Clash of discrete symmetries for the supersymmetric kink on a circle

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We consider the $N=1$ supersymmetric kink on a circle, i.e., on a finite interval with boundary or transition conditions which are locally invisible. For Majorana fermions, the single-particle Dirac Hamiltonian as a differential operator obeys simultaneously the three discrete symmetries of charge conjugation, parity, and time reversal. However, no single locally invisible transition condition can satisfy all three. When calculating sums over zero-point energies by mode number regularization, this gives a new rationale for a previous suggestion that one has to average over different choices of boundary conditions, such that for the combined set all three symmetries are obeyed. In particular it is shown that for twisted periodic or twisted antiperiodic boundary conditions separately both parity and time reversal are violated in the kink sector, as manifested by a delocalized momentum that cancels only in the average.

I. INTRODUCTION

Subtleties in the application of the discrete symmetries charge conjugation $C$, parity $P$, and time reversal $T$ to Majorana fermions have long been a topic of interest [1, 2]. Past discussions generally have dealt with local processes and properties, but the main aim of the present work is to study an anomalous global behavior of these discrete symmetries in a model with a topological structure. For this we consider the simplest possible system: the supersymmetric (susy) kink with what would seem to be natural boundary conditions.

Some time ago the concept of locally invisible boundary conditions was introduced [3, 4]: for a two component Majorana fermion in a kink background in a box of length $L$, the twisted periodic
(TP) and twisted antiperiodic (TAP) boundary conditions

\begin{align*}
\text{TP} : & \quad \psi_1(-L/2) = \psi_2(L/2), \quad \psi_2(-L/2) = \psi_1(L/2) \\
\text{TAP} : & \quad \psi_1(-L/2) = -\psi_2(L/2), \quad \psi_2(-L/2) = -\psi_1(L/2)
\end{align*}

amount to putting the system on a circle without introducing a point where a boundary is present: The kink solution \( \phi_K(x) = \phi_0 \tanh \frac{m x}{2} \) is invariant under the simultaneous transformation \( x = L/2 \to x = -L/2 \) and \( \phi_K \to -\phi_K \). Thus the points \( x = \pm L/2 \) may be identified. The action for the susy kink

\[
\mathcal{L} = -\frac{1}{2} (\partial_\mu \phi)^2 - \frac{1}{2} U^2(\phi) - \frac{1}{2} \bar{\psi} \gamma^\mu \partial_\mu \psi - \frac{1}{2} U'(\phi) \bar{\psi} \psi
\]

with \( U(\phi) = U(-\phi) \) is invariant under the transformation

\[
\phi \to -\phi, \quad \psi \to e^{i\alpha} \gamma^3 \psi,
\]

which is compatible with the Majorana condition for \( \alpha = 0 \) or \( \pi \) whereas for Dirac fermions an arbitrary phase would be allowed. Here we use a Majorana representation of the Dirac matrices with \( \gamma^0 = -i\sigma_2, \gamma^1 = \sigma_3, \gamma^3 = \sigma_1 \). In these terms, the TP and TAP boundary conditions in \( \text{[1]} \), \( \text{[2]} \) are simply \( \psi \to \pm \gamma^3 \psi \), clearly satisfying \( \text{[4]} \). As a consequence there is no visible boundary (meaning no locally observable discontinuity or cusp) at \( x = \pm L/2 \). Note that it is not necessary in these considerations to assume that the center of the kink is located at the point \( x = 0 \). That will be helpful later on in defining the parity operation in a simple manner, but for any other purpose the matching point for the transition or jump conditions \( \text{[4]} \) may be chosen arbitrarily, as befits a locally invisible boundary.

The TP and TAP boundary conditions arise naturally if one begins with a kink-antikink system with periodic (P) boundary conditions, and looks at the values of \( \psi_1, \psi_2 \) between the kink and antikink. One finds then that for P conditions for the kink-antikink system, the fermions satisfy either TP or TAP conditions. In this article we also consider a natural extension of these ideas: we begin with antiperiodic (AP) boundary conditions for the kink-antikink system, and find then that if the fermionic modes are written as plane waves \( e^{-i(\omega t - k x)} \) far away from the kink-antikink system, then in between the kink and antikink they satisfy imaginary twisted periodic and antiperiodic (iTP and iTAP) boundary conditions

\begin{align*}
i\text{TP} : & \quad \psi_1(-L/2) = i\psi_2(L/2), \quad \psi_2(-L/2) = i\psi_1(L/2) \\
i\text{TAP} : & \quad \psi_1(-L/2) = -i\psi_2(L/2), \quad \psi_2(-L/2) = -i\psi_1(L/2)
\end{align*}

where \( \psi_{1,2} \) now refer to the fermionic mode functions as opposed to the complete field. If one prefers to avoid working with complex boundary conditions for the Majorana fermions, one may take the real and imaginary parts of the distorted plane waves, but this then leads to the nonlocal boundary conditions \((-\partial_x^2 + m^2)^{1/2} \psi_1(-L/2) = \pm (\partial_x - m)\psi_2(L/2)\) and similar conditions for \( \psi_2(-L/2) \). In the following we consider only the algebraic boundary conditions \( \text{[3]} \) and \( \text{[4]} \). For periodic boundary conditions on the kink-antikink system, one finds only the real boundary conditions for a single kink given in \( \text{[1]} \) and \( \text{[2]} \), whether one uses complex or real mode functions.

In the trivial sector, P and AP boundary conditions are invisible boundary conditions, and, having introduced iTP/iTAP it seems only natural to also include iP and iAP boundary conditions

\begin{align*}
i\text{P} : & \quad \psi_1(-L/2) = i\psi_1(L/2), \quad \psi_2(-L/2) = i\psi_2(L/2) \\
i\text{AP} : & \quad \psi_1(-L/2) = -i\psi_1(L/2), \quad \psi_2(-L/2) = -i\psi_2(L/2).
\end{align*}
With imaginary boundary conditions, one finds a generalized Majorana identity, in which the adjoint of the field for one of the two boundary conditions is equal to the field for the other boundary condition, so that only if one averages over both conditions is it meaningful to describe the fermions as Majorana particles.

In Ref. [4], it was found that for a single kink one has to consider suitable averages over subsets of the mentioned boundary conditions to obtain the correct susy kink mass, because for particular individual cases one encounters localized boundary energy. This localized energy is due to boundary conditions which distort the field at the boundary and may be called visible boundary conditions. In the kink sector, the P/AP and iP/iAP boundary conditions are visible, whereas in the trivial sector, the twisted versions are visible.

To cancel out localized boundary energy, one needs to average over the results of a twisted and an untwisted boundary condition. In this paper, we shall show that there is a reason to average also over the two twisted boundary conditions, because a single (real) twisted boundary condition breaks parity \( P \) (as well as \( T \)), giving rise to delocalized momentum proportional to the ultraviolet cutoff, which cancels only in the average. (In the case of imaginary boundary conditions, a similar phenomenon arises with iP/iAP in the trivial sector.) This was overlooked in Ref. [4], which had assumed parity-invariance for the spectrum and incorrectly claimed the appearance of delocalized energy.

One might expect that one can find other boundary conditions in the kink sector which preserve parity. Indeed, the invisible boundary conditions iTP, and iTAP have a \( P \) and \( T \) invariant spectrum, but instead violate \( C \) (and thus \( CPT \)), so that these mode functions do not allow one to build a local quantum field theory with Majorana fields. Because \( C \) selects different locally invisible boundary condition from \( P \) and \( T \), it follows that there is no choice which preserves all three symmetries simultaneously. This obstruction occurs despite the fact that the action as a local expression in Bose and Fermi fields is invariant under all the symmetries. Hence, one encounters here a phenomenon which we call with some hesitation a discrete symmetry anomaly, induced by the kink. There is no local counterterm which can remove this anomaly. One can, of course, choose as boundary conditions \( \psi = 0 \) in which case there are no problems with the discrete symmetries, but then one has localized boundary energy, and our aim here is to study the discrete symmetries in the presence of invisible boundary conditions, which means with the kink put on a circle.

The possibility that a nontrivial structure of spacetime can lead to anomalies in discrete symmetries has been studied before. For example, in Ref. [10] a \( CPT \) anomaly was claimed to arise by compactification of some dimensions of (3+1) spacetime.

In our example, both a nontrivial space-time and a nontrivial field topology is present. In Ref. [11], it was found that in 2+1 dimensions there arise chiral fermions living on a susy kink domain wall; these fermions are massless in 2+1 dimensions (their energy is equal to the momentum along the domain wall) and they correspond to fermionic zero modes of the susy kink in 1+1 dimensions. In this case the spectrum is again parity-nonsymmetric (the massless fermions on the domain wall move in one direction but not in the other) but now this is not due to boundary conditions but rather due to the presence of the kink, in accordance with the general results of Refs. [7, 8]. In Ref. [9] the connection between instantons and the breaking of supersymmetry and the discrete symmetries \( C, P, T \) was considered.

Our paper is organized as follows. In Sect. [12] we discuss how the symmetries \( C, P \) and \( T \) act on the boundary conditions in the kink and in the trivial sector. In Sect. [13] we work out the fermionic spectra for the 16 sets of boundary conditions (8 sets in the kink sector, and 8 sets in the trivial sector). We also determine how the total mass and momentum of the kink depend on the choice of boundary conditions. We regulate by mode regularization, i.e., requiring equal numbers of modes in the trivial and kink sector, counting fermionic zero modes according to the rules derived in Ref. [4]. In Sect. [14] we comment on our results.
II. DISCRETE SYMMETRIES AND THEIR IMPLEMENTATION

For the single-particle Dirac Hamiltonian

\[ H = i\hbar \sigma_1 \partial_x + \hbar \sigma_2 m \phi_K(x)/\phi_0, \]

one has simple and unique representations of the three symmetry operations, charge conjugation \( C \), parity \( P \), and time reversal \( T \), which leave this differential operator invariant. \( C \) at the single-particle level is an antiunitary operation which reverses the sign of \( H \), and because in this representation \( H \) is purely imaginary the transformation is accomplished by simple complex conjugation of fermion wave functions: \( C = K \). For \( P \), which must include the transformation \( x \to -x \), a subtlety arises because this operation by itself turns the kink into an antikink. Therefore, in the kink sector, one must require for the action of parity on the classical bosonic field \( \phi_K(x) \to -\phi_K(-x) = \phi_K(x) \).

In the kink background the combined transformation reverses the derivative term but not the mass field \( \phi \). Of course, in the trivial sector, the action of parity on the (constant) classical background
discrete operations on fermion wavefunctions is the same in the trivial sector as it is in the kink sector. Of course, in the trivial sector, the action of parity on the (constant) classical background field \( \phi_0 \) is simply to preserve it. Thus, to keep the background invariant one treats the background field as scalar in the trivial sector but pseudoscalar in the kink sector.

While the discrete transformations can be defined consistently for the differential operator, we still need to look at their effects on the matching or boundary conditions. Let us write these conditions in a general form which covers all the choices described above:

\[ \psi(x = -L/2) = \Gamma e^{i\alpha} \psi(x = +L/2). \]

The twisted boundary conditions which we now analyse correspond to \( \Gamma = \gamma^3 = \sigma_1 \). The conditions could be applied at any point (see \[3\] for the details of the precise procedure), but let us choose symmetric placement around the center of the kink to make the action of the parity symmetry as simple as possible. Evidently we obtain the four different possibilities mentioned above by choosing \( \alpha = 0, \pi, \pi/2, -\pi/2 \), respectively. The action of \( C \) takes \( e^{i\alpha} \) to \( (e^{i\alpha})^* \), so that only \( \alpha = 0, \pi \) (TP and TAP) are left unchanged. For parity, because of the interchange of left and right boundaries along with the presence of the matrix \( \sigma_2 \), one has \( e^{i\alpha} \to -(e^{i\alpha})^{-1} \), so that only \( \alpha = \pm \pi/2 \) (iTAP and iTAP) are left unchanged. For \( T \), the matrix \( \sigma_3 \) implies \( e^{i\alpha} \to -(e^{i\alpha})^* \), and again \( \alpha = \pm \pi/2 \) (iTAP and iTAP) are left unchanged.\(^1\)

The purely real TP and TAP conditions commute with \( C \), but \( T \) and \( P \) each interchange TP with TAP. Consequently, with one of these conditions by itself only \( C \) holds: It is possible to choose wave functions which are real, and a fermion field operator which is Hermitean, but (positive-energy) waves of positive and negative wavenumber \( k \) are not degenerate with each other. This means that an implicit assumption of \([1]\), that the energy spectrum is the same for \( k > 0 \) and \( k < 0 \), is not correct \([10]\). In \([1]\) the spectrum for negative \( k \) was not computed explicitly, and this led to a false conclusion that the energy spectra for TP and TAP are different. In fact, it is easy to check that for each solution with \( k \) of one sign for TP there is a degenerate solution with \( k \) of the opposite sign for TAP. A further assertion of \([1]\) resulting from the assumed difference in spectra is that there exists a delocalized energy for either TP or TAP alone. This also is false \([11]\), but as will be shown below there indeed is a delocalized quantity, a net momentum proportional to the ultraviolet cutoff energy \( \Lambda \).

\(^1\) We use the passive point of view according to which we equate \([1]\) to \( \psi'(-L/2) = M \psi'(L/2) \) and solve for \( M \).
On the other hand, with iTP and iTAP conditions, \( P \) and \( T \) symmetries leave the conditions invariant, but \( C \) interchanges them. Once again, to have all three symmetries one must use an average over the two boundary conditions. This time, if one just chooses one of these boundary condition there is a difference in energy spectrum from the other boundary condition (but the spectra are each parity-symmetric). Now a new difficulty arises, that it is impossible to write a Hermitean Majorana field, because a positive energy state with positive momentum does not have an equal negative energy partner with negative momentum. A different way to reach the same conclusion is to consider the operation \( CPT \), which is a well-accepted symmetry for local quantum field theory.\(^2\)

Evidently this symmetry leaves the field Hamiltonian density invariant only for the TP and TAP conditions, which therefore are the ones uniquely allowed as consistent conditions in quantum field theory. For these conditions to achieve vanishing delocalized momentum one must average over TP and TAP, while for iTP and iTAP implementing \( CPT \) symmetry forces averaging over the two sets. Thus the notion of averaging over sets of boundary conditions, as introduced in \(^1\), does have merit, but detailed claims in the original rationale for this construction needed major revision, as we have just described.

For completeness, we should examine the effects of the discrete symmetries in the trivial sector. Now, invisible boundary conditions have the unit matrix in place of the matrix \( \sigma_1 \). One sees immediately that the \( P \) and \( AP \) conditions satisfy all three discrete symmetries, while \( iP \) and \( iAP \) do not satisfy any. This means that one could implement the discrete symmetries with either \( P \) or \( AP \), but implementation for imaginary conditions would require both \( iP \) and \( iAP \).

To describe the discrete symmetries as transformations on the Majorana field we need a dictionary relating these transformations to those already discussed for the the single particle wave functions. For charge conjugation this is

\[
U_C \psi(x,t) U_C^{-1} = \psi^\dagger(x,t)
\]  

(10)

so that the Majorana condition becomes simply the hermiticity or self adjointness of the field \( \psi \). Note that what had been an antiunitary operation taking \( H \) into its negative for the single-particle description now is a unitary operation leaving the Hamiltonian density \( \mathcal{H}(x,t) \) invariant. This result depends critically on the fact that \( \mathcal{H} \) includes a commutator of \( \psi \) with \( \psi^\dagger \), which reverses sign under charge conjugation. For parity we have\(^3\)

\[
U_P \psi(x,t) U_P^{-1} = i\sigma_2 \psi(-x,t)
\]  

(11)

identical with the single-particle rule. For time reversal one finds the greatest subtlety, because this operation remains antiunitary:

\[
V_T \psi(x,t) V_T^{-1} = \sigma_3 \psi^*(x,-t)
\]  

(12)

The subtlety has to do with defining complex conjugation for the raising and lowering operators \( a^\dagger \) and \( a \) appearing in the mode expansion of the field. The simplest assumption is that this operation leaves the operators invariant, but instead each one could be multiplied by a different phase factor. In that case, the phase factor would have to be explicitly compensated in the action of \( V_T \) on each raising or lowering operator. It is easy to verify that these new definitions are consistent with

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\(^2\) There has been recent interest in anomalous \( CPT \) violation in chiral theories in 4 dimensions \(^{11,12}\) and in 2 dimensions \(^{13}\). We consider the present work (which does not include chiral gauge couplings) complementary to those studies, but the chiral nature of the twisted boundary conditions suggests that there may be a connection to the anomaly in explicitly chiral theories.

\(^3\) As is the case for Majorana fermions in 4 dimensions \(^{14}\), \( P^2 = -1 \).
the earlier analysis of the relation between discrete symmetries and boundary conditions, with the obvious proviso that the boundary conditions now are applied to the field exactly as they previously were applied to the wave functions.

The issues discussed here all arise because we are dealing with Majorana fermions. How would the discussion change if one considered instead an \( N = 2 \) theory, with Dirac fermions? Now the field \( \psi \) no longer need be equivalent to its charge conjugate, so it might seem that one could choose just one boundary condition instead of averaging over a pair. It is enticing to imagine that the Dirac fermion charge could be coupled to a \( U(1) \) gauge field, so that the phase \( \alpha \) in (9) would reflect a magnetic flux threading the circle. However, for no choice of \( \alpha \) would the spectrum obey all three discrete symmetries, just as we found already; that deduction holds regardless of the assumption \( N = 1 \) or \( N = 2 \). Thus we still require a pair of boundary conditions if the symmetries all are to be obeyed simultaneously. In the \( N = 2 \) theory however, continuous values of \( \alpha \) are allowed, and except for the values considered before any other would break all three symmetries, as one would expect for arbitrary irrational flux through the circle. The \( N = 2 \) theory exhibits the Jackiw-Rebbi half-fermion charge localized at the kink \([13]\), and it is amusing that this is consistent with the possibility of tunneling between kink and antikink \([14]\), as the latter also would possess charge one-half. The physical interpretation of this analysis, when combined with what we saw earlier, seems to be that the problem of the kink on a circle ‘knows’ that it really is half of the kink-antikink problem on a doubled circle. Thus the discrete symmetries which are obeyed for half an Aharonov-Bohm quantum of flux through the large circle also are obeyed for one-quarter flux through the small circle, but only when one averages over a suitable pair (iTP and iTAP) of boundary conditions.

III. MODE NUMBER REGULARIZATION OF FERMIONIC CONTRIBUTIONS TO THE ONE-LOOP SUSY KINK MASS

We now turn to the explicit calculation of the fermionic contributions to the susy kink mass at one-loop order in mode number regularization, extending and partially correcting the results presented in Ref. \([4]\).

The \( \phi^4 \)-kink model corresponds to using \( U(\phi) = \sqrt{\lambda/2}(\phi^2 - \phi_0^2) \) in the Lagrangian \([3]\), but the following discussion applies (mutatis mutandis) to other models such as sine-Gordon, where \( U \propto \sin(\gamma \phi/2) \).

In the trivial vacuum, one has \( U(\phi_0) = 0 \) and \( U'(\phi_0) = 2\sqrt{\lambda} \phi_0 = m \), whereas with the nontrivial kink background field \( \phi_K(x) = \phi_0 \tanh(m(x - x_0)/2) \) one has the Bogol’nyi equation \( U'(\phi_K) = -\partial_x \phi_K \) and \( U''(\phi_K) = m \phi_K/\phi_0 \), leading to a fluctuation equation for the fermionic mode functions governed by the differential operator \([8]\).

The fermionic mode functions will be written

\[
\psi(x, t) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} e^{-i\omega t}
\]  

so that the Dirac equation becomes

\[
- i\omega \psi_1 = (\partial_x - U') \psi_2, \quad - i\omega \psi_2 = (\partial_x + U') \psi_1.
\]  

The fermionic contribution to the one-loop quantum mass of a kink is given by sums over zero-point energies according to

\[
M_f^{(1)} = -\frac{\hbar}{2} \left[ \sum \omega_K - \sum \omega_V \right] + \Delta M_f
\]  

where the indices $K$ and $V$ refer to kink and trivial vacuum, respectively, and $\Delta M_f$ is the fermionic contribution to the counter-term due to renormalizing the theory in the trivial vacuum. A minimal renormalization scheme that can be chosen is to require that tadpoles vanish and all other renormalization constants are trivial.\(^4\) This gives

$$\Delta M_f = -\frac{2}{3} \Delta M_b = -\frac{m\hbar}{2\pi} \int_{-\Lambda}^{\Lambda} \frac{dk}{\sqrt{k^2 + m^2}}. \quad (16)$$

In (global)\(^5\) mode regularization the spectrum of fluctuations about a kink (and in the trivial vacuum) is discretized by considering an interval of (large) length $L$ and choosing boundary conditions. The sums in (15) are then cut off at a given large value $N$ of the number of modes, which according to the principle of mode regularization is chosen to be the same in the trivial and in the kink sector.\(^6\)

As argued in Ref.\(^4\), this requires fixed boundary conditions, meaning that they are identical for the trivial and the kink sector. But because invisible boundary conditions in one sector are visible ones in the other, it becomes necessary to average over boundary conditions such that boundary energies cancel in the average.

The correct answer this average has to give is, as has been established by a variety of methods \(^3, 4, 13, 20, 21, 22, 23, 24, 25\),

$$M_f^{(1)} = -M_b^{(1)} - \frac{\hbar m}{2\pi} \quad (17)$$

where $M_b^{(1)}$ is the bosonic contribution, so that there is in total a nonvanishing negative correction for the susy kink mass $M_f^{(1)} = M_f^{(1)} + M_b^{(1)}$ which is in fact entirely due to an interesting anomalous contribution to the central charge operator \(^22, 26, 27\).

A. Quantization conditions

To explicitly compute the difference of the sums in Eq. (15) for the various boundary conditions discussed in Sect. 1, we have to derive the quantization conditions on an interval of length $L$. For ease of comparison with Ref.\(^4\), Sect. VB, we let the spatial coordinate run from 0 to $L$ and put the center of the kink at $x = L/2$.

We shall have to consider carefully both the discrete and continuous\(^7\) spectrum.

1. Trivial sector

If one puts

$$\psi_1 = e^{ikx} + ae^{-ikx} \quad (18)$$

\(^4\) For a thorough discussion of more general renormalization schemes in this context see Ref.\(^4\).

\(^5\) See Refs.\(^10, 15\) for a local variant which avoids the subtleties discussed here as well as allowing one to calculate the local energy distribution.

\(^6\) The proper regularization of these sums is a highly delicate matter. In particular, a simple energy cutoff, which has frequently been employed in the early literature \(^16, 17, 18\), turns out to lead to results inconsistent with the exact integrability of sine-Gordon models \(^19\). If, however, one uses a smooth energy cut-off, one obtains an extra term in the mode sums which is independent of the details of the smoothing, and this then yields the correct result \(^20\).

\(^7\) More precisely the part of the discretized spectrum that becomes continuous in the limit $mL \to \infty$.\]
then it follows from the Dirac equation (14) with $U' \equiv m$ that

$$\psi_2 = -[e^{i(kx + \frac{\theta}{2})} - ae^{-i(kx + \frac{\theta}{2})}]$$

where we define $\theta$ such that

$$e^{\frac{\theta}{2}} = \frac{k - im}{\omega}, \quad \omega = \pm \sqrt{k^2 + m^2}. \quad (20)$$

So $\theta = -2\arctan(m/k)$, but the branch of the arctan is fixed such that (for positive frequencies $\omega$) $\theta$ goes from $-2\pi$ to 0 as $k$ runs from $-\infty$ to $+\infty$. This conforms with the definition adopted in [3] but deviates from Ref. [4]. The definition (20) has the advantage of avoiding explicit sign functions $\text{sgn}(k)$ in the quantization conditions.

The quantization conditions for untwisted P and AP boundary conditions are simply $kL = 2\pi n$ and $kL = 2\pi n + \pi$; iP and iAP have $kL = 2\pi n - \pi/2$ and $kL = 2\pi n + \pi/2$, respectively. Notice that iP and iAP in the trivial sector each have a set of solutions which is not symmetrical under $k \rightarrow -k$.

The twisted boundary conditions read $\psi_1(0) = \rho \psi_2(L)$ and $\psi_2(0) = \rho \psi_1(L)$, where $\rho = e^{i\alpha} = +1, -1, +i, -i$ for TP, TAP, iTP, and iTAP, respectively. Plugging these conditions into (18) and (19) and solving for $a$ gives

$$\frac{-\rho e^{i(kL + \frac{\theta}{2})} - 1}{-\rho e^{-i(kL + \frac{\theta}{2})} + 1} = a = \frac{-e^{i\frac{\theta}{2}} - \rho e^{ikL}}{\rho e^{-ikL} - e^{-i\frac{\theta}{2}}}. \quad (21)$$

Multiplying out, this gives

$$(\rho^2 - 1)(e^{i\frac{\theta}{2}} + e^{-i\frac{\theta}{2}}) = 2\rho(e^{ikL} - e^{-ikL}). \quad (22)$$

For $\rho^2 = 1$, (TP and TAP), this is equivalent to $\sin kL = 0$, i.e. $kL = \pi n$, with $n \neq 0$, because $n = 0$ corresponds to the trivial solution $\psi_1 = \psi_2 = 0$.

The imaginary twisted periodic/antiperiodic boundary conditions (iTP/iTAP) have $\rho^2 = -1$, and one finds for $\rho = \pm i$ the two sets of solutions $a)$ $kL = 2\pi n - \frac{\theta}{2} \pm \frac{\pi}{2}$, $b)$ $kL = 2\pi n + \frac{\theta}{2} \pm \frac{\pi}{2}$. (For these conditions the numerator and denominator on one side of (21) vanish, but not on the other side.) To every solution with $k$ there is one with $-k$, but the two correspond to the same solution (up to normalization) so it suffices to consider $k \geq 0$; $k = 0$ has again $a = -1$ such that $\psi_1 = \psi_2 = 0$ everywhere and therefore must not be counted.

There are also potentially zero modes, $\omega = 0$, and approximately-zero modes, $\omega \approx 0$, which have to be treated separately. For $\omega = 0$, the solutions to the Dirac equation read

$$\psi_1 = \begin{pmatrix} a_1 e^{-mx} \\ a_2 e^{mx} \end{pmatrix}, \quad (23)$$

where $a_1$ and $a_2$ are determined by the boundary conditions.

Only TP and TAP give nontrivial solutions for $a_1$ and $a_2$ and thus are compatible with these solutions. There is one such zero mode for each of these boundary conditions.

The imaginary twisted boundary conditions iTTP/iTAP on the other hand have almost-zero modes $\omega^2 = 4m^2 e^{-2mL}$ for $mL \rightarrow \infty$, with the positive-frequency solution satisfying iTTP, and the negative-frequency one satisfying iTAP. To verify this, one can use the ansatz

$$\psi_1 = e^{-\kappa x} + ae^{\kappa x}, \quad -i\omega \psi_2 = (m - \kappa)e^{-\kappa x} + a(m + \kappa)e^{\kappa x} \quad (24)$$

with $\omega^2 = m^2 - \kappa^2$ and make the approximation $\kappa \approx m$ which becomes valid in the limit $mL \rightarrow \infty$.

The untwisted boundary conditions P, AP, iP, and iAP have neither zero nor almost-zero modes in the trivial sector.
FIG. 1: The quantization conditions for the fermionic modes in the case of TP boundary conditions obtained from solving $\delta + \frac{\theta}{2} = 2\pi n + \pi - kL$ for positive $\omega$. The spectrum is clearly not invariant under $k \rightarrow -k$.

2. Kink sector

In the kink sector, one has asymptotic expressions

\begin{align}
\psi_1 &= \begin{cases} 
  e^{i(kx - \frac{\delta}{2})} + ae^{-i(kx - \frac{\delta}{2})}, & x \approx 0 \\
  e^{i(kx + \frac{\delta}{2})} + ae^{-i(kx + \frac{\delta}{2})}, & x \approx L
\end{cases} \\
\psi_2 &= -\begin{cases} 
  e^{i(kx - \frac{\delta}{2} - \frac{\theta}{2})} - ae^{-i(kx - \frac{\delta}{2} - \frac{\theta}{2})}, & x \approx 0 \\
  e^{i(kx + \frac{\delta}{2} + \frac{\theta}{2})} - ae^{-i(kx + \frac{\delta}{2} + \frac{\theta}{2})}, & x \approx L
\end{cases}
\end{align}

where $\delta = -2 \arctan(3mk/(m^2 - k^2))$ is the phase shift function also appearing for bosonic fluctuations. So $\psi_1$ behaves as the latter, while $\psi_2$ has a modified phase shift $\delta + \theta$.

For $\delta(k)$ we adopt the convention that $\delta(k \rightarrow \pm \infty) \rightarrow 0$ so that there is a discontinuity at $k = 0$ which in accordance with Levinson’s theorem is $2\pi$ times the number of bound states. For $\theta$ we however keep the definition of Eq. (20), which has the advantage of avoiding a separate treatment of positive and negative values of $k$.

We begin with discussing the untwisted boundary conditions.

The (real) P and AP conditions can be satisfied either for a) $a = 1$ and $kL = 2\pi n + \pi - \delta - \theta$ or b) $a = -1$ and $kL = 2\pi n + \pi - \delta$, where only positive $n$ need to be considered to obtain a complete set of solutions and solutions with $k = 0$ have to be excluded, for they correspond to $\psi_1 = \psi_2 = 0$. Because these quantization conditions involve only $e^{i\theta}$ rather than $e^{i\theta/2}$, in this (and only in this) case it would make no difference to define $\theta$ such as to vanish for $k \rightarrow \pm \infty$, as done for example in Ref. [19] (which obtained an incorrect result for the susy kink mass only because there is a localized boundary energy contribution [4], as we shall see shortly).

The imaginary untwisted boundary conditions iP and iAP on the other hand have identical quantization conditions, which are given by the two sets a) $kL = 2\pi n + \frac{\pi}{2} - \delta - \frac{\theta}{2}$, $n \geq 1$, b) $kL = 2\pi n - \frac{\pi}{2} - \delta - \frac{\theta}{2}$, $n \geq 2$. Again, only positive $n$ need to be considered since (in contrast to iP/iAP in the trivial sector) $k \rightarrow -k$ does not lead to further independent solutions.
TABLE I: Summary of fermionic quantization conditions, numbered in conformity with Ref. [4] where applicable, and the number of (almost-)zero modes ($n_z$) in each case. An upper index ± to the number $n_z$ indicates that these modes are only almost-zero modes; an index + or − indicates that only the positive or negative frequency mode, respectively, is compatible with the given boundary condition (b.c.).

| $i$ | b.c. | sector | $k_L$ | $n_z$ |
|-----|------|--------|-------|-------|
| 1 | P | trivial | $2\pi n$, all $n$ | 0 |
| 2 | AP | trivial | $2\pi n + \pi$, all $n$ | 0 |
| 3 | P | kink | a) $2\pi n - \delta - \theta$, $n \geq 1$ | 2 |
| | | | b) $2\pi n - \delta$, $n \geq 2$ | |
| 4 | AP | kink | a) $2\pi n + \pi - \delta - \theta$, $n \geq 1$ | 2± |
| | | | b) $2\pi n + \pi - \delta$, $n \geq 1$ | |
| 1'I | iP | trivial | $2\pi n - \pi/2$, all $n$ | 0 |
| 2'I | iAP | trivial | $2\pi n + \pi/2$, all $n$ | 0 |
| 3'I=4'I | iP/iAP | kink | a) $2\pi n + \pi/2 - \delta - \theta/2$, $n \geq 1$ | 2± |
| | | | b) $2\pi n + \pi/2 - \theta/2$, $n \geq 2$ | |
| 5=6'I | TP/TAP | trivial | a) $2\pi n$, $n \geq 1$ | 1 |
| | | | b) $2\pi n + \pi$, $n \geq 0$ | |
| 7 | TP | kink | $2\pi n + \pi - \delta - \theta/2$, all $n$, $n \neq 0$, $-1$ | 1 |
| 8 | TAP | kink | $2\pi n - \delta - \theta/2$, all $n$, $n \neq 0$, $-1$ | 1 |
| 5'I | iTP | trivial | a) $2\pi n + \pi/2 - \theta/2$, $n \geq 0$ | 1⁺ |
| | | | b) $2\pi n + \pi/2 + \theta/2$, $n \geq 1$ | |
| 6'I | iTAP | trivial | a) $2\pi n - \pi/2 - \theta/2$, $n \geq 1$ | 1⁻ |
| | | | b) $2\pi n - \pi/2 + \theta/2$, $n \geq 1$ | |
| 7'I | iTP | kink | $2\pi n + \pi/2 - \delta - \theta/2$, all $n$, $n \neq 0$, $-1$ | 1⁺ |
| | | | b) $2\pi n - \pi/2 - \theta/2$, all $n$, $n \neq 0$, $+1$ | 1⁻ |

Turning now to the twisted boundary conditions, the TP ones lead to $kL = 2\pi n + \pi - \delta - \theta/2$. As shown in Fig. [4], this has solutions for all $n$ except $n = 0$, $-1$, and the set of these solutions is not symmetric under $k \rightarrow -k$. The solutions generated by the latter transformation instead obey TAP boundary conditions, which require $kL = 2\pi n - \delta - \theta/2$.

The imaginary twisted boundary conditions iTP/iTAP differ from TP/TAP simply by an additional term $-\pi/2$ on the r.h.s. of the quantization conditions (for positive-frequency solutions). For iTP the exemptions are $n = 0$, $-1$ as with TP. For iTAP, $n = 0$ has to be excluded, while $n = \pm 1$ corresponds to the threshold mode $k = 0$, $\omega = m$, which is proportional to $(\psi_1, \psi_2) = (1 - 3 \tanh^2(mx/2), -2i \tanh(mx/2))$, and thus consistent with iTAP boundary conditions (it does not appear in any of the other boundary conditions). Thus $n = \pm 1$ has to be counted only once.

In contrast to TP/TAP, the sets of allowed $k$-values for iTP and iTAP are each symmetric under $k \rightarrow -k$ (while the corresponding solutions are linearly independent), but a positive-frequency solution with momentum $k$ for iTP or iTAP has a negative-frequency partner only for the other of the two imaginary twisted boundary conditions.

For the counting of modes in the next subsection we also need to know how many zero modes there are for each boundary condition in the kink sector. For real boundary conditions these have been discussed in Ref. [4] and are recapitulated in Table I, which summarizes the results of this subsection. The imaginary boundary conditions iP and iAP each have a pair of approximately-zero modes; however, for iTP there is only one approximately-zero mode with positive frequency, while the complex conjugated negative-frequency mode satisfies iTAP boundary conditions. (For iTP
and iTAP boundary conditions, one can take \( \psi_1 \) real and \( \psi_2 \) purely imaginary as this is consistent with the Dirac equation, while for iP and iAP both \( \psi_1 \) and \( \psi_2 \) are complex combinations of two real solutions.

Finally, in the kink sector there is one bound state with energy squared \( \omega_B^2 = \frac{3}{4}m^2 \). One can verify that on a finite interval it is possible to satisfy any of the boundary conditions considered by slightly increasing or decreasing the value of \( \kappa_B \) in \( \omega_B^2 = m^2 - \kappa_B^2 \). This is easy to see for P, AP, iTP, and iTAP boundary conditions where the mode functions \( \psi_1 \) and \( \psi_2 \) are antisymmetric and symmetric around the kink center, respectively; for TP, TAP, iP, and iAP, we have verified the compatibility of the boundary conditions numerically. By contrast, the situation is more complicated for the zero modes, because there \( \kappa_0 \) can only be decreased from its maximal value \( \kappa_0 = m \). Increasing \( \kappa_0 \) would turn \( \omega^2 \) negative, but the Hamiltonian is self-adjoint with a Hermitean inner product.

### B. Mode sums

#### 1. Real boundary conditions

Evaluating (13) with an equal number of modes in the trivial and in the kink sector, one thus obtains for P and AP boundary conditions

\[
M_f^{(1)}(P) = \frac{\hbar}{2} \sum_{n=-N}^{N} \omega_1 - \frac{\hbar}{2} \sum_{n=1}^{N} \omega_{3a} - \frac{\hbar}{2} \sum_{n=2}^{N} \omega_{3b} - 0 - \frac{\hbar \omega_B}{2} + \Delta M_f
\]

\[
= -\frac{\hbar \omega_B}{2} + \hbar m + \hbar \int_0^\Lambda \frac{dk}{2\pi} \omega' \left( \delta + \frac{\theta}{2} \right) + \Delta M_f
\]

(27)

and

\[
M_f^{(1)}(AP) = \hbar \sum_{n=0}^{N} \omega_2 - \frac{\hbar}{2} \sum_{n=1}^{N} \omega_{4a} - \frac{\hbar}{2} \sum_{n=2}^{N} \omega_{4b} - 0 - \frac{\hbar \omega_B}{2} + \Delta M_f = M_f^{(1)}(P),
\]

(28)

where the sums for the trivial sectors are written first, with \( \omega_i = \sqrt{\frac{k_i^2}{\hbar^2} + m^2} \) according to Table III; explicit zeros indicate the presence of (almost-)zero modes. This leads to

\[
M_f^{(1)}(P) = M_f^{(1)}(AP) = M_f^{(1)} + \frac{\hbar m}{4},
\]

(29)

implying that there is a finite amount of boundary energy equivalent to the contribution of one half of that of a low-lying continuum mode. Since P and AP are invisible boundary conditions in the trivial sector, this must be attributed to the kink sector.

For fixed TP and TAP boundary conditions, we find (correcting Ref. [10])

\[
M_f^{(1)}(TP) = \frac{\hbar}{2} \sum_{n=1}^{N} \omega_{5a} + \frac{\hbar}{2} \sum_{n=0}^{N} \omega_{5b} - \frac{\hbar}{2} \sum_{n=1}^{N} \omega_{7} - \frac{\hbar}{2} \sum_{n=2}^{N} \omega_{7} - \frac{\hbar \omega_B}{2} + \Delta M_f
\]

\[
= -\frac{\hbar \omega_B}{2} + \frac{\hbar m}{2} + \hbar \int_0^\Lambda \frac{dk}{2\pi} \omega' \left( \delta + \frac{\theta}{2} \right) + \Delta M_f = M_f^{(1)} - \frac{\hbar m}{4}
\]

(30)

and

\[
M_f^{(1)}(TAP) = \frac{\hbar}{2} \sum_{n=1}^{N} \omega_{6a} + \frac{\hbar}{2} \sum_{n=0}^{N} \omega_{6b} - \frac{\hbar}{2} \sum_{n=1}^{N} \omega_{8} - \frac{\hbar}{2} \sum_{n=2}^{N} \omega_{8} - \frac{\hbar \omega_B}{2} + \Delta M_f
\]

\[
= -\frac{\hbar \omega_B}{2} + \frac{\hbar m}{2} + \hbar \int_0^\Lambda \frac{dk}{2\pi} \omega' \left( \delta + \frac{\theta}{2} \right) + \Delta M_f = M_f^{(1)}(TP).
\]

(31)
TP/TAP are invisible boundary conditions in the kink sector, so that any boundary energy must now be attributed to the trivial sector. As one can see, it has equal magnitude but opposite sign than in the results for P/AP, in agreement with the discussion in Ref. [4]. (Twisting the fermions from P in the trivial sector to TP in the kink sector, the localized boundary energy does not change.) However, because \( M_f^{(1)}(TAP) = M_f^{(1)}(TP) \), there is no delocalized boundary energy in the sense of Ref. [4].

Taking the average of the results of one of the untwisted and one of the twisted boundary conditions eliminates the localized boundary energy and yields the correct result (17).

In Ref. [3] it was found that mode number regularization with the completely invisible “topological” boundary conditions of P in the trivial sector and TP in the kink sector produces the correct finite part, but leaves an infinite (but \( m \)-independent) term corresponding to the contribution of one half of that of a continuum mode with \( k = \Lambda \). The latter is removed by the derivative regularization method proposed in Ref. [3]. For mode regularization to give finite results it is crucial to have fixed boundary conditions. The localized boundary energies that this produces has then to be eliminated by averaging over one twisted and one untwisted boundary condition.

However, taking either TP or TAP for the twisted boundary condition, parity \( P \) is not a symmetry and thus the one-loop correction to the momentum in the kink sector need not be zero. The momentum operator is diagonal asymptotically far away from the kink, and one obtains for TP

\[
P_f^{(1)}(TP) = \frac{\hbar}{2L} \left( \sum_{n=1}^{N \omega_1} + \sum_{n=-2}^{-(N+1)} \right) [2\pi n + \pi - \delta - \theta/2]
\]

\[
= \frac{\hbar}{2} \int_{0}^{\Lambda} \frac{dk}{2\pi} [\delta - \theta/2] + \frac{\hbar}{2} \int_{-\Lambda}^{0} \frac{dk}{2\pi} [-\delta - \theta/2] = +\frac{\hbar}{4} \Lambda
\]

and, for TAP,

\[
P_f^{(1)}(TAP) = \frac{\hbar}{2L} \left( \sum_{n=1}^{N \omega_1} + \sum_{n=-2}^{-(N+1)} \right) [2\pi n - \delta - \theta/2]
\]

\[
= \frac{\hbar}{2} \int_{0}^{\Lambda} \frac{dk}{2\pi} [\delta - \theta/2] + \frac{\hbar}{2} \int_{-\Lambda}^{0} \frac{dk}{2\pi} [-2\pi - \delta - \theta/2] = -\frac{\hbar}{4} \Lambda
\]

Both results correspond to the contribution of one-half of a high-energy mode \(|k| = \Lambda\), but with opposite sign. So there is an infinite amount of “delocalized momentum”, which cancels only in the average over TP and TAP.

2. Imaginary boundary conditions

As discussed in Sect. [4], the imaginary versions of the above boundary conditions have the problem that each of iP, iAP, iTP, and iTAP separately break \( C \) and make it impossible to define Majorana quantum fields. In fact, \( CPT \) is equally violated.

Nevertheless, it may make sense to consider these boundary conditions in an averaged sense. Summing over positive frequencies only one has for iP

\[
M_f^{(1)}(iP) = \frac{\hbar}{2} \sum_{n=-N}^{N} \omega_1 + \frac{\hbar}{2} \sum_{n=1}^{N} \omega_{3a'} + \frac{\hbar}{2} \sum_{n=2}^{N} \omega_{3b'} - 0 - \frac{\hbar \omega_B}{2} + \Delta M_f
\]

\[
= -\frac{\hbar \omega_B}{2} + 2 \times \frac{\hbar m}{2} + \hbar \int_{0}^{\Lambda} \frac{dk}{2\pi} \left[ \delta + \frac{\theta}{2} \right] + \Delta M_f = M_f^{(1)} + \frac{\hbar m}{4},
\]
and the same for $M_f^{(1)}(iAP)$ because $\sum_{N}^N \omega_{1'} = \sum_{N}^N \omega_{2'}$ and (3')=(4') according to Table I. The iP/iAP results for the one-loop energies thus coincide with the corresponding results for P/AP.

Analogously, for iTP one obtains

$$M_f^{(1)}(iTP) = 0 + \frac{\hbar}{2} \sum_{n=0}^N \omega_{5a'} + \frac{\hbar}{2} \sum_{n=1}^N \omega_{5b'} - 2 \times \frac{\hbar}{2} \sum_{n=2}^N \omega_{7'} - \frac{\hbar \omega_B}{2} + \Delta M_f$$

and (3')=(4') according to Table I. The iP/iAP results for the one-loop energies thus coincide with the corresponding results for P/AP.

Although $C$ is broken, the two results coincide, so there is still no delocalized boundary energy in the sense of Ref. [4].

Because $P$ is intact with either iP or iTAP, there is also no delocalized momentum as with real twisted boundary conditions. However, iP/iAP in the trivial sector now break $P$ (whereas the kink sector is symmetric under $k \to -k$), and one finds that there is delocalized momentum associated with the trivial sector,

$$P_f^{(1)}(iP) = \frac{\hbar}{2L} \sum_{n=-N}^N (2\pi n - \frac{\pi}{2}) = -\frac{\hbar}{4} \Lambda$$

and

$$P_f^{(1)}(iAP) = \frac{\hbar}{2L} \sum_{n=-N}^N (2\pi n + \frac{\pi}{2}) = \frac{\hbar}{4} \Lambda.$$
preserved $CPT$, but break both $\mathcal{P}$ and $\mathcal{T}$. The imaginary variants $iTP$ and $iTAP$ on the other hand respect $\mathcal{P}$ and $\mathcal{T}$, but violate $\mathcal{C}$ and therefore even $CPT$, so that these boundary conditions cannot be used for local quantum field theory, although this obstruction is effectively removed by averaging over $iP$ and $iAP$, or $iTP$ and $iTAP$. The cancellation of local boundary energy in the mode regularization scheme requires averaging over the results obtained with one twisted and one untwisted boundary condition, where these conditions have to be used both in the trivial and in the kink sector.

For compatibility with the Euler-Lagrange variational principle, one should require that boundary terms due to partial integrations cancel. In our case these “boundary field equations” read

$$
\psi_1(-L/2)\delta\psi_2(-L/2) + \psi_2(-L/2)\delta\psi_1(-L/2) = \psi_1(L/2)\delta\psi_2(L/2) + \psi_2(L/2)\delta\psi_1(L/2).
$$

(39)

It is easy to see that the real boundary conditions $\mathcal{P}$, $\mathcal{AP}$, $\mathcal{TP}$, and $\mathcal{TAP}$ all satisfy this requirement, but the imaginary versions $iP$, $iAP$, $iTP$, and $iTAP$ each violate it.

This means that none of the imaginary boundary conditions can be used in a Lagrangian formulation with Majorana fermions, although the Hamiltonian (8) with a Hermitean inner product is still self-adjoint. The same conclusion was reached by looking at the spectrum (derived from bulk field equations and imposing the boundary conditions). The problem with imaginary boundary conditions then turned out to be that for a given momentum $k$ and positive frequency $\omega$ there is no corresponding mode in the spectrum with $-k$ and $-\omega$, and no Majorana field can be built.

To avoid this problem, one would have to switch to complex fermions by giving up supersymmetry, as in the original Jackiw-Rebbi model [13], or go to $N=2$ susy models. Neither possibility has been explored in this paper.

We summarize our assertions about averaging over invisible boundary conditions to restore all three discrete symmetries. In the trivial sector, one may average over $\mathcal{P}$ and $\mathcal{AP}$ or $i\mathcal{P}$ and $i\mathcal{AP}$, or both sets. However, because $\mathcal{P}$ and $\mathcal{AP}$ separately obey all symmetries, there is no need to average if one chooses one of these real periodic boundary conditions. In the kink sector, one may average over $\mathcal{TP}$ and $\mathcal{TAP}$ or $i\mathcal{TP}$ and $i\mathcal{TAP}$, or both sets. Any of these is an acceptable method to restore the symmetries, but this time there is no single boundary condition which simultaneously satisfies all three, so that averaging over at least one pair is necessary. That fact is the main point of our work.

The idea that one must average over a set of boundary conditions to restore a symmetry is known in string theory, where the spinning string maintains modular invariance (large general coordinate transformations) and unitarity and supersymmetry only if one sums over all spin structures (the requirement that fermions on a closed surface are periodic or antiperiodic in spacelike or timelike directions) [29].

We close with some speculative remarks. The fact that no locally invisible boundary condition for the fermionic quantum fluctuations satisfies all three symmetries $\mathcal{C}$, $\mathcal{P}$, and $\mathcal{T}$ simultaneously, whereas the classical action is $\mathcal{C}$, $\mathcal{P}$, and $\mathcal{T}$ invariant, suggests that we are dealing with a discrete anomaly. The origin of this effect is the global structure (analogous to a Möbius strip in our case [3]), whereas the usual chiral anomaly is a local effect. Clearly, one should not confuse this with the anomalies due to instantons, where the effective action contains terms of the form $\psi^4 + \bar{\psi}^4$; these preserve parity but break chiral invariance.

Whether or not the striking loss of simultaneous $\mathcal{C}$, $\mathcal{P}$, and $\mathcal{T}$ invariance should be called an anomaly in the sense of the chiral anomaly, it certainly satisfies the definition of an anomaly as a ‘clash of quantum consistency conditions’ [30].
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