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Symmetry-protected topological invariant and Majorana impurity states in time-reversal invariant superconductors

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We address the question of whether individual nonmagnetic impurities can induce zero-energy states in time reversal invariant topological superconductors, and define a class of symmetries which guarantee the existence of such states for a specific value of the impurity strength. These symmetries allow the definition of a position space topological $\mathbb{Z}_2$ invariant, which is related to the standard bulk topological $\mathbb{Z}_2$ invariant. Our general results are applied to the time reversal invariant p-wave phase of the doped Kitaev-Heisenberg model, where we demonstrate how a lattice of impurities can drive a topologically trivial system into the non-trivial phase.

Local impurities in superconductors (SCs) give rise to astonishing physics.[1–8] Magnetic impurities in s-wave SCs lead to pair-breaking, and can induce a quantum phase transition to a metallic state with gapless superconductivity near the transition point.[8] Due to Anderson's theorem, nonmagnetic impurities have little influence on s-wave SCs.[9] However, in unconventional SCs, where the sign of the order parameter depends on the direction of momentum, scattering by impurities leads to pair-breaking since the momentum direction of the paired electrons is changed without changing the phase.[1,2] Thus, impurities give rise to subgap states and can be used to probe high-T_c superconductivity.[1–3]

Here, we focus on impurity bound states in time reversal (TR) invariant odd-parity SCs. These SCs belong to symmetry class DIII of the Altland-Zirnbauer classification[10] and come in two variants, characterized by a $\mathbb{Z}_2$ topological invariant $\mathcal{Q}$.[11–18] The topologically non-trivial SC has protected Majorana boundary modes. It turns out that $\mathcal{Q}$ also predicts the pattern of ground state degeneracies on a torus, when switching between periodic and anti-periodic boundary conditions.[19] Denoting a pair of states $(|\psi\rangle, T|\psi\rangle)$ related by time reversal T as a Kramers pair, ground states are different depending on whether the number of unpaired Kramers pairs below the Fermi level is even or odd, designated in the following as even or odd "Kramers parity". Single band odd-parity SCs have $\Delta(-\boldsymbol{k}) = -\Delta(\boldsymbol{k})$,[16] hence their order parameter vanishes at all TR invariant momenta (TRIM) $\boldsymbol{K}$ with $\boldsymbol{K} = -\boldsymbol{K}$ up to reciprocal lattice vectors, such that for each TRIM below the Fermi level there is one unpaired Kramers pair. The Kramers parity is thus determined by the number of TRIM enclosed by the Fermi surface, and odd-parity SCs where this number is odd are topologically non-trivial.[16,17]

Zero-energy bound states in SCs are intriguing Majorana states.[19–22] Thus, it may be interesting to artificially create them by tuning an impurity potential, but it is also important to understand how to avoid accidental zero-energy states from nonmagnetic disorder, which may interfere with protocols using protected Majorana zero-energy states,[23] occurring for instance in the center of a vortex.[24,25] In this paper, we derive conditions for the existence of zero-energy impurity states in TR invariant SCs. To this end, we deduce conditions for the existence of a position-space topological invariant $\mathcal{Q}_{\mathrm{DIII}}$, which for gapped translationally invariant systems is equivalent to $\mathcal{Q}$ and the Kramers parity. We show that upon introduction of a local impurity potential into the system, the conditions for the existence of $\mathcal{Q}_{\mathrm{DIII}}$ also guarantee the emergence of zero-energy impurity bound states for a suitably chosen impurity strength. In particular, we find that the existence of symmetries protects zero-energy impurity bound states, such that disorder may introduce states with energies less than the thermal energy even at low temperatures. When an impurity bound state moves through the Fermi level, it changes the Kramers parity and $\mathcal{Q}_{\mathrm{DIII}}$ but not $\mathcal{Q}$, since it is spatially localized and insensitive to boundary conditions. However, a lattice of impurities hosts extended states, and we show that partially moving such an impurity band through zero energy can, for a broad range of potential strengths, turn a topologically trivial SC into a non-trivial one.

Model: We consider a general TR invariant Bogoliubov-de Gennes Hamiltonian in symmetry class DIII[10] for an N-site lattice in the position space basis

$$H = \frac{1}{2}\,(c^\dagger, c)\,\mathcal{H}\begin{pmatrix} c \\ c^\dagger \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^\star & -h^T \end{pmatrix}, \tag{1}$$

where $c = (c_\uparrow, c_\downarrow)$, $c_\sigma = (c_{1,\sigma}, \ldots, c_{N,\sigma})$ and $c_{i,\sigma}$ annihilates a fermion with spin σ on site i. Hermiticity of the Hamiltonian and Fermi statistics require $h = h^\dagger$, $\Delta = -\Delta^T$. Hamiltonians in DIII obey both the particle-hole (PH) symmetry $\{P, \mathcal{H}\} = 0$, $P = \tau_1 K$ and TR symmetry $[T, \mathcal{H}] = 0$, $T = i\sigma_2 K$. Here $\boldsymbol{\tau}$ and $\boldsymbol{\sigma}$ denote the Pauli matrices in PH and spin space, respectively, and K is the operator of complex conjugation. Together, these symmetries give rise to the chiral symmetry $\{C, \mathcal{H}\} = 0$, $C = iPT = \tau_1 \otimes \sigma_2$.[11] Hence, every eigenvector $|\psi\rangle$ with energy E has a Kramers partner $T|\psi\rangle$ with energy E, a PH partner $P|\psi\rangle$ and a 'chiral' partner $C|\psi\rangle$ both with energy $-E$.

We describe a local nonmagnetic impurity at site i_0 by the Hamiltonian

$$H(u)=H+H_{\mathrm{imp}}(u),\quad H_{\mathrm{imp}}(u)=u\sum_{\sigma}c^{\dagger}_{i_0,\sigma}c_{i_0,\sigma}\quad. \tag{2}$$

Results: To get insight into the existence of zero-energy impurity states, we note that in the absence of superconductivity $H_0(u)=H(u,\Delta=\mathbf{0}_{2N})$ has a zero-energy eigenvalue for a critical impurity strength u^0_{c}.[26] Without accidental degeneracies, the zero-energy eigenspace is spanned by the mutually orthogonal states $|\psi^0\rangle, T|\psi^0\rangle, P|\psi^0\rangle$ and $C|\psi^0\rangle$. We now ask whether these states are split by a superconducting coupling $H_\Delta=H-H_0$ in first order degenerate perturbation theory, and argue that such a splitting is evidence for an avoided crossing, and thus the absence of a zero-energy state in the full problem. Due to TR and PH symmetry, H_Δ cannot couple $|\psi^0\rangle$ to $T|\psi^0\rangle$ or $P|\psi^0\rangle$, but the coupling to $C|\psi^0\rangle$ is finite in general and leads to an energy splitting.[27] However, in the presence of a unitary symmetry U, which commutes with $H_0(u)$ and H_Δ and anticommutes with C, the coupling between $|\psi^0\rangle$ and $C|\psi^0\rangle$ vanishes: since $U|\psi^0\rangle=\lambda|\psi^0\rangle$ with $|\lambda|=1$, we find that $\langle\psi^0|H_\Delta C|\psi^0\rangle=\langle\psi^0|U^\dagger H_\Delta CU|\psi^0\rangle$, and from $\{H_\Delta C,U\}=0$ it follows that $\langle\psi^0|H_\Delta C|\psi^0\rangle=-\langle\psi^0|H_\Delta C|\psi^0\rangle$. Consequently, $\langle\psi^0|H_\Delta C|\psi^0\rangle$ vanishes, and there is no energy splitting. This fundamental impact of such a symmetry U on the energy E_{imp} of the impurity bound state is illustrated in FIG. 1. There we depict $E_{\mathrm{imp}}(u^{-1})$ obtained from T-matrix[1] calculations for two models: First for the doped Kitaev-Heisenberg (KH) model,[28,29] which, as we will demonstrate, has additional symmetries protecting the zero-energy crossings, and second for the case where we added to this model Rashba spin-orbit coupling and modified the order parameter $\Delta(\boldsymbol{k})$ in order to break all these symmetries.

In order to understand the existence of zero-energy states in the full problem, we note that the determinant $\det[\mathcal{H}(u)]$ can be expressed as a product of the eigenvalues of $\mathcal{H}(u)$. Thus, if the system without impurity is gapped, a zero of $\det[\mathcal{H}(u)]$ for a critical impurity strength u_{c} indicates the existence of a zero-energy impurity bound state. As $\mathcal{H}(u)$ is local in u, and since there is a spin and particle-hole degree of freedom at each lattice site, one finds that $\det[\mathcal{H}(u)]$ is a fourth order polynomial in u. For a general Hamiltonian in class DIII, it is difficult to determine under which conditions this polynomial has zeros for a real valued impurity strength u_{c}. In the following, we reduce the problem to the analysis of a first order polynomial by considering the Pfaffian of redundant sub-blocks of $\mathcal{H}$. This will allow us to show non-perturbatively that the presence of a symmetry with $[\mathcal{H},U]=0$ and $\{C,U\}=0$ indeed ensures the existence of a zero-energy impurity bound state.

We first use the transformation $V=[\mathbf{1}_{4N}+(i\tau_2)\otimes\sigma_2\otimes\mathbf{1}_N]/\sqrt{2}$, which diagonalizes C, to bring $\mathcal{H}$ into a block off-diagonal form

$$V^\dagger\mathcal{H}V=\begin{pmatrix}\mathbf{0}_{2N} & D\\ D^\dagger & \mathbf{0}_{2N}\end{pmatrix}\quad, \tag{3}$$

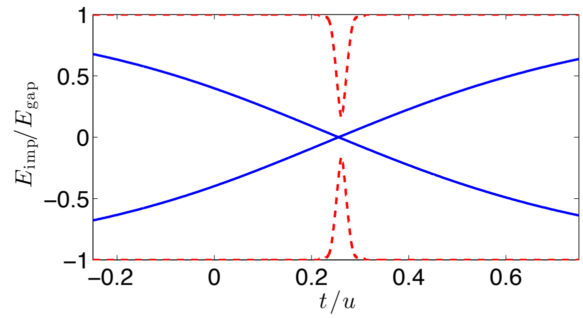

FIG. 1. Two prototypical behaviors of the energy of an impurity state $E_{\mathrm{imp}}/E_{\mathrm{gap}}$ as a function of the inverse impurity strength t/u. The solid blue line shows a symmetry protected zero-energy crossing, whereas the dashed red line shows an avoided crossing, because the symmetry is absent. The relevant symmetries are listed in TAB. I. Both systems are in the topologically non-trivial phase. The blue curve is computed for the TR invariant p-wave phase of the doped Kitaev-Heisenberg model (parameters: $\mu=1.3\,t,\eta=0.05\,t$); for the red curve anisotropic Rashba spin-orbit coupling with $(\kappa_x,\kappa_y,\kappa_z)=(0,1,2)$ and $\lambda_{\mathrm{R}}=0.89\,\eta$ was added.

with $D\equiv h\sigma_2+\Delta=-D^T$. Because D is antisymmetric, $\mathrm{Pf}(D)$ exists and $|\,\mathrm{Pf}(D)|^4=\det\mathcal{H}$, such that zero-energy eigenvalues of $\mathcal{H}$ occur whenever $\mathrm{Pf}(D)=0$. Since u appears only in one entry in the upper and lower triangle of the matrix $D(u)$ respectively, $\mathrm{Pf}[D(u)]=z(u-u_{\mathrm{c}})$ is a linear complex function with $z,u_{\mathrm{c}}\in\mathbb{C}$. If u_{c} is real, the complex phase of $\mathrm{Pf}[D(u)]$ does not depend on u and the system is bound to have a single zero-energy crossing of Kramers pairs at u_{c}. We stress that in general there is no reason for u_{c} to be real, such that no value of the real control parameter u would yield zero-energy states. In the following, we will show that u_{c} is indeed real provided that a symmetry of the Hamiltonian exists which anticommutes with the chiral operator C.

Every possible unitary transformation U satisfying $\{U,C\}=0$ has the property[27]

$$V^\dagger UV=\begin{pmatrix}\mathbf{0}_{2N} & W\\ W^\star & \mathbf{0}_{2N}\end{pmatrix}. \tag{4}$$

with W unitary due to the unitarity of U and V. Provided that U is a symmetry of $\mathcal{H}$ with $[\mathcal{H},U]=0$ it follows that

$$[\mathrm{Pf}(D)]^\star=\frac{(-1)^N}{\det W}\,\mathrm{Pf}(D)\quad. \tag{5}$$

Here, we first used the general properties $[\mathrm{Pf}(B)]^*=(-1)^N\,\mathrm{Pf}(B^\dagger)$ and $\det(A)\,\mathrm{Pf}(B)=\mathrm{Pf}(ABA^T)$ of the pfaffian to write $[\mathrm{Pf}(D)]^\star=\frac{(-1)^N}{\det W}\,\mathrm{Pf}(WD^\dagger W^T)$. By utilizing $WD^\dagger=DW^\star$, which is equivalent to the symmetry condition $[\mathcal{H},U]=0$, and the unitarity of W, we then arrive at Eq. (5). This equation implies that $\sqrt{(-1)^N/\det W}\,\mathrm{Pf}(D(u))$ is a real valued function, and therefore u_c is real. This demonstrates that in the presence of a symmetry U the existence of the zero-energy states is guaranteed for a suitably chosen impurity strength u_c.

To get some intuition about possible symmetries, we first specialize to a situation where U can be decomposed into a product $U = \tau_\mu \otimes \sigma_\nu \otimes R$ of an internal transformation $\tau_\mu \otimes \sigma_\nu$ and a lattice transformation R, which satisfies $R^T = R^{-1}$ as it is a permutation of lattice sites. Then, the condition $\{U, C\} = 0$ implies that not all 16 combinations $\tau_\mu \otimes \sigma_\nu$ can be used to construct symmetries U, but only the eight combinations listed in TAB. I. Next, we expand $h = \sum_{\nu=0}^{3} \sigma_\nu \otimes h_\nu$ into a spin-independent single-particle part h_0 and spin-orbit couplings h_1, h_2, h_3, and decompose $\Delta = i \sum_{\nu=0}^{3} \sigma_\nu \sigma_2 \otimes d_\nu$ into a singlet component d_0 and triplet components d_1, d_2, d_3. Then, for every allowed choice of $\tau_\mu \otimes \sigma_\nu$, a subset of the h_ν, d_ν anticommutes with R, and the remaining h_ν, d_ν commute with R, see TAB. I. In the particularly simple case where U does not contain a lattice transformation, i.e. $R \equiv \mathbf{1}_N$, the anticommutation condition $\{\,\cdot\,, R\} = 0$ implies that the respective h_ν, d_ν vanish identically, whereas the commutation relation $[\,\cdot\,, R] = 0$ is trivially satisfied.

Now we are in a position to treat the special case of impurity bound states in spin-polarized SCs (belonging to symmetry class D[10]) as a first application of our formalism. The specific choice $U = \tau_0 \otimes \sigma_3 \otimes \mathbf{1}_N$ implies that the matrices h_1, h_2, d_0, d_3, which couple up and down spins, have to vanish, see first row in TAB. I. Then, the Hamiltonian matrix decomposes into two uncoupled blocks $\mathcal{H} = \mathcal{H}^\uparrow \oplus \mathcal{H}^\downarrow$, related by TR symmetry $\mathcal{H}^\downarrow = T\mathcal{H}^\uparrow T^{-1}$. Each of the blocks $\mathcal{H}^\sigma$ is not TR symmetric but still obeys PH symmetry and thus can be an arbitrary member of symmetry class D. From our analysis it follows, that $\mathcal{H}^\uparrow$ hosts a zero-energy impurity bound state for a suitably chosen impurity strength while $\mathcal{H}^\downarrow$ provides its Kramers partner. This generalizes the result for p-wave SCs obtained in Ref. 4 to arbitrary spin-polarized SCs in all spatial dimensions. The symmetries in rows two and three of TAB. I imply a decomposition into two class D blocks as well, with spins polarized in y- and x-direction, respectively.

The symmetry $U = \tau_3 \otimes \sigma_0 \otimes \mathbf{1}_N$ in the fourth row of TAB. I requires the absence of superconductivity. Hence, the coupling between the particle and the hole-sector vanishes, and the Hamiltonian decomposes into two spin-1/2 TR invariant systems belonging to symmetry class AII.[10] Thus, we have shown that every gapped system in AII hosts zero-energy impurity bound states for a suitably chosen impurity strength. The last four rows of TAB. I are formally obtained by multiplying the first four rows with the chiral operator C. In the context of electronic SCs, there is no obvious example for their use.

More generally, $R \neq \mathbf{1}_N$, and the symmetry U realizes a combination of a lattice transformation and a rotation in spin and particle hole space which is required to keep a spin-orbit coupling $L \cdot S$ of angular momentum and spin invariant. An important example are spatial reflections

TABLE I. We list all eight types of unitary symmetry operators of the form $U = \tau_\mu \otimes \sigma_\nu \otimes R$ with $R^T = R^{-1}$ which satisfy $\{U, C\} = 0$ and hence guarantee the existence of zero-energy impurity bound states. The symmetry condition $[\mathcal{H}, U] = 0$ implies that the matrices h_ν, d_ν defined by the expansions $h = \sum_{\nu=0}^{3} \sigma_\nu \otimes h_\nu$, $\Delta = i \sum_{\nu=0}^{3} \sigma_\nu \sigma_2 \otimes d_\nu$ are restricted by (anti-)commutation relations with R. Namely the h_ν, d_ν listed in the second [third] column have to anticommute [commute] with R. $R = \mathbf{1}_N$ implies that matrices in the second [third] column vanish [are unrestricted].

U	$\{\,\cdot\,, R\} = 0$	$[\,\cdot\,, R] = 0$
$\tau_0 \otimes \sigma_3 \otimes R$	h_1, h_2, d_0, d_3	h_0, h_3, d_1, d_2
$\tau_3 \otimes \sigma_2 \otimes R$	h_1, h_3, d_0, d_2	h_0, h_2, d_1, d_3
$\tau_0 \otimes \sigma_1 \otimes R$	h_2, h_3, d_0, d_1	h_0, h_1, d_2, d_3
$\tau_3 \otimes \sigma_0 \otimes R$	d_0, d_1, d_2, d_3	h_0, h_1, h_2, h_3
$C(\tau_0 \otimes \sigma_3 \otimes R)$	h_0, h_3, d_1, d_2	h_1, h_2, d_0, d_3
$C(\tau_3 \otimes \sigma_2 \otimes R)$	h_0, h_2, d_1, d_3	h_1, h_3, d_0, d_2
$C(\tau_0 \otimes \sigma_1 \otimes R)$	h_0, h_1, d_2, d_3	h_2, h_3, d_0, d_1
$C(\tau_3 \otimes \sigma_0 \otimes R)$	h_0, h_1, h_2, h_3	d_0, d_1, d_2, d_3

about a mirror plane, accompanied by the appropriate spin rotation.[30–33] We discuss specific examples for such symmetries in the context of the doped KH model.

The presence of a symmetry U is sufficient but not necessary for the existence of zero-energy impurity states. There are conditions not related to symmetries for which $\mathrm{Pf}(D)$ has a real zero for some impurity potential.[27] However, while such conditions can be satisfied in single-particle Hamiltonians, they are expected to be less robust than symmetry conditions when the single-particle Hamiltonian is obtained from a self-consistent mean field approximation to an interacting Hamiltonian which already includes the impurity potential.

Exploiting the constant phase of $\mathrm{Pf}(D)$ in the presence of a symmetry U, we define a topological invariant $\mathcal{Q}_{\mathrm{DIII}} = \mathrm{sgn}[\sqrt{(-1)^N/\det W}\,\mathrm{Pf}(D)]$, which changes whenever one Kramers pair crosses the Fermi energy. To establish a connection between $\mathcal{Q}_{\mathrm{DIII}}$ and the widely used bulk topological invariant $\mathcal{Q}$ for translationally invariant odd-parity single band SCs, we define $D(\boldsymbol{k}) = h(\boldsymbol{k})\sigma_2 + \Delta(\boldsymbol{k})$ for each momentum $\boldsymbol{k}$ in analogy to Eq. (3). For a TRIM $\boldsymbol{K}$, $\Delta(\boldsymbol{K}) = \mathbf{0}_2$ and $h(\boldsymbol{K}) = \xi(\boldsymbol{K})\sigma_0$ where $\xi(\boldsymbol{K})$ is the single-particle energy with respect to the Fermi energy. Hence, $D(\boldsymbol{K})$ is antisymmetric and in agreement with Sato[16]

$$\mathcal{Q} = \prod_{\boldsymbol{K} \in \mathrm{TRIM}} \mathcal{W}(\boldsymbol{K}), \tag{6}$$

where $\mathcal{W}(\boldsymbol{K}) \equiv \mathrm{sgn}[i\,\mathrm{Pf}\,D(\boldsymbol{K})] = \mathrm{sgn}\,\xi(\boldsymbol{K})$, so that $\mathcal{Q}$ counts the number parity of TRIM below the Fermi level and thus the Kramers parity. Consequently, $\mathcal{Q}_{\mathrm{DIII}} = \mathcal{Q}$ for these systems.[34] It is straightforward to generalize our definitions to multiband SCs as well. We will make use of this generalization to demonstrate that a lattice of impurity states can drive a SC into a topologically

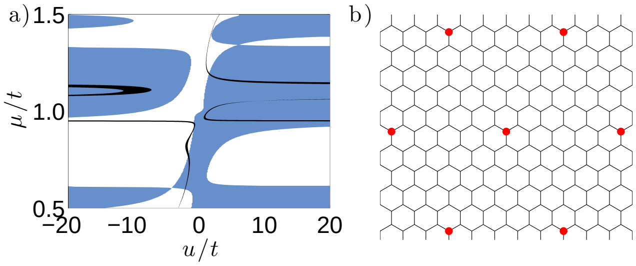

FIG. 2. a) Phase diagram of $\mathcal{Q}$ for an impurity lattice with impurity distance $a_{\rm imp} = 5$ in the TR invariant p-wave phase of the doped KH model as a function of the impurity strength u and the chemical potential μ. Blue denotes the topologically trivial phase $\mathcal{Q} = +1$ whereas white denotes the non-trivial phase $\mathcal{Q} = -1$. Black denotes regions where the system is gapless.[34] b) Impurity lattice for $a_{\rm imp} = 5$; red dots mark impurity sites.

non-trivial phase.

Impurities in the doped KH model: We illustrate our general results by applying them to the TR invariant $p_x \pm ip_y$-wave phase of the doped KH model on the honeycomb lattice,[28,29,36–38] which is paradigmatic for a number of interesting topological phases.[39] This phase is a two-dimensional analogue of the B phase of superfluid ^{3}He and undergoes a topological phase transition at a critical value of the chemical potential.[36] Consider, therefore, the mean field Hamiltonian

$$H_{\rm KH} = -\mu \sum_{\boldsymbol{k},s,\sigma} f^\dagger_{\boldsymbol{k},s,\sigma} f_{\boldsymbol{k},s,\sigma} - \sum_{\boldsymbol{k},\sigma} [t(\boldsymbol{k}) f^\dagger_{\boldsymbol{k},1,\sigma} f_{\boldsymbol{k},2,\sigma} + \text{h.c.}] + \sum_{\boldsymbol{k},\sigma} \left\{ [-\sigma d^x(\boldsymbol{k}) + i d^y(\boldsymbol{k})] f^\dagger_{\boldsymbol{k},1,\sigma} f^\dagger_{-\boldsymbol{k},2,\sigma} + \text{h.c.} \right\} \quad (7)$$

where $f_{\boldsymbol{k},s,\sigma}$ annihilates a fermion with spin σ on sublattice s, μ is the chemical potential, $t(\boldsymbol{k}) = t(e^{i\boldsymbol{\delta}_x\cdot\boldsymbol{k}} + e^{i\boldsymbol{\delta}_y\cdot\boldsymbol{k}} + e^{i\boldsymbol{\delta}_z\cdot\boldsymbol{k}})$ is the nearest neighbor hopping and $d^x = 3i\eta(e^{i\boldsymbol{\delta}_x\cdot\boldsymbol{k}} - e^{i\boldsymbol{\delta}_y\cdot\boldsymbol{k}})/\sqrt{6}, d^y = i\eta(e^{i\boldsymbol{\delta}_x\cdot\boldsymbol{k}} + e^{i\boldsymbol{\delta}_y\cdot\boldsymbol{k}} - 2e^{i\boldsymbol{\delta}_z\cdot\boldsymbol{k}})/\sqrt{2}, d^z = 0$ are the components of the $\boldsymbol{d}$ vector describing $p_x \pm ip_y$ spin-triplet pairing; for small $\boldsymbol{k}$, $\boldsymbol{d} \sim (k_x, k_y, 0)$. Here, η characterizes the superconducting gap and $\boldsymbol{\delta}_{x,y,z}$ are the nearest neighbor vectors.

In Eq. (7) we chose the spin quantization axis such that only equal-spin particles are paired, hence $[\mathcal{H}_{\rm KH}, \sigma_3] = 0$ which is a non-spatial symmetry protecting zero-energy states, cf. TAB. I. From the interacting Hamiltonian[29] the p-wave phase inherits symmetries acting on spin and spatial degrees of freedom.[40] Of these symmetries only the three mirror symmetries M_γ with respect to the x, y or z-links satisfy Eq. (4), for example $M_z = \tau_0 \otimes \sigma_1 \otimes R_z$ where R_z is the matrix for the mirror permutation of the lattice sites with respect to a z-link. Hence, also the M_γ protect the zero-energy crossings shown in FIG. 1. It is instructive to add Rashba spin orbit coupling $H_{\rm R} = i\lambda_{\rm R} \sum_{\langle ij\rangle,\alpha\beta} f^\dagger_{i\alpha} \left[\kappa_\gamma \left(\boldsymbol{\sigma} \times \hat{\boldsymbol{\delta}}_\gamma\right)_z\right]_{\alpha\beta} f_{j\beta}$, with $\hat{\boldsymbol{\delta}}_\gamma = \boldsymbol{\delta}_\gamma/|\boldsymbol{\delta}_\gamma|$ to the Hamiltonian while disregarding the effects that this coupling would have if the order parameter was calculated self-consistently. For $\lambda_{\rm R} \neq 0$ this breaks the non-spatial symmetry $[\mathcal{H}_{\rm KH}+\mathcal{H}_{\rm R}, \sigma_3] \neq 0$, but keeps all spatial symmetries intact if $\kappa_\gamma = 1$, $\gamma = x, y, z$. Anisotropic Rashba coupling with $\kappa_z \neq 1$ breaks all mirror symmetries except for M_z. By choosing different values for all three κ_γ one breaks all relevant symmetries and thus avoids the impurity induced zero-energy crossing. This is illustrated in FIG. 1.

In order to demonstrate that *extended* impurity states not only change $\mathcal{Q}_{\rm DIII}$ but also $\mathcal{Q}$, we consider a triangular lattice of impurities with lattice constant $a_{\rm imp} = 5$, amounting to an impurity density of 2% [see FIG. 2 b)]. We calculate $\mathcal{Q}$ by evaluating $\mathcal{W}(\boldsymbol{K})$ at the four TRIM as well as the Chern number $C_{\rm imp}$ of each spin-resolved impurity band formed by overlapping impurity subgap states, and confirm that $\mathcal{Q}(u) = (-1)^{C_{\rm imp}}\mathcal{Q}(0)$. Due to three-fold rotational symmetry of $H_{\rm KH}$[40] $\mathcal{W}(M) \equiv \mathcal{W}(M_1) = \mathcal{W}(M_2) = \mathcal{W}(M_3) \neq \mathcal{W}(\Gamma)$, where M_i denotes the M-points and Γ denotes the origin of the Brillouin zone. $\mathcal{W}(M)$ as well as $\mathcal{W}(\Gamma)$ are the sign of linear functions in u respectively and thus change independently of each other at critical values $u_{\rm c}^M$ and $u_{\rm c}^\Gamma$ respectively. Hence, one can change $\mathcal{Q} = \mathcal{W}(\Gamma)\mathcal{W}(M)$ by tuning u. In FIG. 2 a) we show the phase diagram of $\mathcal{Q}$ versus impurity strength u and chemical potential μ. The clean system is in the topologically trivial [non-trivial] phase for $\mu < \mu_{\rm c} \simeq 0.993\, t$ [$\mu > \mu_{\rm c}$]. At each value of μ two transitions occur at $u_{\rm c}^M$ and $u_{\rm c}^\Gamma$ respectively and the complicated dependence of $u_{\rm c}^M$ and $u_{\rm c}^\Gamma$ on μ gives rise to an intricate diagram. Remarkably, it is possible to render the system non-trivial by tuning u to values of the order of the hopping t.

Conclusion: We described symmetries which guarantee the existence of zero-energy impurity bound states in TR invariant SCs for a critical value of the impurity strength. The same symmetries allow the definition of the position space topological $\mathbb{Z}_2$ invariant $\mathcal{Q}_{\rm DIII}$ which we related to the bulk $\mathbb{Z}_2$ invariant $\mathcal{Q}$. The relevance of our findings was demonstrated for the TR invariant p-wave phase of the doped KH model, where symmetries protect the zero-energy crossings and a lattice of impurities can change the bulk topological order of the system. Finally, we have shown that TR invariant topologically non-trivial SCs can be made robust against low-energy impurity states by strongly breaking all additional symmetries. This improves prospects for protocols utilizing topologically protected Majorana zero-energy states.

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[1] A. V. Balatsky, I. Vekhter, and Jian-Xin Zhu, Rev. Mod. Phys. **78**, 373 (2006).
[2] H. Alloul, J. Bobroff, M. Gabay, and P. J. Hirschfeld, Rev. Mod. Phys. 81, 45 (2009).
[3] E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan, H. Eisaki, S. Uchida, and J. C. Davis, Nature (London) **411**, 920 (2001).
[4] J. D. Sau, and E. Demler, Phys. Rev. B **88**, 205402 (2013).
[5] H. Hu, L. Jiang, H. Pu, Y. Chen, and X.-J. Liu, Phys. Rev. Lett. **110**, 020401 (2013).
[6] K. Maki and E. Puchkaryov, Europhys. Lett. **45**, 263 (1999).
[7] G. Khaliullin, R. Kilian, S. Krivenko, and P. Fulde, Phys. Rev. B **56**, 11882 (1997).
[8] A. A. Abrikosov and L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **39**, 1781 (1960) [Soviet Phys.-JETP 12, 1243 (1961)].
[9] P. W. Anderson, J. Phys. Chem. Solids **11**, 26 (1959).
[10] A. Altland and M. R. Zirnbauer, Phys. Rev. B **55**, 1142 (1997); M. R. Zirnbauer, J. Math. Phys. **37**, 4986 (1996).
[11] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B **78**, 195125 (2008).
[12] A. Kitaev, arXiv:0901.2686 [cond-mat.mes-hall].
[13] X.-L. Qi, T. L. Hughes, S. Raghu, and S.-C. Zhang, Phys. Rev. Lett. 102, 187001 (2009).
[14] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[15] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[16] M. Sato, Phys. Rev. B **79**, 214526 (2009).
[17] L. Fu and E. Berg, Phys. Rev. Lett. **105**, 097001 (2010).
[18] More generally, the topological invariant in three dimensions is a $\mathbb{Z}$-invariant.[11] $\mathcal{Q}$ is the parity of this $\mathbb{Z}$-invariant.[16,17]
[19] N. Read and D. Green, Phys. Rev. B **61**, 10267 (2000).
[20] A. Y. Kitaev, Physics-Uspekhi **44**, 131 (2001).
[21] D. A. Ivanov, Phys. Rev. Lett. **86**, 268 (2001).
[22] F. Wilczek, Nature Physics 5, 614 (2009).
[23] I. C. Fulga, B. van Heck, M. Burrello, T. Hyart, Phys. Rev. B **88**, 155435 (2013).
[24] N. B. Kopnin and M. M. Salomaa, Phys. Rev. B **44**, 9667 (1991).
[25] G. E. Volovik, JETP Letters **70**, 609 (1999).
[26] The normal state single-particle Hamiltonian $H_0(u)$ in the limit $u \to -\infty$ has one additional Kramers pair occupied compared to the limit $u \to +\infty$. Thus, upon continuously tuning u from large negative to large positive values, at least one Kramers pair has to cross the Fermi level at zero energy.
[27] Supplemental material.
[28] A. Kitaev, Ann. Phys. **321**, 2 (2006).
[29] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009); J. Chaloupka, G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **105**, 027204 (2010).
[30] Y. Ueno, A. Yamakage, Y. Tanaka, and M. Sato, Phys. Rev. Lett. **111**, 087002 (2013).
[31] F. Zhang, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **111**, 056403 (2013).
[32] C.-K. Chiu, H. Yao, and S. Ryu, Phys. Rev. B **88**, 075142 (2013).
[33] T. Morimoto and A. Furusaki, Phys. Rev. B **88**, 125129 (2013).
[34] The gap can close at momenta away from the TRIM, such that $\mathcal{Q}_{\mathrm{DIII}}$ cannot be defined whereas $\mathcal{Q}$ still is well-defined, cf. (6). This indicates gapless topological superconductivity.[35]
[35] M. Sato and S. Fujimoto, Phys. Rev. Lett. **105**, 217001 (2010).
[36] T. Hyart, A. R. Wright, G. Khaliullin, and B. Rosenow, Phys. Rev. B **85**, 140510 (2012).
[37] S. Okamoto, Phys. Rev. B **87**, 064508 (2013).
[38] D. D. Scherer, M. M. Scherer, G. Khaliullin, C. Honerkamp, and B. Rosenow, Phys. Rev. B **90**, 045135 (2014).
[39] T. Hyart, A. R. Wright, and B. Rosenow, Phys. Rev. B **90**, 064507 (2014).
[40] Y.-Z. You, I. Kimchi, and A. Vishwanath, Phys. Rev. B **86**, 085145 (2012).