Spin helix of magnetic impurities in two-dimensional helical metal

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Abstract – The surface state of a topological insulator dubbed as helical metal is a unique metallic system, which exhibits one single Dirac cone and spin-momentum locking. We show that the behaviors of magnetic impurities embedded in this kind of surface states manifest the uniqueness of helical metals among other conventional Dirac materials such as graphene. We find there is a significant Dzyaloshinskii-Moriya (DM) term among the effective interactions between impurity spins mediated by the conduction electrons. For a chain of impurity spins, we show that such a DM interaction gives rise to a single-handed spin helix state, the handedness of which is locked with the sign of the Fermi velocity of the emergent Dirac fermions. We also point out that the polarization of impurity spins can be controlled via electric voltage for dilute magnetic-impurity concentration.

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Introduction. – It is now known that a three-dimensional (3D) insulators with time reversal symmetry can be classified into two categories: ordinary and topological insulator (TI) [1–5]. Though both of them are fully gapped in the bulk, TI has metallic surface states robust against any time-reversal–invariant perturbations. These metallic surface states dubbed as “helical metal” can be described by a two-dimensional (2D) massless Dirac equation. Comparing to other emergent relativistic materials such as single-layer graphene, the surface states of TIs have two unique features. One is that the number of Dirac nodes is odd. In fact, according to the no-go theorem [6], the Dirac nodes always appear in pairs in a conventional 2D lattice such as graphene. The surface state of TI can invalidate the no-go theorem because a pair of Dirac nodes is separated onto two opposite surfaces. A TI with single Dirac cone has been theoretically studied and experimentally observed by angle-resolved photo-emission spectroscopy [7–11]. The other feature is that electron spin and momentum are intimately locked in helical metal, originated from strong spin-orbit coupling. Evidence of the spin-momentum locking has also been observed in recent experiments [12–15].

The intrinsic properties of helical metals could be possibly reflected by some phenomena such as the Kondo effect, superconductivity, etc., which have received considerable attention recently [16–20]. In this letter we point out a novel feature in Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between impurity spins in helical metal, which manifests directly the two features of TI mentioned above. Firstly, due to the spin-momentum locking of the conduction electron, we show the induced RKKY interaction must contain an anisotropic Dzyaloshinskii-Moriya (DM) term by both symmetry analysis and perturbation calculation, which is usually absent in systems like graphene [21–23]. Since the emergent Dirac Hamiltonian of a helical metal is a pure spin-orbit coupling, the magnitude of the DM term is of the same order of the conventional RKKY one. Secondly, the DM term can lead to a single-handed spin helix if the impurities are aligned into a chain, the handedness of which depends on the sign of the Fermi velocity $v_F$ of the helical metal. For strong TIs with a single Dirac cone attached to each surface, $v_F$ is fixed, therefore the
corresponding spin helix must be single-handed. The spin helix is illustrated in fig. 1, where two types of Dirac fermions are considered and the spin helices are perpendicular (fig. 1(a)) and parallel (fig. 1(b)) to the impurity chain, respectively. This is a hallmark of a strong TI, and could be possibly detected by spin-polarized scan tunneling microscopy, or optical measurement like the magneto-optic Kerr effect.

**Model.** We start from the Hamiltonian of the conduction electrons with only one Dirac cone

$$
\hat{H}_0^a = \sum_\mathbf{k} \left( \hbar v_F \mathbf{k} \cdot \mathbf{\sigma} - E_F \right) \hat{c}_\mathbf{k},
$$

with Fermi energy $E_F$ and Pauli matrix $\mathbf{\sigma}$. Via a unitary transformation $\hat{a}_\mathbf{k} = \left[ \hat{c}_\mathbf{k} \uparrow + \text{sgn}(v_F) \hbar \mathbf{v}_\mathbf{F} \cdot \hat{c}_\mathbf{k} \downarrow \right] / \sqrt{2}$ with $\theta_\mathbf{k}$ the angle of vector $\mathbf{k}$ and $s = \pm 1$, it can be diagonalized as $\hat{H}_0^a = \sum_{s = \pm 1} (\hbar v_F |k - E_F|) \hat{a}_\mathbf{k}^s \hat{a}_\mathbf{k}^s$. In practice, the recently discovered TI material, e.g., Bi$_2$Se$_3$ has surface state described by a Rashba-type Hamiltonian [8,9]

$$
\hat{H}_0^b = \sum_\mathbf{k} \left( \hbar v_F (\mathbf{k} \times \mathbf{\sigma}) \right)_z - E_F \hat{c}_\mathbf{k},
$$

which is related to $\hat{H}_0^b$ by a rotation of $\mathbf{k}$ around the $z$-axis by $\pi/2$. In the following we will focus on $\hat{H}_0^b$.

Suppose there are $N_{imp}$ impurity spins located at $\mathbf{r}_n$ denoted by $\mathbf{S}_n$, which interact with the conduction electrons via the following spin-spin coupling:

$$
\hat{H}_I = \sum_{n=1}^{N_{imp}} \lambda_0 \hat{S}_n^z \hat{S}_n^z + \lambda_\pm \left[ \hat{S}_n^x \hat{S}_{n'}^x + \hat{S}_n^y \hat{S}_{n'}^y \right],
$$

where $\hat{S}_n^x,y,z(\mathbf{r})$ are the spin operators of the conduction electron at $\mathbf{r}$. The coupling constants are assumed to be isotropic in the $xy$-plane, $\lambda_\pm \equiv \lambda_{\pm} \hat{z}$, but may differ from the $z$-component. The total Hamiltonian is simply the sum $\hat{H} = \hat{H}_0^b + \hat{H}_I$.

Before proceeding with the discussion of the effective interaction between impurity spins, we follow RKKY [24–26] to divide $\hat{H}_I$ into two parts: $\hat{H}_{10}$ and $\hat{H}_{11}$. $\hat{H}_{10}$ consists of the diagonal term of $\hat{S}_n^z \hat{a}_\mathbf{k}$ and can be written as

$$
\hat{H}_{10} = \lambda_0 \sum_\mathbf{k} (\mathbf{e}_\mathbf{k} \cdot \hat{S}_n^z) \left( \mathbf{e}_\mathbf{k} \cdot \hat{S}_{imp} \right),
$$

where $\mathbf{e}_\mathbf{k} = \mathbf{k} / \mathbf{k}$, $\hat{S}_n^z = \hat{S}_n^z \mathbf{\sigma}$, and $\hat{S}_{imp} = \mathbb{V}^{-1} \sum_{n=1}^{N_{imp}} \hat{S}_n$ is the density of impurity spin. And the remaining part denoted by $\hat{H}_{11}$ is off-diagonal. Notice that for the helical Hamiltonian, the current of the conduction electrons is proportional to their spins, for instance, $\mathbf{J} = e v_F \sum_\mathbf{k} \hat{S}_n$ for $\hat{H}_0^a$, therefore $\hat{H}_{10}$ actually implies a direct coupling between the electric current and the impurity spins, which provides a mechanism to control the impurity spins through the electric voltage for dilute impurity concentration.

**RKKY interaction.** For simplicity we focus on the case of two impurities at $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. The results given below via the symmetry analysis are also valid for the many-impurity case as long as we consider two-body interactions. The RKKY interaction can be obtained by integrating out the degree of freedom of conduction electrons, followed by an expansion to the second order of the coupling parameters $\lambda_{\alpha \beta}$ [24–26].

The effective interaction between impurity spins thus obtained contains only the even-order terms for time-reversal-invariant system.

To the lowest order, the most general form of the interaction is $\hat{H}_{r\text{kkky}}(\mathbf{r}_{12}) = \sum_{\alpha_1 \alpha_2} \Gamma_{\alpha_1 \alpha_2} (\mathbf{r}_{12}) \hat{S}_{\alpha_1}^0 \hat{S}_{\alpha_2}^0$ with $\mathbf{r}_{12} \equiv \mathbf{r}_1 - \mathbf{r}_2$. Without spin-orbit coupling and as in the usual case, only terms with $\alpha_1 = \alpha_2$ can exist due to a rotational symmetry in spin space. However, the situation is quite different for the helical metal, since $\hat{H}_0^a$ is invariant only under a joint rotation in both spin and orbital space, which allows more terms as will soon become clear. Let us consider a global rotation around the $z$-axis by $\varphi$ defined as

$$
\mathbf{R}_{\alpha_1 \alpha_2} \equiv \exp[i \varphi (\mathbf{e}_z \cdot \hat{S}_{\text{cond}})] \times \exp[i \varphi (\mathbf{e}_z \cdot (\hat{S}_1 + \hat{S}_2))]
$$

$$
\times \exp[i \varphi (\mathbf{e}_z \cdot \hat{L})],
$$

with total spin of conduction electrons $\hat{S}_{\text{cond}} = \int \mathbf{d} \mathbf{r} \mathbf{e}_z \hat{c}(\mathbf{r}) / 2$ and orbital angular momentum $\hat{L} = \int \mathbf{d} \mathbf{r} \left( \mathbf{r} \times \mathbf{p} \right) \hat{c}(\mathbf{r})$. Under this rotation, $\hat{H}_0^b$ is obviously invariant, but $\hat{H}_I(\mathbf{r}_1, \mathbf{r}_2) \rightarrow \hat{H}_I(\mathbf{r}'_1, \mathbf{r}'_2)$ with $\mathbf{r}' \equiv e^{-i \varphi (x \mathbf{p}_x - y \mathbf{p}_y)} \mathbf{r} e^{i \varphi (x \mathbf{p}_x - y \mathbf{p}_y)}$, which breaks the rotational symmetry. However since the energy behaves like a scalar, one expects $\hat{H}_{r\text{kkky}}(\mathbf{r}_{12}) = \hat{H}_{r\text{kkky}}(\mathbf{r}'_{12})$, then we are left with is to construct $\mathbf{R}_{\alpha_1 \alpha_2}$-invariants with vectors $\mathbf{e}_\alpha(\equiv \mathbf{e}_{\mathbf{r}_1 / \mathbf{r}_2}, \mathbf{S}_1$ and $\mathbf{S}_2$.

There are many such $\mathbf{R}_{\alpha_1 \alpha_2}$-invariants terms, most of which can be further eliminated by the following two symmetries. The first one is exchanging $\mathbf{r}_1$ and $\mathbf{r}_2$ which obviously leaves $\hat{H}$ invariant. Thus terms like $\mathbf{e}_z \cdot (\hat{S}_1 \times \hat{S}_2)$ are not allowed. The second one is a global rotation $\mathbf{R}_{\alpha_1 \alpha_2}$ around axis $\mathbf{e}_{\mathbf{r}_1 / \mathbf{r}_2}$ by $\pi$

$$
\mathbf{R}_{\alpha_1 \alpha_2} \equiv \exp[i \pi (\mathbf{e}_{\mathbf{r}_1} \times \hat{S}_{\text{cond}})] \times \exp[i \pi (\mathbf{e}_{\mathbf{r}_2} \cdot (\mathbf{S}_1 + \mathbf{S}_2))]
$$

$$
\times \exp[i \pi (\mathbf{e}_{\mathbf{r}_1} \cdot \hat{L})],
$$

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\[
\frac{Z}{Z_0} \approx \exp \left\{ \frac{\beta}{2} \sum_{k_{i1},k_{j2}} \sum_{m,n} \left[ \sum_{x,y,z} \lambda_a F_{k_{i1};k_{j2}}^{a}(1 - f_{k_{j2}m}) \right] \right\},
\]

(9)

which rules out invariants like \([e_{12} \times (S_1 \times S_2)]\), that changes sign under the rotation \(R_{e_{12} \pi}\). Hence, we are left with the following two terms in addition to the conventional ones: \((e_{12} \cdot (S_1 \times S_2))\) and \((e_{12} \cdot S_1)(e_{12} \cdot S_2))\). One then constructs the effective Hamiltonian of impurity spins as

\[
\hat{H}_{\text{RKKY}}(r_{12}) = \Gamma_0(r_{12})[\lambda_{s}^{2}(\hat{S}_1 \cdot \hat{S}_2) + \lambda_{s}^{2}(\hat{S}_2 \cdot \hat{S}_1) + \lambda_{s}^{2}(\hat{S}_1 \cdot \hat{S}_2)]
\]

\[
+ \Gamma_1(r_{12})[e_{12} \cdot (\hat{S}_1) (e_{12} \cdot \hat{S}_2)]
\]

\[
+ \Gamma_{\text{DM}}(r_{12})\lambda_{s} \lambda_{s} [e_{12} \cdot (\hat{S}_1 \times \hat{S}_2)],
\]

(7)

where the \(\Gamma_0\)-term is just the conventional RKKY terms.

**Derivation of \(\Gamma_{\text{0,1,DM}}\).** – The coefficients \(\Gamma_{0,1,DM}\) in eq. (7) can be computed following RKKY’s second-order perturbation [24–26]. Let us consider the following generalized partition function:

\[
Z = T_{\text{cond}} e^{-\beta (H_0 + \hat{H}_1)},
\]

(8)

which is partially traced over conduction electrons. To the quadratic order of \(\lambda_{s,\pm}\), we obtain

\[
\text{see eq. (9) above}
\]

where \(Z_0\) is the partition function of conduction electrons, \(F_{k_{s}} = [1 + e^{\beta(v_F |k| - E_f)}]^{-1}\) is the Fermi distribution function, and the \(F\)-functions take the forms

\[
F_{k_{i1},k_{j2},s}^{x} = \frac{1}{4} t_{sgn}(v_F)(-1|k_{i1} s_{2e} + s_{2e} e_{i1}),
\]

\[
F_{k_{i1},k_{j2},s}^{y} = \frac{i}{4} t_{sgn}(v_F)(s_{2e} e_{i1} - s_{2e} e_{i1}),
\]

\[
F_{k_{i1},k_{j2},s}^{z} = \frac{1}{4} t_{(1 - s_{2e} e_{i1})},
\]

(10)

which depend only on \(\theta_{k_{i1},2}\), the angle of \(k_{i1,2}\). By comparing with eq. (7), one can extract the coefficients \(\Gamma_{0,1,DM}\) from eq. (9) straightforwardly. After integrating over \(\theta_{k_{i1,2}}\), we have \(\Gamma_0 = -2[A(r) - B(r)]\), \(\Gamma_1 = -4B(r)\) and \(\Gamma_{\text{DM}} = -2C(r)\), where the functions \(A, B\) and \(C\) read, in the zero temperature limit,

\[
A(r) = \frac{1}{8|v_F|^2} \sum_{s_{1},s_{2}} \int x_1 dx_1 \int x_2 dx_2 \left\{ \begin{array}{c} J_0(x_1) J_0(x_2) \\ \theta(x_F - x_1) \theta(x_2 - x_F) \end{array} \right\},
\]

(11)

where \(x \equiv kr, x_F = k_F r\), \(\theta(x)\) is the Heaviside step function, and \(J_{0,1}(x)\) are the first and second-order Bessel functions, respectively. Note that \(\Gamma_0(r)\) has already been obtained in ref. [18], which agrees with ours. It is the \(\Gamma_1\) and \(\Gamma_{\text{DM}}\) terms that have not been addressed before, and the physics discussed in this letter is essentially coming from them.

The numerical results of \(\Gamma_{0,1,DM}(r)\) are plotted in fig. 2 where a cutoff is set for \(x\) and the Cauchy principle integration is understood when singularities are encountered in eq. (11). Despite of the oscillation of the conventional RKKY interaction with respect to \(r\) for large \(k_F\), it is interesting to note that the DM interaction is of the same order of the conventional ones, and depends on the sign of \(v_F\), as seen from the expression of \(C(r)\) in eq. (11).

**Single-handed spin helix.** – To reveal the effect of the DM interaction, we focus on the simple case of a one-dimensional chain of impurities aligned with equal spacing \(d\) along the \(x\)-axis, and the corresponding Hamiltonian
reads
\[ H_{\text{imp}} = \sum_n ( - J_z \hat{S}_n^z \hat{S}_{n+1}^z - J_y \hat{S}_n^y \hat{S}_{n+1}^y + J_x \hat{S}_n^x \hat{S}_{n+1}^x ) + J_{DM} ( \hat{S}_n^z \hat{S}_{n+1}^y - \hat{S}_n^y \hat{S}_{n+1}^z ) , \]
(12)
where \( J_z = -\Gamma_0(d)\lambda_0^2, \ J_y = -\Gamma_0(d)\lambda_0^3, \ J_x = [\Gamma_0(d) + \Gamma_1(d)]\lambda_0^4 \), and \( J_{DM} = -\Gamma_{DM}(d)\lambda_0^4 \). Here we consider the case for \( k_F \) close to the Dirac point, where we can neglect the oscillation of the effective coupling constants and simply assume \( J_{y,z} > J_x > 0 \) as can be read off in fig. 2(b) for \( r \approx 1 \). The other situations including two-dimensional arrays of magnetic impurities are left for future studies.

In this case, the spins lie in the \( yz \)-plane in the classical limit. Therefore, we can introduce two variables \( \theta_n \) and \( \hat{\rho}_n \) to describe the spin rotation in the \( yz \)-plane and the amplitude fluctuation along the \( x \)-axis, which satisfy the commutation relation \([\theta_n, \hat{\rho}_m] = i\delta_{mn} \), and are related to \( \hat{S}_n \) through
\[ \hat{S}_n^x = \hat{\rho}, \]
\[ \hat{S}_n^y + i\hat{S}_n^z = e^{i\theta}[(S - \hat{\rho})(S + \hat{\rho} + 1)]^{1/2}, \]
\[ \hat{S}_n^z - i\hat{S}_n^y = [(S - \hat{\rho})(S + \hat{\rho} + 1)]^{1/2}e^{-i\theta}. \]
(13)
One may verify these equations satisfying the angular-momentum algebra, and \( \hat{S}^2 = S(S + 1) \). In the continuum limit the effective Hamiltonian for the dynamics of impurity spins can be written as
\[ \dot{H}_{\text{imp}} = \int dx [ - D_1 \cos(\partial_y \theta) + D_2 \cos(2\theta) + D_3 \sin(\partial_x \theta) + D_0 \hat{\rho}^2 ] \]
with \( [\theta(x), \hat{\rho}(x')] = i\delta(x - x') \). The parameters are given by \( D_0 = J_y d, \ D_1 = (J_z + J_y)S(S + 1)/(2d), \ D_2 = (J_z - J_y)S(S + 1)/(2d) \) and \( D_3 = J_{DM}S(S + 1)/d \).

We first consider the isotropic case, i.e., \( J_z = J_y \). The \( \theta(x) \)-field has a helical background (see fig. 1(a)), with helical angle \( \eta \) satisfying \( \tan(\eta d) = 2J_{DM}/(J_z + J_y) \). The sign of \( \eta \) is the same as that of \( J_{DM} \), and its amplitude is saturated to \( \pi/2d \) as \( J_{DM} \) is large enough as shown in the lower panel in fig. 3. Replacing \( \theta(x) \) in eq. (14) with \( \eta x + \hat{\theta}(x) \), we have \( \dot{H}_{\text{imp}} = \int dx [ - \sqrt{D_1^2 + D_2^2} \cos(\partial_y \theta) + D_0 \hat{\rho}^2 ] \) describing the quantum fluctuation upon the helical background. The low-energy excitations can be obtained by expanding \( \cos(\partial_y \theta) \) to the second order of \( \hat{\rho} \), which leads to a linear spectrum in \( k \) as \( \omega_k = d(2D_0)^{1/2}(D_1^2 + D_2^2)^{1/4} |k| \).

Next we consider the effect of spin anisotropy, i.e. \( J_z \neq J_y \). Without loss of generality, we assume \( J_z > J_y \) (if \( J_z < J_y \), one can shift \( \theta \rightarrow \theta + \pi/2 \) to get positive \( D_2 \)). In this case the Hamiltonian becomes a sine-Gordon (SG) model
\[ \dot{H}_{\text{imp}} \approx \int dx \left\{ \frac{u}{2} [K^{-1}(\partial_y \theta)^2 + K\hat{\rho}^2] + h\partial_x \theta + D_2 \cos(\sqrt{8}\pi \theta) \right\}, \]
(15)
which is written in the standard form by rescaling \( \theta \) and \( \hat{\rho} \) in order to use the well-known results in the literature, e.g. in refs. [27,28]. The coefficients take the form
\[ u = d\sqrt{J_z(J_z + J_y)S(S + 1)}, \]
\[ K = \frac{1}{\pi} \frac{J_z}{(J_z + J_y)S(S + 1)}, \]
\[ h = \sqrt{2\pi J_{DM}S(S + 1)}. \]
(16)
In case \( K > 1 \), the cosine term is irrelevant, so that the system is massless and the spin helix takes place for any finite \( h \). However, in case \( K < 1 \), the theory turns out to be massive, and a critical value of \( |J_{DM}| \) exists, only above which the spin helix can occur in forms of massive soliton excitations of the \( \theta \)-field [27,28] which connect different classical vacua of the SG model. In our case, since \( 0 < J_z < J_y \), we are in the region of \( K < 1 \). A schematic phase diagram for this case is given in the upper panel of fig. 3, where the left helix, non-helical and right helix regions belong to different topological sectors of the sine-Gordon model with negative, zero, and positive topological charges, respectively.

Our analysis of the DM interaction so far is focused on \( H_{\text{imp}}^0 \), where the spin helix is in the \( yz \)-plane perpendicular to the impurity chain. For the helical metal described by \( H_{\text{imp}}^0 \), the RKKY interaction can be obtained by rotating \( e_{12} \) around the \( z \)-axis by \( \pi/2 \) in eq. (7). As a consequence, the \( \Gamma_0 \)-term is invariant, the \( \Gamma_1 \)-term becomes \( \Gamma_1(r_{12}) \lambda_1^2(e_{12} \times \hat{S}_1)_1(e_{12} \times \hat{S}_2)_2 \), and the \( \Gamma_{DM} \)-term becomes \( \Gamma_{DM}(r_{12})\lambda_1^4\lambda_1^2(e_{12} \times (\hat{S}_1 \times \hat{S}_2))_2 \). Notice that \( (e_{12} \times \hat{S}_1)_1(e_{12} \times \hat{S}_2)_2 = \hat{S}_1^x \hat{S}_2^x + \hat{S}_1^y \hat{S}_2^y - (e_{12} \cdot \hat{S}_1)(e_{12} \cdot \hat{S}_2) \), therefore the \( \Gamma_1 \)-term simply changes the coefficients of the first
two terms of eq. (7). Only the change of the $\Gamma_{DM}$-term is essential, which makes the spin rotate in the $xz$-plane instead of the $yz$-plane as illustrated in fig. 1(b).

**Summary.** – The surface state of TI is metallic with strong spin-orbit coupling, in which the magnetic impurities coupled with conductance electrons can be polarized by electric voltage. There is also an effective interaction between impurity spins mediated by the conduction electrons, which includes a DM interaction with the same order of amplitude of the isotropic RKKY interactions. For a 1D chain of impurities, this could lead to a single-handed spin helix, and the handedness is locked with the sign of the Fermi velocity $v_F$ of the emergent Dirac particles.

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