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Fluctuation-induced Néel and Bloch skyrmions at topological insulator surfaces

Flavio S. Nogueira,1,2 Ilya Eremin,2,3 Ferhat Katmis,4,5 Jagadeesh S. Moodera,4,6 Jeroen van den Brink,1,7 and Volodymyr P. Kravchuk1,8

1Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstraße 20, DE-01069 Dresden, Germany
2Institut für Theoretische Physik III, Ruhr-Universität Bochum, Universitätsstraße 150, DE-44801 Bochum, Germany
3National University of Science and Technology MISiS, 119049 Moscow, Russia
4Francis Bitter Magnet Laboratory and Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
5Department of Physics, Middle East Technical University, TR-06800 Ankara, Turkey
6Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
7Institute for Theoretical Physics, TU Dresden, DE-01069 Dresden, Germany
8Bogolyubov Institute for Theoretical Physics of National Academy of Sciences of Ukraine, 03680 Kyiv, Ukraine

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Ferromagnets in contact with a topological insulator have become appealing candidates for spintronics due to the presence of Dirac surface states with spin-momentum locking. Because of this, bilayer Bi2Se3-EuS structures, for instance, show a finite magnetization at the interface at temperatures well exceeding the Curie temperature of bulk EuS. Here, we determine theoretically the effective magnetic interactions at a topological insulator-ferromagnet interface above the magnetic ordering temperature. We show that by integrating out the Dirac fermion fluctuations an effective Dzyaloshinskii-Moriya interaction and magnetic charging interaction emerge. As a result, individual magnetic skyrmions and extended skyrmion lattices can form at the interfaces of ferromagnets and topological insulators, the first indications of which have been very recently observed experimentally.

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Introduction. The spin-momentum locking property of three-dimensional topological insulators (TIs) [1,2] makes them promising candidate materials for future spin-based electronic devices. One important consequence of spin-momentum locking in TIs is the topological electromagnetic response, which arises from induced Chern-Simons (CS) terms [3] on each surface [4]. This happens, for instance, when time-reversal (TR) symmetry is broken, which renders the surface Dirac fermions gapped. This can be achieved, for example, by a proximity effect with a ferromagnetic insulator (FMI) [5–15]. In this case, a CS term is generated if there are an odd number of gapped Dirac fermions, which is achieved only in the presence of out-of-plane exchange fields [11]. The realization of several physical effects related to the CS term that have been predicted in the literature critically depends on growing technologies required for the fabrication of heterostructures involving both strong TIs and FMIs. Recently, high-quality Bi2Se3-EuS bilayer structures have been shown to exhibit proximity-induced ferromagnetism on the surface of Bi2Se3 [6,16,17]. Other successful realizations of stable ferromagnetic TI interfaces were demonstrated recently [18,19]. In addition, it was shown that the interface of FMI and TI can have a magnetic ordering temperature much higher than the bulk ordering temperature [5], indicating that topological surface states can strongly affect the magnetic properties of a proximity-coupled FMI.

These experimental advances motivate us to investigate the effective magnetic interactions that result from the fluctuating momentum-locked Dirac fermion surface states of a TI in contact with an FMI.

We show that even in the absence of any spontaneous magnetization, at temperatures above the Curie temperature of the FMI, intriguing topologically stable magnetic textures, i.e., skyrmions, are induced as a result of quantum fluctuations of the Dirac fermions at the interface. In fact, we demonstrate that integrating out Dirac fermions coupled to a FMI thin film generates a Dzyaloshinskii-Moriya interaction (DMI), that, depending on the form of the Dirac Hamiltonian, favors either Néel- or Bloch-type skyrmions [20–23]. However, skyrmions induced in TI-FMI structures feature in addition a “charging energy,” due to the generation of a term proportional to the square of the so-called magnetic charge $\mathbf{V} \cdot \mathbf{n}$, where $\mathbf{n}$ denotes the direction of the magnetization [24]. An important feature of our finding is that the Dirac fermions that are integrated out are not gapped, since there is no spontaneous magnetization above $T_c$ that would lead to a gap in the Dirac spectrum. Furthermore, the generated DMI is only nonzero if the chemical potential does not vanish. We obtain the phase diagram for the skyrmion solutions and identify the region of stability for skyrmion lattices in the presence of the magnetic charging energy. We determine this region numerically by analyzing the excitation spectrum of the skyrmion solution. An important discovery is that the magnetic charging energy modifies the phase diagram significantly in the case of DMIs favoring Néel skyrmions, a situation relevant for Bi2Se3-EuS interfaces. Our theoretical findings support conceptually the recent experimental observation of a skyrmion texture at a ferromagnetic heterostructure of Cr-doped Sb2Te3 [19]. Having a skyrmion profile on a TI surface will cause significant changes in the conductance that may be observed in transport measurements [25].
heterostructure has the general form
\[ H_{\text{Dirac}}(n(r)) = |d| \langle \nabla n \rangle - J_0 n(r) \cdot \sigma, \]
where \(r = (x, y, z)\), \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) is a vector of Pauli matrices, and \(J_0\) is the interface exchange coupling. The operator \(d\) is a function of the momentum operator \(-i\hbar \nabla\). Here, we consider the two possibilities leading to a Dirac spectrum,
\[ d_1 = -i\hbar \nu_F \nabla \times \mathbf{z}, \quad d_2 = -i\hbar \nu_F \nabla \times \mathbf{z}, \]
with the latter arising in TIs such as Bi\(_2\)Se\(_3\), Bi\(_2\)Te\(_3\), and Sb\(_2\)Te\(_3\) [26]. Experimentally, in order for the effective Hamiltonian (1) to give a valid low-energy description of the physics at the interface, the TI must be at least 7 nm thick. The end result will be that \(d_1\) induces a DMI of the type \(n \cdot (\nabla \times n)\), which is often referred to as a bulk DMI, but for clarity we call it a Bloch DMI. Instead, \(d_2\) leads to a different type of DMI, \(\sim n \cdot [(\mathbf{z} \times \nabla) \times n] = (\mathbf{n} \cdot \nabla) n_z - n_i (\nabla \cdot n)\), in the magnetic literature sometimes known as surface DMI, but to which we refer to as Néel DMI.

The effective energy \(E_{\text{eff}}\) of the system is obtained by integrating out the Dirac fermions \(c = (c^\uparrow, c^\downarrow)\) in the partition function,
\[ e^{-\beta E_{\text{tot}}(n)} = e^{-\beta \rho_s L \int d^3x \langle \mathcal{D} n \rangle^2} \times \int \mathcal{D} c^\dagger \mathcal{D} c e^{-\int_0^{\beta \omega_F} d\tau \int d^3r c^\dagger i n_{\uparrow \downarrow} + \mathcal{H}_{\text{Dirac}}(n(r))]}, \]
where \(\rho_s\) is the magnetization stiffness of the FMI, \(L\) is the film thickness, and the integration is over the film area \(S\). Due to the nonzero \(z\) component of the magnetization, the above model yields a gapped Dirac spectrum for \(T < T_c\) with spin-wave excitations, which give rise to a Chern-Simons term [10]. However, this gap does not occur for \(T > T_c\). In the following, we assume that the gap vanishes for \(T > T_c\) and we obtain the corresponding corrections to the free energy after integrating out the gapless Dirac fermions.

**Effective free energy and induced DMI.** The noninteracting Green’s function for a spin-momentum locked system can be written in general as
\[ G_{\alpha\beta}(\omega_n, k) = G(\omega_n, k) \delta_{\alpha\beta} + F(\omega_n, k) \cdot \sigma_{\alpha\beta}, \]
where \(\omega_n = (2n + 1)\pi/\beta\) is the fermionic Matsubara frequency.

From the Hamiltonian (1) and the functional integral in (3), we have
\[ G(\omega_n, k) = \frac{i \omega_n + \mu}{(i \omega_n + \mu)^2 - d^2(k)}, \]
\[ F(\omega_n, k) = -\frac{d(k)}{(i \omega_n + \mu)^2 - d^2(k)}, \]
where \(d(k)\) is either \(d_1\) or \(d_2\) from Eq. (2) in momentum space. Integrating out the fermions and expanding the free-energy expression up to \(J_0^2\), we obtain, after a long but straightforward calculation, the following correction to the effective free-energy density [27],
\[ \delta F_{\text{Dirac}}^{\text{mag}} = \frac{s}{2} \langle [\mathbf{V} n(r)]^2 + [\mathbf{V} \cdot n(r)]^2 \rangle + i \frac{a}{2} n(r) \cdot [d(-i\hbar \nabla) \times n(r)], \]
where \(\mathbf{V} = \sum_{i=x,y,z} (\nabla n_i)^2\) defines the usual exchange term, and we have defined \(s = \beta J_0^2/[24\pi \cos^3(\beta \mu/2)]\) and \(a = J_0^2(8\pi \nu_F)^{-1} \tan(\beta \mu/2)\). We can drop the constant term \(F_{\text{Dirac}}(0)\) from the free energy, since it does not depend on the field. Thus, we can safely write \(F_{\text{Dirac}}^m = \delta F_{\text{Dirac}}\). The above expression features a DMI induced by Dirac fermion fluctuations. In addition, a contribution \(\sim (\mathbf{V} \cdot n)^2\) is also generated. We will see below that the presence of this term leads to interesting physical properties when \(d_2\) is replaced for \(d_1\) in Eq. (7), modifying in this way the behavior of Néel skyrmions. Note that differently from the case where the Dirac fermion is gapped [15], no intrinsic anisotropy is generated by the Dirac fermions. At the same time, we note that the form of \(\delta F_{\text{Dirac}}^m\), including the DMI term will persist also below \(T_c\), as long as the chemical potential is outside the gap, meaning that the TI surface is metallic, despite the generated mass \(m\) for the Dirac fermions.

**Effective magnetic energy in an external field.** The contributions from the FMI and Dirac fermions allow one to recast the effective energy for a thin ferromagnetic layer in the form
\[ E_{\text{eff}} = L \int S \left[ A \langle (\mathbf{V} n)^2 + (\mathbf{V} \cdot n)^2 \rangle + D\bar{\delta}_{\text{DMI}} + M_s H(1 - n_i) \right] dS, \]
where \(A = \rho_s + s/(2L)\) is the effective magnetization stiffness including the fluctuations due to the Dirac fermions. We assumed that the sample lies in the presence of an external magnetic field \(H\) applied perpendicular to it. We have also introduced the parameter \(\epsilon = s/(2AL) = s/(2\rho_s L + s)\). The DM coupling is given by \(D = a/(2L)\). The DM interaction has the possible forms \(\bar{\delta}_{\text{DMI}} n = n \cdot (\mathbf{V} \times n)\) or \(\bar{\delta}_{\text{DMI}} n = n \cdot (\mathbf{V} \times n)\), depending on whether \(d_1\) or \(d_2\) arises in the Dirac Hamiltonian (1). The latter is more adequate for Bi\(_2\)Se\(_3\)-EuS samples [13]. The ab initio results from Ref. [28] indicate that \(J_0\) is largely enhanced due to Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions at the Bi\(_2\)Se\(_3\)-EuS interface, ranging from 35 to 40 meV. Using \(J_0 = 35\) meV one can estimate that at room temperature \(\epsilon \in [0.05, 0.63]\) meV, and therefore \(\epsilon \in [0.08, 0.51]\) for a 1-nm-thick film and \(\mu \in (0, 0.1)\) eV [29]. Note that \(\epsilon\) strongly depends on the value of \(\mu\), which can be reduced by doping.

Although the temperature fluctuations usually destroy skyrmions in thin films, the individual skyrmions [30–32] as well as skyrmion lattices [33] are observed in various multilayer structures for room temperatures. Therefore, in experiments, it is reasonable to use a multilayer structure in the form of the periodically repeated stack TI/FMI/NI, where NI is a normal insulator. In the following, we neglect the influence of the thermal fluctuations on the magnetization structure, which holds when model (8) is applied for a multilayer structure.

Before studying the energy functional (8), let us emphasize that while the DMI is absent for the case of a vanishing chemical potential, the term \((\mathbf{V} \cdot n)^2\) is always there, even if \(\mu = 0\). Thus, this term is a unique feature of thin-film FMIs proximate to a three-dimensional TI. In fact, it has been recently demonstrated that it is also induced for \(\mu = 0\) at zero temperature when the surface Dirac fermions are gapped by the proximity effect to the FMI [15].
Ground states of system (8) are well studied for the case \( \epsilon = 0 \) [34–38]. The uniform saturation along the field is the ground state with \( E_{\text{eff}} = 0 \) for large fields and weak DM interactions, and a one-dimensional (1D) structure in the form of a periodical sequence of \( 2\pi \) domain walls is the ground state with \( E_{\text{eff}} < 0 \) for small fields and strong DM interactions.

The criterion for the periodical state appearance is negative energy of a single domain wall, which reads \( d > d_c = 8/\pi \), where \( d = \sqrt{2D/M_s H} \) is a dimensionless DM constant. In the vicinity of the boundary \( d \approx d_c \), an intermediate phase in the form of a two-dimensional (2D) periodical structure (skyrmion lattice) forms the ground state [20,21,34,39]. An isolated skyrmion [21,22,35,40] may appear as a topologically stable excitation of the uniformly saturated state. The skyrmions and domain walls are of Bloch and Néel types for the DM excitation of the uniformly saturated state.

Here, we study how the ground states and individual skyrmions are changed when \( \epsilon > 0 \). Since \( \mathbf{V} \cdot \mathbf{n} \equiv 0 \) for any domain wall and skyrmion of the Bloch type (induced by \( \epsilon^{\text{DMI}} \)), the influence of the term \((\mathbf{V} \cdot \mathbf{n})^2\) is not significant in this case. However, it drastically changes the ground-state diagram and stability of the static solutions for the case of \( \epsilon^{\text{DMI}} \). In this case, \( d_c = \sqrt{N} \epsilon = (8/\pi) \int_0^1 \sqrt{1 + \epsilon (2 \xi^2 - 1)} d \xi \) and the period of the 1D structure is increased with \( \epsilon \) [27]. Energy per period is \( E_{\text{DMI}}(d, \epsilon) \approx \alpha E(d, \epsilon) \), where \( \alpha \) is determined by the implicit relation \( d(d^0(\epsilon) = E(4/\xi) \sqrt{\epsilon} / 4 \), with \( E(k) \) being the complete elliptic integral of the second kind [41] (note that \( \epsilon < 0 \). For the case \( \epsilon^{\text{DMI}} \) the 1D periodical structure is not affected by \( \epsilon \) and one has \( d_c = d_c^0(0) \) and \( E_{\text{DMI}}(d) = E_{\text{DMI}}^0(d, 0) \) [27].

Skyrmion solutions. Here, we consider the topologically stable excitations of the saturated state \( \mathbf{n} = 2 \). First, we utilize the constraint \( \mathbf{n}^2 = 1 \) by expressing the direction of the magnetization in spherical coordinates, \( \mathbf{n} = \sin \theta \cos \varphi \mathbf{\hat{r}} + \sin \theta \sin \varphi \mathbf{\hat{\varphi}} + \cos \theta \mathbf{\hat{z}} \). One can show [27] that for the case \( \epsilon^{\text{DMI}} \) the total energy (8) has a local minimum if \( \phi = \chi \) and function \( \theta = \theta(\rho) \) is determined by the equation

\[
(1 + \epsilon \cos^2 \theta) \nabla_\rho^2 \theta - \sin \theta \cos \theta \left( \frac{1 + \epsilon}{\rho^2} + \epsilon \theta^2 \right) \\
+ d \frac{\sin^2 \theta}{\rho} - \sin \theta = 0,
\]

where we introduced the polar frame of reference \((\rho, \chi)\) with the radial distance \( \rho \) measured in units of \( \ell = \sqrt{2A/\left(M_s H^2\right)} \) and \( \nabla_\rho^2 f = \rho^{-1} \partial_\rho (\rho \partial_\rho f) \) denotes the radial part of the Laplace operator. Equation (9) must be solved with the boundary conditions \( \theta(0) = \pi, \theta(\infty) = 0 \). A number of examples of skyrmion profiles determined by Eq. (9) for various values of parameters \( d \) and \( \epsilon \) are shown in Fig. S2 [27]. Note that the skyrmion size is mainly determined by the parameter \( d \), while the parameter \( \epsilon \) weakly modifies the details of the skyrmion profile. For the case \( \epsilon^{\text{DMI}} \) the equilibrium solution is \( \phi = \chi + \pi / 2 \) and the corresponding equation for the profile \( \theta(\rho) \) coincides with (9) when \( \epsilon = 0 \). Note that in this case Eq. (9) is reduced to the well-known skyrmion equation [23,34,40].

In order to analyze the stability of the obtained static solutions we study the spectrum of the skyrmion eigenexcitations by means of the methods commonly applied for skyrmions [38,42] as well as for other two-dimensional magnetic topological solitons [43–47]. Namely, we introduce small, time-dependent deviations \( \theta = \theta_0 + \delta \) and \( \phi = \phi_0 + \delta \sin \theta_0 \), where \( \delta, \phi_0 < 1 \) and \( \theta_0 = \theta_0(\rho) \), and \( \phi_0 \) denotes the static profile. The linearization of the Landau-Lifshitz equations, \( \partial_t \theta = \frac{\partial E}{\partial \theta}, \partial_t \phi = \frac{\partial E}{\partial \phi} \), introduces instability in the form \( \delta \theta = f(\rho) \cos(\omega t + m \chi + \chi_0), \delta \phi = g(\rho) \sin(\omega t + m \chi + \chi_0), \) where \( m \) is a azimuthal quantum number and \( \chi_0 \) is an arbitrary phase. Here, \( \tau = 2 \Omega_0 \) is the dimensionless time, where \( \Omega_0 = \gamma H \) is the Larmor frequency with \( \gamma \) being the gyromagnetic ratio. The eigenfrequencies \( \omega \) and the corresponding eigenfunctions \( f, g \) are determined by solving the Bogoliubov–de Gennes eigenvalue problem [27]. The numerical solution was obtained for a range of \( d \) and a couple of values of \( \epsilon \). A number of bounded eigenmodes with \( \omega < 1 \) are found in the gap. Eigenfrequencies of the radially symmetric \((m = 0)\) and elliptic \((m = 2)\) modes are shown in Fig. 1, where we compare both types of DM terms [48]. If \( \epsilon = 0 \), the spectra are identical for both cases, in particular, the well-known elliptical instability [35,38] takes place due to the softening of the elliptic mode in the region \( d > d_c \), where the uniformly saturated state is thermodynamically unstable [38]. For the case \( \epsilon^{\text{DMI}} \) the \( \epsilon \) term shifts the elliptical instability to the larger values of \( d \) with the condition \( d > d_c^0(\epsilon) \) kept, while in the case \( \epsilon^{\text{DMI}} \) the effect of the \( \epsilon \) term is negligible.

Remarkably, the \( \epsilon \) term influences oppositely on the breathing mode \((m = 0)\), for different DM types. For the case \( \epsilon^{\text{DMI}} \) the eigenfrequency \( \omega_0 \) is increased and for small \( d \) the breathing mode is pushed out from the gap into the magnon.

**FIG. 1.** Eigenfrequencies of two localized modes, namely, radially symmetric \((m = 0)\) and elliptic \((m = 2)\), are found by means of a numerical solution of the eigenvalue problem for different DM terms. Modes which do not demonstrate instability are not shown. Stability/instability regions are indicated for the case \( \epsilon = 1 \).
continuum. As a result, the small-radius skyrmions are free of the bounded states. This is in contrast to the case $\delta_{\text{DMI}}$, when the breaching mode eigenfrequency is rapidly decreased, resulting in a radial instability for small $d$. In order to give some physical insight into the latter effect, we consider the model where the skyrmion profile is described by the linear ansatz \[ \theta(x) = \Phi_1 \delta(x) \] and \[ \Phi = x + \Phi_1. \] Here, the variational parameters $R$ and $\Phi$ describe the skyrmion radius and helicity, respectively, and $H(x)$ is the Heaviside step function.

For this model, total energy \( (8) \) with \( \delta_{\text{DMI}} = \delta_{\text{DMI}}^0 \) reads

\[
\frac{E_{\text{tot}}^N}{2\pi AL} = e_\text{ex} + e_\text{ex} \cos^2 \Phi - 2\delta \cos \Phi R + R^2 e_\text{H},
\]

where the constants $e_{\text{ex}} \approx 6.15$ \[ [49], e_\text{ex} = e_{\text{ex}} - \pi^2/2 \text{, and } e_\text{H} = 1 - 4/\pi^2 \text{ originate from the exchange, $e$-term, and Zeeman contributions, respectively. Here, } \delta = d\pi/4. \]

The energy expression \( (10) \) shows that the equilibrium helicity $\Phi$ is determined by the competition of the $e$ term, which tends to $\Phi = \pm\pi/2$ (Bloch skyrmion), and the DM term, which tends to $\Phi = 0$ (Néel skyrmion). At the same time, the equilibrium skyrmion radius is determined by the competition of the DM and Zeeman terms, and for the Bloch skyrmion one has $R = 0$. Thus, the skyrmion collapse is expected with the $\epsilon$ increasing. Indeed, the minimization of the total energy \( (10) \) with respect to the both variational parameters results in the critical value $\epsilon_c = \delta^2/(e_\text{ex}e_\text{H})$: If $\epsilon < \epsilon_c$, then the equilibrium values of the variational parameters $R_0 = \delta/e_\text{H}$ and $\Phi_0 = 0$ determine the Néel skyrmion; if $\epsilon > \epsilon_c$, the minimum of energy \( (10) \) is reached for $R_0 = 0$ and $\Phi_0 = \pm\pi/2$. The latter corresponds to a collapsed Bloch skyrmion. In other words, a stable Néel skyrmion exists for the case $\epsilon < \epsilon_c$. Surprisingly, there are no intermediate states with $0 < \Phi_0 < \pi/2$ when $\epsilon > \epsilon_c$.

**Skyrmion lattice.** In order to estimate the region of existence of the skyrmion lattice we use the circular cell approximation \[ [34], when the lattice cell is approximated by a circle of radius $R$ and the boundary condition $\theta(R) = 0$ is applied. The skyrmion profile is described by the same linear ansatz as for the case of an isolated skyrmion. Minimizing the energy \( (10) \) per unit cell $E_{\text{tot}}^N = E_{\text{tot}}^N/(\pi R^2)$, one obtains the following equilibrium values of the variational parameters $\Phi_0 = 0$, $R_0^N(\epsilon) = (e_\text{ex} + e_\text{ex})/\delta$, and the corresponding equilibrium energy reads $E_{\text{tot}}^N(\epsilon) = 2\pi R^2\epsilon_\text{H} - \delta^2/(e_\text{ex} + e_\text{ex})$. For the case $\delta_{\text{DMI}} = \delta_{\text{DMI}}^0$ the same procedure results in the $\epsilon$-independent values $\Phi_0^N = \pi/2$, $R_0^N = R_0^N(0)$, and $E_{\text{tot}}^N = E_{\text{tot}}^N(0)$.

Comparing the energies of three states, namely, the energy of the uniform magnetization along field $E = 0$, energy of the 1D periodical state (per period) $E_{\text{1D}}$, and energy of the skyrmion lattice per unit cell $E_{\text{tot}}^N$, we determine the phase diagram of the ground states (see Fig. 2). Note that for $\epsilon > \epsilon_\text{ex} \approx 0.98$ the skyrmion lattice is not a ground state. Given the dependence of $\epsilon$ with the exchange coupling $J_0$, temperature, and chemical potential, the skyrmion lattice phase is likely to occur for a not too high-temperature range as compared to the Curie temperature of EuS. The dimensionless DM parameter $d$ can then be tuned by the external field to attain the interval shown under the green area of Fig. 2(a).

**Conclusions.** We have shown that the effective magnetic energy for a TI-FMI heterostructure exhibits a Dzyaloshinskii-Moriya term induced by tracing out the surface Dirac fermions proximate to the FMI. A unique feature of the effective energy as compared to other DM systems is the presence of an additionally induced magnetic capacitance energy, given by a term proportional to the square of the magnetic charge $\mathbf{V} \cdot \mathbf{n}$. Despite having a small magnitude in realistic samples, the interplay between this term and the DM one yields a phase diagram with interesting phase boundaries in the case of a Néel DMI, which is the situation relevant for, e.g., Bi$_2$Se$_3$ samples proximate to a FMI. Our theory is directly relevant for very recently synthesized TI-ferromagnetic thin-film heterostructures, in some of which the formation of a skyrmionic magnetic texture has been observed \[ [19].\]


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[24] In contrast to the weak contribution from the nonlocal energy of the volume magnetostatic charges, which for a thin film scales quadratically with the thickness, the considered “magnetic charging energy” is linear with the thickness and, therefore, it cannot be neglected.


[29] For EuS we would have $\rho_s = S^2 [J_1 + J_2/2]/a_0 \approx 0.29$ meV/nm, where $S = 7/2$ is the spin of the Eu atom, $J_1/a_0 = 0.228$ K and $J_2/a_0 = -0.118$ K are the nearest- and next-nearest-neighbor exchange energies, respectively, and for the lattice spacing $a_0 = 5.968$ Å [50].


[48] The stability analysis was performed for zero temperature. However, thermally induced magnons would only result in additional damping for bounded skyrmion modes.

[49] The exact value is $e_{ex} = [\pi^2 + \gamma_0 - \text{Ci}(2\pi) + \ln(2\pi)]/2$, where $\gamma_0$ is the Euler constant and $\text{Ci}(x)$ denotes the cosine integral function (see Ref. [34]).