A first theoretical realization of honeycomb topological magnon insulator

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Abstract

It has been recently shown that in the Heisenberg (anti)ferromagnet on the honeycomb lattice, the magnons (spin wave quasiparticles) realize a massless two-dimensional (2D) Dirac-like Hamiltonian. It was shown that the Dirac magnon Hamiltonian preserves time-reversal symmetry defined with the sublattice pseudo spins and the Dirac points are robust against magnon–magnon interactions. The Dirac points also occur at nonzero energy. In this paper, we propose a simple realization of nontrivial topology (magnon edge states) in this system. We show that the Dirac points are gapped when the inversion symmetry of the lattice is broken by introducing a next-nearest neighbour Dzyaloshinskii–Moriya (DM) interaction. Thus, the system realizes magnon edge states similar to the Haldane model for quantum anomalous Hall effect in electronic systems. However, in contrast to electronic spin current where dissipation can be very large due to Ohmic heating, noninteracting topological magnons can propagate for a long time without dissipation as magnons are uncharged particles. We observe the same magnon edge states for the XY model on the honeycomb lattice. Remarkably, in this case the model maps to interacting hardcore bosons on the honeycomb lattice. Quantum magnetic systems with nontrivial magnon edge states are called topological magnon insulators. They have been studied theoretically on the kagome lattice and recently observed experimentally on the kagome magnet Cu(1-3, bdc) with three magnon bulk bands. Our results for the honeycomb lattice suggest an experimental procedure to search for honeycomb topological magnon insulators within a class of 2D quantum magnets and ultracold atoms trapped in honeycomb optical lattices. In 3D lattices, Dirac and Weyl points were recently studied theoretically, however, the criteria that give rise to them were not well-understood. We argue that the low-energy Hamiltonian near the Weyl points should break time-reversal symmetry of the pseudo spins. Thus, recovering the same criteria in electronic systems.

Keywords: topological magnon insulators, magnon edge states, magnon spintronics

(Some figures may appear in colour only in the online journal)

1. Introduction

Topological properties of fermion band theory have dominated research in condensed matter physics and other areas over the past decade or so [1–6]. Recently, it has been shown that the magnon bulk bands of Heisenberg (anti)ferromagnet on the honeycomb lattice exhibit Dirac points at the corners of the Brillouin zone (BZ) [7]. The low-energy Hamiltonian near these points realizes a massless 2D Dirac-like Hamiltonian with Dirac nodes at nonzero energy. This system preserves pseudo spin time-reversal (T) symmetry. It was also shown that the Dirac points are robust against magnon–magnon interactions and any perturbation that preserves the pseudo spin T-symmetry of the Bogoliubov Hamiltonian.

In this paper, we provide evidence of non-trivial topology (magnon edge states) in the magnon bulk bands of Heisenberg (anti)ferromagnet and XY model on the honeycomb lattice, when a gap opens at the Dirac points. We show that
the simplest practical way to open a gap at the Dirac points is by breaking the inversion symmetry of the lattice, which subsequently breaks the pseudo spin $T$-symmetry of the Bogoliubov Hamiltonian. We show that this can be achieved by introducing a next-nearest neighbour Dzyaloshinskii–Moriya (DM) interaction. The opening of a gap at the Dirac points leads to magnon edge states reminiscent of Haldane model in electronic systems [8]. In the case of XY model, we observe the same topological effects with magnon edge states propagating in the vicinity of the magnon bulk gap. Remarkably, the resulting Hamiltonian for the XY model maps to interacting hardcore bosons. Therefore, these magnon edge states can be simulated numerically. As magnons are uncharged particles, noninteracting topological magnons can propagate for a long time without dissipation, thus they are considered as a good candidate for magnon spintronics [9–13]. The topological properties of these Dirac magnons are not just analogues of fermion band theory. They are called topological magnon insulators [14, 15] and has been recently observed on the kagome magnet Cu(1-3, bdc) [16]. For the topological magnon insulators [14, 15] and has been recently observed, they can actually be searched for in many magnets. These are called magnon spintronics and the Weyl points lead to magnon edge states reminiscent of Haldane model, which has been realized experimentally in optical fermionic lattice [19].

In 3D quantum magnets, Dirac and Weyl points are possible in the magnon excitations. Recently, Weyl points have been investigated in quantum magnets using 3D Kitaev fermionic model [20]. Weyl points were recently shown to occur in the magnon excitations of breathing pyrochlore lattice antiferromagnet [21]. In this case, the criteria that give rise to them seem to be unknown in fermionic systems. Here, we show that the resulting Bogoliubov Hamiltonian has the form of Weyl Hamiltonian in electronic systems and that the Weyl points should break the pseudo spin $T$-symmetry by expanding the Bogoliubov Hamiltonian near the non-degenerate dispersive band-touching points and projecting onto the bands. Hence, the criterion for Weyl nodes to exist in electronic systems also applies to magnons.

2. Honeycomb Dirac magnon

In 2D quantum spin magnetic materials, non-degenerate band-touching points or Dirac points require at least two energy branches of the magnon excitations. Therefore, ordered quantum magnets that can be treated with one sublattice are devoid of Dirac points. The simplest two-band model that exhibits Dirac nodes is the Heisenberg ferromagnet on the honeycomb lattice [7]. The Hamiltonian is governed by

$$H = -\sum_{\langle lm \rangle} J_{lm} S_l \cdot S_m, \quad (1)$$

where $J_{lm}$ depends on the bonds along the nearest neighbours. As mentioned above, equation (1) describes several realistic compounds [17, 18]. For simplicity we take $J_{lm} = J > 0$. The ground state of equation (1) is a ferromagnet with two-sublattice structure on the honeycomb lattice; see figure 1. This is equivalent to Heisenberg antiferromagnet by flipping the spins on one sublattice. In many cases of physical interest, magnon excitations are studied by linear spin wave theory via the standard linearize Holstein Primakoff (HP) transformation. This is an approximation valid at low-temperature when few magnons are excited.

The momentum space Hamiltonian is given by

$$H = \sum_{k} \Psi_k ^\dagger \cdot \mathcal{H}_0 \cdot \Psi_k, \quad \Psi_k = (a_k, b_k^*), \quad (2)$$

where $\mathcal{H}_0$ is an identity $2 \times 2$ matrix, and $\sigma_\mu = (\sigma_\mu \pm i\sigma_5)/2$ are Pauli matrices acting on the sublattices; $z = 3$ is the coordination number of the lattice and $v_z = JS$. The structure factor $\gamma_k$ is complex given by

$$\gamma_k = \frac{1}{\varepsilon_k} \sum_{\mu} e^{i k \cdot \delta_\mu}, \quad (3)$$

where $\delta_\mu$ are the three nearest neighbour vectors on the honeycomb lattice, $\delta_1 = (\hat{x}, \sqrt{3} \hat{y})/2$, $\delta_2 = (\hat{x}, -\sqrt{3} \hat{y})/2$ and $\delta_3 = (-\hat{x}, 0)$. The eigenvalues of equation (2) are given by

$$\epsilon_k = 3v_z (1 \pm |\gamma_k|), \quad (4)$$

The energy bands have Dirac nodes at the corners of the BZ reminiscent of graphene model. In contrast to graphene, the Dirac nodes occur with a nonzero energy $3v_z \gamma_k$ as shown in figure 2(a). In addition to the Dirac nodes, there is a zero energy mode in the lower band, which corresponds to a Goldstone mode due to the spontaneous symmetry breaking of SU(2) rotational symmetry of the quantum spin Hamiltonian.

**Figure 1.** The honeycomb lattice (left) and the Brillouin zone (right). The reciprocal lattice vectors are $b_1 = 2\pi(1, \sqrt{3})/3a$ and $b_2 = 2\pi(1, -\sqrt{3})/3a$. 

\[ \text{Figure 1. The honeycomb lattice (left) and the Brillouin zone (right). The reciprocal lattice vectors are } b_1 = 2\pi(1, \sqrt{3})/3a \text{ and } b_2 = 2\pi(1, -\sqrt{3})/3a. \]

\[ \text{Figure 1. The honeycomb lattice (left) and the Brillouin zone (right). The reciprocal lattice vectors are } b_1 = 2\pi(1, \sqrt{3})/3a \text{ and } b_2 = 2\pi(1, -\sqrt{3})/3a. \]
As many physical systems are anisotropic, it is important to note that with spatial anisotropy $J_{lm} = J$, several Dirac points can be obtained by tuning the anisotropy in each bond. The density of states per unit cell as a function of energy is shown in figure 2(b) for the two energy bands in equation (4). The interesting properties of this system are manifested near the Dirac points. There are only two inequivalent Dirac points located at $K_{\pm} = \{2\pi/3, \pm 2\pi/3, \sqrt{3}\}$ as shown in figure 1. In the case of Heisenberg antiferromagnet, only a single Dirac point occurs at $k = 0$ [7]. Expanding equation (2) near $K_{\pm}$ we obtain a linearized model

$$\mathcal{H}(q) = 3\nu_0 + \tilde{v}_j(\sigma q_j - \tau \sigma q_j),$$

where $q = k - K_{\pm}$, $\tilde{v}_j = v_j/2$, and $\tau = \pm$ describes states at $K_{\pm}$. Thus, the low-energy excitation spectrum near the Dirac points is similar to the Bloch Hamiltonian of graphene model. Let us now compute the specific heat at a constant volume described in terms of the HP bosons, an ordered state must be assumed. Hence, the system must contain an even number of half integral spins with $T^2 \equiv (-1)^N$, where $N$ is even. Thus, magnons behave like bosons. However, in the pseudo spin space $T$-operator can be defined for the Bogoliubov Hamiltonian, $T = i\sigma K$ where $K$ denotes complex conjugation and $T^2 = -1$. This pseudo spin symmetry is preserved provided Dirac points exist in the BZ.

### 3. Honeycomb topological magnon insulator

#### 3.1. Heisenberg ferromagnetic insulator

Topological magnon insulators are the analogues of topological insulators in electronic systems. They are characterized by the existence of edge state modes when a gap opens at the Dirac points. For the honeycomb ferromagnets, a next-nearest neighbour interaction of the form $H = -J'\sum_{\langle ij \rangle} S_i \cdot S_j$ ($J' > 0$) only shifts the positions of the Dirac points as it contributes a term of the form $v'_j (6 - g_k)\sigma_0$, where $v'_j = J' S$, and $g_k = 2\sum_n \cos k \cdot \rho_n$. The next-nearest neighbour vectors are

(Images and references for figures 2 and 3 are not included in this text.)
\[ \rho_1 = -\frac{(3\hat{x}, \sqrt{3}\hat{y})}{2}, \quad \rho_2 = (3\hat{x}, -\sqrt{3}\hat{y})/2, \quad \rho_3 = (0, \sqrt{3}\hat{y}). \]

The simplest realistic way to open a gap at the Dirac points is by breaking the inversion symmetry of the lattice, which in turn breaks the \( T \)-symmetry of the Bogoliubov Hamiltonian. This can be achieved by introducing a next-nearest neighbour DM interaction \( H_{\text{DM}} = \sum_{\langle\langle lm\rangle\rangle} D_{lm} \cdot \mathbf{S}_l \times \mathbf{S}_m, \) \( (9) \)

where \( D_{lm} \) is the DM interaction between sites \( l \) and \( m \). The total Hamiltonian of a honeycomb ferromagnetic insulator can be written as

\[ H = -J \sum_{\langle\langle lm\rangle\rangle} \mathbf{S}_l \cdot \mathbf{S}_m - J' \sum_{\langle\langle lm\rangle\rangle} \mathbf{S}_l \cdot \mathbf{S}_m + \sum_{\langle\langle lm\rangle\rangle} D_{lm} \cdot \mathbf{S}_l \times \mathbf{S}_m. \] \( (10) \)

In the HP bosonic mapping, we obtain

\[ H = -v_0 \sum_l (b_l^\dagger b_l + \text{h.c.}) - v_1 \sum_l (e^{i\phi_{lm}} b_l^\dagger b_l + \text{h.c.}) + v_0 \sum_l b_l^\dagger b_l, \] \( (11) \)

where \( v_0 = z\nu + z'\nu', \quad v_D = DS, \quad v_1 = \sqrt{v_D^2 + v_0^2}, \) and \( z' = 6 \) is the coordination number of the NNN sites. We have assumed a DM interaction along the \( z \)-axis. The phase factor \( \phi_{lm} = \nu_{lm}\phi \), where \( \phi = \arctan(D/J') \) is a magnetic flux generated by the DM interaction on the NNN sites, similar to the Haldane model with \( \nu_{lm} = \pm 1 \) as in electronic systems. The total flux enclosed in a unit cell vanishes as depicted in figure 3. In contrast to electronic systems, the phase factor \( \phi \) depends on the parameters of the Hamiltonian. The Bogoliubov Hamiltonian is given by

\[ \mathcal{H}_{\text{B}}(\mathbf{k}) = \mathcal{H}_0 + \mathcal{H}_1, \] \( (12) \)

where \( \mathcal{H}_0 = 3\sqrt{3}v_0 (\sigma_0 + \tau\sigma_z) + m\tau\sigma_z, \)

\( \mathcal{H}_1 = 3v_0 \sigma_0 + \nu(t\sigma_x + \tau\sigma_y) + \nu_D \sigma_z, \)

\( \mathcal{H}_2 = 3v_0 \sigma_0 + \nu(t\sigma_x + \tau\sigma_y) + \nu_D \sigma_z, \)

\( \mathcal{H}_3 = 3v_0 \sigma_0 + \nu(t\sigma_x + \tau\sigma_y) + \nu_D \sigma_z, \)

\( \mathcal{H}_4 = 3v_0 \sigma_0 + \nu(t\sigma_x + \tau\sigma_y) + \nu_D \sigma_z, \)

where \( m = 3\sqrt{3}v_0. \) This model can be regarded as the bosonic analogue of Haldane model in electronic systems [8]. In fermionic systems, there is a topological invariant quantity which is quantized when the Fermi energy lies between the gap, such that the lower band is occupied. In the bosonic model, there is no Fermi energy and not all states are occupied. The bosons can condense at the Goldstone mode in the lower band. However, the topological invariant quantity is, in principle, independent of the statistical property of the particles. It merely predicts edge states in the vicinity of the bulk gap. In the magnon excitations the Chern number \( m_1 = \text{sign}(m) \) simply predicts a pair of counter-propagating magnon edge states in the vicinity of the bulk gap as shown in figures 4(a) and (b) for \( \phi = \pi/2 \) and \( \phi = \pi/4 \) respectively. Hence, the Heisenberg (anti)ferromagnet on the honeycomb lattice realizes topological magnon insulator with magnon edge states propagating at the edge of the sample as depicted in figure 5. As mentioned above, the propagation of magnon edge states differs from those in electronic systems. Therefore, they are useful in many technological devices and magnon spintronics. Besides, they can be accessible in many accessible quantum magnetic systems.
3.2. XY ferromagnetic insulator: hardcore bosons

Dirac points occur in a variety of quantum honeycomb ferromagnetic insulators. Let us consider the XY model on the honeycomb lattice

$$H = -2J \sum_{\langle \langle \rangle \rangle} \left( S_i^x S_j^x + S_i^y S_j^y \right).$$  \hspace{1cm} (14)

The ground state of this model is an ordered ferromagnet or Néel state in the xy plane. Choosing $S_i^z$ quantization axis, the momentum space Hamiltonian in linear spin wave theory is generally written as

$$H = E_0 + \sum_{\mu, \nu} \bar{\Psi}_\mu^\dagger(k) \mathcal{H}(k) \cdot \bar{\Psi}_\nu + \text{const.},$$  \hspace{1cm} (15)

where $\mu, \nu$ label the sublattices. Equation (15) can be written as

$$H = E_0 + \sum_{k} \bar{\Psi}_k^\dagger \cdot \mathcal{H}(k) \cdot \bar{\Psi}_k + \text{const.},$$  \hspace{1cm} (16)

where $\Psi_k^\dagger = (\psi^\dagger_k, \bar{\psi}^\dagger_k)$, $\bar{\Psi}_k^\dagger = (b_k^\dagger b_{k\nu}^\dagger \cdots b_{k\nu}^\dagger)$, and $N$ is the number of sublattice. $E_0 = E_z = S \sum_{kl} \mathcal{A}_{kl}(k)$, and

$$\mathcal{H}(k) = \mathcal{A}(k) + \mathcal{B}(k) + \mathcal{C} \otimes \mathcal{B}^*(k),$$  \hspace{1cm} (17)

where $\mathcal{A}(k)$ and $\mathcal{B}(k)$ are $N \times N$ matrices. This Hamiltonian is diagonalized by a matrix $\mathcal{U}(k)$ via the transformation $\Psi_k^\dagger \rightarrow \mathcal{U}(k) \bar{\Psi}_k$, which satisfies the relation

$$\mathcal{U}^\dagger \mathcal{H}(k) \mathcal{U} = \epsilon(k),$$

$$\mathcal{U}^\dagger \eta \mathcal{U} = \eta,$$  \hspace{1cm} (18)

with $\eta = \text{diag}(I_{N \times N}, -I_{N \times N})$. $\mathcal{P}(k)$ contains the Bogoliubov operators $\alpha_k$ and $\beta_k$ and $\epsilon(k)$ is the eigenvalues. This is equivalent to taking the Bogoliubov Hamiltonian $\mathcal{H}_B(k) = \eta \mathcal{H}(k)$, where

$$\mathcal{H}_B(k) = \mathcal{A}(k) + \mathcal{B}(k) + \mathcal{C} \otimes \mathcal{B}^*(k),$$

and $\mathcal{B}_\pm(k) = (\mathcal{B}(k) \pm \mathcal{B}^*(k))/2$.

The eigenvalues of $\mathcal{H}_B(k)$ are given by $\eta_\epsilon(k) = \{\epsilon_\nu(k), -\epsilon_\nu(k)\}$, where

$$\epsilon_\nu(k) = \sqrt{A_\nu^2(k) - B_\nu^2(k)},$$  \hspace{1cm} (20)

$A_\nu$ and $B_\nu$ are the eigenvalues of $\mathcal{A}(k)$ and $\mathcal{B}(k)$ respectively. For the XY model $\mathcal{H}_B(k)$ is given by

$$\mathcal{H}_B(k) = 3\nu[\sigma_\nu \mathcal{A}(k) + i\sigma_\nu \mathcal{B}(k)],$$  \hspace{1cm} (21)

with $\mathcal{A}(k) = \tau_0 - \mathcal{B}(k)$ and $\mathcal{B}(k) = (\tau_2 \gamma_k + \text{h.c})/2$. The positive eigenvalues (equation (20)) are given by

$$\epsilon_\nu(k) = 3\nu \sqrt{1 + |\gamma_k|^2}.$$  \hspace{1cm} (22)

The magnon excitations exhibit Dirac nodes at $K \pm \pm$ with an energy of $3\nu$. To generate a gap, we follow the same approach above. For simplicity, we ignore an external magnetic field and a NNN isotropic interaction $J'$. Hence, the DM interaction that would open a gap has to be parallel to the $x$-quantization axis,

$$H_{DM} = D \sum_{\langle \langle \rangle \rangle} \nu_{lm}(S_i^x S_j^x - S_i^y S_j^y),$$  \hspace{1cm} (23)

In the HP bosonic mapping, this corresponds to a magnetic flux of $\phi = \pi/2$. In the $S_z$ quantization axis, $S_x$ and $S_y$ are off-diagonals. The momentum space Hamiltonian is given by

$$\mathcal{H}_{DM}^B(k) = -\nu_D \sigma_0 \tau_0 \rho_k.$$  \hspace{1cm} (24)

The positive eigenvalues of the full Hamiltonian are given by

$$\epsilon_{\pm}(k) = \left[ \sqrt{\nu_D^2 \rho_k^2 + \left( \frac{3\nu |\gamma_k|}{2} \right)^2} - \left( \frac{3\nu |\gamma_k|}{2} \right)^2 \right]^{1/2}.$$  \hspace{1cm} (25)

At $K \pm$, a gap of magnitude $|\Delta| = 2|m|$ is generated as shown in figure 6(a). Similar to the Heisenberg model, there exist magnon edge states in the vicinity of the bulk gap as depicted in figure 6(b).

Surprisingly, equations (14) and (23) actually map to interacting hardcore bosons on the honeycomb lattice via the Matsubara–Matsuda transformation [22] $S_i^x \rightarrow (b_i^\dagger + b_i)/2$;
Hamiltonian can be cast into the form of equation (19). From this equation, we see that the momentum space Hamiltonian resembles that of electronic systems.

In addition to Weyl nodes obtained along the BZ paths for \( K > 0 \) and \( J \neq J' \) [21], there is additional non-degenerate band-touching points at the corners of the BZ. The system should realize Dirac Hamiltonian at the corners of the BZ as shown above and also a Weyl Hamiltonian near the Weyl points. To check whether pseudo spin \( T \)-symmetry is preserved or broken at the Dirac or Weyl points respectively, one should follow the approach outlined above. Basically, one has to expand \( \mathcal{A}(k) \) and \( \mathcal{B}_{A}(k) \) near the band-touching points and project the resulting Hamiltonian onto the bands. In principle, the Bogoliubov Hamiltonian (equation (19)) near the Weyl points should break \( T \)-symmetry. Therefore, one recovers the usual criteria for Weyl semimetals [5]. In contrast to 2D systems, a gap is not needed to observe edge states in 3D Weyl magnons. Edge states exist in 3D Weyl magnons provided the momentum lies between the Weyl nodes [21].

4. Conclusion

In summary, we have shown that physical realistic models of honeycomb quantum spin magnets exhibit nontrivial topology in the magnon excitations. In 2D ordered honeycomb quantum magnets, we showed that the non-degenerate band-touching points (at the corners of the Brillouin zone) in the magnon excitation spectrum realize a massless Dirac Hamiltonian. Opening of a gap at the Dirac points requires the breaking of inversion symmetry of the lattice. This leads to nontrivial topological magnon insulator with magnon edge states propagating on the edges of the material, similar to topological insulators in electronic systems. These magnon edge states also manifest in hardcore bosons on honeycomb lattice. The hardcore boson model proposed in equations (26) and (27) should be studied by numerical approach to further substantiate the existence of magnon edge modes in this system. Since there are many physical 2D honeycomb quantum magnetic materials in nature, these results suggest new experiments in ordered quantum magnets and ultracold atoms in honeycomb optical lattices, to search for magnon Dirac materials and topological magnon insulators on the honeycomb lattice. For 3D ordered quantum magnets, Weyl points are possible in the magnon excitations [21]. We argued that the Bogoliubov Hamiltonian near the Weyl points should yield a low-energy Hamiltonian that breaks time-reversal symmetry of the pseudo spins. At nonzero temperature and external magnetic field, there is a possibility of topological magnon Hall effect [25, 26] and spin Nernst effect [25], similar to the kagome, Lieb, and pyrochlore lattices [25, 26]. The analysis of magnon Hall effect for the honeycomb lattice will be reported elsewhere.

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