Exceptional-point avatar of Majorana fermions in one dimension

Sourin Das\textsuperscript{1,2} and Indubala I Satija\textsuperscript{3} \textsuperscript{∗}

\begin{itemize}
\item \textsuperscript{1}Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India
\item \textsuperscript{2}Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany
\item \textsuperscript{3}School of Physics, Astronomy and Computational Sciences, George Mason University, Fairfax, VA 22030, USA
\end{itemize}

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Majorana bound states appearing in 1-D $p$-wave superconductor ($PWS$) are found to result in exotic quantum holonomy of both eigenvalues and the eigenstates. Induced by a degeneracy hidden in complex Bloch vector space, Majorana states are identified with a pair of exceptional point ($EP$) singularities. Characterized by a collapse of the vector space, these singularities are defects in Hilbert space that lead to Möbius strip-like structure of the eigenspace and singular quantum metric. The topological phase transition in the language of $EP$ is marked by one of the two exceptional point singularity degenerating to a degeneracy point with non singular quantum metric. This may provide an elegant and useful framework to characterize the topological aspect of Majorana fermions and the topological phase transition.

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Dirac’s prediction of antiparticles in 1928 stands as one of the most extraordinary triumphs of physics. The mathematical elegance of Dirac’s theory, which is consistent with the general principles of relativity and quantum theory, testifies the symmetry and simplicity that underlies the laws of nature. In 1937, Majorana guided by similar considerations discovered that charge-neutral fermions could be their own antiparticles\textsuperscript{[1]}.

Presently, Majorana fermions occupy a central place in many vibrant frontiers of modern physics. These include neutrino physics, supersymmetry, dark matter, and superconductivity which offer possibilities where Majorana Fermions may be found\textsuperscript{[1]}. Following a pioneering work by Kitaev\textsuperscript{[2]}, the one-dimensional $p$-wave superconducting quantum wire has emerged as an ideal system for theoretical and experimental exploration of Majorana Fermions\textsuperscript{[3]}. Appearance of a zero energy Majorana bound state protected by a gap appearing exactly at the two ends of the 1-D system (which disappeared for periodic boundary condition) was shown to be a hallmark of this topologically nontrivial phase. Using a sophisticated formulation of the problem this phase was characterised by a $Z_2$-index\textsuperscript{[2]}.

In this Letter, we lay down an independent route for identifying the presence of Majorana bound states in terms of exceptional point ($EP$)\textsuperscript{[4,5]}. It is shown that a pair of degenerate zero energy sub-gap states appears for the case of periodic boundary $PBC$ provided one extends the Hilbert space to include complex valued Bloch wave vectors (call it $k = k_r + ik_i$ where $k_r$, $k_i \in \mathbb{R}$). Of course the complex-$k$ leads to a situation which is described by an non-Hermitian Hamiltonian. The zero energy eigenstates of this non-Hermitian Hamiltonian embedded in the $k_r - k_i$ plane are shown to have square root singularity. Encircling these degeneracy point in $k$-space once results in swapping of eigenvectors and encircling twice results in return of the eigenvectors back to itself except for acquire a nontrivial phase. The existence of a nontrivial phase as one encircles the degeneracy is an example of the geometrical phenomenon of anholonomy that relates to the inability of a variable to return to its original value after a cyclic evolution. In contrast to the Berry phase which is an anholonomy in the eigenvector space, the non-Hermitian anholonomy can exist both in eigenvalue and the eigenvector space, exhibiting branch point singularity in the complex $k$-plane. Such anholonomy are popularly referred to as exotic quantum holonomy\textsuperscript{[9]}.

There have been some earlier studies of non-Hermitian systems. Seminal work by Bender\textsuperscript{[10]} had set a stage for the importance of such systems as it was argued that the complex domain being huge compared to the real domain and thus opens new possibilities such as new type of unitary evolution. Recent study of graphene in arm chair geometry\textsuperscript{[11]} has used this approach and shown the existence of $EP$s in the system. In a different type of analysis, analytic continuation of the energy in complex plane provided new insight about topological edge modes in quantum Hall systems\textsuperscript{[12]}. In a similar spirit, the central focus here is to establish a direct connection between the $EP$ and the Majorana fermions. We begin with the Hamiltonian for the 1-D $PWS$ given by

\begin{equation}
H = \sum_{n} 2w c_{n+1}^\dagger c_n + \Delta c_{n+1}^\dagger c_n + c.c. + \mu (c_{n}^\dagger c_{n} - 1/2). \tag{1}
\end{equation}

Here $w$ is the nearest-neighbour hopping amplitude, $\Delta$ the superconducting gap function (assumed real), and $\mu$ the on-site chemical potential. A quantum phase transition occurs as one tunes $\mu$ form $\mu > 1$ (topologically trivial) to $\mu < 1$ (topological nontrivial) with $\mu = 1$ being the point of transition\textsuperscript{[2]}. In the Bogoliubov basis, the system reduces to a collection of 2-level systems for the case $PBC$ given by

\begin{equation}
H(k) = (\cos k - \mu) \sigma_y - \Delta \sin k \sigma_x , \tag{2}
\end{equation}

Where $\sigma_x$ and $\sigma_y$ are the Pauli sigma matrices. The energy spectrum, labeled by the Bloch index $k$ and the corresponding eigenvectors are given by,

\begin{equation}
E_k^\pm = \pm \sqrt{(\mu - \cos k)^2 + \Delta^2 \sin^2 k} . \tag{3}
\end{equation}
The energy spectrum of the system is in general gapped that vanishes at a critical value, \( \mu_c = 1 \). Kitaev show that for \( \mu_c < 1 \) the system has a two fold degenerate manybody ground state or no degeneracy depending up on if we impose \( \text{OBC} \) or \( \text{PBC} \) hence establishing it as a topological phase. He also showed that the degeneracy is directly related to appearance of Majorana mode at each of the two ends of the 1-D \( \mathcal{PW}S \) with \( \text{OBC} \). In this letter we show an independent route to this topological degeneracy with in the \( \text{PBC} \) by extending the \( k \)-space to include complex eigenvalues though this renders the \( H(k) \) non-Hermitian. We begin by noting that for complex \( k = k_r + i k_i \) the \( E_{E_{k}}^{\pm} = 0 \) condition has a legitimate solution (which was not the case of real \( k \)) for a pair of \( k = k_0^\pm \) given by

\[
e^{i k_0^\pm} = \frac{\mu \pm \sqrt{\mu^2 - (1 - \Delta^2)}}{1 + \Delta} .
\] (4)

Note that, we obtain exactly two independent zero energy solutions for \( \text{PBC} \) in the complex plane whose analytic forms are identical to the basis states found by Kitaev \[2\] spanning the zero energy subspace containing the Majoranas in the \( \text{OBC} \) case with \( \mu_c < 1 \). Hence our approach lays down an independent route for visualising the topological degeneracy without the need for applying the \( \text{OBC} \) on 1-D \( \mathcal{PW}S \). In this approach the degeneracy appears purely in the complex \( k \)-plane.

To analyze these degeneracies further lets us rewrite Eq.\([5]\) in an explicit non-Hermitian matrix form

\[
H(k) = \begin{pmatrix} 0 & A_k \\ B_k & 0 \end{pmatrix} ,
\] (5)

where \( A_k = -a_k + ib_k, B_k = -a_k - ib_k \) and \( a_k = \Delta \sin k, b_k = \mu - \cos k \). The eigenvalues of \( H(k) \) are given by \( E_{E_{k}}^{\pm} = \pm \sqrt{A_k^2 + B_k^2} \) and the zero energy solution corresponds to either \( A_k = 0 \) or \( B_k = 0 \). One can immediately see from Eq.\([5]\) that the \( H(k) \) for the zero energy sector either forms a \( 2 \times 2 \) Jordan block \([13]\) for \( B_k = 0, A_k \neq 0 \) or a matrix which is connected to a \( 2 \times 2 \) Jordan block by a similarity transformation for \( B_k = 0, B_k \neq 0 \). Existence of similarity transformation between \( H \) for the case of \( A_k = 0, B_k \neq 0 \) and \( H \) for \( B_k = 0, A_k \neq 0 \) implies that they correspond to the same physical situation and hence we could choose to work with any one of them. The Jordan form corresponds to matrices which are tridiagonal and they can not be diagonalised any further. The \( 2 \times 2 \) Jordan block has two degenerate eigenvalues but its eigenstates collapse to a single state and hence do not span a two-dimensional space. Therefore, in the manifold of eigenstates parametrised by complex valued \( k, k = k_0^\pm \) represents a topological defect as the collapsed eigenspace corresponding to \( k_0^\pm \) can not be continuous deformation to the two-dimensional eigenspace corresponding to rest of the values of \( k \). These topological defects manifest themselves as square-root singularities as we expand eigenvector and eigenvalue of \( H(k) \) about \( k_0^\pm \) leading to a Möbius strip like topology. Such singularities are popularly referred to as exceptional point (EP)\([5]\) or non-Hermitian degeneracies\([6–8]\). Eigenstates spanning the Hilbert space of non-Hermitian \( H(k) \) as in Eq.\([5]\) are the bi-orthogonal vectors given by

\[
| R, \pm \rangle = \frac{1}{\sqrt{2}} \left( \pm \sqrt{A_k/B_k}, 1 \right) ,
\] (6)

where the respective dual vectors are defined as

\[
\langle L, \pm | = \frac{1}{\sqrt{2}} \left( \pm \sqrt{B_k/A_k}, 1 \right) ,
\] (7)

corresponding to \( E_{E_{k}}^{\pm} \). Here \( L, R \) refer to left and right eigenvectors. These vectors satisfy the bi-orthonormalization relation\([14, 15]\)

\[
\langle L, \pm | R, \pm \rangle = 1 \quad ; \quad \langle L, \pm | R, \mp \rangle = 0 .
\] (8)

Though such a normalization procedure works very well for non-Hermitian Hamiltonians in general but it runs into trouble at the exceptional point due to the nontrivial topology associated with the \( \mathcal{EP} \). For concreteness lets take \( A_k = 0 \) as the degeneracy condition. We note that, up to overall normalisations and phases, for \( A_k = 0 \), \( | R, \pm \rangle = (0, 1) \) and \( \langle L, \pm | = (1, 0) \). Hence tuning to the degeneracy point results in collapse of two-dimensional Hilbert space to a one-dimensional space as \( | R, + \rangle \) and \( | R, − \rangle \) become parallel to each other at this point. This is nothing but a manifestation of the non-diagonalizability of \( H(k) \) at the exceptional point. Also note that now the dual vectors at \( \mathcal{EP} \) has become mutually orthogonal, i.e. \( \langle L, \pm | R, \pm \rangle = 0 \) and they no more comply to the normalisation defined in Eq.\([8]\). To study the behaviour of the wavefunction in the vicinity of the exceptional point, we need to perform a systematic perturbative expansion which allows for an expansion of \( H(k) \) around the \( \mathcal{EP} \). The first hurdle in this direction is to identify the eigen-vectors of the unperturbed Hamiltonian, i.e. the Hamiltonian at the \( \mathcal{EP} \) which serve as a natural basis for performing the perturbation theory. Due to the collapse to the Hilbert at \( \mathcal{EP} \) we have to first engineer a consistent way of reconstructing a two-dimensional Hilbert space around the \( \mathcal{EP} \). The \( A_k = 0 \) degeneracy condition leads to a pair of \( \mathcal{EP} \) at \( k = k_0^\pm \) where we will further focus only on \( k = k_0^+ \) (call it \( k_0 \) henceforth) as the perturbation theory around both \( \mathcal{EPs} \) have the same analytic form. For simplifying notation we rename \( \langle L, \pm | \) and \( | R, \pm \rangle \) at \( k = k_0^+ \) as \( \langle L, \mathcal{EP} | \) and \( | R, \mathcal{EP} \rangle \). Note that the \( ± \) sign is redundant owing to the collapse of Hilbert space at the \( \mathcal{EP} \). Following Ref.\([14]\) an associated Jordan vector (call it \( | R(a), \mathcal{EP} \rangle \)) is identified which essentially facilitates a systematic perturbative expansion around \( \mathcal{EP} \). Now a two-dimensional space can be identified which is spanned by the following two linearly independent vectors,

\[
| R, \mathcal{EP} \rangle = (0, 1) , \quad | R(a), \mathcal{EP} \rangle = (-1/2a_{k_0})(1, 0) .
\] (9)

The corresponding duals can be identified as,

\[
\langle L, \mathcal{EP} | = (-2a_{k_0})(1, 0) , \quad \langle L(a), \mathcal{EP} | = (0, 1) ,
\] (10)

which are subjected to the new set of orthonormalization condition

\[
\langle L, \mathcal{EP} | R(a), \mathcal{EP} \rangle = 1 , \quad \langle L(a), \mathcal{EP} | R, \mathcal{EP} \rangle = 1
\]

\[
\langle L, \mathcal{EP} | R, \mathcal{EP} \rangle = 0 , \quad \langle L(a), \mathcal{EP} | R(a), \mathcal{EP} \rangle = 0.
\]
Note that these orthogonality and normalisation condition are distinct form that defined in Eq.(8) which are valid for a general diagonalizable non-Hermitian 2 × 2 Hamiltonian.

A systematic expansion of \( H(k) \) around the \( \mathcal{EP} \) to leading order in \( k - k_0 \) which confirms to a form \( H(k) = H(k_0) + H'(k - k_0) \) is given by

\[
H(k) = -2i\alpha_{k_0} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & A'_k \\ B'_k & 0 \end{pmatrix} (k - k_0),
\]

where \( A'_k = -\mu\Delta + i(1 - \Delta^2)\sin k_0, B'_k = -\mu\Delta - i(1 + \Delta^2)\sin k_0 \) are first derivatives of \( A_k, B_k \) at \( k = k_0 \). Note that the leading correction \( H' \) to the non-diagonalizable Hamiltonian at \( \mathcal{EP} \) is a diagonalisable matrix. The leading order expansion of eigenstates and eigenvalues in \( k - k_0 \) consistent with the Schrödinger equation for the form of \( H(k) \) as in Eq.(11) is given by

\[
|\pm, \theta\rangle = \frac{1}{N}\{ |R, \mathcal{EP}\rangle + \zeta_\pm \sqrt{r}|R(a), \mathcal{EP}\rangle e^{i\frac{\theta}{2}} \},
\]

\[
E_{\pm}(\theta) = \pm \zeta \sqrt{r} e^{i\frac{\theta}{2}},
\]

where \( k - k_0 = re^{i\theta}, \zeta_\pm = \pm \sqrt{(L, \mathcal{EP})|H'|R, \mathcal{EP}} = \sqrt{-2\Delta \sin k_0(-\mu\Delta + i(1 - \Delta^2)\sin k_0)} \) and the normalization is given by \( N = \sqrt{2\zeta_+ \sqrt{r} e^{i\frac{\theta}{2}}} \). The dual vectors corresponding to \(|\pm\rangle\) are identified as

\[
|\mp\rangle = N^{-1}\{ (L, \mathcal{EP}) + \kappa_\pm \sqrt{r} \langle L(a), \mathcal{EP}\rangle e^{i\frac{\theta}{2}} \},
\]

which satisfy the orthonormalization condition,

\[
\langle \pm | \pm \rangle = 1, \quad \langle \pm | \mp \rangle = 0,
\]

hence indicating that once we are away form the \( \mathcal{EP} \) the standard formulation of normalization condition of bi-orthogonal vectors given in Eq.(8) holds. The over line of dual vectors is chosen to emphasize the fact that these are not the same as \(|\pm\rangle\). Note that this expansion in Eq.(13) is unconventional as it is not a Taylor series expansion but rather a power series expansion\([14] \) in terms of \( \sqrt{k - k_0} \). Also this expansion reveals the fact that any infinitesimal deviation from wavefunction at the \( \mathcal{EP} \) induced by a small perturbation is always given in terms of the associated Jordan vector \(( |R, \mathcal{EP}\rangle )\) and hence is unique for developing a systematic perturbation theory around the \( \mathcal{EP} \).

We note that the eigenvalues exchange themselves \((E_{\pm}(\theta) \to E_{\mp}(\theta))\) as we go once around the \( \mathcal{EP} \), i.e. \( \theta \to \theta + 2\pi \) and they return to themselves as we go around twice \((\theta \to \theta + 4\pi)\). The branch geometry of energy associated with these non-Hermitian degeneracies (see Fig.1) are to be contrasted with that of diabolic geometry\([17] \) that is associated with degeneracies of the Hermitian Hamiltonian of a two-level system. Also, the eigenvectors exchange themselves up to phase \( |\pm, \theta\rangle \to -i|\mp, \theta\rangle \) as \( \theta \to \theta + 2\pi \). One going around twice, the states return to themselves \(( |\pm, \theta\rangle \to - |\pm, \theta\rangle \) except for the negative sign. This negative sign is nothing but a topological phase of \( \pi \) which is considered as an hallmark of an exceptional point\([9] \) confirming a Möbius strip-like topology. It is important to note that the \( \theta \) dependence of the normalisation constant \(N \sim e^{i\theta/4}\) contributes nontrivially to recover the correct anholonomy of the state \(|\pm, \theta\rangle\) as a function of \( \theta \). Based on the analysis presented above we conclude that the zero energy states obtained in 1-D \( PWS \) subjected to \( PBC \) and complex \( k \)-space extension indeed corresponds to a pair of \( \mathcal{EPs} \).

![FIG. 1. The figure shows a parametric plot in \( r, \theta \) depicting the geometric view of the pair of \( \mathcal{EP} \) in \( E^\pm \) in the complex \( k_r - k_i \) plane where \( k_r = r \cos(\theta) \) and \( k_i = r \sin(\theta) \) for the case of \( \Delta = 0.4 \) and \( \mu = 0.9 \) which corresponds to a pair of \( \mathcal{EP} \) at \( k_r = \pm 0.19 \) and \( k_i = 0.42 \). The two white lines represents the branch cuts starting at the two \( \mathcal{EP} \) and going off to infinity. The origin of \( k_i \)-axis is shifted to \( k_i = 0.42 \) for a symmetric view.](image)
of the non-Hermitian Hamiltonian given by
\[ g_{ij} = \frac{1}{2} \left\{ \langle \partial_i \psi | \partial_j \psi \rangle - \langle \partial_j \psi | \psi \rangle \langle \psi | \partial_i \psi \rangle + i \leftrightarrow j \right\}. \]  
(16)

To evaluate \( g_{ij} \) in the neighbourhood of \( \mathcal{EP} \) we prefer to use the cartesian coordinate corresponding to \( k - k_0 = k_1 + i k_2 \) and we reparametrized \( | \pm, \theta \rangle \) as \( | \pm, (k_1, k_2) \rangle \). It is straightforward to show that \( \partial_{k_1} \pm, (k_1, k_2) \rangle = -\{1/(4(k - k_0))\} \mp, (k_1, k_2) \rangle \) and \( \partial_{k_2} \pm, (k_1, k_2) \rangle = -\{1/(4(k - k_0))\} \mp, (k_1, k_2) \rangle \) which implies that the second term in the expression of \( g_{ij} \) is identically zero while the first term leads to \( g_{ij} \approx 1/(k - k_0)^2 \). This singular behaviour of the quantum metric in the neighbourhood of the \( \mathcal{EP} \) is again a hallmark of the \( \mathcal{EP} \).[14]

Now we turn to the issue the of phase transition. It is know that the transition point correspond to \( \mu = 1 \). At the transition point the two zero energy solution appear at \( k_0^+ = 0 \) and \( k_0^- = i \log \{(1 + \Delta)/(1 - \Delta)\} \) (from Eq.(4)). Using Eq.(13) it is straight forward to check that \( k_0^- \) indeed corresponds to an exceptional point. On the other hand at \( k_0^+ = 0 \), we note that \( a_{k_0} = \Delta \sin k_0^+ = 0 \) which leads to vanishing of the coefficient of the Jordan block itself in Eq.(11). Hence the exceptional point corresponding to \( k_0^- \) vanishes exactly at \( \mu = 1 \).

To understand what physics takes over the \( \mathcal{EP} \) corresponding to \( k = k_0^+ \), we perform an expansion of \( H(k) \) around this point to leading order in \( k - k_0^+ \) at \( \mu = 1 \) which gives
\[ H(k) = -\Delta \sigma_x k. \]  
(17)

This implies that we have a null hamiltonian exactly at \( k = k_0^+ = 0 \) representing a perfect level crossing. The corresponding eigenvectors are,
\[ | R, \pm \rangle = \frac{1}{\sqrt{2}} \left( 1 \pm \frac{i}{\Delta} k, 1 \right). \]  
(18)

Although the linear dispersion hints towards a close resemblance of the present situation to the diabolic points representing accidental degeneracies of two level of a Hermitian Hamiltonian[17] and a related monopole singularity, we note that the corresponding eigenvectors (see Eq.(18)) clearly rule out any topological singularity. In other words, in this non-Hermitian Hamiltonian systems, conical interactions do not result in Diabolic points[17] hence in turn indicates absence of any monopole singularity. To see this more clearly, note that the eigenfunction in Eq.(15) results in a quantum metric which is independent of \( k_0 - k_1 \) with no singularities in the \( k_0 - k_1 \) plane as derivatives of \( | R, \pm \rangle \) with respect to \( k_0, k_1 \) are both constant. This is in sharp construct with the singular quantum metric associated with the \( \mathcal{EP} \) shown above.

To conclude, in the space of complex-\( k \) the quantum phase transition is marked by the conversion of one of the two \( \mathcal{EP} \)s to trivial degeneracy (as seen in Fig. 11) and then back to \( \mathcal{EP} \) as we cross the transition. Degeneration of a pair of \( \mathcal{EP} \) into one exceptional and one trivial degeneracy at the critical point of the topological phase transition unveils a new scenario quite distinct from popularly observed bifurcation of a diabolic point[17] into two \( \mathcal{EP} \)s associated with gap closing discussed in earlier studies[4]. This characterization of topological phase transition is one of the key results of our paper. We further note from Eq.(4), for \( \mu > 1 \) we have \( \Im \{3m(k_0^+)\} < 0 \), \( \Im \{3m(k_0^-)\} > 0 \) and for \( \mu < 1 \) we have \( \Im \{3m(k_0^+)\} > 0 \), \( \Im \{3m(k_0^-)\} > 0 \) and \( \Im \{3m(k_0^-)\} = 0 \) at \( \mu = 1 \). Here \( \Im \{m\} \) represents imaginary part. Hence \( \text{sgn}\{3m(k_0^+)\} \) (\( \text{sgn} \) is signum function) define a \( Z_2 \) valued quantum number which changes form \(-1 \) to \(+1 \) across the transition. And the count of Majorana fermion pairs in our formulation is simply given by \( \langle 1/2 | \text{sgn}\{3m(k_0^+)\} | 1 + \text{sgn}\{3m(k_0^-)\} \rangle \) which is zero for \( \mu > 1 \) (non-topological phase) and is one for \( \mu < 1 \).

Discussion: It is conceivable that the non-topological phase (\( \mu > 1 \)) would be fragile as the gap could disappear in the presence of perturbation like disorder[20]. Hence it is natural to ask how the \( \mathcal{EP} \) appearing in non-topological phase react to presence of disorder as this could provide a clear difference between exceptional point appearing on two side of the transition in our study. This will be topic of future study[21]. Lastly we would would like to point out that engineering situation between exceptional point appearing on two side of the transition in our study. This will be topic of future study[21]. Lastly we would would like to point out that engineering situation between exceptional point appearing on two side of the transition in our study. This will be topic of future study[21]. Lastly we would would like to point out that engineering situation between exceptional point appearing on two side of the transition in our study. This will be topic of future study[21].

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