Strong zero modes and eigenstate phase transitions in the XYZ/interacting Majorana chain

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Abstract
I explicitly construct a strong zero mode in the XYZ chain or, equivalently, Majorana wires coupled via a four-fermion interaction. The strong zero mode is an operator that pairs states in different symmetry sectors, resulting in identical spectra up to exponentially small finite-size corrections. Such pairing occurs in the Ising/Majorana fermion chain and possibly in strongly disordered many-body localized phases. The proof here shows that the strong zero mode occurs in a clean interacting system, and that it possesses some remarkable structure—despite being a rather elaborate operator, it squares to the identity. Eigenstate phase transitions separate regions with different strong zero modes.

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(Some figures may appear in colour only in the online journal)
properties of full spectrum undergo a sharp transition as couplings are varied [3]. Such transitions need not involve the ground state; one proposal of [3] is a change between types of statistics governing all energy-level spacings.

One substantial complication in understanding eigenstate phase transitions in the MBL context is that properties of the full spectrum (e.g. the eigenstate thermalization hypothesis) are typically subtle. Complicating the analysis further is that strongly disordered couplings are typically needed to obtain the novel physics. Thus unfortunately the dominant tools utilized in these studies are intuition and numerical analysis.

I discuss in this paper an eigenstate phase transition that has the virtues of being fairly easy to characterize, and tractable analytically. This transition is for a strong zero mode, an operator that commutes with the Hamiltonian, up to corrections that fall off exponentially in system size [4–6]. I prove that a strong zero mode occurs in an interacting system without disorder, with interesting consequences for the energy spectrum.

The canonical example of a strong zero mode is in the Ising/Majorana quantum chain in the ordered phase with free boundary conditions on both ends. The strong zero mode pairs each state in the even-fermion-number sector with one in the odd, requiring their energies are the same up to exponentially small finite-size corrections [4, 7]. It therefore results in a much stronger constraint on the energy spectrum that the constraint of (topological) order, where only pairing of ground states is necessary. This behavior is robust; the pairing persists when the couplings are allowed to vary spatially, as long as the strong zero mode operator remains normalizable (i.e. when acting on any normalizable state it gives another one). The strong zero mode and hence the pairing go away precisely at the quantum phase transition between spin/topological order and disorder, so in this case eigenstate and quantum phase transitions occur at the same coupling.

There have been suggestions that the strong zero mode does not survive the inclusion of interactions, unless the disorder is strong enough to create an MBL phase [3, 8, 9]. This is true in some cases. The three-state Potts chain has in a trivially solvable limit a threefold analog of the pairing, but the strong zero mode disappears for arbitrarily small interactions, although the spin/topological order and a ‘weak’ zero mode remain [5, 6, 10, 11]. The splitting between would-be degenerate energy levels here depends on the system size via a power law.

On the flip side, there is some evidence for a strong zero mode once chiral interactions are included in the three-state Potts chain [5, 6]. An operator can be constructed to all orders in perturbation theory that seems to fit the bill [5], but it has not yet been proven to be normalizable. Moreover, perturbative arguments show that the splitting in pairs of low-lying excited states remains exponentially small in system size [6]. In addition, the pairing survives to at least first order in perturbation theory when interactions are included in the Ising/Majorana case [12]. In the case studied in this paper, the left of figure 1 below provides another compelling suggestion that sometimes the pairing survive interactions.

In this paper I promote the latter suggestion to a proof. By explicit construction I find a strong zero mode in a clean system with strong interactions, the XYZ spin chain with free boundary conditions or equivalently, two Majorana chains coupled by a particular four-fermion interaction. As apparent from (2) below, the operator involves many terms, but the form is quite elegant. I show that is normalizable by using brute force to derive a striking property: its square is the identity operator! These properties indicate that the strong zero mode is a fundamental property of the system.
The definition of a strong zero mode

Given a quantum Hamiltonian $H$ acting on a $L$-site chain with open boundary conditions, a strong zero mode $\Psi$ is an operator satisfying [13]

- $[H, \Psi] \to 0$ as $L \to \infty$, with finite-size corrections operators whose expectation values vanish as $u^L$ with $|u| < 1$.
- $[\Psi, \mathcal{D}] = 0$, where $\mathcal{D}$ generates a discrete symmetry, i.e. $[H, \mathcal{D}] = 0$ and $\mathcal{D}^m = 1$ for some integer $m > 1$.
- $\Psi^n \propto I$, the identity operator, for some integer $n > 1$.

Since $\mathcal{D}$ commutes with $H$, the eigenstates of the latter can be grouped into sectors labelled by the eigenvalues of the former (which necessarily are roots of unity). The last two conditions then require that acting with $\Psi$ on a state in one sector must give a state in another. Combining this with the first condition means acting with $\Psi$ on an eigenstate of $H$ gives a different state with the same energy, up to corrections going to zero exponentially fast as $L \to \infty$. The last condition guarantees that $\Psi$ is normalizable, meaning that when acting on any normalizable state, it returns a normalizable one. This condition possibly could be

*Figure 1.* Spectra of the XXZ spin chain $J_x = J_y = 1$ in $D_x = \pm 1$ sectors for ten sites; on the right the energy is rescaled for easier comparison. In the left plots $J_z = 4$ so that the model is ordered, whereas in the right ones $J_z = 1/2$ so that it is critical. Only in the ordered case is a pairing between the states apparent.
relaxed, but here and elsewhere (e.g. for free parafermions [14]), it holds. Since this property seems highly non-trivial and fundamental, it seems worthy to emphasize it via this definition. It is worth noting that in general the strong zero mode is not a symmetry—the spectrum is only asymptotically degenerate unless the finite-size corrections to $[H, \Psi]$ exactly vanish.

The XYZ chain

The XYZ chain is an integrable strongly interacting quantum spin chain [15]. The Hilbert space is a chain of $L$ two-state systems and the Hamiltonian is

$$H = \sum_{j=1}^{L-1} (J_x \sigma_x^j \sigma_x^{j+1} + J_y \sigma_y^j \sigma_y^{j+1} + J_z \sigma_z^j \sigma_z^{j+1}),$$

where $\sigma_\alpha^j$ for $\alpha = x, y, z$ is the Pauli matrix $\sigma^\alpha$ acting on the two-state system at the $j$th site. For $J_z = \pm J_x$, this is the XXZ chain, and $J_x = J_y = J_z$ the antiferromagnetic spin-$1/2$ Heisenberg chain. The operators $D_\alpha = \prod_{j=1}^L \sigma_\alpha^j$ implement a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. When $|J_x|$ is the largest coupling, the model is ordered with the corresponding discrete symmetry spontaneously broken [15]. Critical lines separate the different orderings; they occur when $|J_x| = |J_y| \geq |J_z|$ for any $\alpha = \beta \neq \gamma$.

A Jordan–Wigner transformation maps the Hamiltonian to a fermion one [16]. Any two of the three terms in (1) can be mapped to fermion bilinears, but the third is then a four-fermion term. Thus when one coupling vanishes, the model is free, and turns out to have the same spectrum as two copies of the Ising chain [16]. The two copies are dual to each other, meaning that when one copy is in the ordered/topological phase, it has a strong edge zero mode [4], while the other is disordered and does not.

As in the Ising/Majorana chain [4], the strong edge zero mode is apparent in a trivially solvable limit. When $J_x = 0$, any basis state $|\zeta\rangle$ in the basis where all $\sigma_\alpha^j$ are diagonal is an eigenstate of the Hamiltonian. The symmetry operator $D_x$ then flips all spins, so $D_x|\zeta\rangle = |\zeta\rangle$. Therefore $|\zeta\rangle + D_x|\zeta\rangle$ and $|\zeta\rangle - D_x|\zeta\rangle$ are distinct eigenstates of both $D_x$ and $H$ having the same energy. Since the operator $\sigma_\alpha^j$ anticommutates with $D_x$, it must map between the two: $\sigma_\alpha^j (|\zeta\rangle + D_x|\zeta\rangle) = \pm (|\zeta\rangle - D_x|\zeta\rangle)$. Therefore in this limit $\Psi(0) = \sigma_\alpha^j$ is a strong zero mode localized at the edge.

Computing the finite size spectra using exact diagonalization strongly suggests that the strong zero mode here survives interactions. The plots for $L = 10$ in the XXZ case for two values of $J_z$ are plotted in figure 1. The ordered case shows clear evidence for pairing between $D_x = \pm 1$ sectors. Further checks indicate that as $L$ is increased to 14 (in the sector with vanishing $S_z = \sum_{j=1}^L \sigma_z^j$), the splitting between pairs does indeed fall off exponentially.

The main result

Before its proof, I state the main result. Letting $X = J_y/J_x$, $Y = J_z/J_x$ and

$$\langle a_d^\dagger \rangle = Y^{a-d}(1 - X^{-2})\sigma_z^d \sigma_z^d + X^{a-d}(1 - Y^{-2})\sigma_y^d \sigma_y^d,$$

the exact strong edge zero mode for $X^2 < 1$, $Y^2 < 1$ is

$$\Psi = \sum_{S=0}^\infty \sum_{a,b} (XY)^{S-1} \sigma_b^\dagger \prod_{i=1}^{S} \langle a_{2i-1} a_{2i} \rangle,$$

(2)
where the second sum is over all sets of $2S+1$ positive integers obeying $0 < a_1 < a_2 < \cdots < a_{2S} < b$; if $S = 0$ the product is 1. Terms involving the operator $\sigma_{L+1}^z$ are at least order $L/2$ in $X$ and/or $Y$.

Despite the elegance of this expression, the gargantuan number of terms makes it far from obvious that $\tilde{\Psi}^2$ is proportional to the identity operator. Nevertheless, by brute force I prove in the supplemental information (stacks.iop.org/jpa/49/30LT01/mmedia) that for $X^2 < 1$ and $Y^2 < 1$

$$\Psi^2 = \frac{1}{(1 - X^2)(1 - Y^2)}.$$  

The strong zero mode is normalizable except when $X^2 = 1$ and/or $Y^2 = 1$, the critical lines. Thus eigenstate phase transitions occur at the same couplings as the conventional quantum phase transitions. If a coupling, say $X^2$, is increased past 1, then $|J_x|$ becomes the largest coupling, and the entire analysis can be repeated with $J_x \leftrightarrow J_z$. A strong zero mode therefore exists everywhere except along the critical lines; different orderings are associated with different strong zero modes.

**Strong zero mode for $J_x = 0$**

When any of the three couplings vanishes, the XYZ Hamiltonian can be written in terms of fermion bilinears. The strong zero mode is then a linear combination of fermion operators, because commuting a fermion bilinear with any linear combination returns another linear combination. Computing the strong zero mode (and all the raising/lowering operators [14, 16]) is then rather simple.

It is not difficult to find this strong zero mode in this limit directly, but as a warm-up for the general case it is useful to compute it by iteration. Taking $|J_z| > |J_y|$ and $J_x = 0$, the $Z_2$ ordering arises from the operator $V = J_Z \sum_{j=1}^{L-1} \sigma_j^x \sigma_{j+1}^x$ dominating $H$. The zeroth order contribution to the strong zero mode, $\Psi^{(0)} = \sigma_1^z$, necessarily commutes with $V$, but not with $H_0 = H|_{J_x=0}$.

$$[H_0, \sigma_1^z] = J_z [\sigma_1^x \sigma_2^y, \sigma_1^y] = 2i J_z \sigma_1^x \sigma_2^y.$$  

The iterative method relies on finding an operator that gives a cancelling contribution when commuted with $V$. Here

$$[V, \sigma_1^x \sigma_2^y \sigma_3^z] = J_z [\sigma_1^x \sigma_2^y, \sigma_1^x \sigma_2^y \sigma_3^z] = 2i J_z \sigma_1^x \sigma_2^y$$

yields the first correction to the zero mode. Adding this to the zeroth order term and taking the commutator with $H_0$ yields an order $J_y^2$ expression, which can be cancelled by a second correction:

$$[H_0, \sigma_1^x - Y \sigma_1^x \sigma_2^y \sigma_3^z] = -2i J_y Y \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^y = -[V, Y^2 \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^y].$$

The pattern now is obvious. It is easy to show directly that

$$\Psi|_{J_x=0} = \sum_{k=0}^{\infty} (-Y)^k \sigma_2^y \prod_{j=1}^{2k+1} \sigma_j^y$$

obeys

$$\lim_{L \to \infty} [H_0, \Psi]|_{J_x=0} = 0.$$
When $X = 0$, the full expression (2) reduces to (4), which indeed is a sum of Majorana fermion operators.

For the zero mode to be meaningful, it must be normalizable. Because each term in the sum in (4) anticommutes with the others, $\Psi^2$ is proportional to the identity:

$$\Psi^2 |_{J_x=0} = 1 + Y^2 + Y^4 + \cdots = (1 - Y^2)^{-1},$$

where the series converges and can be resummed when $Y^2 < 1$, i.e. $|J_x| < |J|$. This zero mode therefore exists throughout the $z$-ordered region; only at the critical point $|J_x| = |J|$ is it not normalizable. If $|J| < |J_x|$ instead, then the entire calculation goes through with $y \leftrightarrow z$. Thus whenever the $J_x = 0$ model is ordered, it possesses a strong zero mode.

### Strong zero mode by iteration

The iterative approach works for $J_x \equiv 0$ as well, although it requires considerably more effort. Two pieces of notation useful for this analysis are

$$\left\{\left\{ f(X, Y) \right\} \right\}_{23} = f(X, Y) \sigma^a_2 \sigma^b_3,$$

$$\left\{\left\{ f(X, Y) \right\} \right\}_{23} = f(X, Y) \sigma^a_2 \sigma^b_3 + f(X, Y) \sigma^a_3 \sigma^b_2,$$

where $f$ is some function of $X$ and $Y$. Any function symmetric in $X$ and $Y$ can be pulled out of or put into the double brackets, e.g. $[[XYf(X, Y)]] = XY[[f(X, Y)]]$.

Proceeding as with $J_x = 0$, it is easy to verify that

$$[H, \sigma^a_1] = [J_z][Y]_{12} = [V, \left\{ \left\{ Y \right\} \right\}_{12} \sigma^a_3].$$

The first correction to the strong zero mode is therefore $\Psi^{(1)} = \left\{ \left\{ Y \right\} \right\}_{12} \sigma^a_3$. Iterating again yields

$$[H, \sigma^a_1 - \{ \{ Y \} \}_{12} \sigma^a_3] = -[V, \hat{\Psi}^{(2)}],$$

where the putative second-order correction is

$$\hat{\Psi}^{(2)} = \{ \{ Y \} \}_{12} \{ \{ Y \} \}_{34} \sigma^a_3 - \{ \{ XY \} \}_{13} \sigma^a_4.$$

I say putative because at next order a complication arises. Commuting the last term in (8) with $H$ gives

$$[H, \{ \{ XY \} \}_{13} \sigma^a_4] = -J_z \sigma^a_1 \{ \{ XY^2 \} \}_{12} \sigma^a_3 + \cdots.$$

The right-hand side does appear in a commutator with $V$, but only in combination with another term:

$$[V, \{ \{ f \} \}_{23}(\alpha \sigma^a_1 + \beta \sigma^a_3)] = J_z(\beta - \alpha)(1 - \sigma^a_1 \sigma^a_3)[f]_{23}.$$

Thus any commutator of $V$ will yields the product $[[XY^2]]_{13} (1 - \sigma^a_1 \sigma^a_3)$, which does not arise in $[H, \hat{\Psi}^{(2)}]$. The way forward is to note any function of the $\sigma^a_j$ commutes with $V$. Thus at any given order, one can add such a function to the zero mode, and the effects will only be felt at the next order, after the commutation with the full $H$ is done. Namely, if the second-order correction is modified to be $\Psi^{(2)} = \hat{\Psi}^{(2)} + XY\sigma^a_3$, the commutation relation (7) is still satisfied, but $[H, \Psi^{(2)}]$ now includes the desired combination:

$$[H, XY \sigma^a_3 - \{ \{ XY \} \}_{13} \sigma^a_3] = J_z(1 - \sigma^a_1 \sigma^a_3)[xy^2]_{123} + \cdots.$$

With this modification, a $\Psi^{(3)}$ obeying $[H, \Psi^{(2)}] = -[V, \Psi^{(3)}]$ can indeed be found.
The iteration proceeds straightforwardly by doing such modifications; it turns out one needs to include a term \((X^2)^m \sigma_{n+1} \) in \(\Psi^{(2a)}\). An important consequence of the modifications is that they make \(\Psi^2\) proportional to the identity operator order by order. Although the number of terms grows exponentially, staring at the results for a while leads to (2).

**The proof**

Here I prove that the expression (2) satisfies

\[
\lim_{L \to \infty} [H, \Psi] = 0. \tag{9}
\]

For the proof, the XYZ Hamiltonian is split into pieces:

\[
H = J_j \sum_{j=1}^{L-1} (T_j + V_j)
\]

\[
V_j \equiv \sigma_j^x \sigma_{j+1}^x, \quad T_j \equiv X \sigma_j^x \sigma_{j+1}^x + Y \sigma_j^y \sigma_{j+1}^y.
\]

Each term in the sum (2) is labelled as \(\psi_{(a)_{(b)_{(c)}}}\). It is convenient to separate out of this the pieces \(\psi_{(a)_{(b)}}\), which has the added restriction that \(a_1 < 2 < \cdots < a_{2j} < p\).

For the proof, the XYZ Hamiltonian is split into pieces:

\[
H = J_j \sum_{j=1}^{L-1} (T_j + V_j)
\]

where

\[
T_j \equiv X \sigma_j^x \sigma_{j+1}^y + Y \sigma_j^y \sigma_{j+1}^x.
\]

The factors of \(XY\) in front are precisely the relative factors appearing in \(\psi\), so the corresponding contributions to \(\psi_{(a)_{(b)}}\) sum to zero for any \(\eta_p\). The only other contributions with no \(\sigma_j^x\) arise from the commutators with \(a_{2j} = b - 1\):

\[
[T_{b-1}, \eta_p (p b - 1) \sigma_{b+1}] = - \eta_p [Y (X - 1)]_{p b},
\]

\[
[XY, \eta_p (p b - 1) \sigma_{b+1}] = X Y \eta_p [Y (X - 1)]_{p b},
\]

where \(l\) in \(\eta_p\) obeys \(l = S - 1\). Again, the relative factors of \(XY\) are exactly as they occur in the expansion of \(\psi\), and again, the commutators cancel for any \(p\) and \(\eta_p\). Thus all terms in \([H, \Psi]\) with no explicit \(\sigma_j^x\) cancel.

A given term in \([H, \Psi]\) containing \(\sigma_j^x [pq]\) has an ‘inside’ \(\sigma_j^x\) when \(p < r < q\), and ‘outside’ otherwise. Two canceling pairs with outside \(\sigma_j^x\)

\[
[T_{p q}, (p q) j] = \sigma_j^x [X^{p-q+1} (1 - Y^2)]_{p+1, q},
\]

\[
[V_{p q}, (p + q) j] = - \sigma_j^x [X^{p-q+1} (1 - Y^2)]_{p+1, q},
\]

where \(q \geq p + 2\). Any terms in \([H, \Psi]\) with outside \(\sigma_j^x\) can be obtained by multiplying the above commutators by any \(\eta_p \psi^{(a)}\), so all terms with no inside \(\sigma_j^x\) cancel.
The analogous terms with an inside $\sigma^z$ are

$$
\begin{align*}
[T_p, \langle p + 1 \mid q \rangle] &= \sigma^z_{p+1}[[X^{p+q+2}(1 - Y^{-2})]]_{p,q}, \\
[V_p, \langle p \mid q \rangle] &= -\sigma^z_{p+1}[[X^{p-q}(1 - Y^{-2})]]_{p,q}, \\
[T_{q-1}, \langle p \mid q - 1 \rangle] &= -\sigma^z_{q-1}[[Y^{p-q+2}(1 - X^{-2})]]_{p,q}, \\
[V_{q-1}, \langle p \mid q \rangle] &= \sigma^z_{q-1}[[Y^{p-q}(1 - X^{-2})]]_{p,q}.
\end{align*}
$$

The sum $S$ of these four commutators is zero only if $q = p + 2$. However, when $q > p + 2$, an inside $\sigma^z$ arises from

$$
[T_r, \langle p \mid r \rangle \langle r + 1 \mid q \rangle] = (1 - X^{-2})(1 - Y^{-2}) \times (\sigma^z_{r+1}[[Y^{p-r}X^{r-q+2}]]_{p,q} - \sigma^z_{r}[[Y^{p-r+1}X^{r-q+1}]]_{p,q}),
$$

for any $p < r < q - 1$. Summing these over all such $r$ gives $-S$, cancelling the original four. Multiplying these by any $p \mid q \rangle \langle r \mid s \rangle$ means that all the commutators with an inside $\sigma$ cancel; note that $[V_r, \langle p \mid r \rangle \langle r + 1 \mid q \rangle] = 0$.

This analysis accounts for all non-vanishing terms in $[H, \Psi]$, and shows all cancel. Thus (9) indeed holds.

**$\Psi$ as a symmetry operator**

The boundary conditions used in (1) are free at each end. An interesting and useful fact is that if the boundary conditions at the far end are instead fixed, $\Psi$ commutes with $H$ without taking $L \to \infty$. Precisely, the Hamiltonian is modified to $\tilde{H} = H + \sum_r V_r$, so that the spin on the site $L + 1$ is fixed: no term in $\tilde{H}$ can flip it, but it still interacts with the spin at site $L$. Letting $\tilde{\Psi}$ be $\Psi$ with the additional requirement that that $b \leq L + 1$, the preceding proof then shows that $[\tilde{H}, \tilde{\Psi}] = 0$.

Thus, with free boundary conditions at one end and fixed at the other, $\tilde{\Psi}$ indeed generates a symmetry. The catch is that flipping the spins changes the fixed boundary condition, so $D$ no longer generates a symmetry. The pairing becomes trivial: the energies with boundary condition $\sigma^z_{L+1} = 1$ are identical to those with $\sigma^z_{L+1} = -1$. Thus acting with $\tilde{\Psi}$ no longer results in degeneracies.

**Finite-size effects**

This observation allows the finite-size correction to $[H, \Psi] \to 0$ to be determined. Since $[\tilde{H}, \tilde{\Psi}] = 0$, it follows that $[H, \Psi_L] = [\tilde{H} - \sum_r V_r, \Psi_L] = -L[\sigma^z_L \sigma^z_{L+1}, \Psi_L]$. Non-vanishing contributions to this commutator must have $a_{22} = L$ and $b = L + 1$. These are necessarily at least order $L/2$ in $X$ and $Y$, with the leading contributions those from $X = 0$ or $Y = 0$, as in (4). This and the normalizability condition (3) ensure that the finite-size corrections do indeed go to zero exponentially fast.

However, the precise bounding seems difficult to determine. One complication is that $(\Psi_L)^2$ is not proportional to the identity, although perhaps it could be modified to make it so. Since $\Psi_L$ commutes with $\tilde{H}$, $\Psi_L^2$ must as well. Therefore, $\Psi_L^2$ may involve powers of $\tilde{H}$, but since the XYZ chain is integrable, it may involve the commuting higher Hamiltonians as well. Understanding this may provide a route to a much nicer proof of (3) than than horrible brute force one in the supplemental information.
Conclusion

I have found the strong zero mode in the clean XYZ chain. An important issue left mostly unexplored is the role the integrability plays. Although very probably the integrability is why the explicit expression is so elegant (and why it could be found straightforwardly by iteration), it is not clear whether or not it is necessary for the strong zero mode to exist. The XYZ chain is not integrable when it has disordered couplings; even staggering them breaks the integrability. Nonetheless, low-order calculations indicate that the iterative method still works, but that the expressions become much more complicated. This, along with the work on parafermionic models [5, 6] and on the Ising chain plus interactions [12, 17, 18], gives a good sign that strong zero modes still play an interesting role in non-integrable models.

Moreover, at strong disorder, the resulting MBL phase is argued to also exhibit the same pairing in the spectrum [3, 8, 9]. Since MBL phases are believed to resemble integrable systems, for example in having local integrals of motion [19–21], it would be very interesting if there were a precise correspondence between pairing in clean and very dirty systems. If there is no correspondence, then the interesting question is: what happens at weak disorder? The XYZ case analysed here, the eigenstate and quantum phase transitions here occur at the same couplings. The MBL case, however, hints that this correspondence may not be true in general.

A tool that may prove useful in answering these and other questions is the entanglement spectrum [22]. This is much easier to compute numerically than the energy spectrum, and it would be interesting to understand if the pairing and the strong zero mode occur in this context as well.

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