0(\phi)$ is the many-body ground state energy. Corresponding results are presented in Fig. 1.

The spectrum of $\hat{\mathcal{H}}_{\text{BdG}}$ is shown in the lower panels for the topological (left and middle) and the nontopological (right) phase. In the topological phase, there are zero-energy bound states (light-blue curves) that emerge from the Majorana states localized at the far ends of the finite-length chains. The solid red curves emerge from the hybridization of the dot states with the adjacent Majorana states. In the nontopological phase, the subgap states are gapped. As a consequence of Kramers theorem, the subgap states are twofold degenerate at ϕ equal to integer multiples of π . At other flux values, time reversal is broken by the phase bias and the subgap states are non-degenerate. The top panel of Fig. 1 shows the Josephson current for values of μ both in the topological ($\mu < 2\lambda$) and the nontopological ($\mu > 2\lambda$) phases. In the topological phase, the Josephson current jumps at $\phi = \pi$ (up to finite-size effects), reflecting the level crossing of the subgap states. (Note that we assume complete equilibration over fermion parities.) The nontopological phase exhibits the usual smooth behavior.

For a nonzero interaction U , the Josephson current can be calculated by evaluating $G_{d,\sigma}^{(21)}(i\omega_n)$ using quantum

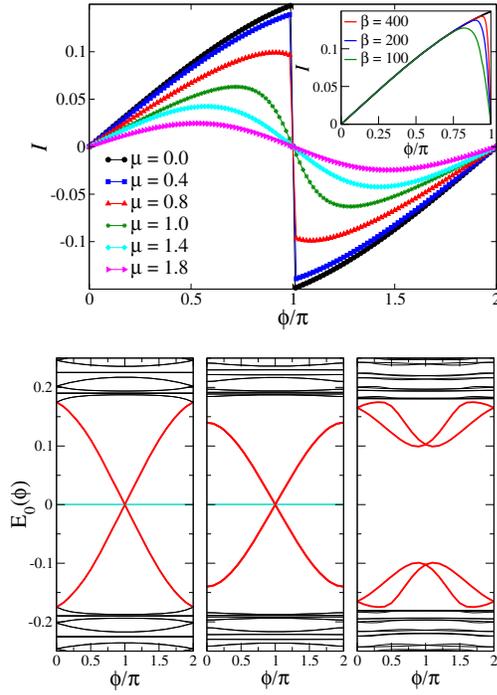


FIG. 1. Top: Josephson current vs ϕ for a quantum dot at $T = 0$ with $U = 0$, $t' = t$, $\lambda = t/2$, $\Delta = t/5$, and values of μ in the topological ($\mu < t$) as well as the nontopological ($\mu > t$) phase. The wires have $N = 500$ sites. Inset: Josephson current at finite temperature. Red, blue, and green lines correspond to $\beta = 400, 200$, and 100 , respectively. The $T = 0$ case is plotted in black for reference. Bottom: Spectrum of $\hat{\mathcal{H}}_{\text{BdG}}$ for $\mu = \epsilon_d = 0$ (left), $\mu = 0$, $\epsilon_d = t$ (middle), and $\mu = -\epsilon_d = 1.8$ (right). Other parameters are as they are in the top panel. Energies are measured in units of $t = 1$.

Monte Carlo simulations [39]. Previous works on S-QD-S junctions [12,15,16] as well as normal wires coupled to correlated dots and molecules [40,41] proved this strategy to be accurate and reliable. We perform a Shiba transformation, mapping H to a particle-number conserving Hamiltonian with negative U [15]. The Green function of the transformed problem is then calculated by the algorithm introduced in Refs. [42,43]. Inversion of the Shiba transformation leads to $G_{d,\sigma}(i\omega_n)$, which enters the Josephson current (6). Results for a half-filled configuration (i.e., $\langle n_{d\uparrow} + n_{d\downarrow} \rangle = 1$) are shown in Fig. 2.

The nontopological case (bottom panel) shows the expected 0-to- π transition. When coupling the quantum dot to superconducting leads, the local moment persists when Δ is larger than the Kondo temperature T_K , but becomes Kondo screened by the quasiparticle states for $\Delta \ll T_K$. For a particle-hole symmetric configuration, the Kondo temperature of the junction is given by $k_B T_K = \sqrt{\delta U/2} \exp(-\pi U/8\delta)$ [44] with the hybridization parameter $\delta \sim \pi(t')^2 \sqrt{1 - \mu^2/(2t)^2}/(2t)$. Consequently, there is a 0- π transition as U increases. For $U = t$, the dot is in the

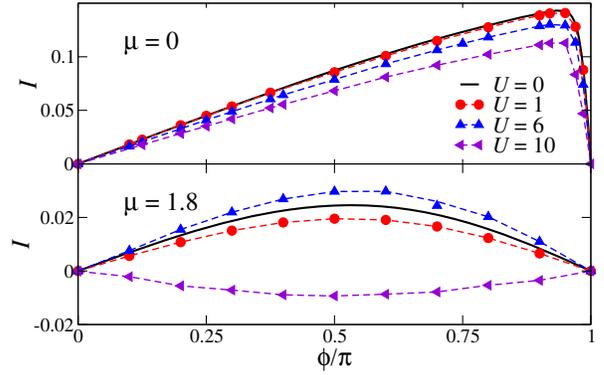


FIG. 2. Josephson current for an interacting quantum dot at $\beta = 400$ with $t' = t$, $\epsilon_d = -U/2$, $\lambda = t/2$, $\Delta = t/5$. The upper (lower) panel corresponds to the topological (nontopological) phase. The values of U and μ are indicated in the figure. Energies are expressed in units of $t = 1$.

intermediate valence regime, while for $U = 6t$ and $U = 10t$, it would be in the Kondo regime when attached to normal leads. In our case, $k_B T_K \sim \Delta$ for $U \sim 8.5t$, consistent with the observed transition between 0- and π -junction behavior between $U = 6t$ and $U = 10t$.

It is our central observation that there is no corresponding 0- π transition when the superconducting leads are in the topological regime. Instead, the current-phase relation remains similar to the noninteracting case for all interaction strengths U . In particular, the abrupt dependence at a phase difference of $\phi = \pi$, while slightly smoothed by finite temperature, becomes more pronounced as the number of sites increases, as in the noninteracting case (cp. the inset of Fig. 1). These results suggest that the impurity spin is efficiently screened in the topological case, despite the presence of the superconducting gap. This robust screening of the spin of the quantum dot originates from its interaction with the subgap states emerging from the Kramers pairs of Majorana states of the adjacent left and right wires.

Effective Hamiltonian.—To arrive at this conclusion, we interpret our numerical results in the context of an effective Hamiltonian. Consider a singly occupied, interacting quantum dot coupled to two time-reversal-invariant topological superconductors. For simplicity, we assume that the superconducting gap is large compared to the Kondo temperature so that we can neglect hybridization with the quasiparticle continuum. Then, we only need to consider the hybridization with the subgap states originating from the Majorana bound states. We can project out the empty and doubly occupied dot states by employing a Schrieffer-Wolff transformation [45] (see also [37] for similar considerations). This yields an effective Hamiltonian in the eight-dimensional subspace spanned by the two eigenstates of the quantum dot spin \mathbf{S}_d and the two states for each of the superconducting leads that are associated with the Kramers pair of Majorana operators.

Here, we sketch the derivation of this Hamiltonian (for details, see [38], Sec. III).

In a first step, we project the tunneling Hamiltonian H_c to the subgap states of the wires, giving $H_c = t_{\text{eff}} e^{i\phi/4} \sum_{\sigma} (\Gamma_{L,\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} \Gamma_{R,\sigma}) + \text{H.c.}$, where $t_{\text{eff}} \lesssim t'$ and the Bogoliubov operators for the zero-energy modes satisfy $\Gamma_L^{\dagger} = \Gamma_{L,\uparrow}^{\dagger} = i\Gamma_{L,\downarrow}$, and $\Gamma_R^{\dagger} = \Gamma_{R,\uparrow}^{\dagger} = -i\Gamma_{R,\downarrow}$ (see [46,38], Sec. II). Focusing on the particle-hole symmetric point $\varepsilon_d = -U/2$, and eliminating the empty and doubly occupied states of the quantum dot by a Schrieffer-Wolff transformation, we obtain (see [38], Sec. III for details, including more general configurations)

$$H_{\text{eff}} = J \left\{ S_d^z \left[(n_L + n_R - 1) + i \sin \frac{\phi}{2} (\Gamma_L^{\dagger} \Gamma_R - \Gamma_R^{\dagger} \Gamma_L) \right] + i \cos \frac{\phi}{2} (S_d^- \Gamma_L^{\dagger} \Gamma_R^{\dagger} - S_d^+ \Gamma_R \Gamma_L) \right\}, \quad (7)$$

where $J = 4t_{\text{eff}}^2/U$ and we defined the occupations $n_{\alpha} = \Gamma_{\alpha}^{\dagger} \Gamma_{\alpha}$. A convenient basis for this Hamiltonian is $|\sigma, n_L, n_R\rangle$ with $n_{\alpha} = 0, 1$ and $\sigma = \uparrow, \downarrow$. Note that n_{α} also labels the polarization of the fractional spins.

The Hamiltonian H_{eff} is easily diagonalized. It conserves the number parity of $n = n_L + n_R$. For $n = 1$, the terms involving S_d^{\pm} do not contribute and we find doubly degenerate eigenstates that are linear superpositions of $|\sigma, 1, 0\rangle$ and $|\sigma, 0, 1\rangle$ with energy $\pm J/2 \sin(\phi/2)$. For even occupations n , we have two phase-independent states with degenerate eigenenergies $J/2$ corresponding to $|\uparrow, 1, 1\rangle$ and $|\downarrow, 0, 0\rangle$ as well as a pair of nondegenerate states with energies $-J/2 \pm J \cos(\phi/2)$, which are linear combinations of the states $|\uparrow, 0, 0\rangle$ and $|\downarrow, 1, 1\rangle$.

At all phase differences, the ground state is an equal-probability superposition of $|\uparrow, 0, 0\rangle$ and $|\downarrow, 1, 1\rangle$. These states describe configurations with overall zero spin. Indeed, in both states the quantum-dot spin of $\hbar/2$ is pointing opposite to the fractional spins of $\hbar/4$ of the two adjacent superconductors. Thus, these configurations can be interpreted as an effective singlet configuration of the quantum dot spin and the fractional spins of the topological superconductors.

Similar to the singlet formation via hybridization with the quasiparticle continuum of nontopological superconductors [19], this singlet formation with the fractional spins quenches the π -junction behavior. Indeed, the low-energy spectrum emerging from the Schrieffer-Wolff treatment predicts a Josephson energy that is minimal at phase differences equal to integer multiples of 2π . Moreover, we also see that there is a cusp in the ground state energy at a phase difference of π . Both of these results are consistent with our numerical results that incorporate the hybridization with the quasiparticle continuum above the superconducting gap.

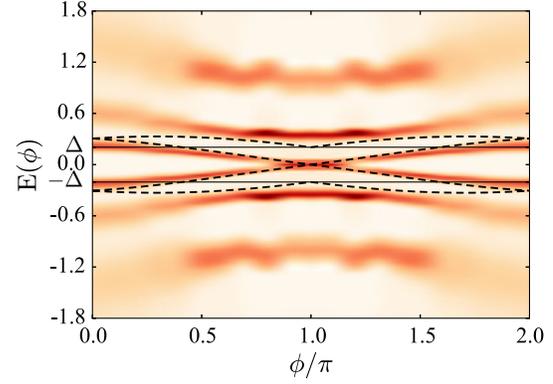


FIG. 3. Local density of states (LDOS) at the quantum dot obtained by QMC. The black dashed lines are the predictions for the peaks in the density of states on the basis of H_{eff} with $J = 0.2$. The amplitude of the superconducting gap $\Delta = 0.2$ is indicated in thin lines. Other parameters are $U = 4t$, $J = 0.2$, $\lambda = 0.5t$, $t' = t$, $\mu = 0$, and $\beta = 400$.

In Fig. 3, we benchmark our low-energy Hamiltonian with results for the LDOS at the quantum dot $\rho(\omega) = -2 \sum_{\sigma} \text{Im}[G_{d,\sigma}^R(\omega)]$. The latter was calculated by analytically continuing the Monte Carlo data to the real frequency axis. Results are shown in the color plot. The low-energy spectrum obtained from H_{eff} is shown as solid lines for comparison. The peaks in the LDOS reflect the energy necessary to add or remove one particle. Thus, the peak positions can be estimated from H_{eff} by the energy difference between the odd-parity eigenstates and the ground state, which yields $\pm[J/2 + J|\cos(\phi/2)| \pm J/2 \sin(\phi/2)]$. We find that our numerics is qualitatively consistent with the predictions of H_{eff} , although the numerics is performed in a regime where the addition spectrum already hybridizes with the quasiparticle continuum. Apart from shifts in energy, the hybridization lifts the degeneracies at $\phi = 0$ and 2π . Besides the low-energy features that are qualitatively described by H_{eff} , the numerical results also exhibit high-energy features at $\pm U/2$, which are associated with the charge-transfer peaks of the impurity Anderson model.

TRITOPS-QD-TRITOPS Josephson junctions combine topological superconductivity with time-reversal symmetry and electron-electron interactions. While this is superficially similar to quantum spin Hall Josephson junctions including interactions either within the edge states [47,48] or through coupling to an interacting quantum dot [49,50], these two types of Josephson junctions are governed by remarkably different physics. Quantum spin Hall Josephson junctions exhibit an 8π -periodic Josephson effect that can be interpreted as resulting from the tunneling of $e/2$ charges enabled by the formation of Z_4 parafermions or from a spin transmutation as a consequence of the fermion parity anomaly [49]. In contrast, the present system has a Josephson effect that is 4π periodic and results from an effective singlet formation with two fractional spins.

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