Topological phases of antiferromagnetic insulator

Ying-Lin Li[1]   Chung-Yu Mou[1,2]

[1]Center for Quantum Science and Technology and Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 300, R.O.C.

[2]Institute of Physics, Academia Sinica, Nankang, Taiwan, R.O.C.

1 Introduction

In this paper, the topological phases of a three dimensional tilted antiferromagnetic insulator featured Dresselhaus and Rashba spin-orbit couplings are explored. In contrast to previous studies that rely on assumed Néel order to classify topological properties, we acknowledge the potential impact of spin-orbit interactions on the Néel orde. Employing self-consistent magnetic order calculations, we observe distinctive spin arrangements under Dresselhaus and Rashba couplings. After the spin orders are confirmed under different interactions, the topological phases of the three dimension systems are classified by Z_4 index with inversion symmetry or nonsymmorphic symmetry protection.

2 Theoretical Model

Starting from a 3D topological insulator in cubic lattice with the Dresselhaus coupling or the Rashba coupling, there are two Hamiltonians[1, 3].

$$h_D(k) = \nu_F \tau^x \otimes (\sin k_x \sigma^x + \sin k_y \sigma^y + \sin k_z \sigma_z) \\ +[m + t(\cos k_x + \cos k_y + \cos k_z)]\tau^z. \quad (1)$$

$$h_R(k) = \nu_F(\tau^x \sigma^y \sin k_x - \tau^x \sigma^x \sin k_y + \tau^y \sin k_z) \\ +m + t(\cos k_x + \cos k_y + \cos k_z)]\tau^z. \quad (2)$$

In the Eq.1,2, τ_i and σ_i, two sets of Pauli matrices, denote the orbit and the spin degrees of freedom.v_F is the Fermi velocity. Both of the system are non-trivial in the region $\frac{1}{3} < \frac{t}{m} < 1$. In order to discuss the order of spin, the Hubbard model and Hund's rule should be consider.

$$\begin{aligned} H_U &= \sum_i U_a n_{i,a\uparrow} n_{i,a\downarrow} + U_b n_{i,b\uparrow} n_{i,b\downarrow} \\ H_H &= \sum_{i;m\neq m'} U' n_{im\sigma} n_{im',\bar{\sigma}} + \sum_{i;m<m'} (U' - J) n_{im\sigma} n_{im'\sigma} \\ &+ \sum_{i,m\neq m'} J C^\dagger_{im\uparrow} C^\dagger_{im'\downarrow} C_{im\downarrow} C_{im'\uparrow} + \sum_{i;m\neq m'} J' C^\dagger_{im\uparrow} C^\dagger_{im\downarrow} C_{im'\downarrow} C_{im'\uparrow}. \end{aligned}$$

To be general, there are different Hubbard U parameter in two orbits, labeled by U_a and U_b. The subscript m in Hund's model is label orbit. Thus, the total Hamiltonian are $H_D = h_D + H_U + H_H$ and $H_R = h_R + H_U + H_H$

For the purpose of figuring out the spin arrangement of topological insulator with spin-orbital coupling, the system is considered half filling and in strong Hubbard coupling, the ground state is that charges are single occupying in each orbit. By doing the canonical transformation, the Hamiltonian is reorganized to a spin model so that the mean field theory is used to find the spin order of ground state.

2.1 Canonical transformation

After doing the canonical transformation, the Hamiltonian is given by

$$\begin{aligned} H =& v_F^2\left(\frac{1}{U_a} + \frac{1}{U_b}\right)[(S^x_{i,a}S^x_{j,b} + S^x_{i,b}S^x_{j,a}) + (S^y_{i,a}S^y_{j,b} + S^y_{i,b}S^y_{j,a}) + (S^z_{i,a}S^z_{j,b} + S^z_{i,b}S^z_{j,a}) \\ &+ \frac{3}{4}(n_{i,a}n_{j,b} + n_{i,b}n_{j,a})] + \frac{24t^2}{U_a}(S^x_{i,a}S^x_{j,a} + S^y_{i,a}S^y_{j,a} + S^z_{i,a}S^z_{j,a} - \frac{1}{4}n_{i,a}n_{j,a}) \\ &+ \frac{24t^2}{U_b}(S^x_{i,b}S^x_{j,b} + S^y_{i,b}S^y_{j,b} + S^z_{i,b}S^z_{j,b} - \frac{1}{4}n_{i,b}n_{j,b}) \\ &- 2J(S_{i,a} \cdot S_{i,b} + S_{j,a} \cdot S_{j,b}) + (2U' - J)\left(\frac{n_{i,a}n_{i,b}}{2} + \frac{n_{j,a}n_{j,b}}{2}\right), \end{aligned}$$

where this is Dresselhaus interaction considered and due to the expectation of antiferromagnetic field, i,j label the sublattice in the unit cell and a,b label the two orbits on site.

2.2 Result of self-consistent calculation

By the mean field theory, $\langle S^{x,y,z}_{i,a}\rangle, \langle S^{x,y,z}_{i,b}\rangle \langle S^{x,y,z}_{j,a}\rangle$ and $\langle S^{x,y,z}_{j,b}\rangle$ are computed for Dresselhaus coupling and Rashba coupling, respectively. Firtly, the transition for both situations are checked, $T_c/t \approx 3$, see Fig.1(a)(b) .

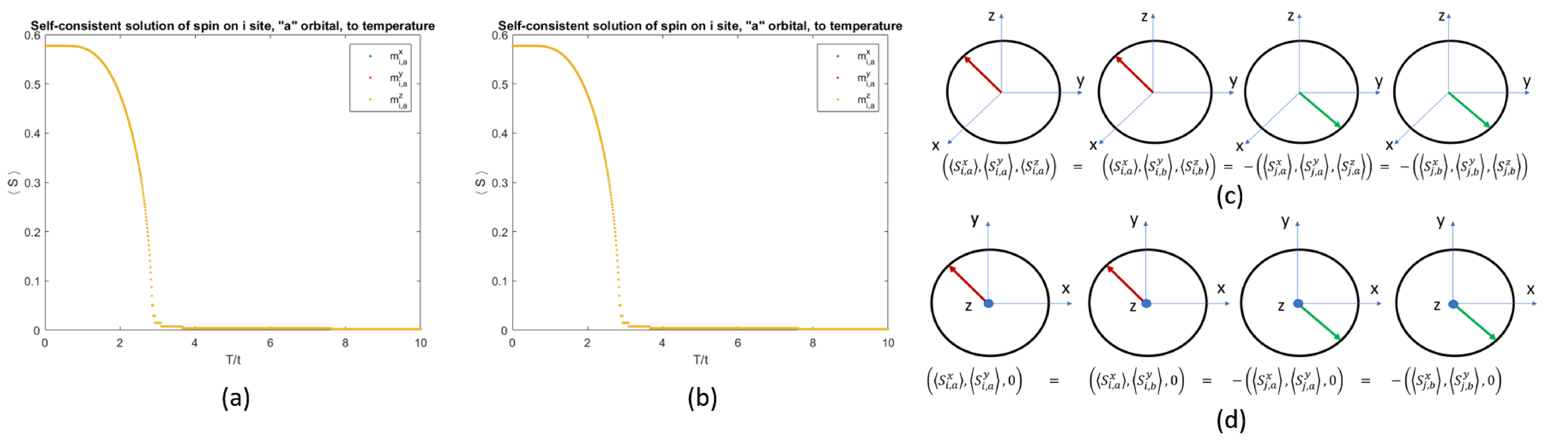

Figure 1: The Magnetic Order Parameter of orbit a on site i with Respect to Temperature for (a)Dresselhaus coupling and (b)Rashba coupling. The order parameters, $m^{x,y,z}_{i,a}$ overlap due to the initial value for both figures. As temperature increases, the spin orders decrease to zero. $T_c/t \approx 3$ for both situations. (c)The spin order under the Dresselhaus interaction. There are free energy degeneracy in 3D real space, due to the rotational symmetry. The spins, on the same site but different orbits, direct in the same direction. The spins between nearest neighbor sites are parallel in opposite direction.(d)The spin order under the Rashba interaction.The data are checked by random 1000 sets of initial value undert=1, T=0.05, U_a=U_b=10, v_F=0.5 and J=0.5

For Dresselhaus case,the spin arrangement is antiferromagnetic between different sites, nearest neighbor, i,j and ferromagnetic for the same site but at different orbits, a,b, see Fig.1(c) For Rashba case, the order of spins is antiferromagnetic in x-y plane between nearest neighbor site, i,j and ferromagnetic in x-y plane for the same site but at different orbits, a,b, see Fig.1(d)

Furthermore, at small t<0.019, between nearest neighbor site, the spin arrange antiferromagnetic pointing any direction in x-y plane and ferromagnetic in z direction so the spins are tilted under rashba spin-orbital coupling, see Fig.3.

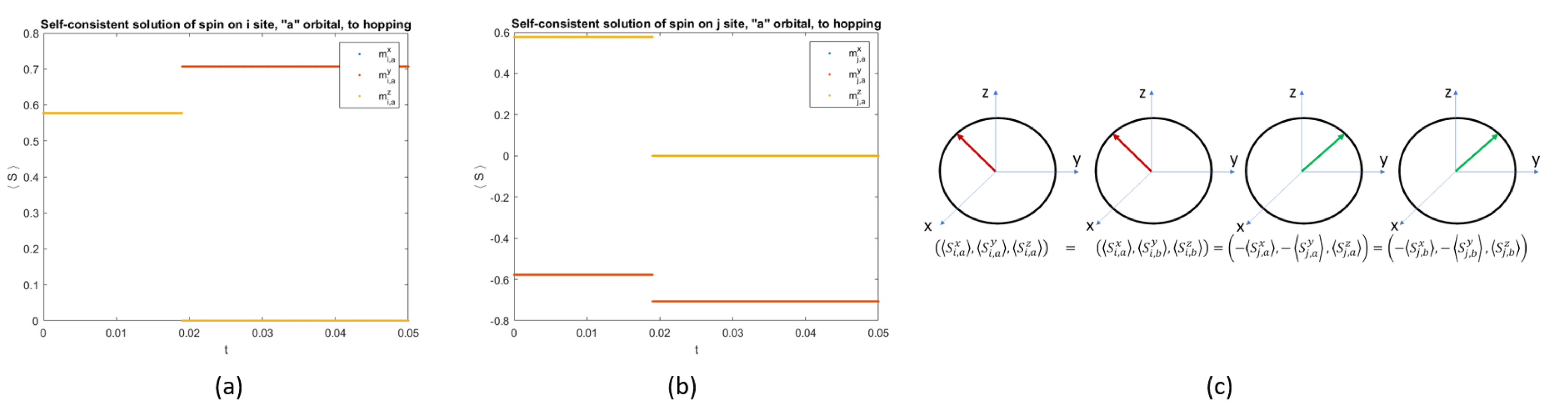

Figure 2: (a)the spin order of i site on orbit a and (b)the spin order of j site on orbit a with respect to t. When t<0.019, $\langle S^x_{i,a}\rangle = \langle S^y_{i,a}\rangle = \langle S^z_{i,a}\rangle = 0.577$ but the $-\langle S^x_{j,a}\rangle = -\langle S^y_{j,a}\rangle = \langle S^z_{j,a}\rangle = 0.577$, (c)antiferromagnetic in x-y plane and ferromagnetic in z direction. For larger t, $\langle S^z_{i,a}\rangle = \langle S^z_{j,a}\rangle = 0$ and antiferromagnetic in x-y plane, $\langle S^x_{i,a}\rangle = \langle S^y_{j,a}\rangle = -\langle S^x_{i,a}\rangle = -\langle S^y_{j,a}\rangle$.

3 Z_4 Index and the Nonsymmorphic Topological Insulator

For the antiferromagnetic spin configuration, the system is protected by inversion symmetry and the spin tilted case, the system is protected by nonsymmorphic symmetry, glide reflection symmetry, and both of them can be classify by Z_4 index[4, 2].

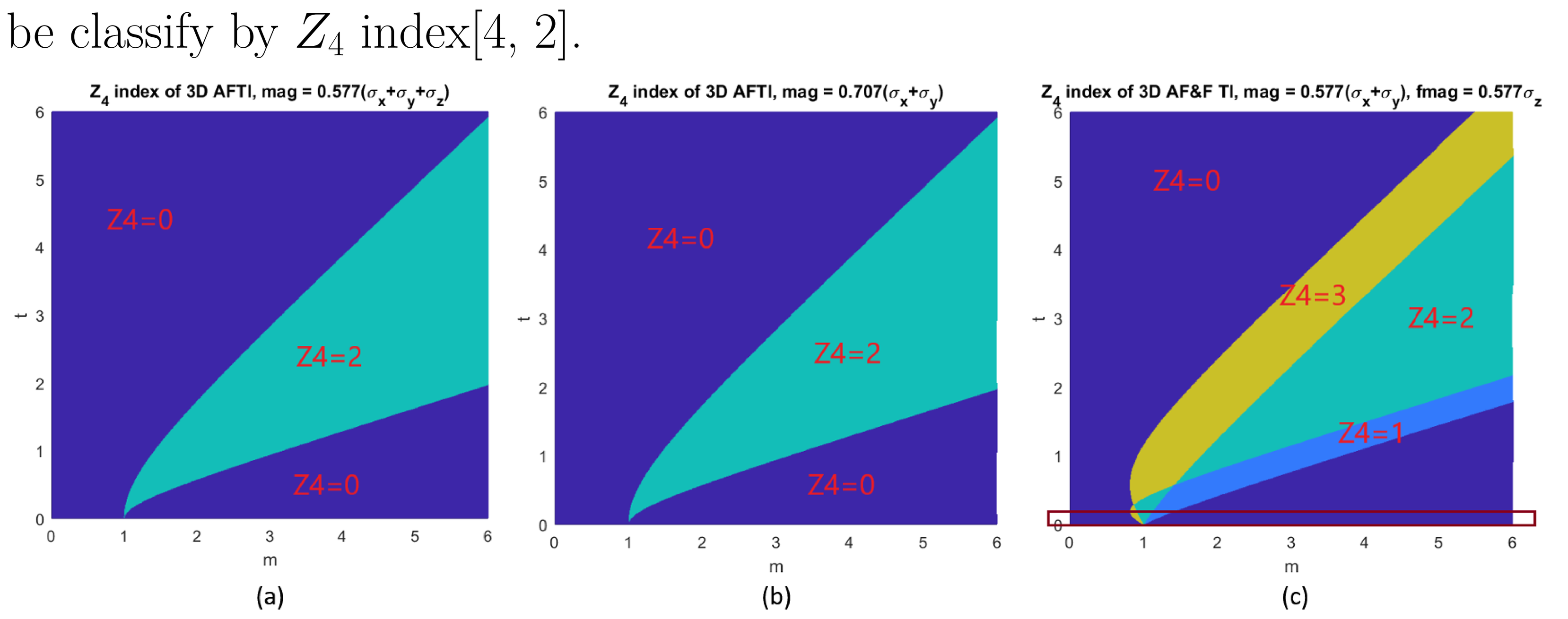

Figure 3: Z_4 index phase diagram (a)for the Dresselhaus case, the spin configuration exhibits antiferromagnetic order, proceted by inversion symmetry, (b)for the Rashba case, the spins antiferromagnetically aligning in the xy-plane, protected by inversion symmetry, (c)for a small interaction controlled by hopping parameter with Rashab coupling, the spin tilting, protected by nonsymmorphic symmetry.

4 Conclusions

In the previous research, the antiferromagnetic topological insulator in three dimension are specified by Z_2 index. However, under our general spins an-ferromagnetically alignment, the Z_4 will be well define. Furthermore, When $Z_4 = 2$, topological non-trivial phase, the system is a higher-order topological insulator with gapless hinge states. As a result, with the Dresselhaus coupling or Rashba coupling, the system is a an-ferromagnetic topological crystalline insulator.

References

[1] Pavan Hosur, Shinsei Ryu, and Ashvin Vishwanath. Chiral topological insulators, superconductors, and other competing orders in three dimensions. *Phys. Rev. B*, 81:045120, Jan 2010.

[2] Heejae Kim, Ken Shiozaki, and Shuichi Murakami. Glide-symmetric magnetic topological crystalline insulators with inversion symmetry. *Phys. Rev. B*, 100:165202, Oct 2019.

[3] Roger S. K. Mong, Andrew M. Essin, and Joel E. Moore. Antiferromagnetic topological insulators. *Phys. Rev. B*, 81:245209, Jun 2010.

[4] Ari M. Turner, Yi Zhang, Roger S. K. Mong, and Ashvin Vishwanath. Quantized response and topology of magnetic insulators with inversion symmetry. *Phys. Rev. B*, 85:165120, Apr 2012.