Topological Classification of One-Dimensional Chiral Symmetric Interfaces

Supplemental Material

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S1. PROOF OF THEOREM (5)

We consider the 2D substrate with the embedded scattering interface, described by the Hamiltonian $\mathcal{H}(k_x) = \mathcal{H}_0(k_x) + \mathcal{H}_V(k_x)$. The scattering interface is assumed to be concentrated to site $y = 0$, which could be a chain of impurities. Alternatively, as explained in the main text, if the interface has a larger width we can partition the y coordinates into supercells of the width of the interface, such that integer y label the position of the supercells, and the y dependence within each supercell is taken into account as internal matrix index such as spin or particle-hole degrees of freedom. For an interface in the form of a chain, the supercell matches the unit cell. Since $\mathcal{H}_V(k_x)$ is restricted to $y = 0$ we can write $\mathcal{H}_V(k_x) = H_V(k_x) \otimes P_{y=0}$, where P_y projects onto supercell y.

Let $\{|y\rangle\}$ form an orthonormal basis of 1D wavefunctions localised at cell y such that $\langle y|\,\mathcal{A}(k_x)\,|y'\rangle$ reduces any operator $\mathcal{A}(k_x)$ to a matrix of internal degrees of freedom only. We restrict ourselves to substrates that are fully translationally invariant, so $\langle y|\,\mathcal{H}_0(k_x)\,|y'\rangle = \langle y+n|\,\mathcal{H}_0(k_x)\,|y'+n\rangle$ for all y, y', n. Consider a global symmetry of the Hamiltonian $\tilde{\Lambda}$ such that $\tilde{\Lambda}^{-1}\mathcal{H}(k_x)\tilde{\Lambda} = \pm\mathcal{H}(\pm k_x)$, where the $\pm$ are chosen depending on the type of symmetry. As $\tilde{\Lambda}$ is global, it acts site-wise [S1], i.e. the symmetry is of the form $\tilde{\Lambda} = \Lambda \otimes \mathbb{1}_y$, where Λ is an operator that acts on the degrees of freedom within a supercell and $\mathbb{1}_y$ is the identity acting on the y cell coordinate. The action of the symmetry on the Hamiltonian gives

$$\tilde{\Lambda}^{-1}\big[\mathcal{H}_0(k_x) + \mathcal{H}_V(k_x)\big]\tilde{\Lambda} = \pm\big[\mathcal{H}_0(\pm k_x) + \mathcal{H}_V(\pm k_x)\big]. \tag{S1}$$

As $\mathcal{H}_V$ is local to the interface, there exists a $y^* > 0$ such that $\langle y'|\,\mathcal{H}_V(k_x)\,|y''\rangle = 0$ for $|y'|, |y''| > y^*$, but also that $\langle y'|\,\tilde{\Lambda}^{-1}\mathcal{H}_V(k_x)\tilde{\Lambda}\,|y''\rangle = 0$ as $\tilde{\Lambda}$ acts only locally. Therefore for such y', y''

$$\begin{aligned}&\langle y'|\,\tilde{\Lambda}^{-1}\big[\mathcal{H}_0(k_x) + \mathcal{H}_V(k_x)\big]\tilde{\Lambda}\,|y''\rangle \\ &= \pm\,\langle y'|\,\big[\mathcal{H}_0(\pm k_x) + \mathcal{H}_V(\pm k_x)\big]\,|y''\rangle\,,\end{aligned} \tag{S2}$$

reduces to

$$\langle y'|\,\tilde{\Lambda}^{-1}\mathcal{H}_0(k_x)\tilde{\Lambda}\,|y''\rangle = \pm\,\langle y'|\,\mathcal{H}_0(\pm k)\,|y''\rangle\,. \tag{S3}$$

Due to the translational invariance of $\mathcal{H}_0(k_x)$ the latter equality holds for any y', y'', and it follows that

$$\tilde{\Lambda}^{-1}\mathcal{H}_0(k_x)\tilde{\Lambda} = \pm\mathcal{H}_0(\pm k). \tag{S4}$$

This means that $\tilde{\Lambda}$ is a symmetry for $\mathcal{H}_0(k_x)$ separately too. From Eq. (S1) it follows in turn that

$$\tilde{\Lambda}^{-1}\mathcal{H}_V(k_x)\tilde{\Lambda} = \pm\mathcal{H}_V(\pm k), \tag{S5}$$

so that $\tilde{\Lambda}$ is a symmetry also for $\mathcal{H}_V(k_x)$. It follows further that Λ is a symmetry of $H_V(k_x)$.

Finally from Eq. (4) in the main text, we obtain that if $\tilde{\Lambda}$ is a symmetry of $\mathcal{H}_0(k_x)$, then Λ is a symmetry of $g(\omega = 0, k_x, y)$.

To prove the converse let us assume that Λ is a symmetry of $g(\omega = 0, k_x, y)$. Then $\tilde{\Lambda} = \Lambda \otimes \mathbb{1}_y$ is a symmetry of $\mathcal{H}_0(k_x)$ for the translationally invariant substrate. If furthermore Λ is a symmetry of $H_V(k_x)$, then $\tilde{\Lambda}$ is a symmetry of $\mathcal{H}_V(k_x) = H_V(k_x) \otimes P_{y=0}$. Therefore from Eq. (S1), $\tilde{\Lambda}$ is a symmetry of $\mathcal{H}(k_x)$. This concludes the proof of Theorem (5).

S2. WINDING NUMBER OF TOPOLOGICAL HAMILTONIAN

The winding number can evaluated by writing the Dyson equation for Green's function [Eq. (1) in the main text] as follows

$$\begin{aligned}G(0, k_x, y, y') = g(0, k_x, y)T(0, k_x)g(0, k_x, -y')\\ \times\Big\{\mathbb{1} + \big[g(0, k_x, -y')\big]^{-1}\big[T(0, k_x)\big]^{-1}\\ \times\big[g(0, k_x, y)\big]^{-1}g(0, k_x, y - y')\Big\}.\end{aligned} \tag{S6}$$

where $\mathbb{1}$ is the identity operator, the y label supercells as explained in Sec. S1, and the written G, g and T are matrices in all internal degrees of freedom of a supercell. The inversion of the substrate Green's function and the T-matrix is possible due to the assumption that both are gapped apart from at phase boundaries. The topological Hamiltonian [Eq. (3) in the main text] can then be written as

$$\begin{aligned}H^{top}(k_x, y) = -\Big\{\mathbb{1} + \big[g(0, k_x, -y)\big]^{-1}\big[T(0, k_x)\big]^{-1}\\ \times\big[g(0, k_x, y)\big]^{-1}g(0, k_x, 0)\Big\}^{-1}\\ \times\big[g(0, k_x, -y)\big]^{-1}\big[T(0, k_x)\big]^{-1}\big[g(0, k_x, y)\big]^{-1}.\end{aligned} \tag{S7}$$

To simplify the notation we shall omit the index k_x in most of the following expressions.

A. Case $y = 0$

Let us consider $y = 0$ and set $g = g(0, k_x, 0)$ and $T = T(0, k_x)$. The topological Hamiltonian then becomes

$$\begin{aligned} H^{top}(k_x) &= -\big(\mathbb{1} + g^{-1}T^{-1}\big)^{-1} g^{-1}T^{-1}g^{-1} \\ &= -\big[\mathbb{1} + g^{-1}\big(H_V^{-1} - g\big)\big]^{-1} g^{-1}T^{-1}g^{-1} \\ &= -H_V T^{-1} g^{-1}. \end{aligned} \tag{S8}$$

Theorem (5) guarantees that T, g and H_V, and therefore H^{top}, are all chiral symmetric, admit a simultaneous chiral decomposition, and can be written in the chiral eigenbasis

$$\begin{aligned} H_V = \begin{pmatrix} 0 & h_V \\ h_V^\dagger & 0 \end{pmatrix}, \quad g^{-1} = \begin{pmatrix} 0 & \tilde{g}^{-1} \\ \tilde{g}^{-1\dagger} & 0 \end{pmatrix}, \\ T^{-1} = \begin{pmatrix} 0 & \tilde{T}^{-1} \\ \tilde{T}^{-1\dagger} & 0 \end{pmatrix}, \quad H^{top} = \begin{pmatrix} 0 & h^{top} \\ h^{top\dagger} & 0 \end{pmatrix}, \end{aligned} \tag{S9}$$

where

$$h^{top} = -h_V \tilde{T}^{-1\dagger} \tilde{g}^{-1}. \tag{S10}$$

The minus sign does not affect the winding number which can then be evaluated as

$$\begin{aligned} W(y=0) &= \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk_x \partial_{k_x} \log[\det(h^{top})] \\ &= \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk_x \partial_{k_x} \Big\{ \log[\det(h_V)] + \log[\det(\tilde{T}^{-1\dagger})] \\ &\qquad + \log[\det(\tilde{g}^{-1})] \Big\}. \end{aligned} \tag{S11}$$

Consider a general chiral symmetric operator A with chiral decomposition a and take a change of variable $z = \det(a)$ such that the k_x integration over the first Brillouin zone becomes the z integration over the closed contour $\mathcal{Z} = \{\, z = \det(a(k_x)) \,|\, k_x \in [-\pi, \pi) \,\}$. We can then write the corresponding winding number in the form

$$W_A = \int_{-\pi}^{\pi} \frac{dk_x}{2\pi i} \partial_{k_x} \log\big\{\det\big[a(k_x)\big]\big\} = \oint_{\mathcal{Z}} \frac{dz}{2\pi i z}. \tag{S12}$$

From this expression we see that if we take $a \to a^\dagger$, $\det(a) \to \det(a)^*$ then $\mathcal{Z}$ is inverted about the real axis and the contour is traversed in the opposite direction. This gives an overall minus to the winding number. Therefore the winding number of the topological Hamiltonian becomes

$$W(y=0) = W_{g^{-1}} - W_{T^{-1}} + W_{H_V}. \tag{S13}$$

A locally acting H_V has a zero winding number. But general k_x dependent $H_V(k_x)$ may lead to $W_{H_V} \neq 0$, and thus seemingly to a topological phase transition without gap closure. However, in such a case the change in W_{H_V} is compensated by a simultaneous change in $W_{T^{-1}}$, so that a gap closure still remains mandatory. To see this, we should recall that $-W_{T^{-1}} + W_{H_V}$ represents the winding of $H_V T^{-1} = \mathbb{1} - H_V g$, thus of $\det(\mathbb{1} - h_V \tilde{g}^\dagger)$. This means that the direct winding from H_V is undone but the zeros of T^{-1} are preserved. In case of doubt indeed the foolproof expression to be used for the winding number is $(\mathbb{1} - h_V \tilde{g}^\dagger)$, whereas the T-matrix arises naturally from scattering theory and remains under normal conditions the object of choice.

B. Case $y \neq 0$

When $y \neq 0$, the chiral decomposition of the Hamiltonian is

$$\begin{aligned} h^{top}(y) = &- \Big\{ \mathbb{1} + \big[\tilde{g}(-y)\big]^{-1} \tilde{T}^{-1\dagger} \big[\tilde{g}(y)\big]^{-1} \tilde{g}(0) \Big\}^{-1} \\ &\times \big[\tilde{g}(-y)\big]^{-1} \tilde{T}^{-1\dagger} \big[\tilde{g}(y)\big]^{-1}, \end{aligned} \tag{S14}$$

where $\tilde{g}(y)$ is the chiral decomposition of $g(0, k_x, y)$. The winding number is then evaluated as before. We obtain

$$\begin{aligned} W(y) = &\int_{-\pi}^{\pi} \frac{dk_x}{2\pi i} \\ \times \partial_k \Big\{ &- \log\big[\det\big(\mathbb{1} + \big[\tilde{g}(-y)\big]^{-1} \tilde{T}^{-1\dagger} \big[\tilde{g}(y)\big]^{-1} \tilde{g}(0)\big)\big] \\ &+ \log\big[\det\big(\big[\tilde{g}(-y)\big]^{-1}\big)\big] + \log\big[\det\big(\tilde{T}^{-1\dagger}\big)\big] \\ &+ \log\big[\det\big(\big[\tilde{g}(y)\big]^{-1}\big)\big] \Big\}, \end{aligned} \tag{S15}$$

which gives Eq. (10) in the main text. If we consider the Lehmann representation of the Green's function [S2]

$$G(\omega, k_x) = \sum_n \frac{|E_n(k_x)\rangle \langle E_n(k_x)|}{\omega_+ - E_n(k_x)}, \tag{S16}$$

where E_n and $|E_n\rangle$ are the eigenvalues and eigenmodes of the Hamiltonian and $\omega_+ = \omega + i0^+$, the local Green's function can be written as

$$\begin{aligned} G(\omega, k_x, y, y) &= \langle y |\, G(\omega, k_x) \,| y \rangle \\ &= \sum_n \frac{\langle y | E_n(k_x) \rangle \langle E_n(k_x) | y \rangle}{\omega_+ - E_n(k_x)}. \end{aligned} \tag{S17}$$

For a trivial substrate the in-gap wavefunctions are localised to the interface region and normalisable. Therefore for such wavefunctions $\lim_{|y|\to\infty} \langle y | E_{in-gap}(k_x) \rangle = 0$. Taking thus $|y| \to \infty$ for generic V_m, k_m suppresses any pole from the in-gap modes. The remaining poles are from substrate and therefore gapped as the substrate is trivial. This then means that $W(|y| \to \infty) = 0$ and $H^{top}(k_x, |y| \to \infty)$ is trivial. Examining the form of the winding number we obtain

$$\begin{aligned} W_{T^{-1}} = &- \lim_{|y|\to\infty} \int_{-\pi}^{\pi} \frac{dk_x}{2\pi i} \\ &\times \partial_k \log\Big\{ \det\Big[\mathbb{1} + \big[\tilde{g}(-y)\big]^{-1} \tilde{T}^{-1\dagger} \big[\tilde{g}(y)\big]^{-1} \tilde{g}(0) \Big] \Big\}. \end{aligned} \tag{S18}$$

From the form of the Green's function in Eq. (S6) we see the term that gives the y dependent winding number does not have any poles (as we have assumed the substrate is trivial). As such any change in the winding number as y is varied must be due to zeros in the determinant of this term and so of $G(\omega = 0, k_x, y, y)$.

S3. PROOF OF THE EQUIVALENCE OF THE WINDING NUMBERS OF H AND H^{top}

In this section we prove that the winding numbers obtained for the full Hamiltonian $\mathcal{H}$ and for the topological Hamiltonian H^{top} are equal, up to a fixed sign between them, and hence they are equivalent descriptions of the topological properties of the system.

The substrate is assumed to be translationally invariant with a topologically trivial bulk Hamiltonian $\mathcal{H}_0(k_x, k_y)$. As the scattering interface breaks the translational symmetry in the y direction we switch the description from k_y to positions y and note that the system then becomes one-dimensional with an effective unit cell that contains all y labels. We shall denote the full Hamiltonian in this description $\mathcal{H}(k_x)$ and the substrate Hamiltonian $\mathcal{H}_0(k_x)$. With the scattering included we have $\mathcal{H}(k_x) = \mathcal{H}_0(k_x) + H_V(k_x) \otimes P_{y=0}$, where $P_{y=0}$ denotes the projection onto $y = 0$. The following proof will rely on the assumption stated in the main text that $\det[g(\omega = 0, k_x, y = 0)] \neq 0$, and on the the already demonstrated property that $W_{H^{top}}$ can only change when a pole of the T-matrix passes through $\omega = 0$. The topology will be characterised through the winding numbers for the different k_x dependent matrices from Hamiltonians or Green's functions.

The proof of the required theorem is broken up into several stages.

(a) *$\mathcal{H}_0(k_x)$ and $[g(\omega = 0, k_x, y = 0)]^{-1}$ are topologically trivial*

We assume that the substrate is trivial, meaning that the relevant 2D topological index of $\mathcal{H}_0(k_x, k_y)$ is zero. This means there is a continuous deformation of $\mathcal{H}_0(k_x, k_y)$ to a trivial spectrally flat (k_x, k_y independent) Hamiltonian. Such a deformation preserves the gap at all k_x, k_y and as such preserves the gap of the 1D Hamiltonian $\mathcal{H}_0(k_x)$. This means that $\mathcal{H}_0(k_x)$ is continuously connected to a trivial spectrally flat phase and so the winding number of $\mathcal{H}_0(k_x)$ is zero.

The eigenvalues of $\mathcal{H}_0(k_x)$ define the poles of $g(\omega = 0, k_x, y = 0)$ and so the zeros of $[g(\omega = 0, k_x, y = 0)]^{-1}$. Since the considered deformation does not produce a gap closure of $\mathcal{H}_0(k_x, k_y)$, it does not produce a gap closure of $[g(\omega = 0, k_x, y = 0)]^{-1}$ either. Since we assume furthermore that initially $\det[g(\omega = 0, k_x, y = 0)] \neq 0$ it is possible to choose a deformation that does not cause $\det[g(\omega = 0, k_x, y = 0)] = 0$ at any point, as this would require for the assumed topologically trivial substrate a fine tuning of the parameters that is avoidable. Hence we can choose a deformation that continuously connects $\mathcal{H}_0(k_x, k_y)$ to a k_x independent Hamiltonian while maintaining an invertible, finite $g(\omega = 0, k_x, y = 0)$ throughout. Hence $[g(\omega = 0, k_x, y = 0]^{-1}$ transforms continuously to a k_x independent matrix too, showing that it is topologically trivial.

(b) *$\mathcal{H}(k_x)$ is trivial if and only if $H^{top}(k_x, y = 0)$ is trivial*

Let $\mathcal{H}(k_x)$ be topologically trivial. Then it can be continuously deformed to the $H_V = 0$ limit (i.e. to the substrate Hamiltonian), as we know it is topologically trivial too. Such a deformation generates no gap closures in $\mathcal{H}(k_x)$ and so no poles of $T(\omega = 0, k_x)$. Therefore the winding number of $H^{top}(k_x, y = 0)$ is preserved and equal to winding number of $H^{top}(k_x, y = 0)|_{H_V=0} = -[g(\omega = 0, k_x, y = 0)]^{-1}$. From item (a) it follows that $W_{H^{top}} = 0$. Conversely, if $H^{top}(k_x, y = 0)$ is topologically trivial it can be deformed continuously to the $H_V = 0$ limit without generation of any pole in $T(\omega = 0, k_x)$. Therefore $\mathcal{H}(k_x)$ can be continuously connected to $\mathcal{H}_0(k_x)$ which is trivial, and consequently $W_{\mathcal{H}} = 0$.

(c) *$|W_{\mathcal{H}}| = |W_{H^{top}}|$*

We shall show that the equality $|W_{\mathcal{H}}| = |W_{H^{top}}|$ follows from the simultaneous fulfilment of the two inequalities $|W_{\mathcal{H}}| \leq |W_{H^{top}}|$ and $|W_{H^{top}}| \leq |W_{\mathcal{H}}|$. We make use of the fact that for any phase with a winding number of modulus $|W|$ deformations of the system parameters to $W = 0$ require at least $|W|$ gap closures, and that there are deformations that pass through exactly $|W|$ gap closures. Let then $|W_{\mathcal{H}}| < |\mathcal{W}_{H^{top}}|$. Then there exists a deformation of $\mathcal{H}(k_x)$ to the trivial $\mathcal{H}_0(k_x)$ by letting $H_V \to 0$ that generates only $|W_{\mathcal{H}}|$ gap closures, and as such exactly $|W_{\mathcal{H}}|$ poles of $T(\omega = 0, k_x)$. However, since $|W_{H^{top}}|$ is strictly larger than this number of gap closures, it is impossible that $H^{top}(k_x, y = 0)$ could then connect to the topologically trivial $H_V = 0$ limit $H^{top}(k_x, y = 0) = -[g(\omega = 0, k_x, y = 0)]^{-1}$. We must conclude therefore that $|\mathcal{W}_{H^{top}}| \leq |W_{\mathcal{H}}|$. The converse is proven by swapping the roles of $\mathcal{H}(k_x)$ and $H^{top}(k_x, y = 0)$.

(d) *$W_{\mathcal{H}} = \pm W_{H^{top}}$ with a fixed $\pm$ sign through the phase diagram*

Consider a pair of Hamiltonians $\mathcal{H}_1(k_x)$ and $\mathcal{H}_2(k_x)$ together with their associated topological Hamiltonians $H_1^{top}(k_x)$ and $H_2^{top}(k_x)$. We assume first that $W_{\mathcal{H}_1} = -W_{\mathcal{H}_2} \neq 0$. We have already proven that then $|W_{H_1^{top}}| = |W_{H_2^{top}}|$ but we wish to show furthermore that $W_{H_1^{top}} = -W_{H_2^{top}}$. Let us assume that $W_{H_1^{top}} = W_{H_2^{top}}$ instead. Then there is a continuous deformation between $H_1^{top}(k_x)$ and $H_2^{top}(k_x)$ that generates no gap closures and thus no poles of $T(\omega = 0, k_x)$. Consequently $\mathcal{H}_1(k_x)$ and $\mathcal{H}_2(k_x)$ must be continuously connected too, which is a contradiction with the assumption $W_{\mathcal{H}_1} = -W_{\mathcal{H}_2}$. Therefore

we must have $W_{H_1^{top}} = -W_{H_2^{top}}$. The converse is proven by the same logic as already applied above, by switching the role of $\mathcal{H}(k_x)$ and $H^{top}(k_x)$. Note that we cannot say anything about the sign between $W_{\mathcal{H}}$ and $W_{H^{top}}$, but as this sign is global to the entire phase diagram it is irrelevant.

As a consequence of items (a)–(d) the two winding numbers $W_{\mathcal{H}}$ and $W_{H^{top}}$ are equivalent, if not equal.

S4. FOURIER TRANSFORM OF LATTICE S-WAVE SUPERCONDUCTOR GREEN'S FUNCTION

The partially Fourier transformed retarded Green's function of a square lattice s-wave superconductor is evaluated. The Hamiltonian of such a 2D superconductor, after taking the gauge transformation $c^\dagger_{x,y,\sigma} \to e^{ik_m\sigma}c^\dagger_{x,y,\sigma}$, where k_m is the spiral wavevector of the magnetic impurity interface, is given by

$$\mathcal{H}_0(k_x,k_y) = \mathcal{H}^\uparrow\sigma^\uparrow + \mathcal{H}^\downarrow\sigma^\downarrow, \tag{S19}$$

where we define $\sigma^{\uparrow,\downarrow} = (\mathbb{1} \pm \sigma^z)/2$, for σ^z the Pauli-z matrix acting on the spin degrees of freedom and

$$\mathcal{H}^\sigma = \epsilon_{k_x,k_y,\sigma}\tau^z + \sigma\Delta\tau^x, \tag{S20}$$

where $\epsilon_{k_x,k_y,\sigma} = -2t(\cos(k_x+\sigma k_m)+\cos(k_y)) - \mu$, the τ^i are the Pauli matrices acting on the particle-hole degrees of freedom, t is the hopping integral, μ the chemical potential, and Δ the superconductor pairing amplitude chosen to be real and positive. The retarded Green's function of the superconductor is given by [S2]

$$g(\omega,k_x,k_y) = [\omega_+ - \mathcal{H}_0(k_x,k_y)]^{-1}, \tag{S21}$$

where $\omega_+ = \omega + i0^+$. The partial Fourier transform of the retarded Green's function is defined as [S3]

$$g(\omega,k_x,y) = \int_{-\pi}^{\pi}\frac{dk_y}{2\pi}e^{ik_y y}g(\omega,k_x,k_y). \tag{S22}$$

For the given Hamiltonian we obtain

$$g(\omega,k_x,y) = g^\uparrow(\omega,k_x,y)\sigma^\uparrow + g^\downarrow(\omega,k_x,y)\sigma^\downarrow, \tag{S23}$$

with

$$g^\sigma(\omega,k_x,y) = \frac{1}{2\pi}\int_{-\pi}^{\pi}dk_y\frac{e^{ik_y y}(\omega_+ + \epsilon_{k,\sigma}\tau^z + \sigma\Delta\tau^x)}{\omega_+^2 - \epsilon_{k,\sigma}^2 - \Delta^2}. \tag{S24}$$

We should notice that since $g(\omega,k_x,k_y) = g(\omega,k_x,-k_y)$ this integral is independent of the sign of y and we can thus replace $y \to |y|$. We then change the integration variable to $z = e^{ik_y}$, with $dz = izdk_y$, such that the integration is over the unit circle S^1 in the positive, anticlockwise direction, and obtain

$$g^\sigma(\omega,k_x,y) = \frac{1}{2\pi i}\oint_{S^1}dz\, z^{|y|-1}\, g(\omega,k_x,z). \tag{S25}$$

As we focus on the in-gap states with $|\omega| < \Delta$, the small $+i0^+$ is of no importance we shall use ω instead of ω_+ henceforth. Focusing on just the denominator in the integrand

$$\begin{aligned} &z(\omega^2 - \epsilon^2_{k_x,z,\sigma} - \Delta^2) \\ &= z\Big\{\omega^2 - \big[-t(z+1/z) - \mu_{k_x}\big]^2 - \Delta^2\Big\} \\ &= z(\omega^2-\Delta^2) - \frac{z}{z^2}\big[t(z^2+1) + \mu_{k_x}z\big]^2 \\ &= \frac{t^2}{z}\Big\{z^2(\tilde\omega^2 - \tilde\Delta^2) - \big[(z^2+1) + \tilde\mu_{k_x}z\big]^2\Big\}, \end{aligned} \tag{S26}$$

where we have defined $\tilde\mu_{k_x} = \tilde\mu + 2\cos(k_x + \sigma k_m)$ and introduced the dimensionless energies $\tilde\omega = \omega/t$, $\tilde\Delta = \Delta/t$, and $\tilde\mu = \mu/t$. The integral then becomes

$$g^\sigma(\omega,k_x,y) = \frac{1}{2\pi i t^2}\oint_{S^1}\frac{dz z^{|y|+1}g^\sigma(\omega,k_x,z)}{z^2(\tilde\omega^2-\tilde\Delta^2) - [(z^2+1)+\tilde\mu_{k_x}z]^2}. \tag{S27}$$

The numerator is given by

$$z^{|y|+1}g^\sigma(\omega,k_x,z) = tz^{|y|}\Big[\tilde\omega z - (\tilde\mu_{k_x}z + z^2 + 1)\tau^z + z\sigma\tilde\Delta\tau^x\Big]. \tag{S28}$$

All the poles are contained within the denominator and we can safely proceed by solving

$$0 = z^2(\tilde\omega^2-\tilde\Delta^2) - \big[(z^2+1)+\tilde\mu_{k_x}z\big]^2, \tag{S29}$$

or

$$z^2(\tilde\omega^2-\tilde\Delta^2) = \big[(z^2+1)+\tilde\mu_{k_x}z\big]^2, \tag{S30}$$

from which the square root leads to the two quadratic equations

$$0 = z^2 + z(\tilde\mu_{k_x} \pm \sqrt{\tilde\omega^2-\tilde\Delta^2}) + 1. \tag{S31}$$

We thus obtain the four roots of the denominator

$$\begin{aligned} z_{\pm_1,\pm_2} = &\frac{1}{2}\Big[\tilde\mu_{k_x} \pm_1 \sqrt{\tilde\omega^2-\tilde\Delta^2}\Big] \\ &\pm_2 \frac{1}{2}\sqrt{\Big(-\tilde\mu_{k_x} \pm_1 \sqrt{\tilde\omega^2-\tilde\Delta^2}\Big)^2 - 4}. \end{aligned} \tag{S32}$$

Then the integral is

$$\begin{aligned} &g^\sigma(\omega,k_x,y) = \\ &\frac{-1}{2\pi i t}\oint_{S^1}\frac{z^{|y|}dz}{(z-z_{+,+})(z-z_{-,+})(z-z_{+,-})(z-z_{-,-})} \\ &\quad\times\Big[\tilde\omega z - (\tilde\mu_{k_x}z + z^2+1)\tau^z + z\sigma\tilde\Delta\tau^x\Big]. \end{aligned} \tag{S33}$$

The total minus sign arises from the negative z^4 coefficient in the denominator. The integral can then be evaluated using Cauchy's residue theorem. In Fig. S1 we show

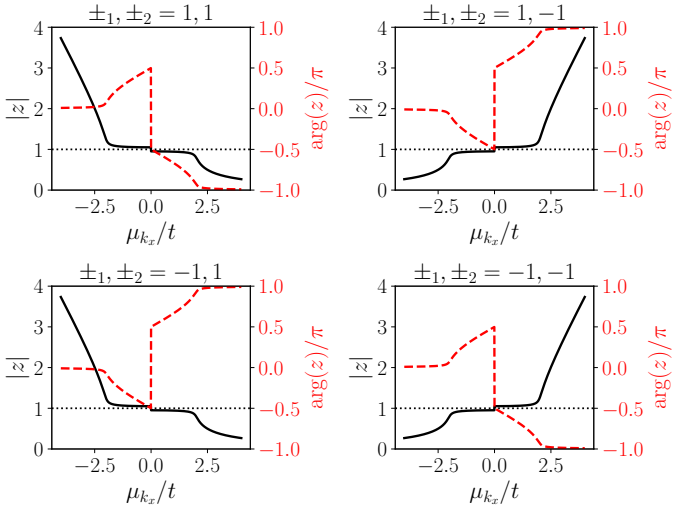

FIG. S1. Modulus (black, solid) and phase (red, dashed) of the poles obtained from Eq. (S31) for $\omega = 0$ and $\Delta = 0.1t$. The black dotted line shows $|z| = 1$. One can verify that as long as $|\omega| < \Delta$, the two poles $z_{\pm,\mathrm{sign}(\mu_{k_x})}$ are within in the unit circle.

the value of the poles for the example of $\omega = 0$ as a function of μ_{k_x}. For $|\omega| < \Delta$ the poles $z_{1,2} = z_{\pm,\mathrm{sign}(\mu_k)}$ lie within the unit circle, and the poles $z_{3,4} = z_{\pm,-\mathrm{sign}(\mu_k)}$ are outside the unit circle. The Green's function then evaluates to

$$g^\sigma(\omega, k_x, y) = \frac{-\xi_-(\tilde{\omega} + \sigma\tilde{\Delta}\tau^x) + i\xi_+\sqrt{\tilde{\Delta}^2 - \tilde{\omega}^2}\tau^z}{t(z_1 - z_2)} \tag{S34}$$

where

$$\xi_\pm = \frac{z_1^{|y|+1}}{(z_1 - z_3)(z_1 - z_4)} \pm \frac{z_2^{|y|+1}}{(z_2 - z_3)(z_2 - z_4)}. \tag{S35}$$

We note that ξ_+ is real and ξ_- purely imaginary as $z_1 = z_2^*$ and $z_3 = z_4^*$. Consequently g^σ is real as expected for a Green's function when ω lies in a range with vanishing density of states. The $\xi_\pm$ functions are non-singular as long as $\Delta \neq 0$. We emphasise that this is the exact Green's function of a square lattice tight binding s-wave superconductor, and no low-energy approximation has been made.

S5. PHASE DIAGRAM

With the explicit form of the Green's function for the impurity chain given by Eq. (1) in the main text, we can solve for the conditions of a phase boundary by finding poles of the T-matrix at $\omega = 0$,

$$\det\left[T^{-1}(0, k_x)\right] = 0. \tag{S36}$$

This equation can be simplified by making use the model's chiral symmetry at $\omega = 0$. We can write the T-matrix in the eigenbasis of the chiral symmetry, using the unitary

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & i & 0 & i \\ 0 & -1 & 0 & 1 \\ i & 0 & -i & 0 \end{pmatrix}, \tag{S37}$$

written in the basis

$$(c_{k_x,y=0,\uparrow}, c_{k_x,y=0,\downarrow}, c^\dagger_{-k_x,y=0,\uparrow}, c^\dagger_{-k_x,y=0,\downarrow}). \tag{S38}$$

This transforms the T-matrix to

$$U^\dagger T^{-1} U = \begin{pmatrix} 0 & \tilde{T}^{-1} \\ \tilde{T}^{-1\dagger} & 0 \end{pmatrix}, \tag{S39}$$

with the notation $T = T(\omega = 0, k_x)$ and

$$\det(T^{-1}) = |\det(\tilde{T}^{-1})|^2. \tag{S40}$$

Defining the notation $g^\sigma_{ij} = [g^\sigma(\omega = 0, k_x, y = 0)]_{ij}$ and using that at $\omega = 0$ we have $g^\sigma_{11} = -g^\sigma_{22}$ and $g^\sigma_{12} = g^\sigma_{21}$, we obtain

$$\tilde{T}^{-1} = \begin{pmatrix} ig^\uparrow_{12} - g^\uparrow_{11} & \frac{i}{V_m} \\ -\frac{i}{V_m} & ig^\downarrow_{12} - g^\downarrow_{11} \end{pmatrix}. \tag{S41}$$

The condition for a phase transition is $\det(T^{-1}) = 0$, which becomes

$$0 = g^\uparrow_{11}g^\downarrow_{11} - g^\uparrow_{12}g^\downarrow_{12} - i(g^\uparrow_{11}g^\downarrow_{12} + g^\downarrow_{11}g^\uparrow_{12}) - \frac{1}{V_m^2}. \tag{S42}$$

The bare Green's function is real as the density of states is zero at $\omega = 0$, and as noted earlier we can omit the infinitesimal shifts $i0^+$. Then the real and imaginary parts split into two equations. The imaginary part gives

$$g^\downarrow_{11}g^\uparrow_{12} = -g^\uparrow_{11}g^\downarrow_{12}. \tag{S43}$$

If $k_m \neq n\pi$ for $n \in \mathbb{Z}$, this has solutions for any set of system parameters, but required $k_x = 0, \pi$. This is because the only differences between the two spin species is the kinetic energy $\cos(k_x + \sigma k_m)$ and the sign of the pairing $\sigma\Delta$. At $k_x = 0, \pi$, the dispersions are equal as $\cos(k_x + \sigma k_m) = \pm\cos(\sigma k_m) = \pm\cos(k_m)$. Therefore $g^\uparrow_{11} = g^\downarrow_{11}$ and $g^\uparrow_{12} = -g^\downarrow_{12}$, and so the above equation is satisfied. When $k_m = 0, \pi$, the above equation is satisfied for any k_x meaning the gap closes and stays closed rather than opening up again.

The real part gives the conditions for the phase transition and along with the symmetry of the spin species at $k_x = 0, \pi$. We find

$$V^*_{m,k_x} = \pm\left\{[g^\uparrow_{11}(k_x)]^2 + [g^\uparrow_{12}(k_x)]^2\right\}^{-1/2}. \tag{S44}$$

giving Eq. (12) in the main text. As gap closures only occur at $k_x = 0, \pi$, the winding number is restricted to

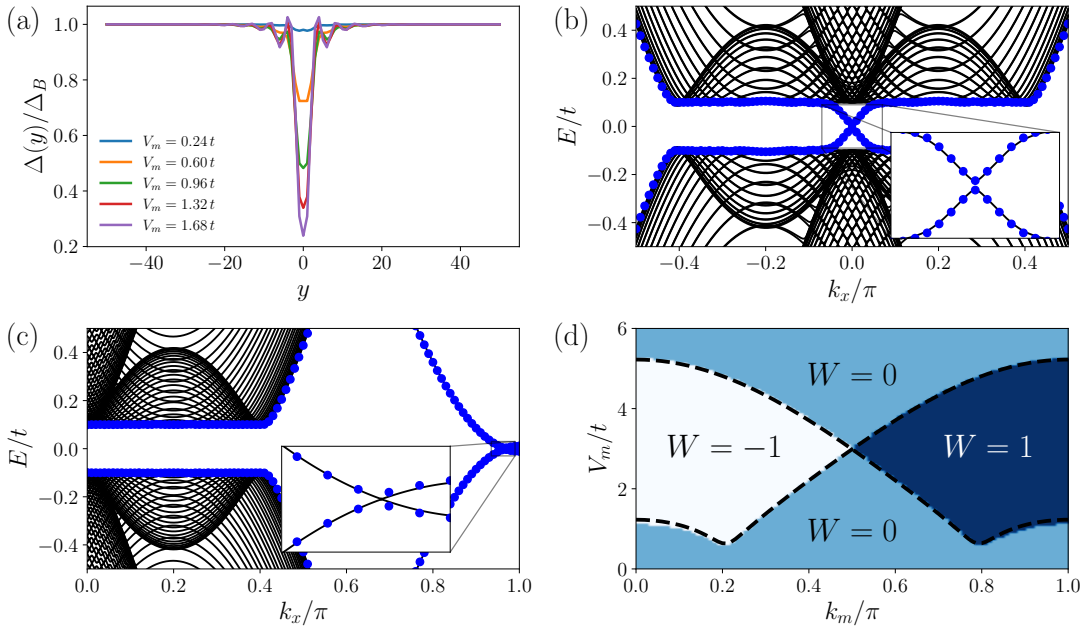

FIG. S2. Results of self-consistent calculations for $N_y = 101$, $\Delta_B = 0.1t$ and $k_F = 0.65$. Panel (a) Shows $\Delta(y)$ for $k_m = k_F$ and various values of V_m. Although the scattering potential has a considerable effect at the impurity site at $y = N_y/2$, the renormalisation of $\Delta(y)$ almost immediately drops to below 10% independently of the scattering strength. Panels (b) and (c) show a comparison of the band structure of the self-consistent solution (black lines) and lowest two eigenvalues of the non-self consistent $\Delta(y) = \Delta_B$ (blue circles) for $k_m = 0.63$, and $V_m = 0.6$ and 4.8 respectively. There is very little difference between the two, particularly around the gap closures at $k_x = 0, \pi$. The insets confirm that there is little change in the electronic structure. Panel (d) shows the phase diagram obtained from Eq. (S48) together with the analytically calculated phase boundaries from Eq. (S44). There is almost perfect agreement.

$W = 0, 1, -1$ and therefore it is sufficient to find its parity. This can written as the sign of the product of the determinants of the chiral decomposition at $k_x = 0, \pi$ [S4]. Using the chiral decomposition above, this is given by

$$\begin{aligned}(-1)^{W(y=0)} &= \prod_{k_x=0,\pi} \text{sign}\left[(g_{11}^{\uparrow})^2 + (g_{12}^{\uparrow})^2 - (V_m)^{-2}\right] \\ &= \prod_{k_x=0,\pi} \text{sign}\left[(V_{m,k_x}^{*})^{-2} - (V_m)^{-2}\right], \end{aligned} \tag{S45}$$

giving Eq. (13) in the main text.

S6. PHASE DIAGRAM OF SELF-CONSISTENT SOLUTION

We describe a self-consistent solution to the superconducting gap equations in the presence of a magnetic interface and show that it makes very little difference to the overall phase diagram. The self-consistency condition is the same that was used in Ref. [S3, S5]. We restrict ourselves to just s-wave pairing as the triplet pairing is extremely weak. We maintain translational invariance along the x-direction. Then the self consistency condition is

$$\Delta(y) = V_P \langle c_{x,y,\uparrow}^{\dagger} c_{x,y,\downarrow}^{\dagger} \rangle = V_P \sum_{k_x} \langle c_{k_x,y,\uparrow}^{\dagger} c_{-k_x,y,\downarrow}^{\dagger} \rangle , \tag{S46}$$

where $\langle \ldots \rangle$ denotes the ground state average. The translational invariance along the x-direction means the pairing is only a function of y. The pairing potential strength V_P is chosen such that the pairing tends to the chosen bulk pairing, Δ_B (i.e. the pairing at $V_m = 0$)

$$V_P = \frac{\Delta_B}{\sum_{k_x} \langle c_{k_x,|y|\to\infty,\uparrow}^{\dagger} c_{-k_x,|y|\to\infty,\downarrow}^{\dagger} \rangle}. \tag{S47}$$

Starting from the initial guess $\Delta(y) = \Delta_B$ we calculate $\langle c_{k_x,y,\uparrow}^{\dagger} c_{-k_x,y,\downarrow}^{\dagger} \rangle$ from direct diagonalisation of the tight-binding matrix. With this result we update V_P through Eq. (S47) to guarantee that $\Delta(y)$ tends to Δ_B at large y. With this we reconstruct the Hamiltonian and iterate until convergence. With the final solution of the tight-binding model we calculate a topological invariant of the bands. As it is computationally heavy to calculate the winding number of a large matrix, we make use of the inversion symmetry to calculate an equivalent invariant. This is defined as

$$\nu = n_0 - n_\pi, \tag{S48}$$

where n_{k_x} is the number of negative non-zero eigenvalues of $P(k_x)\mathcal{I}P(k_x)$ where $\mathcal{I}$ is the inversion symmetry operator. This has been shown to be equal to the number of $\zeta = 1/2$ modes in the entanglement spectrum localised to the edge of the system [S6].

The self consistent solution to the gap is shown in Fig. S2(a) for various V_m. We see that the gap is lowered by around 20% around the magnetic impurity around the critical scattering $V^*_{m,k_x=0} \approx 0.63t$. The residual error of this solution is on the order of $10^{-8}\Delta_B$. We show the band structure for two values of V_m around the phase boundaries in Fig. S2(b)–(c) and compare it to the in-gap bands of the non-self-consistent solution. We again see that around the bottom of the band very little difference is made and the only visible deviations are around the $k_x \approx 2k_F$ where the in-gap bands of the self-consistent solution are slightly lower than the non-self-consistent one. Finally, in Fig. S2(d) we show the phase diagram of the invariant ν defined above with the non-self-consistent phase boundaries overlayed and again we see perfectly agreement up to the pixel size. We conclude that self-consistency has so little effect on all relevant results such that it can be safely ignored.

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