Magnetic fluctuations in topological insulators with ordered magnetic adatoms: Cr on Bi_2Se_3 from first principles

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We consider a system consisting of a topological insulator with an array of magnetic adatoms interacting with the surface states of electrons. We find that the indirect coupling of the magnetic impurities results in a ferromagnetic ordering of the magnetic moments and is also responsible for the unusual linear dispersion of the surface magnons. We also show that the interaction of magnons with surface electrons essentially renormalizes the electron energy spectrum. The renormalized spectrum is nonlinear and can be characterized by a negative effective mass of electrons and holes for any $k \neq 0$. The electron velocity near the Dirac point depends on the electron-magnon coupling.

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I. INTRODUCTION

The interest in topological insulators (TIs) is to a large extent driven by an amazing connection between the time-reversal symmetry, the topology of the energy bands in the bulk, and the existence of gapless electron modes at the surface of spin Hall insulators and semiconductors with strong spin-orbit interaction [1], allowing for numerous potential applications. Therefore, it is important to study how the properties of TIs are changed when the time-reversal symmetry is broken. For example, this may be brought about by magnetic impurities [2–9].

A further interesting situation is that of periodically ordered magnetic impurities at the surface of a TI [10]. In this case the translation symmetry is still preserved. Magnetic impurities arranged in this way and interacting with conduction-band electrons (a model also referred to as the Kondo lattice) possess a ground state and excitation spectra that are completely different from those in the clean surface case [11,12]. While the physics of individual impurities is by now rather well understood, the properties of TIs in the presence of such a lattice have yet to be analyzed in full detail.

It is known that the interaction between magnetic impurities at the surface of a typical TI can be long ranged and ferromagnetic, which eventually leads to a ferromagnetic ordering. [2,4,7,13] In turn, as the time-reversal symmetry is obviously broken in the ferromagnet, it drives the appearance of a gap in the spectrum of surface electrons. Another interesting study has found a pronounced helicoidal arrangement of spins due to a strong Dzyaloshinskii-Moriya coupling induced by the interaction of the impurity spins with the conduction-band electrons [14].

In this paper we would like to advance the knowledge in this area by fully analyzing the lowest-lying excitation spectrum of the system with a special emphasis on surface magnons and their coupling to the conductance-band electrons, which opens the way for a range of applications of TIs in magnonics [14]. We find that the spectrum of surface magnons at low temperatures is linear, which is very unusual for ferromagnets. Calculating the electron self-energy for the process of spin-wave emission by electrons, we find that the electron energy spectrum can be strongly modified by the magnons, so that the velocity of electrons depends on the electron-magnon coupling.

II. MAGNETIC IMPURITY AT THE Bi_2Se_3 (0001) SURFACE

The three-dimensional (3D) topological insulator features linear dispersion of surface metallic states forming a Dirac cone with a crossing point around the Fermi level [1]. First-principles calculations reproduce correctly the main band-structure features of these systems, as ishown in Fig. 1 for Bi_2Se_3, which is a representative example of a 3D TI. We see that the Bi_2Se_3 surface band structure, calculated with the first-principles pseudopotential VASP code [15], demonstrates linear dispersion of the bands near the point $\bar{\Gamma}$ of the Brillouin zone.

To make our model with magnetic adatoms close to reality, we consider first the properties of a single magnetic impurity (e.g., a Cr atom) at the surface of Bi_2Se_3, which can be obtained from first-principles simulations. We use a self-consistent Green function method within multiple-scattering theory [16], which takes into account properly the boundary conditions for a cluster embedded into a semi-infinite system. The magnetic anisotropy energy (MAE) was computed using the Lloyd formula, which takes into account the energy change of the valence electrons [17,18].

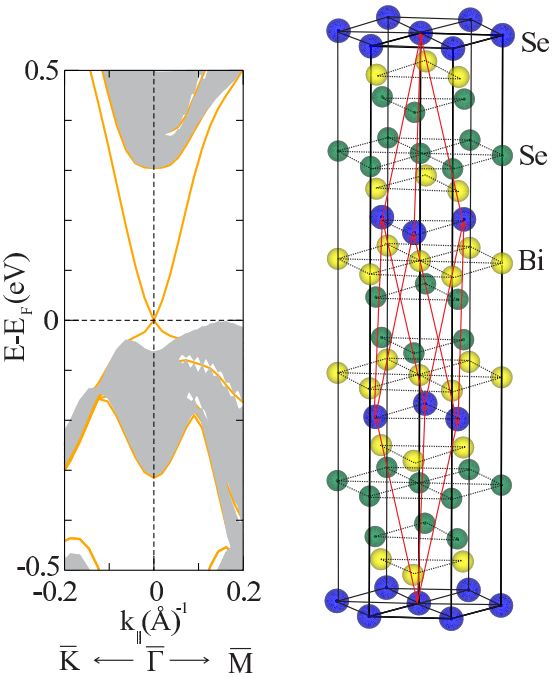

FIG. 1. (Color online) Surface band structure (left panel) of the topological insulator Bi_2Se_3 (0001), the crystal structure of which is depicted on the right panel.

Here we consider Cr adatoms on the Bi_2Se_3 (0001) surface and investigate their electronic and magnetic properties. According to recent experiments, the distribution of transition metal impurities on the surface of a topological insulator can depend on the deposition temperature [19–21]. With a low-temperature deposition, the transition metal impurities can occupy two different interstitial sites on Bi_2Se_3 (0001), while with a high-temperature deposition they substitute for Bi atoms in the subsurface layers.

According to our single-impurity calculations, the density of state (DOS) of Cr substituting for Bi atoms features a strong peak at the Fermi level in the majority-spin channel, while the minority-spin channel is almost unoccupied [see the spin-resolved local DOS of chromium on Bi_2Se_3 (0001) in Fig. 2 (red area), calculated using a scalar-relativistic approach]. The Cr impurities possess magnetic moments of $3.79\mu_B$ and $3.78\mu_B$ for both out-of- and in-plane magnetization directions.

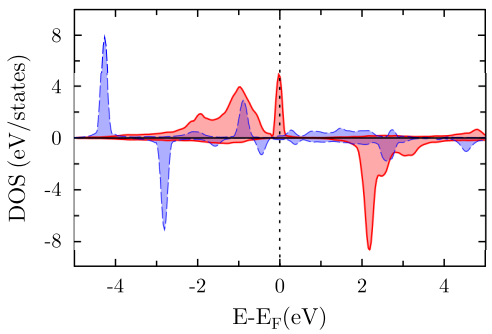

FIG. 2. (Color online) Spin-resolved densities of states of Cr atoms on the Bi_2Se_3 (0001) surface.

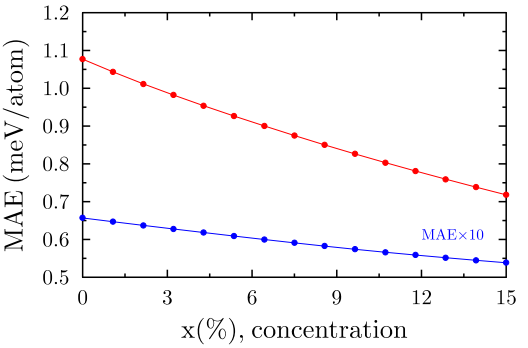

FIG. 3. (Color online) Calculated MAE of Bi_2Se_3 (0001) surfaces doped with Cr atoms, which substitute for Bi atoms (red line) or are located in the surface interstitial position (blue line). $x = 0\%$ corresponds to the case of a single impurity.

In the case of the interstitial surface impurities, the magnetic moment is significantly smaller, $0.71\mu_B$ and $0.70\mu_B$ for both out-of- and in-plane magnetization directions, and the DOS is characterized by sharp impuritylike peaks in both spin channels (the blue area in Fig. 2). Our calculations of the MAE reveal the out-of-plane magnetization direction for both cases (see Fig. 3), which is in good agreement with results of recent first-principles calculations [10]. This opens the band gap, which was estimated in our calculations at 5% chromium concentration to be 4.5 meV and 1.2 meV for the substitutional and interstitial Cr impurities, respectively.

Using a first-principles Green function method within the coherent potential approximation, we investigated magnetic coupling between Cr impurities on the Bi_2Se_3 (0001) surface in the low- and moderate-concentration regimes (0.01%–15%). To calculate the exchange constants entering the Heisenberg Hamiltonian, we applied the magnetic force theorem as it is implemented within multiple-scattering theory [22]. Our calculations reveal two important results: (i) the system is ferromagnetic ($T_C = 25$ K and $T_C = 10$ K in the cases of the substitutional and interstitial impurities for 5% chromium concentration), and (ii) the MAE is significantly smaller than the energy of magnetic interaction between magnetic impurities, which was estimated from our first-principles calculations to be between 0.1 and 8.0 meV/per pair; see Fig. 4.

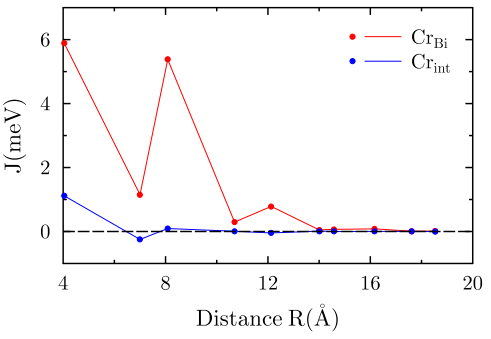

FIG. 4. (Color online) Calculated exchange interaction between Cr atoms on the Bi_2Se_3 (0001) surface, which substitute for Bi atoms (red line) or are located in the surface interstitial position (blue line). Calculations were obtained for the case $x = 5\%$.

Thus, due to the on-site magnetic anisotropy, one can rather anticipate ferromagnetic ordering of the Cr moments provided they are coupled by RKKY interaction, even in the case of anisotropic exchange coupling (see [2,13] and the discussion in Ref. [4]).

III. MODEL OF AN ARRAY OF MAGNETIC ADATOMS

Now we would like to discuss the properties of a multi-impurity system. We consider the model of surface electrons in a TI with a linear energy spectrum interacting with magnetic impurities distributed homogeneously at the surface. The Hamiltonian of the free electrons has the form

$$\mathcal{H}_0 = -iv(\sigma_x\partial_x + \sigma_y\partial_y), \tag{1}$$

where $\boldsymbol{\sigma}$ are the spin Pauli matrices. This effective model captures correctly the energy structure of Bi_2Se_3 near the Dirac point [2], particularly of the surface electrons of a TI with strong spin-orbit interaction. In the absence of this interaction, the material is an ordinary insulator, for which there are no gapless surface states. The Hamiltonian describing the coupling of surface electrons to the spin density distribution $\mathbf{S}(\mathbf{r})$ associated with magnetic impurities is

$$\mathcal{H}_{\rm int} = \frac{\lambda_l}{2}[\sigma_+ S_-(\mathbf{r}) + \sigma_- S_+(\mathbf{r})] + \lambda_t \sigma_z S_z(\mathbf{r}), \tag{2}$$

where $S_\pm(\mathbf{r}) = S_x(\mathbf{r}) \pm iS_y(\mathbf{r})$, while λ_l and λ_t are the longitudinal and transverse coupling constants, respectively. As follows from *ab initio* calculations, this model corresponds to a Cr adatom at the surface of Bi_2Se_3.

Now we assume that the magnetic impurities form a superlattice at the surface of the topological insulator. Such substructures can emerge during the self-organization of adatoms resulting, e.g., from the strain fields generated by the adatoms [23]. Also, ordered adatom structures can be produced by nanostructuree formation [24].

The spin superlattice in itself is assumed to possess no dynamics. Then the full Hamiltonian is the sum of (1) and (2). Coupling to electrons with coupling constants λ_l and λ_t induces long-ranged interactions of spins. It is known that indirect RKKY interaction between magnetic impurities in the TI is usually ferromagnetic and long ranged, leading to ferromagnetic ordering at low temperatures [2,13]. Our *ab initio* calculations also confirm this result. The anisotropy of the RKKY interaction leads to preferably out-of-plane ferromagnetic ordering as we found for Cr on Bi_2Se_3 and was shown in the model with a linear energy spectrum [2,4,13]. However, as pointed out in Ref. [4], for some λ_l/λ_t larger than a critical value, it is possible that spin-glass ordering is energetically favorable. The existence of small on-site anisotropy makes ferromagnetic ordering more probable even at a large ratio of longitudinal and transverse coupling.

The ferromagnetic ordering usually results in a gap in the electronic spectrum of surface electrons. This gap can be very small if the mean value of the ordered spin component is small enough due to low dimensionality and fluctuations. Here we consider the correction to the electron energy spectrum due to the interaction between electrons and the fluctuating magnetization. Such magnetic density fluctuations (spin waves) can be strong in the vicinity of the Curie temperature T_C (critical fluctuations) and at $T > T_C$ (paramagnons). At low temperatures $T \ll T_C$ these spin waves can be rather weak. Nonetheless, due to the 2D geometry of the system they are still very important.

In order to access the electronic dynamics we can integrate out the spin degrees of freedom. This is possible because spin-1/2 fields can be represented by ordinary fermions, which enter the total Hamiltonian linearly [25]. In order to perform this program we need the correlation functions of spins, which we accessed by mean-field theory concepts, assuming a finite average magnetization in the spin subsystem.

In ferromagnets with a long-range interaction of magnetic moments, the spin correlations have been studied by Vaks *et al.* [26] (see also Ref. [27]). The diagram technique for calculating the magnetic correlators presented there is justified not only at $T \ll T_C$ but also at temperatures close to T_C provided that the effective radius of the interaction, r_0, is large. At low temperatures, when the magnetic fluctuations are simple spin waves, one can take the spin density propagator in the following form (it corresponds to the time-ordered Green function of magnons after a small shift $\omega \to \omega + i\delta\,\mathrm{sgn}\,\omega$ to the complex plane):

$$D_{+-}(\mathbf{q},\omega) = \frac{S_z}{\omega + S_z[V(\mathbf{q}) - V(0)] - KS_z}, \tag{3}$$

where we take the magnetization along the z axis and S_z is the average value of the z component of the spin density. The function $V(\mathbf{q})$ in Eq. (3) is the Fourier transform of the interaction between the spins, which is the electron-mediated exchange interaction related to the coupling presented by Eq. (2). The last term in the denominator of (3) is the one-site anisotropy of the spin Hamiltonian. We introduced explicitly the anisotropy K to make this model closer to the results of *ab initio* simulations. In accordance with Eq. (3), the spectrum of the surface spin waves, corresponding to the poles of the spin correlator, is given by $\omega(\mathbf{q}) = S_z[V(0) - V(\mathbf{q})] + KS_z$.

IV. EXCHANGE INTERACTION AND SPIN WAVES

In the standard loop approximation we can find the energy of magnetic interaction between $\mathbf{S}(\mathbf{r})$ and $\mathbf{S}(\mathbf{r}')$ as

$$E_{ij}^{\rm int}(\mathbf{r}-\mathbf{r}') = S_i(\mathbf{r})\,S_j(\mathbf{r}')\,\chi_{ij}(\mathbf{r}-\mathbf{r}'), \tag{4}$$

where $\chi_{ij}(\mathbf{r}-\mathbf{r}')$ is the magnetic susceptibility. Its Fourier transformation is

$$\chi_{ij}(\mathbf{q}) = -i\lambda_{l,t}^2 \mathrm{Tr}\int \frac{d\varepsilon}{2\pi}\frac{d^2\mathbf{k}}{(2\pi)^2}\,\sigma_i G_0(\mathbf{k}+\mathbf{q},\varepsilon)\,\sigma_j G_0(\mathbf{k},\varepsilon), \tag{5}$$

where $G_0(\mathbf{k},\varepsilon)$ is the Green function corresponding to Hamiltonian (1) of the free-electron gas at the surface of a topological insulator. Note that we do not include here the gap Δ, assuming that its value is rather small, so that the characteristic interaction radius r_0 is large, $r_0 \simeq v/\Delta \gg a$, where a is the spin superlattice constant. We also assume the chemical potential of surface electrons to be located at the band-crossing point $\mu = 0$. It turns out that the transverse fluctuations of the moments are the only ones which remain gapless at low

temperatures. Thus they are by far the strongest ones and that is why we consider only them in what follows.

Using Eq. (5), calculating the trace over spins, and integrating over energy, we find $\chi_{ij}(\mathbf{q}) = \delta_{ij} V(\mathbf{q})$, where

$$V(\mathbf{q}) = -\frac{\lambda_t^2}{8\pi^2 v} \int_0^{2\pi} d\theta \int_0^{k_{\max}} \frac{k dk}{|\mathbf{k}+\mathbf{q}| + k}, \tag{6}$$

$k_{\max}$ is the cutoff of the electron energy spectrum, and θ is the angle between the vectors $\mathbf{k}$ and $\mathbf{q}$. It gives us the constant part $V(0) = -\lambda^2 k_{\max}/4\pi v$. Since the integral over k for $V(\mathbf{q}) - V(0)$ converges at large k, and assuming $q/k_{\max} \ll 1$, we can calculate it by taking $k_{\max} \to \infty$. Then we get $V(\mathbf{q}) - V(0) = -\lambda_t^2 C_0 q/8\pi^2 v$, where

$$C_0 = -\int_0^{\infty} dx \int_0^{\pi} d\theta \, \frac{y-x}{y+x} \simeq 1.2434, \tag{7}$$

and $y = (x^2 + 2x\cos\theta + 1)^{1/2}$. Then using (6) and (7) we find

$$V(\mathbf{q}) = -\frac{\lambda_t^2 C_0}{8\pi^2 v}\left(q + \frac{2\pi k_{\max}}{C_0}\right). \tag{8}$$

Thus, we obtain the spectrum of surface spin waves,

$$\omega(q) = \frac{\lambda_t^2 C_0 S_z q}{8\pi^2 v} + K S_z, \tag{9}$$

which turns out to be a linear function of the wave vector q even though the magnetic ordering is ferromagnetic. The anisotropy makes a gap but the linearity of the magnon spectrum is preserved.

One can compare Eq. (8) to the known result [2] in coordinate representation at large R, $V(R) \simeq -C/R^3$ with $C = \text{const} > 0$, where the minus sign reflects the ferromagnetic coupling. After Fourier transformation it gives

$$V(\mathbf{q}) = -C \int_{R>a_0} e^{-i\mathbf{q}\cdot\mathbf{R}} \frac{d^2\mathbf{R}}{R^3} \simeq -2\pi C\left(q + \frac{1}{a_0}\right). \tag{10}$$

Thus, both approaches lead to the same result.

V. ELECTRON SELF-ENERGY

Now we can use the spin correlator of Eq. (3) and calculate the electron self-energy related to the coupling to magnons,

$$\Sigma(\mathbf{k},\varepsilon) = i\lambda_t^2 \int \frac{d\omega}{2\pi} \frac{d^2\mathbf{q}}{(2\pi)^2} \, \sigma_- \, G_0(\mathbf{k}-\mathbf{q}, \varepsilon - \omega)\, \sigma_+ \times D_{+-}(\mathbf{q},\omega). \tag{11}$$

The real part of the self-energy allows for the computation of corrections to the energy spectrum. Correspondingly, the imaginary part of Eq. (11) describes the processes of magnon emission and absorption by electrons.

It is convenient to use the unitary transformation $U = \exp(\frac{i\pi\sigma_y}{4}) \exp(\frac{i\varphi\sigma_z}{2})$ with $\tan\varphi = k_y/k_x$, which diagonalizes Hamiltonian (1), $\widetilde{\mathcal{H}}_0 = U\mathcal{H}_0 U^{-1} = \text{diag}\,(vk, -vk)$. The corresponding transformation of the Pauli matrices is $U\sigma_\pm U^{-1} = e^{i\varphi}(\sigma_z \pm i\sigma_y)$. The electron self-energy in the new basis is (all matrix elements are equal),

$$\widetilde{\Sigma}(\mathbf{k},\varepsilon) = (1+\sigma_x)\,\Sigma_{\mathbf{k}\varepsilon}, \tag{12}$$

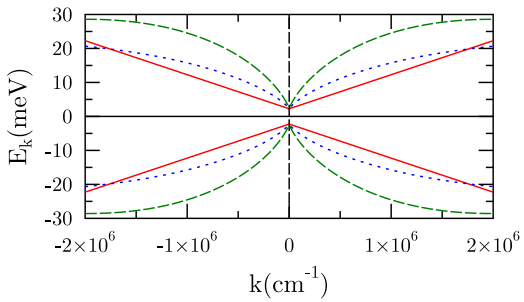

FIG. 5. (Color online) The energy spectrum of electrons renormalized due to the coupling to magnons calculated for various ξ: $\xi = 0.00$ (red solid line), $\xi = 0.02$ (blue dotted line), and $\xi = 0.04$ (green dashed line). The gap $\Delta = \lambda_t \langle S_z \rangle \approx 4.5$ meV is due to magnetization.

where we denoted

$$\Sigma_{\mathbf{k}\varepsilon} = i\lambda_t^2 \int \frac{d\omega}{2\pi} \frac{d^2\mathbf{q}}{(2\pi)^2} \, [G_0^+(\mathbf{k}-\mathbf{q}, \varepsilon-\omega) + G_0^-(\mathbf{k}-\mathbf{q}, \varepsilon-\omega)] D_{+-}(\mathbf{q},\omega), \tag{13}$$

$G_0^{\pm}(\mathbf{k},\varepsilon) = (\varepsilon \mp \varepsilon_{\mathbf{k}} + i\delta\,\text{sgn}\,\varepsilon)^{-1}$, and $\varepsilon_{\mathbf{k}} = v|\mathbf{k}|$. Calculating the real and imaginary parts of (13) we find

$$\begin{aligned} \text{Im}\,\Sigma_{\mathbf{k}\varepsilon} &\approx -32\varepsilon\left(\xi \tan^{-1}\left[\frac{q_{\max}}{2k}\frac{(\xi+1)}{\sqrt{\xi(\xi+2)}}\right] + \frac{\xi^2}{\xi+1}\sqrt{\xi(\xi+2)}\right), \\ \text{Re}\,\Sigma_{\mathbf{k}\varepsilon} &\approx 16\xi\varepsilon \ln[q_{\max}(\xi+1)/2k]. \end{aligned} \tag{14}$$

where $q_{\max}$ is a cutoff in the magnon spectrum and $\xi = \lambda_t^2 C_0 S_z/8\pi v^2$ is the dimensionless constant. Using the self-energy (12) we can find the renormalized energy spectrum by diagonalizing again the Hamiltonian with the self-energy correction, $\widetilde{\mathcal{H}} = \widetilde{\mathcal{H}}_0 + \widetilde{\Sigma}(\mathbf{k},\varepsilon) \to \widetilde{\widetilde{\mathcal{H}}}$. This leads to

$$\widetilde{\widetilde{\mathcal{H}}} = \sigma_z\left[\Sigma_{\mathbf{k}\varepsilon} + \left(\Sigma_{\mathbf{k}\varepsilon}^2 + v^2k^2\right)^{1/2}\right]. \tag{15}$$

In this equation we should substitute $\Sigma_{\mathbf{k},\varepsilon=vk}$ for the upper energy branch, and $\Sigma_{\mathbf{k},\varepsilon=-vk}$ for the lower branch, as it corresponds to the self-energy at the mass surfaces for positive and negative energies. The constant (independent of k) part of the self-energy is already omitted as it leads to a homogeneous shift of the energy spectrum.

Using (14) we calculated numerically the real and imaginary parts of the function $\Sigma_{\mathbf{k},vk} - \Sigma_{0,0}$ and the energy spectrum corresponding to (15). The renormalized spectrum of electrons is shown in Fig. 5. It demonstrates that the velocity of electrons depends strongly on the coupling to the magnons. Namely, this interaction enhances the velocity at the vicinity of the Dirac point $k = 0$. Besides, as is evident, the energy spectrum is strongly nonlinear. It has the very unusual form of electron and hole bands corresponding to particles with a negative effective mass. The energy gap is solely related to a nonvanishing average magnetization. Figure 6 shows that the broadening of electron states due to the interaction with magnons is rather strong even at a very small coupling. Thus,

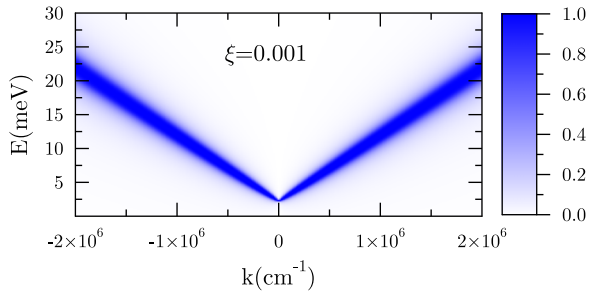

FIG. 6. (Color online) Spectral function of electrons for $\xi = 0.001$. The broadening is proportional to Im $\Sigma_{\mathbf{k}\varepsilon}$.

the electron-magnon interaction has a significant contribution to the momentum relaxation of electrons.

VI. CONCLUSION

Using detailed *ab initio* numerical simulations we have evaluated the electronic and magnetic properties of individual magnetic impurities on the surface of a topological insulator Bi_2Se_3. We find that their magnetic moments are ferromagnetically ordered and they turn out to be polarized perpendicular to the TI surface.

In the second step we set up a microscopic model for an array of such impurities interacting with the topological surface state electrons. Using an approach which takes into account the finite magnetization expectation value of the lattice S_z, we succeeded in computing the excitation spectra of the electronic degrees of freedom as well as of the magnons. Our main results are the linear spectrum of surface spin waves in the magnetic system and the nonlinear renormalized energy spectrum of surface electrons near the crossing point.

Our calculations demonstrate that one-site spin anisotropy does not affect the linearity of the magnon spectrum, which is solely due to the peculiarity of the RKKY interaction in graphene. Correspondingly, the anisotropy-induced parallel shift of the magnon dispersion does not affect the electron self-energy.

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