Temperature Induced Spin Density Wave in Magnetic Doped Topological Insulator Bi$_2$Se$_3$

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We study the magnetic properties of Bi$_2$Se$_3$ doped with isoelectronic magnetic impurities. We obtain that at zero temperature the impurities order ferromagnetically, but when raising the temperature the system undergoes a first order phase transition to a spin density wave phase before the system reaches the paramagnetic phase. The origin of this phase is the non-trivial dependence of the spin susceptibility on the momentum. We analyze the coupling of the non-uniform magnetic phase with the Dirac electronic system that occurs at the surfaces of the topological insulator.

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I. INTRODUCTION

Topological insulators (TI) are a newly discovered type of systems which are insulating in the bulk and characterized by the existence of a robust helical gapless Dirac two dimensional electron system at their surface[1–3].

TTI’s are typically band insulators for which strong spin orbit coupling produces an inversion of the bulk band gap. Therefore, in TTI’s the energy gap is related with the spin orbit coupling and that limits its magnitude. The most studied and more promising topological insulator is Bi$_2$Se$_3$, which is a three dimensional TI with a relatively large bulk energy gap $\sim 0.3$eV and with the Dirac point of the surface states located outside the bulk bands[4–6]. Angle resolved spectroscopy[4, 6] and scanning tunneling microscopy[7] experiments have shown the Dirac nature of the surface states of Bi$_2$Se$_3$.

The spin and wavevector of the surface states of a TI are strongly coupled, and the occurrence of a half-quantized Hall effect when an energy gap opens at the surface has been predicted[8, 9]. Due to the protected character of the Dirac states, a gap at the surface should be opened with a perturbation that breaks the time reversal symmetry. This can be done by doping the system with magnetic impurities. At the surface of the TI, because of the large spin-orbit coupling, the interaction between the Dirac-like surface states and the impurities induces a large single ion magnetic anisotropy and polarizes the spin of the impurities perpendicularly to the surface. This spin-orbit coupling translates in the opening of an energy gap at the Dirac point of the surface states[10–12].

From the experimental side, angle resolved photoemission spectroscopy (ARPES) studies on the surface of Fe-doped Bi$_2$Se$_3$ single crystals have confirmed the opening of an energy gap at the Dirac point[20] and the creation of odd multiples of Dirac fermions[21]. Also, recently, experiments in thin films of Cr-doped Bi$_2$Sb$_2$–xTe$_3$, has shown a large anomalous Hall conductance in a magnetically doped topological insulator[22].

However, recent experiments[23] found that the spins of Fe ions deposited on Bi$_2$Se$_3$ orient in plane. Also ARPES experiments[24, 25] found Dirac crossing even in the presence of magnetic impurities in contradiction with earlier experiments and existing theory. On the other hand, recently it has been reported the suppression of the Dirac point spectral weight, both in magnetically doped and undoped TI, suggesting that the observed gap at the Dirac point can not be taken as the sole evidence of a magnetic gap[26]. In addition, density functional theory based calculations[27] find that Co adatoms lying in the Bi$_2$Se$_3$ surface exhibit an energetically stable magnetic moment perpendicular to the surface, whereas for Co atoms located on the interlayer Van der Waals spacing the momentum is in the plane parallel to the surface. All these results indicate the complexity of the interpretation of the ARPES experiments and the possible importance of other effects not included in the Dirac hamiltonian, as crystalline anisotropy or surface reconstruction, might play an important role on the orientation of the magnetic impurities. In this work we use an effective hamiltonian for describing Bi$_2$Se$_3$, which although it does not include microscopic details of the material describes appropriately the basic properties of the Bi$_2$Se$_3$ related with its band structure topology.

In this work we study the phase diagram of magnetically doped Bi$_2$Se$_3$. Bi$_2$Se$_3$ is a layered material formed by five atom layers arranged along the z-direction. We find that at low temperatures the magnetic impurities order ferromagnetically along the z-direction. By raising the temperature, the TI undergoes two transitions: A first order transition from the ferromagnetic to the spin density wave phase, and at higher temperatures a second order transition from the spin density wave phase to the paramagnetic phase. The spin density wave phase has both, the polarization and the wavevector, parallel to the z-direction. We have also studied the effect of the surface states by calculating the magnetization as function of temperature of a slab of Bi$_2$Se$_3$ topological insulator. Here we find that the surface magnetization survives to higher temperatures than the bulk spin density wave phase.

The paper is organized as follow, in Section II we define the hamiltonian we use for describing the electrical properties of Bi$_2$Se$_3$. In Section III we calculate the
wavevector dependent paramagnetic spin susceptibility of Bi$_2$Se$_3$ and discuss the interaction between magnetic impurities through the paramagnetic susceptibility. In Section IV we formulate a Landau theory for describing the magnetic order of magnetically doped Bi$_2$Se$_3$, and discover the existence of a ferromagnetic to spin density wave phase transition at finite temperature. In Section V we study the polarization profiles of a magnetically doped Bi$_2$Se$_3$ slab and analyze the effect that the Dirac-like surface states have on the magnetic phases. We finish in Section V with some conclusions and remarks.

II. HAMILTONIAN

The low energy and long wavelength electronic properties of Bi$_2$Se$_3$ topological insulators are described by the four bands $k \cdot p$ Hamiltonian\(^2\),

$$H = E(k) + \mathcal{M}(k) \tau_z \otimes I + A_1 k_z \tau_x \otimes \sigma_z + A_2 (k_x \tau_x + k_y \tau_y) \otimes \sigma_x$$  \hspace{2cm} (1)

where $\sigma_x$ and $\tau_x$ are Pauli matrices, $I$ the unity matrix, $\mathcal{M}(k)=M_0 - B_2(k_x^2 + k_y^2) - B_1 k_z^2$, $k_\pm = k_x \pm ik_y$ and $E(k)=C + D_1 k_x^2 + D_2 (k_x^2 + k_y^2)$. The Hamiltonian is written in the basis $|1> = |p1^+, \uparrow>$, $|2> = -i|p2_-, \downarrow>$, $|3> = |p1^-, \downarrow>$, $|4> = i|p2_-, \uparrow>$, which are the hybridized states of the Se-p orbital and the Bi-p orbital with even (+) and odd (−) parities and spin up ($\uparrow$) and down ($\downarrow$). The Hamiltonian parameters for Bi$_2$Se$_3$ are\(^2\) $M_0 = 0.28$eV, $A_1 = 0.22eVnm$, $A_2 = 0.41eVnm$, $B_1 = 0.10eVnm^2$, $B_2 = 0.566eVnm^2$, $C_0 = 0.0068eV$, $D_1 = 0.013eVnm^2$ and $D_2 = 0.196eVnm^2$. In this basis the spin operators get the form\(^2\) $S_z = I \otimes \sigma_z$, $S_x = \tau_z \otimes \sigma_x$ and $S_y = \tau_z \otimes \sigma_y$.

III. BULK SPIN SUSCEPTIBILITY

The paramagnetic susceptibility obtained from the Hamiltonian Eq[1] has the form

$$\chi_{\mu \nu}(q) = \frac{2}{\Omega} \sum_{k \in V} \sum_{n', \text{empty}} |<n', k| S_{\mu} |n, k>|^2 \varepsilon_{n', k+q} - \varepsilon_{n, k}.$$  \hspace{2cm} (2)

Here $|n, k>$ and $\varepsilon_{n, k}$ are the eigenfunctions and eigenvalues of Hamiltonian Eq[1] and $\Omega$ is the sample volume. In the case of an insulator, this spin susceptibility is caused by the coupling of the valence and conduction band induced by the spin operator\(^3\). The susceptibility is a smooth function of the wavevector and because the system is an insulator there are no anomalies associated with Fermi surfaces. The symmetry of the original Hamiltonian dictates that the non-diagonal elements of the susceptibility tensor are zero and $\chi_{xx} = \chi_{yy} = \chi_{zz}$.

In Fig[1] we plot the $\chi_{xx}$ and $\chi_{zz}$ as a function of $q_z$ and $q_x$. The direct coupling, $A_2 k_z$, between atomic orbitals with opposite parities and opposite $z$-component of the spin, makes that for $k_\pm \neq 0$, occupied and empty states are coupled through $S_z$. Whereas those states are only connected through $S_x$ when $k_\pm \neq 0$. This makes $\chi_{zz}(q) > \chi_{xx}(q)$.

The more important contribution to $\chi_{zz}(q_z)$ comes from regions in the reciprocal space where the matrix elements $<n', k + q_z|S_z|n, k>$, with $n$ occupied and $n'$ empty, reaches the maximum value. This happens when $\mathcal{M}(k)=0$ or $\mathcal{M}(k + q_z)=0$. For a given $k_z$ these conditions define two circular crowns of radius $\sqrt{M_0-B_2 k_z^2}$ and $\sqrt{M_0-B_1(k_z+q_z)^2}$ and thickness $A_2/(2B_2)$. Therefore, the area of the reciprocal space that contributes appreciably to $\chi_{zz}(q_z)$ increases with $q_z$. For larger values of $q_z$ one of the circular crowns collapses to zero and the contributions to the integral decrease. This behavior qualitatively the maximum that $\chi_{zz}$ presents at a wavevector $G \sim \sqrt{M_0/B_1}$.

The existence of a maximum in $\chi_{zz}(q_z)$ at finite $q_z$ is robust against small changes in the parameters of the four bands Hamiltonian. In Fig[2] we plot $\chi_{zz}(q_z)$ for different values of the TI gap. The position of the maximum decreases continuously towards $q = 0$ when $M_0$ decreases and only disappears for small values of $M_0$. In the normal insulator phase, $M_0 < 0$, the maximum always occurs at $q = 0$.

A. Coupling between diluted magnetic impurities

Consider now a TI doped with magnetic impurities of spin $S$. We assume that the number of electrons in the system does not change in the presence of the magnetic impurities. That can be achieved by doping with iso-
electronic magnetic dopants or by adding compensating non-magnetic dopants\cite{31}. In this work we consider the dilute limit, i.e. concentration of impurities smaller than 5%, for which the direct interaction between the spin of the magnetic impurities can be neglected.

However, the electrons spins have a strong exchange coupling, $\frac{S^2}{2}J(|r|)$, with the magnetic impurities spins which, in turn, are equally affected by the exchange field of the electrons. In this form the magnetic impurities in the system interact mediated by electronic states. We treat this interaction in second order perturbation theory\cite{32,33}, that has proved to be a reliable approximation in diluted magnetic semiconductors\cite{33,34}. In this approach the effective exchange parameter between two magnetic impurities separated by a vector $\mathbf{R}$ and spins pointing in the $\nu$-direction is,

$$J_{\nu}(\mathbf{R}) = -\frac{S^2}{4}J_{eff}^2 \Omega \sum_\mathbf{q} \chi_{\nu\nu}(\mathbf{q}) e^{i \mathbf{q} \mathbf{R}}$$

(3)

where $J_{eff} = \int J(|r|)dr$ is the effective exchange coupling between the magnetic impurity and the electron spin.

Because $\chi_{zz} > \chi_{xx}$ in all range of wavevectors, the system has an easy axis of magnetization along the $z$-direction and therefore isoelectronic magnetic impurities in Bi$_2$Se$_3$ will tend to polarize in the $z$-direction. The maximum that the spin susceptibility presents at finite temperature, $\chi_{zz}$, for different values of $M_0$, is given in Table I, for which the direct interaction between the spin of the magnetic dopants\cite{31}. In this work we consider the dilute limit, i.e. concentration of impurities smaller than 5%, for which the direct interaction between the spin of the magnetic impurities can be neglected.

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The phase diagram of a system described by a free energy as that of Eq. 8 depends on the relative magnitudes of the fourth-order potentials [37]. In our case the product of the pre-factors of $m_0^4$ and $m_2^4$ is smaller than the square of the $m_2^2 m_0^2$ pre-factor and there is no phase coexistence in the phase diagram. By increasing the temperature, there is a first order transition from the FM phase to the SDW phase at

$$T^* = \frac{\sqrt{3} T_0 - \sqrt{2} T_G}{\sqrt{3} - \sqrt{2}}.$$ (10)

This is the main result of this work: by heating, a magnetically doped TI undergoes two phase transitions, a FM to SDW first order transition at $T^*$ and a SDW to paramagnetic second order transition at $T_G$. Although at $T=0$, the FM phase has lower energy than the SDW phase, the FM to SDW transition at finite $T$ occurs because the entropy of the SDW increases faster with $T$ than the entropy of the FM phase.

In the next section we analyze how the surface states existing in topological insulators couple to the bulk magnetic polarization.

V. SPIN POLARIZATION OF MAGNETICALLY DOPED TI SLABS

At the surface of a TI there exists a two dimensional Dirac electron gas. Because the chirality of the electron gas, an exchange field perpendicular to the surface opens a gap in the spectra. Then, in order to minimize the energy, a magnetic impurity will polarize perpendicularly to the surface [10–12, 18]. In the diluted limit, surface states mediate an RKKY interaction among the impurities which is always ferromagnetic, whenever the chemical potential resides near the Dirac point [10] [12] [18]. Therefore magnetic impurities at the surface of a TI will order ferromagnetically perpendicular to the surface.

We are going to study numerically the spin polarization as function of temperature and position of a magnetically doped TI slab. The objective here is first to confirm the results obtained with the Landau functional where we consider a unique Fourier component of $\chi_{zz}(q_z)$ and second to analyze the coupling between the surface and the bulk magnetization.

We analyze a TI slab of thickness $L$ and perpendicular to the $z$-direction. We expect the electron affinity of Bi$_2$Se$_3$ to be much larger than its band gap. Therefore, at the surface of the TI we will neglect the penetration of the electron wavefunction into the vacuum. The eigenvalues, $\varepsilon_{n,k}$, and wavefunctions, $\Psi_{n,k}(z)$, are obtained by solving Eq. 4 with $k_z = -i 0_2$ and forcing the wavefunction to vanish at $z = 0$ and $z = L$. This is satisfied expanding $\Psi_{n,k}(z)$ in harmonics,

$$\Psi_{n,k}(z) = \frac{e^{i k r}}{\sqrt{A}} \sqrt{\frac{2}{L}} \sum_{l=1}^{N_{\text{max}}} \sum_{j=1,4} a^l_{n,j}(k) \sin \left( \frac{l}{L} \pi z \right),$$ (11)

where $A$ is the sample area and we choose $N_{\text{max}}$ large enough so that the results do not depend on it.

For $L > 10$nm, the surfaces of the slab are decoupled and the band structure is independent of $L$. In the bulk energy gap region, appear some surface states which are the benchmark of the TI. In Fig. 3 we plot the band dispersion and the shape of the wavefunction of these states. The results we obtain agree completely with previous results [3, 29].

In the slab geometry the momentum in the $z$-direction is not a good quantum number and the paramagnetic susceptibility depends on two position indices $z$ and $z'$. Therefore, in the virtual crystal approximation and in second order perturbation theory, the internal energy of the magnetically doped TI slab is,

$$E = \frac{J}{2L} \int_0^L \int_0^L dz dz' \tilde{\chi}(z, z') m(z) m(z'),$$ (12)

$$\tilde{\chi}(z, z') = \frac{1}{A} \sum_{n, n', k} n_F(\varepsilon_{n,k}) - n_F(\varepsilon_{n',k}) \times \frac{\Psi^*_{n,k}(z) S_z \Psi_{n',k}(z) \times \Psi^*_{n',k}(z') S_z \Psi_{n,k}(z')},$$ (13)

where $n_F(\varepsilon)$ is the Fermi distribution function. $\tilde{\chi}(z, z')$ indicates the coupling between uniform polarized $(x, y)$-planes, located at positions $z$ and $z'$. The interaction between magnetic impurities is mediated by electrons in the system, and because the bulk system is an insulator, the interaction is very short ranged in the $z$-direction, see Fig. 4.

We compute the temperature dependence of the magnetization profile in the mean field approximation. At a given position $z$, the magnetization $m(z, T)$ feels a $(in \ energy\ units)$ magnetic field,

$$B(z) = J \int_0^L dz' \tilde{\chi}(z, z') m(z'),$$ (14)

and the magnetization of an isolated impurity in the pres-
FIG. 4: (Color online) $\tilde{\chi}_{zz}(z,z')$ evaluated at the maximum of the surface wavefunction, $z=1.2$ nm, and at the center of a 20 nm thick slab, as function of $z'$. The first case corresponds to a region near the surface, where the two dimensional Dirac electron system contributes to the response functions. In the latter case the response function is not affected by the surface and it is the bulk response function. In both cases the functions are very peaked at $z=z'$. The negative values of the coupling in the bulk response function is a consequence of the maximum that the response function present at $q_z=G$ in the reciprocal space. Near the surfaces, and because of their metallic character, the magnetic coupling is stronger. This is reflected in the asymmetry of the dashed line, the interaction between planes is larger as closer the planes are to the surface.

FIG. 5: (Color online) Magnetization as a function of temperature for TI slabs of thickness (a) $L=5$ nm, (b) $L=10$ nm and (c) $L=30$ nm. $T_0$ is the bulk FM critical temperature of the topological insulator. The small "step" in the middle of the first order transition that occurs at $L=30$ nm is consequence of an interference effect between the surface magnetization and the bulk SDW phase.

FIG. 6: (Color online) Magnetic polarizations as a function of the position across the topological insulator slab $z$, for different layer thickness and temperatures.

ence of the molecular field is,

$$m(z, T) = \coth \left( \frac{B(z)}{k_B T} \right) - \frac{k_B T}{B} . \quad (15)$$

Solving self-consistently Eq. 14 and Eq. 15, we obtain the magnetization profiles as a function of T.

Because the metallic surface states intermediate a RKKY coupling at the surface, the response function, $\tilde{\chi}(z,z')$ is larger near the surface than in the bulk, see Fig. 4. Therefore, as function of $T$, the absolute value of the magnetization decreases faster in the bulk region than in the surface. However, it is important to note that the surface and the bulk are part of a unique system and therefore there is only a unique critical temperature, corresponding to the transition of the paramagnetic phase.

In Fig. 5 we show the magnetization as function of temperature for TI slabs of thickness $L = 5$ nm, $L = 10$ nm and $L = 30$ nm. We plot the average value of $m(z, T)$, and the value of the magnetization on top of the surface states. In Figure 3 we plot the magnetization profiles for different temperatures and $L = 5$ nm, $L = 10$ nm and $L = 30$ nm.

For $L = 10$ nm and $L = 30$ nm the surfaces are practically decoupled and the central part of the slab behaves as bulk. There is a strong jump in the magnetization at
$T^*$, that indicates the first order FM to SDW transition. In the SDW phase the oscillating magnetization does not contribute to the total magnetization and the magnetization for $T > T^*$ is due to surface states. In Fig. 6(b)-(c), it is apparent at the center of the slab, the abrupt transition from an uniform magnetization phase to a SDW phase. For smaller thickness of the slab, Fig. 6(a), the surface states are coupled and there is no well defined phase. For smaller thickness of the slab, Fig. 6(a), the surface states are coupled and there is no well defined phase. For smaller thickness of the slab, Fig. 6(a), the surface states are coupled and there is no well defined phase. For smaller thickness of the slab, Fig. 6(a), the surface states are coupled and there is no well defined phase. For smaller thickness of the slab, Fig. 6(a), the surface states are coupled and there is no well defined phase. 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VI. FINAL REMARKS AND CONCLUSIONS

In this work we study the phase diagram of magnetically doped Bi$_2$Se$_3$. At low temperatures the magnetic impurities order ferromagnetically along the $z$-direction. By raising the temperature, the TI undergoes two transitions: A first order transition from the ferromagnetic to the spin density wave phase, and at higher temperatures a second order transition from the spin density wave phase to the paramagnetic phase. This results could explain recent experimental results[40] that suggest the existence, as function of the temperature, of two different magnetic phases in Fe doped Bi$_2$Se$_3$.

We have also studied the effect of the surface states by calculating the magnetization as function of temperature of a slab of Bi$_2$Se$_3$ topological insulator. Here we find that the surface magnetization survives to higher temperatures than the bulk spin density wave phase. The existence of a range of temperatures for which the bulk magnetization practically vanishes whereas a finite magnetization exits at the surface, could explain some experimental results that observe a gap at the surface of Bi$_2$Se$_3$ but not bulk magnetism[20, 21].

It is important to analyze the behavior of the phase diagram as function of the gap parameter $M_0$. In Fig. 7 we show the phase diagram of a magnetically doped thick TI slab as a function of $M_0$. For $M_0 < 0$ the system is a normal insulator and there are no surface states. Also the spin orbit coupling is small and the SDW phase does not exist. For $M_0 > 0$ the system is a TI and the gap increases with $M_0$. TI with larger gaps have more metallic surface states and the FM order at the surface is therefore more robust. Also the effective spin orbit coupling is stronger and both $T^*$ and $T_G$ increase with $M_0$. The results of Fig. 7 show that the range of temperatures where the SDW phase exists increases with $M_0$.

Finally we make an estimation of the critical temperature. From the band structure parameters of Bi$_2$Se$_3$, choosing the density of the magnetic impurities to be $5 \times 10^{20}$ cm$^{-3}$, the total angular momentum of a single magnetic ion to be $S = 3/2$ and the effective exchange coupling $J_{eff} = 250$ meV nm$^3$[12] we obtain $T_{Gbulk} = 18K$. This values can change by factors of two by changing the magnetic ions or the density of impurities. It is well known that the mean-field approximations tend to overestimate the transition temperature due to the neglect of the fluctuations. In diluted magnetic semiconductors thermal fluctuations reduce the value of the Curie temperature in near 30%[55], and we expect a similar reduction in topological insulators.

Acknowledgments

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Appendix A: Mean Field Expression for the Entropy.

In this section we obtain an expression for the entropy of a system of classical spins of magnetization $m$, that are coupled with the topological insulator through a general term $E[m]$. The Free Energy of a system of classical spins of magnitude unity in an external magnetic field is

$$F = -\frac{1}{\beta} \ln \left( \frac{2 \sinh(\beta h)}{\beta h} \right) ,$$

from where the magnetization can be calculated as

$$m \equiv m > = \frac{\partial F}{\partial h} = -\frac{1}{\tanh(\beta h)} - \frac{1}{\beta h} . \tag{A2}$$

The entropy of the spin system is then

$$-TS = F - mh = \frac{1}{\beta} \left( -\ln \left( \frac{2 \sinh(\beta h)}{\beta h} \right) - m\beta h \right) . \tag{A3}$$

The total energy of the system is

$$F_{\text{total}} = E[m] - TS = E[m] - \frac{1}{\beta} \left[ \ln \left( \frac{2 \sinh(\beta h)}{\beta h} \right) + m\beta h \right]$$

where $E[m]$ is the change in the electronic energy of the system because of the polarization of the magnetic impurities.

To obtain $h$, we minimize the total free energy with respect to $h$, $\partial F_{\text{total}} / \partial h = 0$. In the limit of small $h$

$$\ln \left( \frac{2 \sinh(\beta h)}{\beta h} \right) \simeq \ln(2) + \frac{(\beta h)^2}{6} - \frac{(\beta h)^4}{180} + ... \tag{A5}$$

In this limit, the minimization condition gives $\beta h = -3m - \frac{4}{5}m^3 + ...$, and the entropy gets the form

$$-TS = -k_B T \ln(2) + \frac{3}{2} k_B T m^2 + \frac{9}{20} k_B T m^4 . \tag{A6}$$

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