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Majorana Bound States without Vortices in Topological Superconductors with Electrostatic Defects

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Vortices in two-dimensional superconductors with broken time-reversal and spin-rotation symmetry can bind states at zero excitation energy. These so-called Majorana bound states transform a thermal insulator into a thermal metal and may be used to encode topologically protected qubits. We identify an alternative mechanism for the formation of Majorana bound states, akin to the way in which Shockley states are formed on metal surfaces: An electrostatic line defect can have a pair of Majorana bound states at the end points. The Shockley mechanism explains the appearance of a thermal metal in vortex-free lattice models of chiral p -wave superconductors and (unlike the vortex mechanism) is also operative in the topologically trivial phase.

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Two-dimensional superconductors with spin-polarized-triplet, p -wave pairing symmetry have the unusual property that vortices in the order parameter can bind a non-degenerate state with zero excitation energy [1–4]. Such a midgap state is called a Majorana bound state, because the corresponding quasiparticle excitation is a Majorana fermion—equal to its own antiparticle. A pair of spatially separated Majorana bound states encodes a qubit, in a way which is protected from local sources of decoherence [5]. Since such a qubit might form the building block of a topological quantum computer [6], there is an intensive search [7–12] for two-dimensional superconductors with the required combination of broken time-reversal and spin-rotation symmetries (symmetry class D [13]).

The generic Bogoliubov–de Gennes Hamiltonian H of a chiral p -wave superconductor is only constrained by particle-hole symmetry, $\sigma_x H^* \sigma_x = -H$. At low excitation energies E (to second order in momentum $\mathbf{p} = -i\hbar\partial/\partial\mathbf{r}$) it has the form

$$H = \Delta(p_x \sigma_x + p_y \sigma_y) + [U(\mathbf{r}) + p^2/2m]\sigma_z, \quad (1)$$

for a uniform (vortex-free) pair potential Δ . The electrostatic potential U (measured relative to the Fermi energy) opens up a band gap in the excitation spectrum. At $U = 0$ the superconductor has a topological phase transition (known as the thermal quantum Hall effect) between two localized phases, one with and one without chiral edge states [14–17].

Our key observation is that the Hamiltonian (1) on a lattice has Majorana bound states at the two end points of a linear electrostatic defect. The mechanism for the production of these bound states goes back to Shockley [18]: The band gap closes and then reopens upon formation of the defect, and as it reopens a pair of states splits off from the band edges to form localized states at the end points of the defect [see Fig. 1]. Such Shockley states appear in systems

as varied as metals and narrow-band semiconductors [19], carbon nanotubes [20], and photonic crystals [21]. In these systems they are unprotected and can be pushed out of the band gap by local perturbations. In a superconductor, particle-hole symmetry requires the spectrum to be $\pm E$ symmetric, so an isolated bound state is constrained to lie at $E = 0$ and cannot be removed by a local perturbation.

We propose the name Majorana-Shockley (MS) bound state for these topologically protected Shockley states. Similar states have been studied in the context of lattice gauge theory by Creutz and Horváth [22,23], for an altogether different purpose (as a way to restore chiral symmetry in the Wilson fermion model of QCD [24]).

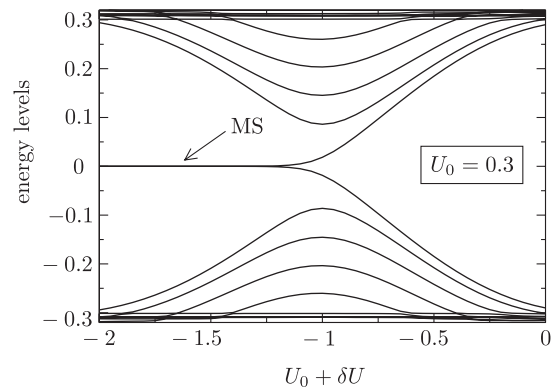


FIG. 1. Emergence of a pair of zero-energy MS states as the defect potential $U_0 + \delta U$ is made more and more negative, at fixed positive background potential $U_0 = 0.3$. (All energies are in units of $\gamma \equiv \hbar\Delta/a$.) The energy levels are the eigenvalues of the Hamiltonian (1) on a square lattice (dimension $100a \times 100a$, $\beta \equiv \hbar^2/2ma^2 = 0.4\gamma$, periodic boundary conditions). The line defect has length $50a$. The dense spectrum at top and bottom consists of bulk states.

Consider a square lattice (lattice constant a), at uniform potential U_0 . The Hamiltonian (1) on the lattice has dispersion relation

$$E^2 = [U_0 + 2\beta(2 - \cos ak_x - \cos ak_y)]^2 + \gamma^2 \sin^2 ak_x + \gamma^2 \sin^2 ak_y. \quad (2)$$

(We have defined the energy scales $\beta = \hbar^2/2ma^2$, $\gamma = \hbar\Delta/a$.) The spectrum becomes gapless for $U_0 = 0, -4\beta$, and -8β , signaling a topological phase transition [25]. The number of edge states is zero for $U_0 > 0$ and $U_0 < -8\beta$, while it is unity otherwise (with a reversal of the direction of propagation at $U_0 = -4\beta$). The topologically nontrivial regime is therefore reached for $-8\beta < U_0 < 0$.

We now introduce the electrostatic line defect by changing the potential to $U_0 + \delta U$ on the N lattice points at $\mathbf{r} = (na, 0)$, $n = 1, 2, \dots, N$. In Figs. 1 and 2, we show the closing and reopening of the band gap as the defect is introduced, accompanied by the emergence of a pair of states at zero energy. The eigenstates for which the gap closes and reopens have wave vector k_x parallel to the line defect equal to either 0 or $\pm\pi/a$.

We have calculated that the gap closing at $k_x = 0$ happens at a critical potential $\delta U = \delta U_0$ given by [26]

$$\delta U_0 = \begin{cases} -\sqrt{U_0(U_0 + 4\beta) + \gamma^2} & \text{for } U_0 > 0, \\ \sqrt{U_0(U_0 + 4\beta) + \gamma^2} & \text{for } U_0 < -4\beta, \\ \text{no finite value otherwise.} & \end{cases} \quad (3)$$

The critical potential δU_π for closing of the gap at $k_x = \pm\pi/a$ is obtained from Eq. (3) by the replacement of U_0 with $U_0 + 4\beta$. The MS states appear for defect potentials

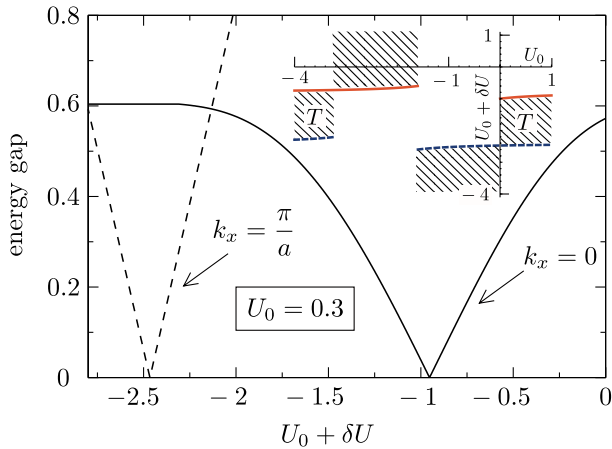


FIG. 2 (color online). Main plot: Closing and reopening of the excitation gap at $U_0 = 0.3$, $\beta = 0.4$ (in units of γ), for states with $k_x = 0$ (black solid curve) and $k_x = \pi/a$ (black dashed curve). The MS states exist for defect potentials in between two gap closings, indicated as a function of U_0 by the shaded regions in the inset. [The (red) solid and (blue) dashed curves show, respectively $U_0 + \delta U_0$ and $U_0 + \delta U_\pi$. The label T indicates the topologically trivial phase.]

$U_0 + \delta U$ in between two subsequent gap closings, as indicated in the inset of Fig. 2. We conclude that MS states exist for any value of U_0 . In contrast, Majorana bound states in vortices exist only in the topologically nontrivial regime [3,27,28].

Our reasoning so far has relied on the assumption of a constant pair potential Δ , unperturbed by the defect. In order to demonstrate the robustness of the Majorana-Shockley mechanism, we have performed numerical calculations that determine the pair potential self-consistently by means of the gap equation [26,29]. In Fig. 3 we show a comparison of the closing and reopening of the band gap as obtained from calculations with and without self-consistency, in the relevant weak pairing regime ($U_0 < 0$). The self-consistency does not change the qualitative behavior. In particular, the gap only closes at $k_x = \pi/a$ for the parameters chosen.

In Fig. 4 we demonstrate that the MS states are localized at the end points of the line defect. The exponentially small, but nonzero overlap of the pair of states displaces their energy from 0 to $\pm E$ (with corresponding eigenstates $\psi_- = \sigma_x \psi_+^*$ related by particle-hole symmetry). The unpaired Majorana bound states ψ_1 and ψ_2 are given by the linear combinations

$$\psi_1 = \frac{1}{2}(1 - i)\psi_+ + \frac{1}{2}(1 + i)\psi_-, \quad (4a)$$

$$\psi_2 = \frac{1}{2}(1 + i)\psi_+ + \frac{1}{2}(1 - i)\psi_-, \quad (4b)$$

shown also in Fig. 4. These states are particle-hole symmetric, $\psi_{1,2} = \sigma_x \psi_{1,2}^*$, so the quasiparticle in such a state is indeed equal to its own antiparticle (hence, it is a Majorana fermion).

If the line defect has a width W which extends over several lattice sites, multiple gap closings and reopenings

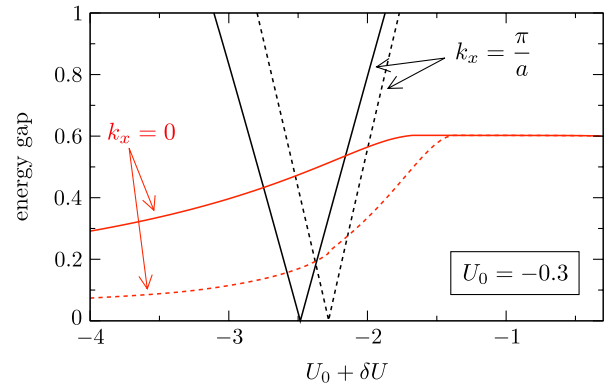


FIG. 3 (color online). Closing and reopening of the excitation gap at $U_0 = -0.3$, $\beta = 0.4$ (in units of γ), for states with $k_x = 0$ [grey (red) curves] and $k_x = \pi/a$ (black curves). The results were obtained from numerical calculations using a constant isotropic pair potential Δ (solid lines) as in Fig. 2 as well as a spatially dependent, anisotropic pair potential $[\Delta_x(\mathbf{r}), \Delta_y(\mathbf{r})]$ determined self-consistently from the gap equation (dashed lines).

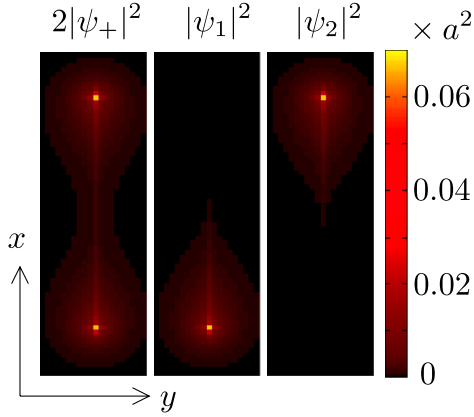


FIG. 4 (color online). Probability density of the paired (ψ_+) and unpaired (ψ_1, ψ_2) Majorana bound states at the end points of a line defect of length $50a$, calculated for $U_0 = 0.1\gamma$, $U_0 + \delta U = -1.3\gamma$, $\beta = 0.4\gamma$.

appear at $k_x = 0$ upon increasing the defect potential $U_0 + \delta U \equiv -(\hbar k_F)^2/2m$ to more and more negative values at fixed positive background potential U_0 . In the continuum limit $W/a \rightarrow \infty$, the gap closes when [26] $qW = n\pi + \nu$, $n = 0, 1, 2, \dots$, with $q = [k_F^2 - (m\Delta)^2]^{1/2}$ the real part of the transverse wave vector and $\nu \in (0, \pi)$ a phase shift that depends weakly on the potential. (Similar oscillatory coupling energies of zero-modes have been found in Refs. [30,31].) The MS states at the two ends of the line defect alternately appear and disappear at each subsequent gap closing.

So far we constructed MS states for a linear electrostatic defect. More generally, we expect a randomly varying electrostatic potential to create a random arrangement of MS states. To test this, we pick $U(\mathbf{r})$ at each lattice point uniformly from the interval $(\bar{U} - \Delta U, \bar{U} + \Delta U)$ and calculate the average density of states $\rho(E)$. The result in Fig. 5 shows the expected peak at $E = 0$. This peak is characteristic of a thermal metal, studied previously in models where the Majorana bound states are due to vortices [32–34]. The peak in the density of states of a thermal metal has a logarithmic profile [15], $\rho(E) \propto \ln|E|$, consistent with our data.

Without Majorana bound states, the chiral p -wave superconductor would be in the thermal insulator phase, with an exponentially small thermal conductivity at any nonzero \bar{U} [3,32,35,36]. Our findings imply that electrostatic disorder can convert the thermal insulator into a thermal metal, thereby destroying the thermal quantum Hall effect. Numerical results for this insulator-metal transition will be reported elsewhere [37].

These results are all for a specific model of a chiral p -wave superconductor. We will now argue that our findings are generic for symmetry class D (along the lines of a similar analysis of solitons in a polymer chain [38]). Let p be the momentum along the line defect and α a parameter that controls the strength of the defect. Assume that the gap

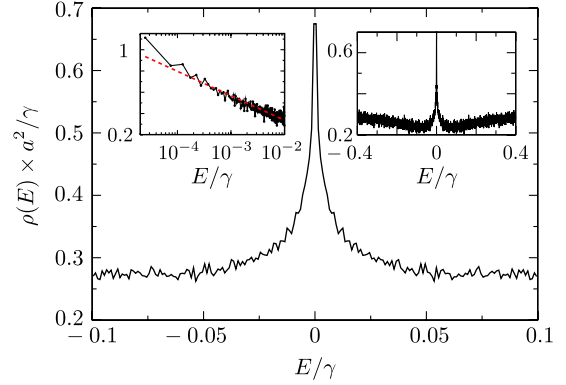


FIG. 5 (color online). Average density of states for a potential that fluctuates randomly from site to site ($\bar{U} = 0.01\gamma$, $\Delta U = 2\gamma$, $\beta = 0.2\gamma$). The lattice has size $400a \times 400a$. The right inset shows the same data as in the main plot, over a larger energy range. The left inset has a logarithmic energy scale, to show the dependence $\rho \propto \ln|E|$ expected for a thermal metal [red dashed line].

closes at $\alpha = \alpha_0$ and at $p = 0$. (Because of particle-hole symmetry the gap can only close at $p = 0$ or $p = \pm\hbar\pi/a$ and these two cases are equivalent.) For α near α_0 and p near 0 the Hamiltonian in the basis of left-movers and right-movers has the generic form

$$H(\alpha) = \begin{bmatrix} (v_0 + v_1)p & -i(\alpha - \alpha_0) \\ i(\alpha - \alpha_0) & -(v_0 - v_1)p \end{bmatrix}, \quad (5)$$

with velocities $0 < v_1 < v_0$. No other terms to first order in $p = -i\hbar\partial/\partial x$ and $\alpha - \alpha_0$ are allowed by particle-hole symmetry, $H(\alpha) = -H^*(\alpha)$.

The line defect is initially formed by letting α depend on x on a scale much larger than the lattice constant. We set one end of the defect at $x = 0$ and increase α from $\alpha(-\infty) < \alpha_0$ to $\alpha(+\infty) > \alpha_0$. Integration of $H[\alpha(x)]\psi(x) = 0$ then gives the wave function of a zero-energy state bound to this end point,

$$\psi(x) = \left(\frac{\sqrt{v_0/v_1 - 1}}{\sqrt{v_0/v_1 + 1}} \right) \exp\left[-\int_0^x \frac{\alpha(x') - \alpha_0}{\sqrt{v_0^2 - v_1^2}} dx' \right]. \quad (6)$$

This is one of the two MS states, the second being at the other end of the line defect. We may now relax the assumption of a slowly varying $\alpha(x)$, since a pair of uncoupled zero-energy states cannot disappear without violating particle-hole symmetry.

In conclusion, we have identified a purely electrostatic mechanism for the creation of Majorana bound states in chiral p -wave superconductors. The zero-energy (midgap) states appear in much the same way as Shockley states in nonsuperconducting materials, but now protected from any local perturbation by particle-hole symmetry. A consequence of our findings is that the thermal quantum Hall effect is destroyed by electrostatic disorder (in marked contrast to the electrical quantum Hall effect). The recent

proposal to realize Wilson fermions in optical lattices [39] also opens the possibility to observe Majorana-Shockley states using cold atoms.

Our analysis is based on a generic model of a two-dimensional class-D superconductor (broken time-reversal and spin-rotation symmetry). An interesting direction for future research is to explore whether Majorana-Shockley bound states exist as well in the other symmetry classes [13]. Since an electrostatic defect preserves time-reversal symmetry, we expect the Majorana-Shockley mechanism to be effective also in class DIII (when only spin-rotation symmetry is broken). That class includes proximity-induced s -wave superconductivity at the surface of a topological insulator [40] and other topological superconductors [41–43].

It would also be interesting to investigate the braiding of two electrostatic defect lines, in order to see whether one obtains the same non-Abelian statistics as for the braiding of vortices [4].

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