A magnetic monopole in topological insulator: exact solution

Yuan-Yuan Zhao and Shun-Qing Shen

Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China

We present an exact solution of a magnetic monopole in a topological insulator. It is found that a magnetic monopole can induce a pair of zero energy modes: one is bound to the monopole and the other is distributed near the surface. For a finite size system, the interference of two states may lift the degeneracy, and the resulting states have one half near the origin and another half around the surface. However, the energy difference decays exponentially with the size of the system. Due to the particle-hole symmetry only one electron can occupy the two states at half filling. The presence of a pair of degenerate zero energy modes does not fully support the realization of the Witten effect in a topological insulator as the charge bound to the monopole can be from zero to one modulus an integer. External fields such as the Zeeman field may remove the degeneracy of two states. In this case, a half charge around the monopole becomes possible.

PACS numbers: 03.65.Vf, 14.80.Va, 14.80.Hv

Topological insulators are electronic materials that behave like insulators or semiconductors in the bulk, but are surrounded by a topologically protected conducting layer near the surface of the materials. One of the predicted features in the materials is the “axion electrodynamics”, as a response to external electromagnetic fields. The idea of axion was first introduced to address the strong charge-parity problem in the physics of strong interaction. It becomes a possible candidate for the dark matter in the universe, and however, has not been confirmed yet experimentally so far. Historically, it was known that an additional term $\theta \epsilon^2 \mathbf{B} \cdot \mathbf{E}$ can be introduced into the Maxwell Lagrangian for electric and magnetic fields, which is time reversal invariant when $\theta = \pi$. This additional term revises both the Gauss’ law and Ampere’s law in the Maxwell’s equations by adding extra terms,

\[
\nabla \cdot \mathbf{D} = \rho_e - \frac{\alpha}{\pi \mu_0 c} \nabla \theta \cdot \mathbf{B},
\]

\[
\nabla \times \mathbf{H} = \partial_t \mathbf{D} + j + \frac{\alpha}{\pi \mu_0 c} (\nabla \theta \times \mathbf{E} + \partial_t \mathbf{B})
\]

where $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$, $\mathbf{H} = \frac{1}{\mu_0} \mathbf{B} - \mathbf{M}$, and $\alpha = \frac{e^2}{2\pi \hbar c}$ is the fine structure constant. One of the fundamental properties in the revised Maxwell’s or axion equations is the Witten effect, which states that a magnetic monopole of unit strength $e_M = \phi_0 = \frac{\hbar c}{e}$ in an axion media must bind an electric charge, $-(n + \frac{\theta}{2\pi})e$, where $e(>0)$ is the elementary charge and $n$ is an integer. Consider a point-like magnetic monopole situated at the origin, which produces a magnetic field, $\nabla \cdot \mathbf{B} = \phi_0 \delta(r)$. We suppose that $\theta = 0$ initially and then increases adiabatically to $\theta = \pi$. $\theta$ is uniform in the space and there is no current in the media. It follows from the axion equations that

\[
\delta \rho_e = \rho_e(\theta = \pi) - \rho_e(\theta = 0) = -\frac{\alpha}{\mu_0 c} \nabla \cdot \mathbf{B} = -\frac{e}{2} \delta(r).
\]

As a magnetic monopole does not induce a half elementary charge in a conventional media of $\theta = 0$, the charge bound to the monopole should be $-e/2$ modulus an integer for a time reversal invariant topological insulator of $\theta = \pi$. Charge fractionalization in condensed matters was extensively discussed for one dimension in 1980s. The quasi-particles in the fractional quantum Hall effect also carry fractional charge. Whether or not a half elementary charge bound by a magnetic monopole could exist in a topological insulator becomes a subtle issue to test the validity of the axion theory for topological insulators. Rosenberg and Franz studied the Witten effect in a crystalline topological insulator numerically, and intended to use it as a criterion to justify whether the system is topologically trivial or non-trivial.

In this paper, we present an exact solution of a magnetic monopole located in the center of a topological insulator sphere, which is described by the modified Dirac-like equation. It is found that there exist a pair of degenerate solutions of zero energy: one is located in the vicinity of the magnetic monopole and the other around the sphere surface, which is characteristic of non-trivial topological insulator. At half filling, only one electron occupies the two degenerate states due to the particle-hole symmetry in the system. The double degeneracy of the zero energy states does not favor or disfavor the Witten effect because the bound charge near the monopole can be from zero to $-e$ modulus an integer charge $-nc$, although it does not exclude a half elementary charge as the Witten effect requires. The degeneracy of the two states can be removed due to the finite size effect for a small sphere. In the case the states are split into two halves, one half is in the vicinity of the monopole, and another half is distributed around the sphere surface. External fields such as the Zeeman splitting can also remove the degeneracy.

The model Hamiltonian for a magnetic monopole in the modified Dirac equation is given by

\[
H = \left( \begin{array}{cc} mv^2 - B \Pi^2 & v \sigma \cdot \Pi \\ v \sigma \cdot \Pi & -mv^2 + B \Pi^2 \end{array} \right)
\]

where $2mv^2$ is the energy gap between the conduction
band and valence band, $v$ is the effective velocity and $B$ is a parameter of dimension of inverse mass. $\sigma_{x,y,z}$ are the Pauli matrices. The canonical momentum operator $\Pi = -i\hbar \nabla + eA$ and $\nabla \times A = \frac{2\pi}{q} D q r / r^3$. $q$ is half of an integer due to the quantization of magnetic charge and $q = \frac{1}{2}$ for a unit monopole. It is known that the vector potential $A$ cannot be written as a single expression in the whole space, and has to be defined as two functions in two overlapping regions to keep singularities. In the absence of the magnetic monopole, the topological properties of this equation have been understood very well. It is topologically non-trivial for $mB > 0$ and trivial for $mB < 0$. A topological quantum phase transition occurs at $mB = \pm \frac{1}{2}$. In the presence of the magnetic monopole, the orbital angular momentum is modified to $L = r \times \Pi - q \hbar \nabla \times r$, which satisfies the algebra $[L_\alpha, L_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} L_\gamma$. The eigenfunctions of $L^2$ and $L_z$ are denoted by $Y_{l,m}$, with the eigenvalues $l(l+1)\hbar^2$ and $l\hbar$. Since both terms in $L$ are orthogonal to each other, $L^2 = |r \times \Pi|^2 + q^2 \hbar^2$ and $l(l+1) \geq |q|^2$. The total angular momentum is defined as $J = L + \frac{1}{2}\sigma$. The total angular momentum $J^2$ and its $z$-component $J_z$ commute with the Hamiltonian, and are good quantum numbers. Thus we can diagonalize simultaneously $H$, $J^2$ and $J_z$. According to the definition, $J$ is the sum of two angular momenta, $L$ and $\frac{1}{2}\sigma$. Thus the eigenvalues of $J^2$ can be $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$, respectively, and the corresponding eigenstates are the linear combination of $Y_{l,\pm l}$ and the eigenvectors for $\sigma_z$. For a minimal $l = |q|$ and $j = |q| - \frac{1}{2}$, the eigenstates are $\eta_{j,j} = \left( -\frac{\sqrt{|q|-m+1}}{\sqrt{2|q|+1}} Y_{q,|q|,j}, \frac{\sqrt{m+1}}{\sqrt{2|q|+1}} Y_{q,|q|,j} \right)$.

Due to the particle-hole symmetry in the model Hamiltonian, the eigenvalues of $\pm E$ appear in pairs. For a half-filled system, we focus on the case of half-filled system, we are interested in the energy level. The eigenvalues of $\rho$ are arbitrary function of the Pauli matrices. The canonical momentum operator is a parameter of dimension of inverse mass. $\sigma$ other cases of in the whole space, and has to be defined as two functions in two overlapping regions to keep singularities. In the absence of the magnetic monopole, the topological properties of this equation have been understood very well. It is topologically non-trivial for $mB > 0$ and trivial for $mB < 0$. A topological quantum phase transition occurs at $mB = \pm \frac{1}{2}$. In the presence of the magnetic monopole, the orbital angular momentum is modified to $L = r \times \Pi - q \hbar \nabla \times r$, which satisfies the algebra $[L_\alpha, L_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} L_\gamma$. The eigenfunctions of $L^2$ and $L_z$ are denoted by $Y_{l,m}$, with the eigenvalues $l(l+1)\hbar^2$ and $l\hbar$. Since both terms in $L$ are orthogonal to each other, $L^2 = |r \times \Pi|^2 + q^2 \hbar^2$ and $l(l+1) \geq |q|^2$. The total angular momentum is defined as $J = L + \frac{1}{2}\sigma$. The total angular momentum $J^2$ and its $z$-component $J_z$ commute with the Hamiltonian, and are good quantum numbers. Thus we can diagonalize simultaneously $H$, $J^2$ and $J_z$. According to the definition, $J$ is the sum of two angular momenta, $L$ and $\frac{1}{2}\sigma$. Thus the eigenvalues of $J^2$ can be $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$, respectively, and the corresponding eigenstates are the linear combination of $Y_{l,\pm l}$ and the eigenvectors for $\sigma_z$. For a minimal $l = |q|$ and $j = |q| - \frac{1}{2}$, the eigenstates are $\eta_{j,j} = \left( -\frac{\sqrt{|q|-m+1}}{\sqrt{2|q|+1}} Y_{q,|q|,j}, \frac{\sqrt{m+1}}{\sqrt{2|q|+1}} Y_{q,|q|,j} \right)$.

We first consider a large radius limit of the sphere, $\rho = kR \gg 1$. In this case it is reduced to a one-dimensional modified Dirac equation by ignoring the term of $\frac{1}{\rho}$ at the end of $r = R$, which has a solution of zero energy near $r = R$ when $mB > 0\frac{1}{2}$. In general, assume that $mB > 0$ and $\lambda = 0$. One obtains a general solution $\psi_{j,m} = \chi_s \otimes \eta_{j,j} f_s(\rho)$

where $\sigma_y \chi_s = s \chi_s$ where $\chi_s^T = \frac{1}{\sqrt{2}}(1, is)$ and $(s = \pm 1)$. For $\zeta^2 \neq 4$ $f_s(\rho) = C_1 e^{-\zeta \rho/2} \frac{1}{\sqrt{\rho}} J_\alpha(\beta \rho) + C_2 e^{-\zeta \rho/2} \frac{1}{\sqrt{\rho}} K_\alpha(\beta \rho)$.

Thus the wave function denoted by $\psi_{j,m}^+(\rho) = \chi_+ \otimes \eta_m f_+(\rho)$ is mainly located in the vicinity of the magnetic monopole. On the other hand, both $J_\alpha(\beta \rho)$ and $K_\alpha(\beta \rho)$ become divergent for a large $\rho$, but convergent for a small $\rho$. For $s = -1$ one has the other solution which vanishes at $\rho_R = kR$

$$f_-(\rho) = C_1 \frac{\sqrt{\rho R}}{\sqrt{\rho e^{\zeta \rho/2}}} \left( \frac{J_\alpha(\beta \rho)}{J_\alpha(\beta \rho)} - \frac{K_\alpha(\beta \rho)}{K_\alpha(\beta \rho)} \right).$$

This solution denoted by $\psi_{j,m}^-(\rho) = \chi_- \otimes \eta_m f_-(\rho)$ is distributed near the sphere surface at $r = R$ and decays exponentially in $\rho_R - \rho$ or $R - r$. This is a surface state of zero energy, and is one of the characteristics of topological insulators. For $\zeta^2 = 4$ and $\beta = 0$, we also have two solutions of zero energy: one is near the origin, $f_+(\rho) = C_3 e^{-\zeta \rho/2} \rho^{\alpha - 1/2}$

with $s = 1$ and the other is around the surface, $f_-(\rho) = C_4 e^{\zeta \rho/2} \rho^{\alpha - 1/2} - \left( \frac{\rho}{\rho_R} \right)^{\alpha + 1/2}$

with $s = -1$.

Except for the two solutions of zero energy, there also exist other states even for $l = |q|$ and $j = |q| - \frac{1}{2}$. We
to the particle-hole symmetry in Eq. (4), below which all zero energy is $4|q|$-fold degeneracy. For $q = \frac{1}{2}$, only one electron occupies these two well-separated and degenerate states. When $mB < 0$, there is no solutions of zero energy near the center and around the surface. Although it is possible that the magnetic monopole can bind a lot of electron charges with the energy below zero, the electron charges accumulated around it must be an integer multiple of the elementary charge $-e$. This is consistent with the fact that the system is topologically trivial with $\theta = 0$. When $mB > 0$, the system is topologically non-trivial. The appearance of the surface state of $E = 0$ is one of the characteristics. If the topological insulator is really an axion media, $\theta$ should be $\pi$. Thus the sign change of $mB$ should accompany the change of $\theta$ from 0 to $\pi$. Therefore if a topological insulator is really an axion media, a half elementary charge must be bound to the magnetic monopole as the Witten effect requires. However, the double degeneracy of the zero energy solutions could make the charge around the monopole from 0 to $-e$. Therefore our exact solutions are neither in favor of nor against the picture of the Witten effect as we couldn’t exclude the possibility of a half elementary charge.

Now we come to consider a sphere of a finite radius $R$. Denote the state near the origin by $\psi^{+}_{j,m}$ and the surface state by $\psi^{-}_{j,m}$. If the radius is large enough such that the two wavefunctions have no overlap in space, $\psi^{+}_{j,m}$ and $\psi^{-}_{j,m}$ are two exact solutions of zero energy. When the radius $R$ is finite and the two wavefunctions overlap in space, the interference of the two wavefunctions may lift the degeneracy of the two states, which is dubbed the finite size effect. As a degenerate perturbation approach, we still use the two functions as the basis. As $\chi_{S}$ are the eigenstates of $\sigma_{S}$, we have the relations $\chi_{S}^{+}\sigma_{S}\chi_{S}^{+} = \chi_{S}^{-}\sigma_{S}\chi_{S}^{-} = 0$. Therefore the expectation values $\langle \psi^{+}_{j,m} | H | \psi^{+}_{j,m} \rangle \equiv 0$. However, $\chi_{S}^{+}\sigma_{S}\chi_{S} = 2$ and $\chi_{S}^{-}\sigma_{S}\chi_{S} = -2is$, then $\Delta = \langle \psi^{+}_{j,m} | H | \psi^{-}_{j,m} \rangle \neq 0$. As a consequence of the first-order degenerate perturbation, the energy eigenvalues become $\pm|\Delta|$ and the two states become

$$
\psi_{\pm} = \frac{1}{\sqrt{2}} \left( \psi^{+}_{j,m} \pm \frac{\Delta}{|\Delta|} \psi^{-}_{j,m} \right).
$$

The values of the $\pm|\Delta|$ are evaluated numerically and plotted in Fig. 2. There are two different cases. For $\zeta^{2} \leq 4$, the gap increases monotonically with decreasing $R$ while for $\zeta^{2} > 4$ the gap oscillates, but the amplitude increases with decreasing $R$. The states $\psi_{\pm}$ are separated into two halves as $\psi^{+}_{j,m}$ and $\psi^{-}_{j,m}$ are orthogonal and well separated in space. The weights of these two parts are exactly equal to $1/2$. When the state with lower energy is occupied, the electron will be split into two parts: one half is near the origin and the other is around the surface as shown in Fig. 3.
To estimate the size of the wave package in real materials, we adopt the fitted parameters from ARPES data for Bi$_2$Se$_3$: $mv^2 = 0.126$eV, $Bk^2 = 21.8$eVÅ$^2$, and $hv = 2.94$eV. As the wave function decays exponentially combining a power law decay from the origin, $\exp[-r/\xi]$ or from the surface, $\exp[-(R - r)/\xi]$, the characteristic length is $\xi \approx 15\text{Å}$. The finite size effect becomes obvious when $R$ is comparable with several $2\xi \approx 30\text{Å}$, which is consistent with the fact that gap opening in the Bi$_2$Se$_3$ thin film with thickness several quintuple layers$^{22}$. Therefore the characteristic length for a finite size effect is quite small.

Rosenberg and Franz claimed that a half electron charge is really bound to a magnetic monopole in a crystalline topological insulator$^{13}$. By repeating their numerical calculation, it is found that what they did is for the case of half filling minus a single electron, i.e., the two zero energy modes are empty. It shows that a half electron charge accumulating around the monopole originates as the collective behaviors of the bulk states and the hydrogen-like bound states around the magnetic monopole, not from a single particle state splitting in the space. At the half filling, the charge accumulated around the monopole are an integer for a finite size system, which has no clue for the Witten effect. From our exact solutions, the double degeneracy of zero energy solutions make the charge distribution around the monopole uncertain: it can change from zero to one continuously. For a small sphere, the degeneracy can be removed, and the charge accumulation near the monopole is an integer according to numerical calculation. In this sense the exact solutions does not support the Witten effect in topological insulator.

Since a half electron charge is possibly accumulated near the monopole in the case of half filling minus one electron, it is possible to remove the degeneracy of the two zero energy modes by means of external fields. Consider a radial magnetic field $B = B_r \hat{r}$. The Zeeman energy term is

$$
\delta H = \mu_{eff} B_r \left( \sigma_r 0 \atop 0 \sigma_r \right),
$$

which breaks the time reversal symmetry. $\sigma_r = \sigma \cdot r/r$ is the Pauli operator along the radial direction. The energy shifts of the two states of zero energy are $\Delta E_\pm = 2\text{sgn}(q)\mu_{eff} \int_0^{\rho_R} dp B_r |f_\pm(p)|^2$. The degeneracy will be removed as the two integrals are usually not equal. For example, if the field appears only near the surface due to the proximity effect of a ferromagnetic layer, it is obvious that $\Delta E_+ = 0$ and $\Delta E_- \neq 0$. However, as the off-diagonal integral is zero, $\langle \psi_{j,m}^+ | \delta H | \psi_{j,m}^- \rangle = 0$, the two states will never be mixed as those due to the finite size effect. Essentially the two states are still located near the origin and the surface separately even in the presence of the Zeeman field. Thus it becomes possible that the charge fractionalization may be realized by the Zeeman field in the topological insulator or due to the proximity effect of a ferromagnetic layer covering around the surface.

In short we have found two exact solutions of zero energy modes for a magnetic monopole with strength $\phi_0$ in a topological insulator: one is located around the monopole and the other is distributed around the surface. At half filling, only one electron occupies the two degenerate states due to the particle-hole symmetry. Thus, the charge accumulated around the monopole is not determined certainly, which is not in agreement with the prediction by the Witten effect in an axion media. However, the external fields such as the Zeeman field may remove the degeneracy of two zero energy modes. It does not exclude the possibility that the half electron charge accumulates around the monopole in a topological insulator.

We would like to thank Hui-Ming Guo for numerical calculations of charge distribution in a lattice model. We also thank Shou-Cheng Zhang for his critical comment. This work was supported by the Research Grant Council of Hong Kong under Grant No.: HKU 7051/11P.

1. J. E. Moore, Nature (London) 464, 194 (2010).
2. M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
3. X. L. Qi and S. C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
4. X. L. Qi, T. L. Hughes and S. C. Zhang, Phys. Rev. B 78, 195424 (2008).
5. R. D. Peccei and H. R. Quinn, Phys. Rev. Lett. 38, 1440 (1977).
6. F. Wilczek, Phys. Rev. Lett. 58, 1799 (1987).
7. E. Witten, Phys. Lett. B 86, 283 (1979).
8. R. Jackiw and C. Rebbi, Phys. Rev. D, 3398 (1976).
9. A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W. P. Su, Rev. Mod. Phys. 60, 781 (1988).
10. S. Kivelson and J. R. Schrieffer, Phys. Rev. B 25, 6447 (1982).
11. R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).
12. J. K. Jain, Phys. Rev. Lett. 63, 199 (1989).
13. G. Rosenberg and M. Franz, Phys. Rev. B 82, 035105 (2010).
14. H. M. Guo, G. Rosenberg, G. Refael, and M. Franz, Phys. Rev. Lett. 105, 216601 (2010).
15. S. Q. Shen, W. Y. Shan and H. Z. Lu, SPIN 1, 33 (2011).
16. H. Z. Lu, W. Y. Shan, W. Yao, Q. Niu, and S. Q. Shen, Phys. Rev. B 81, 115407 (2010).
17. P. A. M. Dirac, Proc. R. Soc. London A 133, 60 (1931).
18. J. J. Sakurai, Modern Quantum Mechanics, Revised Edition, Addison-Weiley, Inc. (1994).
19. Y. Kazawa, C. N. Yang and A. S. Goldhaber, Phys. Rev. D 15, 2287 (1977).
20. Y. M. Shnir, Magnetic Monopole, Springer-Verlag, (2005).
21. B. Zhou, H. Z. Lu, R. L. Chu, S. Q. Shen, and Q. Niu, Phys. Rev. Lett. 101, 246807 (2008).
22. Y. Zhang, K. He, C. Z. Cui, C. L. Song, L. L. Wang, X. Chen. J. F. Jia, Z. Fang, X. Dai, W. Y. Shan, S. Q. Shen, Q. Niu, X. L. Qi, S. C. Zhang, X. C. Ma, and Q. K. Xue, Nat. Phys. 6, 584 (2010).