Spin Susceptibility and Helical Magnetic Orders at the Edges/Surfaces of Topological Insulators Due to Fermi Surface Nesting

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We study spin susceptibility and magnetic order at the edges/surfaces of two-dimensional and three-dimensional topological insulators when the Fermi surface is nested. We find that due to spin-momentum locking as well as time-reversal symmetry, spin susceptibility at the nesting wavevector has a strong helical feature. It follows then, a helical spin density wave (SDW) state emerges at low temperature due to Fermi surface nesting. The helical feature of spin susceptibility also has profound impact on the magnetic order in magnetically doped surface of three dimensional topological insulators. In such system, from the mean field Zener theory, we predict a helical magnetic order.

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I. INTRODUCTION

In the past few years, a new family of materials called topological insulators (TIs) have been theoretically predicted$^{1,2}$ and then experimentally observed$^{2,3}$\footnote{Specifically, in this paper, we are interested in a class of 3D TIs where the surface state consists of a single Dirac cone. Examples are Bi$_2$Te$_3$, Bi$_2$Se$_3$, Sb$_2$Te$_3$, TlBiSe$_2$.$^{10,12,15}$} A TI has a energy gap in the bulk and gapless excitation in the edge/surface, which is due to the nontrivial band topology and protected by time reversal symmetry. TIs possess a nontrivial topological order, which distinguishes them from simple band insulators. In a two dimensional (2D) TI, which is also known as a quantum spin Hall insulator, the edge states form a helical Luttinger liquid.$^{11,12}$ The surface states of three dimensional (3D) TIs form a “helical metal” with Dirac cone like spectrum.$^{4,5,8,9,12,14}$ Examples are Bi$_2$Te$_3$, Bi$_2$Se$_3$, Sb$_2$Te$_3$, TlBiSe$_2$,$^{12,15,16}$ and many other materials.$^{19,20}$ Due to large bandgap and high purity, these materials have great potential for application and scientific research.$^{21,22}$ An important feature is that spin and momentum are closely correlated in the edge/surface states of TIs, which leads to many unusual effects$^{23,24}$ and potential applications in spintronics and quantum computation.$^{25}$

Recently, it was found in Bi$_2$Te$_3$ that the Fermi energy increases from the Dirac point, the shape of Fermi surface gradually changes from a circle, first to a hexagonal shape, and then to a snowflake-like$^{16,26}$ This phenomenon was also found in other 3D TIs with similar structures.$^{15,16,18,20}$ This kind of band structure is theoretically reproduced by Fu from the $k \cdot p$ theory.$^{26}$ For a certain range of energies, the Fermi surface is almost a hexagon, which leads to strong nesting at three wavevectors and possible instability to the formation of SDW states.$^{27}$

In this paper, we study spin susceptibility and magnetic order at the edges/surfaces of TIs when the Fermi surface is nested. We find that due to the one-to-one correspondence between spin state and momentum (“spin-momentum locking”) as well as time reversal symmetry, the spin susceptibility function at nesting wavevector has a strong helical feature. It follows then, a helical SDW state emerges at low temperature due to Fermi surface nesting. We present a mean field theory of the helical SDW state. The helical feature of the spin susceptibility function also has profound impact on the magnetic order in the magnetically doped surfaces of 3D TIs. In such system, from the mean field Zener theory, we predict a helical magnetic order.

II. HAMILTONIAN, SPECTRUM AND EIGENSTATES

We consider the situation where Fermi surface exhibits strong nesting feature. Examples are, the edge states in a 2D TI, and the surface state in the 3D TI Bi$_2$Te$_3$ with Fermi energy in the range of $[0.13, 0.23]$ eV where the Fermi surface is almost a hexagon.$^{10,27}$ The hexagonal shape of Fermi surface also exists in the surface states of many other 3D TIs, such as Bi$_2$Se$_3$, Sb$_2$Te$_3$, TlBiSe$_2$, TlBiTe$_2$ and a recently discovered large class of 3D TIs in Ref. 20. In the following we would call these materials the “Bi$_2$Se$_3$ class”.$^{21}$

The Hamiltonian of the edge states in a 2D TI can be written as$^{11}$

$$H_0 = \sum_{k_{\alpha\beta}} v_0 k |c_{k\alpha}^\dagger \sigma_{z\alpha\beta}^z c_{k\beta}|,$$  \hspace{1cm} (1)

where $v_0$ is the Fermi velocity. The spin orientations of the eigenstates, through proper choosing of the spin coordinates, have been taken as up and down. The eigenenergies and eigenstates are

$$\varepsilon_{\pm}(k) = \pm v_0 |k|, \quad u_{\pm}(k) = \begin{pmatrix} \Theta(\pm k) \\ \Theta(\mp k) \end{pmatrix},$$  \hspace{1cm} (2)

where $\Theta$ is the Heaviside function. The nesting vector is $Q = 2k_F$. 

\hspace{1cm}
where

\( \phi_{\alpha} = k_{x} \sigma_{y} - k_{y} \sigma_{x} \) \quad (3)

and

\( k_{z} = k_{x} \pm i k_{y} \). The eigenenergy and spin states are

\[ \epsilon_{\pm}(k) = \pm \sqrt{v^{2}k^{2} + \gamma^{2}k^{6} \cos^{2}3\theta_{k}} \quad (4) \]

\[ u_{\pm}(k) = \frac{1}{A(k)} \left( \frac{vk(\sin \theta_{k} + i \cos \theta_{k})}{\epsilon_{\pm}(k) - \gamma^{2}k^{3} \cos 3\theta_{k}} \right) \quad (5) \]

with \( k = k(\cos \theta_{k}, \sin \theta_{k}) \), \( A(k) = v^{2}k^{2} + (\epsilon_{+}(k) - \gamma^{2}k^{3} \cos 3\theta_{k})^{2} \). The Hamiltonian is time-reversal invariant. The last term reduces the symmetry from \( C_{6v} \) to \( C_{3v} \). The Hamiltonian describes the surface state of the Bi\(_{2}\)Se\(_{3}\) class of 3D TIs. It is instructive to rescale the Hamiltonian with

\[ H_{0} = E_{s} H'_{0}, \quad k = k_{s}k' \quad (6) \]

where

\[ E_{s} = v \sqrt{v/\gamma} \quad k_{s} = \sqrt{v/\gamma} \quad (7) \]

Then the Hamiltonian becomes

\[ H'_{0} = (k'_{x} \sigma_{y} - k'_{y} \sigma_{x} + \frac{1}{2}(k'_{x}^{3} + k'_{y}^{3}) \sigma_{z} \quad (8) \]

Throughout this paper, we focus on the situation where the Fermi energy \( E_{F} \) is high and the temperature is low, so that states far below the Fermi surface (such as those below the Dirac point) is irrelevant. This regime is easy to achieve in the Bi\(_{2}\)Se\(_{3}\) class of 3D TIs, thanks to the large bandgap and Dirac velocity.

The Hamiltonian for the surface states in 3D TI with a single Dirac cone, is given in Refs. 27 and 28. Keeping only the dominant terms, the Hamiltonian is (with \( x \) and \( y \) axes along the \( \Gamma - K \) and \( \Gamma - M \) directions respectively) \( 27,28 \)

\[ H_{0} = v(k_{x} \sigma_{y} - k_{y} \sigma_{x}) + \frac{\gamma}{2}(k_{x}^{3} + k_{y}^{3}) \sigma_{z}, \quad (3) \]

Obviously, the physical properties are universal in these materials, with exact quantitative scaling by properly recovering the dimension via \( E_{s} \) and \( k_{s} \) within the above model. The parameters, \( v, \gamma, E_{s} \) and \( k_{s} \) of several 3D TIs inferred from experiments are listed in Table I.

| Material       | \( v \) (eV\( \text{Å}^{-1} \)) | \( \gamma \) (eV\( \text{Å}^{-1} \)) | \( E_{s} \) (eV) | \( k_{s} \) (\text{Å}^{-1}) |
|---------------|-----------------|-----------------|-------------|--------------------|
| Bi\(_{2}\)Te\(_{3}\)\(^{a}\) | 2.55            | 250             | 0.26        | 0.1                |
| Bi\(_{2}\)Se\(_{3}\)\(^{b}\) | 3.55            | 128             | 0.59        | 0.17               |
| TlBiSe\(_{2}\)\(^{c}\) | 3.1             | 182             | 0.4         | 0.13               |
| GeBi\(_{2}\)Te\(_{4}\)\(^{d}\) | 2.37            | 99              | 0.37        | 0.15               |
| Bi\(_{2}\)Te\(_{2}\)Se\(_{2}\)\(^{d}\) | 7.25            | 580             | 0.81        | 0.11               |

If the Fermi energy is in the range of \( 0.5E_{s} \leq E_{F} \leq 0.9E_{s} \), the Fermi surface is almost a hexagon, which exhibits strong nesting feature. There are three nesting wave-vectors

\[ Q_{1} = 2k_{0}(1,0), \quad Q_{2} = 2k_{0}(\frac{1}{2}, -\frac{\sqrt{3}}{2}), \quad Q_{3} = 2k_{0}(\frac{1}{2}, \frac{\sqrt{3}}{2}), \quad (9) \]

where \( k_{0} \) is determined by \( \sqrt{v^{2}k_{0}^{2} + \gamma^{2}k_{0}^{6}} = E_{F} \).

At higher Fermi energy, the Fermi surface is distorted to snowflake-like and new nesting wave-vectors emerge. However, at such high Fermi energy usually the bulk conduction band is also occupied, which complicates the situation and is not interested in this paper.

The electron-electron interaction consists of the long-range Coulomb interaction and the short-range Hubbard interaction. The former does not affect the spin susceptibility [to the random phase approximation (RPA) \( 22 \)] and is hence ignored. The onsite Hubbard interaction is written as

\[ H_{U} = -\frac{U}{3} \sum_{\mathbf{q}} \sigma(\mathbf{q}) \cdot \sigma(-\mathbf{q}), \quad (10) \]

where \( \sigma(\mathbf{q}) = \sum_{\mathbf{k},\mathbf{\delta}} c_{\mathbf{k}+\mathbf{q},\alpha}^{\dagger} c_{\mathbf{k},\beta} \sigma_{\alpha\beta} \) with \( \sigma \) being Pauli matrices vector and \( \alpha, \beta \) being spin indices. For positive Hubbard \( U \) (repulsive interaction), Fermi surface nesting leads to the SDW instability and transition into the SDW state at sufficient low temperature. Whereas, for negative \( U \) (attractive interaction), it leads to the charge density wave (CDW) instability and the emergence of CDW state. Here we assume, as in most cases, \( U > 0 \).
III. SPIN SUSCEPTIBILITY AND SDW INSTABILITY

A. Edge states of 2D TIs

The linear spin susceptibility function is

\[ \chi_{\mu\nu}(q,\omega) = i \int_0^\infty dt \langle [\sigma_\mu(q,t), \sigma_\nu(-q,0)] \rangle e^{i(\omega + q\tau)^+} \],

(11)

where \( \mu, \nu = (x, y, z) \) or \( (\pm, z) \) with \( \sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y) \). In the edge of a 2D TI, at the nesting vector \( Q = 2k_F \), the only nonzero terms are \( \chi_+(-Q,\omega) \) and \( \chi_+(Q,\omega) \) as the nesting wavevector connects spin-down and spin-up states. This helical feature of the spin susceptibility function is due to spin-momentum locking as well as time reversal symmetry. The two susceptibility functions are actually related by \( [\chi_+(-Q,\omega)]^* = \chi_+(Q,\omega) \). In the absence of interaction, the spin susceptibility is

\[ \chi_+(Q,\omega) = \sum_k \frac{n_F(\xi_k + Q)}{\omega - \xi_k + Q + i0^+} - n_F(\xi_k) \],

(12)

where \( \xi_k = -E_F \) and \( n_F \) is the Fermi distribution. Including the Hubbard interaction within RPA, one gets

\[ \chi_+(Q,\omega) = \frac{\chi_+(Q,\omega)}{1 - U\chi_+(Q,\omega)} \].

(13)

Due to Fermi surface nesting, the spin susceptibility \( \chi_+(Q,\omega) \) diverges at low temperature. Actually, directly from Eq. (12), one can show that \( \chi_+(Q,0) \approx \frac{1}{\pi} \log(E_F/k_B T) \). That is, the spin susceptibility function is logarithmically divergent with decreasing temperature. This signals the SDW instability. The feature that only \( \chi_+(Q,0) \) diverges indicates a helical SDW order.

The above treatment based on the Fermi-liquid theory is of course invalid for one-dimensional electron system, but it sheds some light on the problem. In the following, we analyze the problem via the bosonization theory.

Following Wu et al., the bosonized Hamiltonian in the presence of Umklapp scattering can be expressed as

\[ H = \frac{1}{2\pi} \int dx \left[ uK(\nabla \theta(x))^2 + \frac{u}{K}(\nabla \phi(x))^2 \right] + \frac{g_\mu}{2(2\pi a)^2} \cos(4\phi(x)), \]

(14)

where the bosonized fermion fields are

\[ \psi_{R,\mu}^\dagger(x) = e^{i\kappa x}e^{-i\phi(x)} \]

(15)

with \( \phi = (\phi_R + \phi_L)/2 \), \( \theta = (\phi_R - \phi_L)/2 \), \( K \) the Luttinger parameter. \( u \) is the renormalized Fermi velocity. \( g_\mu \) is the Umklapp scattering strength. \( a \) is a short-distance cutoff. Due to symmetry reasons, the only possible instabilities are SDW and singlet superconductivity (SC). This is because CDW and triplet SC instabilities pair particles with the same spin, i.e., terms like \( \psi_{R,\mu}^\dagger \psi_{L,\mu} \) for CDW and \( \psi_{R,\mu}^\dagger \psi_{L,\mu} \) for triplet SC, are impossible. The bosonized form of spin operators are

\[ \sigma_+(x) = \psi_{R,\mu}^\dagger(x)\psi_{L,\mu}(x) = \frac{e^{-i2k_F x}}{2\pi a} e^{i\phi(x)}, \]

\[ \sigma_-(x) = \psi_{L,\mu}^\dagger(x)\psi_{R,\mu}(x) = \frac{e^{i2k_F x}}{2\pi a} e^{-i\phi(x)}. \]

(16)

From standard bosonization theory, the Umklapp term becomes relevant when \( K < 1/2 \). Then RG flow will go to a strong coupling fixed point, \( g_\mu \to \infty \), and the \( \phi \) field will become ordered. Depending on the sign of \( g_\mu \), the ordered value of \( \phi \) is

\[ \langle \phi \rangle = \frac{\pi}{4} + \frac{2n\pi}{4}, \quad g_\mu > 0, \]

(17)

\[ \langle \phi \rangle = 0 + \frac{2n\pi}{4}, \quad g_\mu < 0. \]

This signifies a true phase transition. Then the spin operators, which have zero expectation values in the nonordered phase, also acquire nonzero average value across the transition,

\[ \langle \sigma_x \rangle = \langle \sigma_+ + \sigma_- \rangle = \frac{2}{(2\pi a)^2} \cos(2k_F x - \langle \phi \rangle), \]

\[ \langle \sigma_y \rangle = \frac{1}{2(2\pi a)^2} \sin(2k_F x - \langle \phi \rangle) \]

(18)

which shows helical structure and is consistent with the mean field result. We note that very recently a similar calculation has been carried out by Kharitonov considering helical Luttinger liquid in the proximity to a ferromagnet, which also agrees with our result.

B. Surface states of 3D TIs

a. General considerations On the surface of a 3D TI, the nesting vector will connect states which are not Kramers pairs and hence their spin states are not antiparallel. As a consequence, the spin susceptibility is finite in all directions. The free spin susceptibility function in this case is

\[ \chi_{\mu\nu}(Q,0) = \sum_k \frac{n_F(\xi_k + Q)}{\xi_k - \xi_k + Q + i0^+ - g_\mu(k, Q)g_\nu(k, Q)} \]

(19)

where

\[ g_\mu(k, Q) = \langle u_+(k)|\sigma_\mu|u_+(k + Q) \rangle \]

(20)

with \( \mu, \nu = (x, y, z) \). One can note that, \( g_\mu(k, Q)g_\nu(k, Q) \) is a bilinear tensor, where \( g_\mu(k, Q) \) is its eigenvector with eigen-value

\[ \kappa_\mu(k, Q) = \sum_\mu |g_\mu(k, Q)|^2. \]

(21)
Moreover, if
\[ g_0(k, Q) = \langle u_+(k) | u_+(k + Q) \rangle, \]
and
\[ \chi^0(Q, 0) = \sum_k \frac{n_F(\varepsilon_k + Q_+) - n_F(\varepsilon_k)}{\varepsilon_k - Q_+ + i0^+} |g_0(k, Q)|^2, \]
is the charge susceptibility, then
\[ |g_0|^2 + \kappa_g(k, Q) \equiv 2, \quad 1 \leq \kappa_g(k, Q) \leq 2. \]
and a “complementary relation” between the spin- and charge- susceptibility,
\[ \sum_{\mu} \chi^0_{\mu}(Q, 0) + \chi^0_{\mu}(Q, 0) = \chi^0(Q, 0) \]
with \( \chi^0(Q, 0) = \sum_k \frac{n_F(\varepsilon_k + Q_+) - n_F(\varepsilon_k)}{\varepsilon_k - Q_+ + i0^+} \), due to spin-momentum locking. We then introduce the spin density operator
\[ \sigma_g(k, Q) = \frac{1}{\kappa_g(k, Q)} \sum_{\mu, \alpha \beta} g^\mu_{\alpha}(k, Q) c^\dagger_{k\alpha} \sigma^\alpha_{\mu} c_{k+Q\beta}. \]
One can show that
\[ \langle u_+(k) | \sigma_g(k, Q) | u_+(k + Q) \rangle = 1. \]
And, any spin density operator
\[ \sigma_f(k, Q) = \sum_{\mu, \alpha \beta} f^\mu_{\alpha}(k) c^\dagger_{k\alpha} \sigma^\alpha_{\mu} c_{k+Q\beta}, \]
which is perpendicular to \( \sigma_g \), i.e., \( \sum_{\mu} g^\mu_{\alpha}(k) f_{\mu}(k) = 0 \), has
\[ \langle u_+(k) | \sigma_f(k, Q) | u_+(k + Q) \rangle = 0. \]
Therefore, only one spin density susceptibility is nonzero (if only \( k \) and \( k + Q \) states are concerned), which is defined by \( \sigma_g(k, Q) \). This intriguing feature is due to spin-momentum locking.

b. Helical feature Consider, if \( k \) and \( k + Q \) are time reversal pairs states, of which spin orientations are opposite, the spin density operator \( \sigma_g(k, Q) \) is helical, as we learn from the case in the edges of 2D TIs. Unfortunately, here \( g_0(k, Q) \) is \( k \) dependent. Besides, only for some very special \( k \) states, such as \( k_0 = (-k_0, 0) \) and \( k_0 + Q_1 = (k_0, 0) \), the two states are time reversal pairs. If the contributions of all \( k \) states are summed, the helical feature may be smeared out.

To study this case, we calculate the free spin susceptibility function \( \chi^0(Q_1, 0) \) numerically for \( E_F \in [0.5, 0.9] E_\nu \) where the Fermi surface is hexagonal \( Q_1 = (2k_0, 0) \) [see Eq. (3)] connects Fermi Arc 4 and Arc 1 [see Fig. 1(b)]. Our results are presented in Fig. 2. From the calculation, we find that, though the exact helical spin susceptibility is ruled out, the spin susceptibility function still has strong helical feature. Specifically, one of the eigenvalues of the spin susceptibility tensor \( \chi^0_{\mu\nu}(Q_1, 0) \) is much larger than the other two [Fig. 2(b)], which corresponds to a spin density response with helicity very close to unity [Fig. 2(c)]. The helical spin rotating axis is indicated in Fig. 2(a) as \( n_g \), which lies in the \( y-z \) plane with an angle \( \theta_n \) [Fig. 2(c)] between \( y \)-axis.

![FIG. 2. (Color online) (a) Schematic of the spin density response corresponding to the largest eigenvalue of the spin susceptibility tensor \( \chi^0(Q_1, 0) \). \( n_g \) is the helical rotating axis. The blue arrows indicate spins rotating around the \( n_g \) axis. \( n_g \) lies in the \( y-z \) plane with an angle \( \theta_n \) between \( y \) axis. (b) Eigenvalues (positive definite) of the tensor \( \chi^0(Q_1, 0) \) as function of Fermi energy (in unit of \( E_\nu \)). (c) The helicity and the angle \( \theta_n \) as function of Fermi energy. All data are calculated at \( k_B T = 1.3 \times 10^{-3} E_\nu \).](image)
Fermi Arc 4, where the main contribution to spin susceptibility comes, the overlapping factor
\[ \sum_{\mu} f_{\mu} g_{\mu} (k, Q_{1}) \]
is also very large, if \( f_{\mu} = g_{\mu} / \sqrt{\kappa_{\sigma}} \). Calculation indicates that the overlapping factor is very close to unity in the vicinity of Fermi Arc 4. Therefore, the spin density operator \( \sigma \) which maximizes the spin susceptibility function should be
\[ \sigma_{G}^{0}(Q_{1}) = \sum_{\mu} g_{\mu} \sigma_{\mu}(Q_{1}) / \sqrt{\kappa_{\sigma}} \].
This observation is very close to the truth, except that it ignores some delicate part. Although the factor
\[ \xi_{k_{0}+} = \xi_{k_{0}+}^{|Q_{1}| = 0} \]
is peaked at \( k_{0} = (-k_{0}, 0) \) (as \( \xi_{k_{0}+} = \xi_{k_{0}+}^{|Q_{1}| = 0} \)), the dispersion, however, is asymmetric around \( k_{0} \) along the \( k_{z} \) direction, as the spectrum is nonlinear [see Eq. (3) and Fig. 1]. Therefore, the spin density operator which maximize the spin susceptibility, denoted as \( \sigma_{G} \), deviates slightly from \( \sigma_{G}^{0} \). Nevertheless, \( \sigma_{G} \) is very close to \( \sigma_{G}^{0} \) and keeps most of the features of \( \sigma_{G}^{0} \), especially the helical feature. This feature even persists to room temperature, thanks to the large bandgap and Dirac velocity in the Bi_{2}Se_{3} class of 3D TIs.

One can write
\[ G_{1\mu} \approx \frac{1}{\sqrt{2}} g_{\mu}^{0}, \quad \sum_{\mu} |G_{1\mu}|^2 = 1. \] (32)

From Eq. (31), we know that \( G_{1x} \) is a pure imaginary number, whereas \( G_{1y} \) and \( G_{1z} \) are real numbers. Also, \( iG_{1x}, G_{1y}, G_{1z} < 0 \). Hence the helical spin rotation axis is
\[ \mathbf{n}_{\sigma} = (0, \cos \theta_{n}, \sin \theta_{n}) \] (33)
with \( \theta_{n} = \operatorname{Arctan}(G_{1z}/G_{1y}) - \pi/2 \), agreeing with the results in Fig. 2. The helicity is \( 2 \sqrt{G_{1y}^2 + G_{1z}^2 G_{1x}} \). From Eqs. (32) and (31), one can see that the helicity is indeed close to unity.

d. Systematic results
In Fig. 3(a), we plot the largest eigenvalue of the spin susceptibility tensor, \( \chi_{G}^{0}(Q, 0) \), as function of \( |Q| \) with \( Q \) along the \( x \)-direction. It is seen that the spin susceptibility function has a strong peak at the nesting wave-vector \( Q_{1} \), especially when \( E_{F} = 0.7E_{s} \) where the Fermi surface is almost a perfect hexagon. We also plot the spin susceptibility function at a higher temperature \( T = 100 \) K (blue dotted curve) with chemical potential \( 0.7E_{s} \). We find that the nesting and the helical features persist to high temperature. And the largest eigenvalue of the spin susceptibility tensor is still much larger than the other two for \( Q \sim Q_{1} \), at high temperature.

We present a two-dimensional plot of \( \chi_{G}^{0}(Q, 0) \) in Fig. 3(b). It is seen that the spin susceptibility function peaks at regions close to the nesting wavevectors \( \pm Q_{i} \), \( i = (1, 2, 3) \). Spin susceptibility is small at both small and large \( Q \). This is quite different from the situation in a normal two-dimensional electron system, where spin susceptibility at small \( Q \) is large.

\[ \chi_{G}^{0}(Q, 0) = \frac{\chi_{G}^{0}(Q, 0)}{1 - a_{G}U_{G}(Q, 0)}, \] (39)

\[ \chi_{G}^{0}(Q, 0) = \frac{\chi_{G}^{0}(Q, 0)}{1 - a_{G}U_{G}(Q, 0)}, \] (34)

Here
\[ \chi_{G}(Q, 0) = i \int_{0}^{\infty} dt \langle [\sigma_{G}(Q, t), \sigma_{G}(Q, 0)] \rangle e^{i(t+0+)} \] (35)
\[ a_{G} = \frac{1}{2} \left[ 1 + \left| \sum_{\mu} G_{1\mu}^2 \right| \right], \quad \frac{1}{2} \leq a_{G} \leq 1. \] (36)

Here the awkward factor \( a_{G} \) is due to the factor that the spin density \( \sigma_{G}(Q_{1}) \) is not properly normalized. The normalized spin density is
\[ \hat{\sigma}_{G}(Q_{1}) = \sqrt{a_{G}} \sum_{\mu} G_{1\mu} \sigma_{\mu}(Q_{1}). \] (37)

It is more obvious to see this through two specific cases: i) If \( \{G_{1\mu}\} \) is a real vector, e.g., \( (1, 0, 0) \), then \( a_{G} = 1 \). This is the non-helical case. The normalized spin density is just \( \hat{\sigma}_{G} = \sigma_{z} \). ii) If \( \{G_{1\mu}\} = \sqrt{2}(1, i, 0) \), then \( a_{G} = \frac{1}{2} \), which is the helical case. The normalized spin density is then \( \hat{\sigma}_{G} = \sigma_{z} = 1/2(\sigma_{x} - i\sigma_{y}) \). The expectation values of both \( \sigma_{x} \) and \( \sigma_{y} \) are less than or equal to unity, which signals the normalization.

Accordingly, hereafter we use the normalized spin susceptibility function,
\[ \tilde{\chi}_{G} \equiv a_{G} \chi_{G}. \] (38)

One then gets
\[ \tilde{\chi}_{G}(Q_{1}, 0) = \frac{\tilde{\chi}_{G}^{0}(Q_{1}, 0)}{1 - U_{G}(Q_{1}, 0)}, \] (39)
which indicates the SDW instability at low temperature.

f. \( \hat{\chi} \) at other nesting wave-vectors
From the symmetry of the system, the spin susceptibility at other nesting wave-vectors can be obtained. Due to the \( C_3 \) symmetry, \( \hat{\chi}(\mathbf{Q}_2, 0) = \mathcal{P} \hat{\chi}(\mathbf{Q}_1, 0) \mathcal{P} \), and \( \hat{\chi}(\mathbf{Q}_3, 0) = \mathcal{P} \hat{\chi}(\mathbf{Q}_2, 0) \mathcal{P} \) with \( \mathcal{P} \) being the transformation matrix for rotation around the z-axis by \( 2\pi/3 \), i.e., the \( C_3 \) operator. The spin density operators,

\[
\hat{\sigma}_G(\mathbf{Q}_i) = \pm \sum_\mu G_{i\mu}^* \sigma_\mu(\mathbf{Q}_i),
\]

transform as (\( \Theta \) denotes time-reversal operation)

\[
C_3 : \quad \hat{\sigma}_G(\mathbf{Q}_i) \rightarrow \hat{\sigma}_G(\mathbf{Q}_{i+1})
\]

\[
\Theta : \quad \hat{\sigma}_G(\mathbf{Q}_i) \leftrightarrow -[\hat{\sigma}_G(\mathbf{Q}_i)]^\dagger.
\]

The complex vectors \( \{G_{i\mu}\} \) transform as

\[
\mathcal{P}\{G_{i\mu}\} = \{G_{i+1\mu}\}.
\]

IV. MEAN FIELD THEORY OF THE HELICAL SDW STATE

A. Edges of 2D TIs

The mean spin density in the helical SDW state is

\[
\langle \sigma_x \rangle = 2S_0 \cos(Qz), \quad \langle \sigma_y \rangle = -2S_0 \sin(Qz),
\]

where \( S_0 > 0 \) (by properly choosing the coordinate) is the amplitude. It is noted that only the helical SDW with negative helicity (along z-axis) exists. This is due to the unique property of spin-momentum locking in TIs. If \( v_0 \) in Eq. (11) is negative, then only the helical SDW with positive helicity exists.

The properties of the ground state and quasi-particles in the helical SDW state can be explored via the mean field theory. Ignoring unimportant terms, the mean field Hubbard interaction is

\[
H_U = -2U[\langle \sigma_+(-Q) \rangle \langle \sigma_-(Q) \rangle + \langle \sigma_+(-Q) \rangle \langle \sigma_-(Q) \rangle - \langle \sigma_+(-Q) \rangle \langle \sigma_-(Q) \rangle],
\]

with \( \langle \sigma_-(Q) \rangle = \langle \sigma_+(-Q) \rangle = S_0 \). The mean field Hamiltonian is then

\[
H_{MF} = \sum_p \left( \sum_{p+Q} \left( \begin{array}{cc} \xi_{p+Q}^\dagger & B \\ B & \xi_p \end{array} \right) \left( \begin{array}{c} c_{p+Q} \\ c_{p+Q}^\dagger \end{array} \right) + 2US_0^2 \right).
\]

where \( B = -2US_0 \). \( p = k + k_F \) and \( \xi_{p+Q} = -v_0p = -\xi_{p+Q}^\dagger \). The summation \( \sum_p' \) is restricted in the region \(-k_F < p < k_F \) as \(-2k_F < k < 0 \) and \( 0 < k + Q < 2k_F \). Introducing a Bogoliubov transformation,

\[
\eta_p = u_pc_{p+Q}^\dagger - v_pc_{p+Q}, \quad \lambda_p = v_pc_{p+Q}^\dagger + u_pc_{p+Q},
\]

with

\[
\begin{array}{c}
H_{GL} = F_2 + F_4 h \\
F_2 = \frac{1}{2} \sum_{\nu, \mathbf{q}} \hat{\chi}_{\nu, \mathbf{q}}(0) \phi_{\nu}(\mathbf{q})^2.
\end{array}
\]
Here $\tilde{\chi}_{\nu,\nu}$ is the diagonalized and “normalized” [see Eq. (33)] spin susceptibility tensor. $\phi_i(q)$ is the SDW. $F_{4\theta}$ denotes the free-energy to the fourth and higher orders of $\phi$. At sufficient low temperature, $\chi$ and $F_2$ become negative, which drives the system into the SDW state. As

$$\tilde{\chi}_{\nu,\nu}^{-1} = \frac{1 - U\tilde{\chi}_{\nu,\nu}^0}{\tilde{\chi}_{\nu,\nu}^0} = -U + 1/\tilde{\chi}_{\nu,\nu}^0, \quad (51)$$

the SDW with largest $\tilde{\chi}_{\nu,\nu}^0$ will first emerge as temperature is lowered down. According to the discussion in Sec. III B, such spin susceptibility is $\tilde{\chi}_{G}(q_i, 0) [i = (1, 2, 3)]$. Therefore, the first emergent SDW is the helical SDW. As $\tilde{\chi}_{G}(q_i, 0)$ is much larger than the others, there will be a temperature region, where only the helical SDW emerges. The following discussion is restricted in this temperature region. 

Free energy $F_2$ of the concerned helical SDWs is,

$$F_2 = \frac{1}{2} \sum_i \tilde{\chi}_{G}^{-1}(q_i, 0)|\phi_i|^2, \quad (52)$$

with

$$\phi_i \equiv \langle \tilde{\sigma}_G(q_i) \rangle \quad (53)$$

being complex. According to Eq. (11), $F_{GL}$ should be invariant under the symmetry operations:

$$\phi_i \rightarrow \phi_{i+1}, \quad \phi_i \leftrightarrow -\phi_i^* \quad (54)$$

The $C_{3v}$ symmetry also gives another invariant operation,

$$\phi_i \rightarrow \phi_{i-1}. \quad (55)$$

Besides, $F_{GL}$ respects the translational symmetry,

$$\boldsymbol{r} \rightarrow \boldsymbol{r} + \boldsymbol{d} : \phi_i \rightarrow \phi_i e^{i\boldsymbol{Q}\cdot\boldsymbol{d}}. \quad (56)$$

Therefore, the symmetry allowed terms in $F_{GL}$ at the fourth order are,

$$F_4 = \sum_i u_{41}|\phi_i|^4 + u_{42}|\phi_i|^2|\phi_{i+1}|^2. \quad (57)$$

To the sixth order,

$$F_6 = \sum_i u_{61}|\phi_i|^6 + u_{62}|\phi_i|^4|\phi_{i+1}|^2 + |\phi_i|^2|\phi_{i+1}|^4 \nonumber + u_{62}|(\phi_i \phi_2 \phi_3)^2 + (\phi_i^2 \phi_2^2 \phi_3^2)^2|, \quad (58)$$

where the last term appears due to the translational symmetry and $\sum_i Q_i = 0. If these higher order terms determine whether the three SDWs coexist or only one of the SDWs is allowed (the stripe phase). Explicitly, after reorganization, there are terms like $(|\phi_i|^2 - |\phi_{i+1}|^2)^{2n}$ with $n \geq 1$, which prefer the difference $(|\phi_i|^2 - |\phi_{i+1}|^2)$. If those terms are prominent, the stripe phase is favored.

Below, we explore a mean field theory to describe the helical SDW states on the surfaces of 3D TIs. For simplicity, we restrict ourself to the stripe phase, where only one helical SDW exists. The mean field Hubbard Hamiltonian is

$$H_U = -\frac{U}{aG} \sum_i \left[ \tilde{\sigma}_G(q_i) \phi_i^* + (\tilde{\sigma}_G(q_i))^\dagger \phi_i \right] - |\phi_i|^2, \quad (59)$$

The magnitude $|\phi_i|$ is determined by minimizing the Ginzburg-Landau free energy, whereas phase fluctuation of $\phi_i$ correspond to the gapless spin wave excitations (Goldstone modes). In the stripe phase, only one of the three $|\phi_i|$ is nonzero. The mean field Hamiltonian is

$$H_{MF} = \frac{U}{aG} \sum_i |\phi_i|^2 + \sum_{k,i} \left( c_{k+}^\dagger c_{k+Q_i}^\dagger B_{1g(k)} \xi_{k+Q_i} \right) \left( c_{k+} B_{1g(k)} \xi_{k} \right) \xi_{k+Q_i}^2, \quad (60)$$

with

$$g_i(k) = \langle u_+(k)|\tilde{\sigma}_G(q_i)|u_+(k + Q_i) \rangle, \quad B_i = \frac{U}{aG} \phi_i^*. \quad (61)$$

The summation $\sum_i$ is restricted in certain region as $k$ and $k + Q_i$ dictate the same Hamiltonian. For example, for the case where only $\phi_1$ is nonzero, $k$ is restricted in the region where $-Q_1 \leq k_x < 0$ as $Q_1 = (Q_1, 0)$. A significant feature of the Hamiltonian is that both the diagonal and off-diagonal terms are $k$-dependent, which may induce nontrivial Berry curvature in some cases. But we will not discuss this important property here. The mean field Hamiltonian is diagonalized as

$$H_{MF} = \sum_{k,i} \left[ E_{ik} + \eta_{ik} \xi_{ik} + E_{ik} - \lambda_{ik} \xi_{ik} \right] + \frac{U}{aG} \sum_i |\phi_i|^2, \quad (62)$$

via the following Bogoliubov transformation,

$$\eta_{ik} = u_{ik} e^{-i4\phi_k} c_{ik} + v_{ik} c_{ik+Q_i}, \quad \lambda_{ik} = v_{ik} e^{-i4\phi_k} c_{ik} + u_{ik} c_{ik+Q_i+1} \quad (63)$$

with

$$u_{ik} = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{\xi_{ik}^2 + [B_{1g(k)}]^2}}, \quad v_{ik} = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{\xi_{ik}^2 + [B_{1g(k)}]^2}} \quad (64)$$

and $\psi_{ik} = \text{Arg}[B_{1g(k)}]$. $\xi_{ik} = \frac{1}{2}(\xi_{ik}^2 + \xi_{ik+Q_i+1})$. The energy spectrum of the quasi-particle excitation is

$$E_{ik} = \pm \sqrt{\xi_{ik}^2 + [B_{1g(k)}]^2} \pm \frac{1}{2}(\xi_{ik} + \xi_{ik+Q_i+1}). \quad (65)$$

It should be mentioned that although the energy gap is $k$-dependent, it does not close at any $k$. 

V. HELICAL MAGNETIC ORDER IN THE MAGNETICALLY DOPED SURFACES OF 3D TIS

The magnetic order in the magnetically doped surfaces of 3D TIs has attracted a lot of interest.\textsuperscript{33,34} Theoretical investigation\textsuperscript{36} has shown that the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction is always ferromagnetic when the Fermi energy is close to the Dirac point. When a ferromagnetic order emerges, a gap is opened around the Dirac point. Recent experiments confirmed such results in Mn or Fe doped Bi$_2$Se$_3$ and Bi$_2$Te$_3$\textsuperscript{33,34,41,42}.

Here we consider the situation when the Fermi energy is much higher and the Fermi surface is hexagonal (and hence nested). From the discussion in previous sections, we know that the spin susceptibility function is peaked at the nesting wavevector where it is helical. Physically, the effective interaction between two magnetic impurities are mediated by the carrier spin density excited by one of the impurity and felted by another. The spin susceptibility function describes such excitation. The nature of the spin susceptibility thus has profound implication on the effective interaction and the magnetic order.

The above picture can be described well by the mean field Zener theory, which has been shown to be successful in the theory of dilute III(Mn)-V magnetic semiconductors.\textsuperscript{29} The Hamiltonian of the system is

\[
H = H_{STI} - J \sum_{ij} \mathbf{S}_I \cdot \mathbf{s}_i,
\]

where \(H_{STI}\) is the Hamiltonian of carriers in the surfaces of 3D TIs. The last term describes the carrier–magnetic-impurity exchange interaction. \(I\) and \(i\) label magnetic impurities and carriers respectively (with spin \(\mathbf{S}_I\) and \(\mathbf{s}_i\) respectively).

In Zener theory, the equilibrium mean carrier and magnetic-impurity spin densities are calculated by minimizing the Ginzburg-Landau free energy. Under the mean field approximation and neglect higher order correlations, the free energy functional is\textsuperscript{40}

\[
F_{GL}[\phi] = -n_M k_B T \ln \left[ \sum_{j=-S}^{S} \exp(J\phi_j/Lk_B T) \right] + F_c[\phi] - J\phi S B_S (SJ\phi/Lk_B T),
\]

where \(\phi = \sqrt{\sum_\mu |\phi_\mu|^2}\) is the mean carrier spin density. \(L\) is the width of surface channel. The first term in right hand side is the free energy of magnetic impurities with \(S\) being the total spin quantum number of a single impurity. \(n_M\) denotes the density of magnetic impurities. The second and third terms are the free energy of the carrier system. The last term is the energy of carrier spin density under the mean field of the exchange interaction, with \(B_S\) being the Brillouin function.

The underlying physics is that, the increase in carrier spin density \(\phi\) reduces the first and last terms in the Ginzburg-Landau free energy, whereas it costs by increasing \(F_c[\phi]\) as the carrier system is in the paramagnetic state. The equilibrium value of \(\phi\) is determined by minimizing \(F_{GL}[\phi]\). At small carrier spin density (the “linear susceptibility regime”), \(F_c[\phi]\) can be written as

\[
F_c[\phi] = \frac{1}{2L} \sum_{\mathbf{q}} \tilde{\chi}_{\mathbf{q},\nu}^{-1}(\mathbf{q})|\phi_{\nu}(\mathbf{q})|^2
\]

where \(\tilde{\chi}_{\mathbf{q},\nu}\) is the diagonalized and “normalized” [see Eq. (38)] spin susceptibility. It is noted that the spin density \(\phi_{\nu}(\mathbf{q})\) corresponding to the largest \(\tilde{\chi}_{\mathbf{q},\nu}(\mathbf{q})\) is energetically favored as it minimizes \(F_c[\phi]\). In previous sections, we have shown that the largest spin susceptibility is achieved at \(\tilde{\chi}_{G}(\mathbf{Q})\). [see Fig. 3], where the corresponding \(\phi_{G}(\mathbf{Q})\) is a helical spin density wave. Therefore, the energetically favored magnetic order is the helical magnetic order, when Fermi surface is nested.

It should be pointed out that the above equations can also be used to obtain the Curie temperature of the magnetic order\textsuperscript{39,40}

\[
k_B T_C = \frac{S(S + 1) J^2 n_M \tilde{\chi}_{G}(\mathbf{Q}, 0)}{3 L}.
\]

The mean carrier spin density is a stripe helical one at the nesting wave-vector \(\mathbf{Q}\). The spins of magnetic impurities are aligned parallel or anti-parallel to the carrier spin density at their local positions, depending on the sign of the exchange constant \(J\). Explicitly, the mean carrier spin density is

\[
\langle \sigma_\mu(\mathbf{r}) \rangle = \sum_i \langle \sigma_\mu(\mathbf{Q}_i) \rangle e^{i\mathbf{Q}_i \cdot \mathbf{r}} + \text{c.c.},
\]

where

\[
\langle \sigma_\mu(\mathbf{Q}_i) \rangle = \frac{G_{i\mu}}{\sqrt{G_{G}}} \phi_i,
\]

with \(\mu = (x, y, z)\) and \(\phi_i = \langle \phi_{G}(\mathbf{Q}_i) \rangle\) is complex. Here \(G_{G}\) is defined in Eq. (40) and \(G_{i\mu}\) is defined in Eq. (44) [the special case \(i = 1\) is given approximately in Eq. (42)].

The amplitude \(\phi = \langle \phi_i \rangle\) is determined by minimizing \(F_{GL}[\phi]\). There are three energetically favored configurations corresponding to the three \(\mathbf{Q}_i\). For each configuration, the magnetic anisotropy is expected to be very large, as the spin susceptibility tensor \(\tilde{\chi}(\mathbf{Q}_i, 0)\) is highly anisotropic [it has an eigen-value much larger than the other two, see Fig. 2(b)].

According to our calculation, for Mn doped Bi$_2$Te$_3$ surface states with \(E_F \simeq 0.7 eV\), corresponding electron density \(4 \times 10^{12} \text{ cm}^{-2}\), \(\tilde{\chi}_{G} \simeq 0.3 \times 10^{-2} \text{ A}^{-2} \text{ eV}^{-1}\) [see Fig. 3(a)], \(J \simeq 10^2 \text{ eV A}^2 \text{ cm}^{-2}\) the width of surface channel \(L = 50 \text{ Å}\) (inferred from Ref. [10]), \(n_M = 2 \times 10^{-3} \text{ Å}^{-3} \text{ mole fraction}\), \(S = 5/2\), we get \(T_C \simeq 30 \text{ K}\), which is not very low.

It should be pointed out that further investigations on the problem are demanded. On one hand, the carrier–magnetic-impurity exchange interaction, which leads to carrier spin relaxation and shortens the propagating distance of the carrier SDW excited by magnetic impurities,
should be included in the calculation of the spin susceptibility function. On the other hand, the exchange and correlation corrections to the spin susceptibility function should be included. A density-functional calculation will be appreciated. Via such improvement, the magnetization can be calculated at arbitrary temperature, carrier and magnetic-impurity densities. We believe that the helical magnetic order is still favored after those corrections are included, according to the symmetry of the system. We assumed that the electron density can be tuned either by gate-voltage or doping by other dopants besides ferromagnetic impurities, which is in principle achievable in experiments.

Finally, we note that very recently, Ye et al. found that the helical magnetic order emerges in a chain of impurity spins in the surfaces of 3D TIs. And Zhu et al. discussed the RKKY interaction when Fermi surface correlation corrections to the spin susceptibility function should be included. The tunability of inter-particle interaction (and many other properties) in such systems may be utilized to enhance the helical SDW order predicted in this paper.

VI. CONCLUSION

We study spin susceptibility and magnetic order at the edges/surfaces of topological insulators when the Fermi surface is nested. We find that due to spin-momentum locking as well as time-reversal symmetry, spin susceptibility at the nesting wavevector has a strong helical feature. It follows then, a helical SDW state emerges at low temperature due to Fermi surface nesting. The helical feature of spin susceptibility also has profound impact on the magnetic order in the magnetically doped surfaces of 3D TIs. From the Zener theory, to the lowest order, we predicted a helical magnetic order in such system.

The helical SDW order can be probed/determined either directly by spin resolved STM or indirectly by the existence of an energy gap at the Fermi surface via, e.g., ARPES. For spin pump-probe measurements, if a local spin density is excited, it will propagate with certain helicity along the nesting wavevectors. The helical magnetic order in magnetically doped surface of 3D TIs can also be probed directly by spin resolved STM and other magnetic response measurements.

Finally, recent studies indicate that topological insulators can also be achieved in cold-atom systems. The tunability of inter-particle interaction (and many other properties) in such systems may be utilized to enhance the helical SDW order predicted in this paper.

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