Particle-Hole Symmetry Protected Zero Modes on Vacancies in the Topological Insulators and Topological Superconductors on the Honeycomb Lattice

Jing He,1 Ying-Xue Zhu,1 Ya-Jie Wu,1 Lan-Feng Liu,1 Ying Liang,1 and Su-Peng Kou1,∗

1Department of Physics, Beijing Normal University, Beijing, 100875, P. R. China
(Dated: October 28, 2021)

In this paper we study the quantum properties of the lattice vacancy in topological band insulators (TBIs) and topological superconductors (TSCs) on honeycomb lattice with particle-hole symmetry. Each vacancy has one zero mode for the Haldane model and two zero modes for the Kane-Mele model. In addition, in TSCs on honeycomb lattice with particle-hole symmetry, we found the existence of the Majorana zero modes around the vacancies. These zero energy modes are protected by particle-hole symmetry of these topological sates.

Topological band insulators (TBIs) represent a class of novel states of matter characterized by a special band structure: they are the materials that behave like insulators in their interior or bulk while permitting the metallic boundaries. In two dimensions, there are two types of TBIs, the TBIs with time-reversal symmetry (TRS) and those without TRS. For the TBIs without TRS, the Thouless-Kohmoto-Nightingale-Nijs (TKNN) number can be identified to be the topological invariant: While for the TBIs with TRS (quantum spin Hall states in two dimension), people use the $Z_2$ topological invariant to label their properties. On the other hand, recently, people found that superconducting (SC) states with the same local order parameter may have different topological properties, which leading to the concept of “topological superconductivity (TSC)”.

The non-trivial topology of the bulk can also be exposed by introducing topological defects, π-flux, dislocations and vortices, to name a few. Moreover, the interplay of defect topology and topology of the original states result in even richer phases. Previous works have been done on the effect of π-flux and dislocations on the Haldane model which indeed trap zero energy bound states. Moreover, according to the index theorem, a vortex in topological superconductors is predicted to harness a Majorana fermion zero mode inside the vortex core. In turn, such vortices were found to be non-Abelian anyons which are the holy grail of topological quantum computation.

In this paper, we will focus on the effects of different type of defects–vacancies, in two dimensional topological states with particle-hole symmetry on the honeycomb lattice. FIG.1.a is the illustration of a vacancy on the honeycomb lattice. It is known in graphene, zero modes of electrons were found around the vacancies. Here we also found that the lattice defects of the TBIs on honeycomb lattice have nontrivial quantum properties: for the Haldane model each vacancy has one zero mode and for the Kane-Mele model each vacancy has two zero modes. These zero energy modes in TBIs are protected by particle-hole symmetry and the finite energy gap of the electrons. For the graphene system without energy gap, the zero modes (localized states) of electrons around the vacancies are fragile. By adding the perturbations that break the particle-hole symmetry (for example, the staggered potential), these zero modes (localized states) disappear. On the other hand, our results are much different from those in the Ref.[18], in which the effect of lattice vacancies in graphene with intrinsic spin-orbit interaction is studied in a continuum model. And these zero modes around a vacancy cannot be simply regarded as the remnant of the gapless edge states in a continuum effective model as people have done in Ref.[19]. In addition, in TSCs on honeycomb lattice with particle-hole symmetry, we found that there also exists (non-topological) Majorana zero modes around the vacancies.

Vacancies for the Haldane model: We start from the spinless Haldane model, of which the Hamiltonian is defined as

$$H_H = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + h.c.) - t’ \sum_{\langle\langle i,j \rangle\rangle} e^{i\phi_{ij}} \hat{c}_i^\dagger \hat{c}_j + \varepsilon \sum_{i \in A} \hat{c}_i^\dagger \hat{c}_i - \varepsilon \sum_{i \in B} \hat{c}_i^\dagger \hat{c}_i$$

FIG. 1: (Color online) (a) The lattice defect of the honeycomb lattice - vacancy. (b) The particle density of the zero mode around the vacancy of the Haldane model with particle-hole symmetry ($\varepsilon = 0$).

where $t$ and $t’$ are the nearest-neighbor hopping

*Corresponding author; Electronic address: spkou@bnu.edu.cn
and the next-nearest-neighbor hopping, respectively. $e^{i\phi_{ij}}$ is a complex phase of the next-nearest-neighbor hopping, and we set the direction of the positive phase to be clockwise ($|\phi_{ij}| = \frac{\pi}{2}$). $\varepsilon$ is the coefficient of the on-site staggered energy. Using the Fourier transformations, we can get the spectrum of free fermions as $E_k = \pm\sqrt{|\xi_k^0 - \varepsilon|^2 + |\xi_k|^2}$ where

$|\xi_k| = t\sqrt{3 + 2\cos(\sqrt{3}k_y) + 4\cos(3k_x/2)\cos(\sqrt{3}k_y)/2}$ and $\xi_k^0 = 2t'[2\cos(3k_x/2)\sin(\sqrt{3}k_y)/2 + \sin(\sqrt{3}k_y)]$. For this free fermionic system, there are two phases: the TBI state with TKNN number $C = \pm 1$ and the normal band insulator (NI) state. The phase boundary is $2\varepsilon = 6\sqrt{3}t'$.

Firstly we study the particle-hole symmetry of the Haldane model. After doing the particle-hole transformation, $\tilde{c}_{i\in A}^\dagger \leftrightarrow \tilde{c}_{i\in A}$ and $\tilde{c}_{i\in B} \leftrightarrow \tilde{c}_{i\in B}$ together with a complex (or charge) conjugate transformation, the hopping terms are invariant but the staggered potential term is changed. So for the case of $\varepsilon = 0$, the Hamiltonian have the particle-hole symmetry as $H_{\text{H}} = P^\dagger H_{\text{H}} P$ where $P$ is the particle-hole transformation operator for spinless fermion on the honeycomb lattice. Now we have the spectrum symmetry: each energy level of the electrons with positive energy $E$ must be paired with an energy level of the electrons with negative energy $-E$. While for the case of $\varepsilon \neq 0$, the particle-hole symmetry is broken, $H_{\text{H}} \neq P^\dagger H_{\text{H}} P$. However, now, we still have the spectrum symmetry as $E \leftrightarrow -E$. This is because after doing the particle-hole symmetry, the staggered potential changes sign. Due to the translation symmetry, we may do a sublattice transformation as $A \leftrightarrow B$. Then the total Hamiltonian is invariant.

We study the effect of a vacancy on the electronic states. It is obvious that such a defect that breaks translation symmetry is a local distortion of the system and has no topological properties. We can consider a vacancy as a "hole" in the system by removing a site. Due to the non-zero TKNN number, there may exist topologically protected edge states on the boundary of this "hole". It is known that at low energy the dispersion of edge states has a form as $E(k) \sim v_F k$ where $v_F$ is Fermi velocity of edge states. When the size of the hole shrinks, the energy levels of the edge states become discrete and eventually the edge states on the boundary around the "hole" turn into localized states around the vacancy. Because the Haldane model is based on a bipartite lattice, when we remove a site to create a vacancy, there will exist an unpaired electronic state. Due to the spectrum symmetry ($E \leftrightarrow -E$), the corresponding localized unpaired electronic state must have exact zero energy. Such zero mode is protected by the particle-hole symmetry of the TBI.

We calculate the electronic states for the Haldane model with a vacancy for the particle-hole symmetry case ($\varepsilon = 0$) numerically. On a $36 \times 36$ lattice, we found a zero mode near the vacancy in the Haldane model. In FIG. 1.b, we plot the particle density of the zero modes. The particle density is localized around the defect center within a length-scale $\sim (\Delta f)^{-1}$ where $\Delta f$ is the fermion’s energy gap. FIG. 2.a shows the energy levels via $t'$ for the Haldane model with a vacancy. Now the total number of the electronic states for this case is odd. FIG. 2.b shows the density-of-state (DOS) of the electronic states, of which a $\delta$ function is around $\omega = 0$ due to the zero mode of the vacancy.

Besides, we calculate the induced quantum number on a vacancy. From the numerical results, we have found a zero mode on the vacancy for the Haldane model. So a vacancy possesses two localized states which are denoted by $|+\rangle$ and $|-\rangle$ that are the occupied and unoccupied state of fermions, respectively. Around a vacancy, the fermionic operators are expanded as $\hat{\psi}(r,t) = \sum_{k \neq 0} c_k e^{-iE_k t} \Psi_k(r) + \sum_{k \neq 0} d_k^\dagger e^{iE_k t} \Psi_k^\dagger(r) + c_0 \Psi_0(r)$, where $c_k$ and $d_k^\dagger$ are the operators of $k \neq 0$ modes that are irrelevant to low energy physics. $\Psi_0(r)$ is the wave-function of the unpaired zero mode. $c_0$ is the annihilation operator of the zero mode. We define the induced fermion number operators as $\hat{N}_F \equiv \int \hat{\psi}^\dagger \hat{\psi} = d^2 r \ c_0^\dagger c_0 + \sum_{k \neq 0} (c_k^\dagger c_k - d_k^\dagger d_k) - \frac{1}{2}$ where $\hat{\psi}^\dagger \hat{\psi}$ means normal product of $\hat{\psi}^\dagger \hat{\psi}$. So we obtain the eigenvalues of induced fermion number operator as $\hat{N}_F(\pm) = \pm \frac{1}{2} |\pm\rangle$. 

FIG. 2: (Color online) (a) The energy levels with the spectrum symmetry ($E \leftrightarrow -E$): the localized state has zero energy shown by the blue line and the continuum. Spectrum is shown by the blue region (b) The scheme of DOS of electronic states with a vacancy. In non-interacting limit, the contribution of DOS from the vacancy is a $\delta$ function at $\omega = 0$. Here we set $t' = 0.1$. 

We study the effect of a vacancy on the electronic states. It is obvious that such a defect that breaks translation symmetry is a local distortion of the system and has no topological properties. We can consider a vacancy as a "hole" in the system by removing a site. Due to the non-zero TKNN number, there may exist topologically protected edge states on the boundary of this "hole". It is known that at low energy the dispersion of edge states has a form as $E(k) \sim v_F k$ where $v_F$ is Fermi velocity of edge states. When the size of the hole shrinks, the energy levels of the edge states become discrete and eventually the edge states on the boundary around the "hole" turn into localized states around the vacancy. Because the Haldane model is based on a bipartite lattice, when we remove a site to create a vacancy, there will exist an unpaired electronic state. Due to the spectrum symmetry ($E \leftrightarrow -E$), the corresponding localized unpaired electronic state must have exact zero energy. Such zero mode is protected by the particle-hole symmetry of the TBI.
The occupation (or unoccupation) of this zero mode lead to $N_F = \frac{c}{2}$ (or $N_F = -\frac{c}{2}$) fractional electronic charge. Although there is no topological background, an induced fractional charge is trapped around each vacancy in the Haldane model.

In addition, we found the parity effect for the Haldane model with multi-vacancy: for odd number vacancies (for example, 3 vacancies, 5 vacancies...), there exist zero energy modes; while for even number multi-vacancy (for example, 2 vacancies, 4 vacancies...), the localized states will have finite energy. It is also the particle-hole symmetry that enforces a zero energy level together with the pairs of energy levels with finite energy for the case of odd number vacancies. For example, for two separated vacancies, there exist two localized states (quasi-zero-modes) and the localized states slightly split due to the quantum tunneling effect between them. It is obvious that the energy splitting decays exponentially as the distance between two vacancies increases.

We have found the particle-hole symmetry protected zero mode around vacancies in the TBI phase of the Haldane model. Then we add the staggered on-site potential which breaks particle-hole symmetry. When the particle-hole symmetry is broken, the localized state will shift from zero to a finite value. We plot the bound state energy via $\varepsilon$ for the case of $\varepsilon = 0.1t$ in FIG.3. For $\varepsilon < \varepsilon_c = 3\sqrt{3}t'$, in TBI phase, there exist a localized state around the vacancy. For $\varepsilon > \varepsilon_c = 3\sqrt{3}t'$, the ground state is NI phase with trivial quantum properties, then the localized states disappear.

Finally, by varying local disordered potential on a given site $i_0$ gradually, the wave-function evolves from the extended state to the localized state. The Hamiltonian model in Eq.(1) turns into

$$H_{\text{H-V}} = -t \sum_{\langle i \neq i_0, j \neq i_0 \rangle} \left( \hat{c}_i^\dagger \hat{c}_j + h.c. \right) - t' \sum_{\langle \langle i \neq i_0, j \neq i_0 \rangle \rangle} e^{i\phi_{ij}} \hat{c}_i^\dagger \hat{c}_j - \alpha t \sum_{\langle \langle i_0, j \rangle \rangle} \left( \hat{c}_i^\dagger \hat{c}_j + h.c. \right) - \alpha t' \sum_{\langle \langle i_0, j \rangle \rangle} e^{i\phi_{ij}} \hat{c}_i^\dagger \hat{c}_j + V_0 \hat{c}_{i_0}^\dagger \hat{c}_{i_0} \in A. \tag{2}$$

where $V_0 = (1 - \alpha)t/\alpha$. $\alpha$ is a parameter to tune the local disordered potential. In the limit of $\alpha \to 0$, the on-site potential turns into infinite and the hopping parameters turn to zero around the site $i_0$. On the other hand, in the limit of $\alpha \to 1$, the system has translation invariance, of which the Hamiltonian reduces into Eq.(1) of $\varepsilon = 0$. By tuning $\alpha$, we don’t find any quantum phase transition. One extended state will turn into the localized state when there exists arbitrary small disordered potential with $\alpha \neq 0$. See FIG.4.

On the other hand, we studied the properties of the topological defects (the $\pi$-flux on a plaquette of the honeycomb lattice) in the Haldane model and also found a zero mode around it in the TBI phase. The zero modes around the $\pi$-flux are protected by the topological invariant. In TBI phase, the localized state has exact zero energy which is robust against arbitrary perturbation. There also exists an induced fractional charge $N_F = \frac{c}{2}$ around the $\pi$-flux. With the induced fractional charge, each $\pi$-flux carries a statistical angle $\pi/4$.

**Vacancies for the Kane-Mele model:** The Hamiltonian of the Kane-Mele model is similar to that of the Haldane
model as
\[
H_{\text{KM}} = -t \sum_{\langle i,j \rangle, \sigma} \left( \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c. \right) - t' \sum_{\langle i,j \rangle} e^{i\phi_{ij}} \hat{c}_{i,\sigma}^\dagger \sigma_z \hat{c}_j \\
+ \varepsilon \sum_{i \in A, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} - \varepsilon \sum_{i \in B, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} 
\]
where \( \sigma_z \) is the Pauli matrix and \( \sigma \) are the spin-indices representing spin-up (\( \sigma = \uparrow \)) and spin-down (\( \sigma = \downarrow \)) for electrons. Using similar calculations, we found that there exist two zero modes around a vacancy for the Kane-Mele model with \( \varepsilon = 0 \) and there also exists the parity effect for multi-vacancy case. These zero modes are also protected by the particle-hole symmetry. When there exist particle-hole breaking terms, the zero modes turn into the localized modes with finite energy.

Then we calculate the induced quantum number on a vacancy for the Kane-Mele model. Using similar approach, we found that for the TBI phase, the two zero modes around a vacancy correspond to four degenerate energy levels denoted by \( |\uparrow\uparrow\rangle \otimes |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle \otimes |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle \otimes |\downarrow\downarrow\rangle \). Here \( |\sigma_+\rangle \) and \( |\sigma_-\rangle \) are the occupied and unoccupied state, respectively. For the half filling case, the localized states around the vacancy are \( |\uparrow\uparrow\rangle \otimes |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle \otimes |\downarrow\uparrow\rangle \) of which there exists a spin-\( \frac{1}{2} \) moment as
\[
\hat{S}^z |\uparrow\uparrow\rangle \otimes |\downarrow\downarrow\rangle = \frac{1}{2} |\uparrow\uparrow\rangle \otimes |\downarrow\downarrow\rangle,
\]
\[
\hat{S}^z |\uparrow\downarrow\rangle \otimes |\downarrow\uparrow\rangle = -\frac{1}{2} |\uparrow\downarrow\rangle \otimes |\downarrow\uparrow\rangle. 
\]
In Ref.\[24\], people proposed that the Kane-Mele model can be realized in a Silicene based material with honeycomb lattice and strong spin-orbital coupling interaction. Then in this system people can detect the local spin moment by observing uniform spin susceptibility which obeys Curie-Weiss law as \( \chi_s \sim N_{\text{th}}(k_B T)^{-1} \) where \( N_{\text{th}} \) is the vacancy number.

Recently, people have studied the quantum properties of the \( \pi \)-flux in Ref.\[21\], \[22\]. They found there exist two zero modes and induced spin-\( \frac{1}{2} \) moment on the \( \pi \)-flux.

**Vacancies for the TSCs on honeycomb lattice with particle-hole symmetry:** In this part we will consider the effect of a vacancy in a \( C = \pm 1 \) chiral TSCs on honeycomb lattice with particle-hole symmetry. The effective model of the TSC is
\[
H_{\text{TSC}} = H_H + \Delta_{\text{induce}} \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + h.c. 
\]
where \( H_H \) is the Hamiltonian of the Haldane model with \( \varepsilon = 0 \) and \( \Delta_{\text{induce}} \) is the induced SC order parameter due to the proximity effect to an extended s-wave SC order. Now the ground state is really a \( C = \pm 1 \) TSC, of which the topological properties are similar to those of \( p_x + ip_y \) wave pairing TSC. Above effective model has particle-hole symmetry as, \( E \leftrightarrow -E \).

We then studied the properties of a vacancy by solving the Bogoliubov-de Gennes (BdG) equations. On each vacancy, we found a single zero-mode which is described by a real fermion field \( \gamma^\dagger = \int dr [u_0 \psi^\dagger + v_0 \psi] \) obtained as a solution of the BdG equations. When two vacancies fuse (taken to the nearby sites in the honeycomb lattice), the result contains more than one quasi-particle due to the Ising fusion rule \[25\]: \( \sigma \times \sigma = I + \psi \) where \( \sigma \) denotes a vacancy, \( I \) the vacuum and \( \psi \) the fermion. This fusion rule is same to that of the non-Abelian anyons. However, although trapping a Majorana zero mode, the vacancy has trivial quantum statistics and cannot be regarded as a non-Abelian anyon. That is we found a symmetry protected Majorana zero modes in two dimensions without topological defects. So we call it non-topological Majorana mode.

Furthermore, we studied the properties of the \( \pi \)-flux for this system and also found a zero mode around of it in the TSC phase. So in the TSC state, the localized state has exact zero energy which is also robust against arbitrary perturbation. With trapping the Majorana zero modes, each \( \pi \)-flux obeys the non-Abelian statistics.

**Conclusion:** In the end we draw a conclusion. In general, for a TBI or a TSC on a bipartite lattice with particle-hole symmetry, there must exist zero energy modes around a vacancy and the parity effect for multi-vacancy. In this paper we investigate the lattice vacancy by using TBIs and TSCs on honeycomb lattice as examples to show this effect. For the TBIs and TSCs on a \( \pi \)-flux lattice (another two dimensional bipartite lattice), the properties of vacancies are similar to those on honeycomb lattice. As the remnant of the gapless edge state around a "hole" with minimize size, the localized states around the vacancies will have exact zero energy which are protected by the particle-hole symmetry of these topological states. The perturbations breaking particle-hole symmetry will shift the zero energy of the localized state to a finite value. But the induced quantum numbers on the vacancies doesn’t change until the energy gap closes and the quantum transition phase occurs.

Finally we give a table to show the difference between the zero modes around a topological defect (the \( \pi \)-flux) and the the zero modes around a vacancy (non-topological defect) in difference topological states.

Acknowledgments

This work is supported by National Basic Research Program of China (973 Program) under the grant No. 2012CB921704, 2011CB921803, 2011cb00102 and NSF Grant No. 11174035.
|                | The Haldane model | The Kane-Mele model | The TSC on honeycomb lattice |
|----------------|-------------------|---------------------|-----------------------------|
| π-flux vacancy | Abelian anyon with statistical angle π/4 | spin moment | Non-Abelian anyon |
|                | e/2 charge        | spin moment         | Majorana fermion mode       |

TABLE I: In different topological states, the π-flux (topological defect) and the vacancy (non-topological defect) have different properties.

[1] K. V. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. 45, 494 (1980).
[2] R. Prange and S. Girvin, *The Quantum Hall Effect* (Springer, New York, 1987); H. Aoki, Rep. Progr. Phys. 50 (1987) 655.
[3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[4] X. L. Qi and S. C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[5] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
[6] D. J. Thouless, M. Kohmoto, M. P. Nightingale and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
[7] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005); 95, 226801 (2005).
[8] B. A. Bernevig, T. L. Huge and S. C. Zhang, Science 314, 1757 (2006).
[9] G. E. Volovik, Zh. Eksp. Teor. Fiz. 94, 123 (1988) [Sov. Phys. JETP 67, 1804 (1988)].
[10] N. Read and D. Green, Phys. Rev. B 61, 10267 (2000).
[11] C. Weeks, G. Rosenberg, B. Seradjeh and M. Franz, Nature Physics 3, 796 (2007); G. Rosenberg, B. Seradjeh, C. Weeks, M. Franz, Phys. Rev. B 79, 205102 (2009).
[12] V. Juricic, A. Mesaros, R.-J. Slager, and J. Zaanen, Phys. Rev. Lett. 108, 106403 (2012).
[13] S. Tewari, S. Das Sarma, and Dung-Hai Lee, Phys. Rev. Lett. 99, 037001 (2007).
[14] L. Santos, Y. Nishida, C. Chamon, and C. Mudry, Phys. Rev. B 83, 104522 (2011).
[15] R. Roy, arXiv:1001.2371
[16] Vitor M. Pereira, F. Guinea, J. M. B. Lopes dos Santos, N. M. R. Peres, and A. H. Castro Neto, Phys. Rev. Lett. 96, 036801 (2006).
[17] M. M. Ugeda, I. Brihuega, F. Guinea, J. M. Gomez-Rodriguez, Phys. Rev. Lett. 104, 096804 (2010).
[18] M. Inglot and V. K. Dugaev, J. Appl. Phys. 109, 123709 (2011).
[19] W. Y. Shan, J. Lu, H. Z. Lu, and S. Q. Shen, Phys. Rev. B 84, 035307 (2011).
[20] C.N. Yang and S.C. Zhang, Mod. Phys. Lett. B 4, 759 (1990).
[21] S. P. Kou, Phys. Rev. B 78, 233104 (2008).
[22] X. L. Qi and S. C. Zhang, Phys. Rev. Lett. 101, 086802 (2008).
[23] Y. Ran, A. Vishwanath and D. H. Lee, Phys. Rev. Lett. 101, 086801 (2008).
[24] C. C. Liu, W. Feng, and Y. Yao, Phys. Rev. Lett. 107, 076802 (2011).
[25] G. Moore, and N. Read, Nucl. Phys. B 360, 362-396 (1991).