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Magnetoelectric effect induced by electron–electron interaction in three dimensional topological insulators

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ABSTRACT

We compute the magnetoelectric response of an interacting topological insulator in three space dimensions with a short range interaction between electrons in different orbitals. We show that in the presence of interactions and inverted bands the chiral phase is gauged away and replaced by a topological angle (θ-term) which is determined by saddle point of the interacting action and the Fujikawa integration measure. The magnetoelectric response breaks time reversal symmetry which is restored at strong interactions. The effect is equivalent to the one in four dimensions without interaction; it can be observed by measuring the Faraday rotation under external stress.

1. Introduction

When time reversal symmetry is broken the electromagnetic Hamiltonian for a material in $3+1$ dimensions $H=\frac{1}{2}(\epsilon E^2+\frac{1}{\mu}B^2)$ is modified by the term $\delta H=\theta(\frac{e^2}{2\pi h})E\cdot B$ where $0<\theta<\pi$. The value of topological angle θ is determined by an axion field $\theta(\vec{r},t)$ which in the static case becomes $\theta(\vec{r})\approx\theta$ [1–4]. The axion field results from the projection of a higher dimensional Hamiltonian to $3+1$ dimensions. For time reversal invariant systems such as non-interacting topological insulators (*TI*) the axion field is replaced by the topological angle $\theta=\pm\pi$ and the second Chern number in $4+1$ dimensions. Insulators with spin–orbit interactions can give rise to either regular insulators or to topological insulators. The low energy excitations of the insulators such as Bi_2Se_3 and Bi_2Te_3 can be approximated by a two-band model with spin–orbit interactions which respect the time reversal symmetry. One finds that when bands at the Γ point are inverted, the system is a *TI* according to the classification of the second Chern number [5] or band invariants introduced in Ref. [6]. One of the possible experimental evidences came from the Faraday effect, when circularly polarized light passes from a medium with $\theta=0$ (normal insulator) to a medium with $\theta\neq 0$ a rotation of the polarization is expected. Since time reversal symmetry is not broken the rotation must correspond to a topological angle $\theta=\pm\pi$ [1,7,8]. One of the experimental difficulties to observe a quantized response arises from the fact that the experiments are performed in three space dimensions and the second Chern topological invariant exists in four space dimensions.

A formal solution to this problem was given in [7–9] which suggested to use dimensional reduction. One performs the computations in four space dimensions and then compactifies one of the coordinates to a small circle. Other solutions based on a macroscopic polarization on the surface of the sample have been proposed [10,11]. An adiabatic approach to the polarization has been given in [12] for the second Chern number. The relation between the second Chern number and polarization follows from the mathematical physics literature [5]. The second Chern number can be written as an external derivative of a *local three-form*. This means that for different regions we have different three-forms. The use of Stokes theorem allows us to show that the four space dimensional integration of the Chern character [5] is equal to the boundary difference of the three-forms in three dimensions. This result allows us to identify the Chern number with the polarization difference ΔP for a band model with no interactions [9]. Another important result [5,13] is the chiral anomaly. The Dirac equation in three space dimensions does not conserve the γ^5 current J_5^μ, instead we have (the integral over the 4-torus) $\int_{T^4}\partial_\mu J_5^\mu=\Delta P$. Therefore the presence of a coupling field of the form $\gamma^5\varphi$ can generate a polarization term ΔP as obtained in the band model without interactions in four space dimensions. The relation between the topological angle θ and quantization has been discussed in [14]. Only recently the effect of interactions on *TI* has been considered [15]. The effect of an applied magnetic field on the surface of a *TI* gives rise to a simple relation between the Faraday and Kerr rotations [16].

The main purpose of this Letter is to present a derivation for the magnetoelectric response of *TI* in three space dimensions. This is an extension of the work in Ref. [17]. We obtain this result using

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an explicit two-body orbital interaction for insulators with inverted bands. The interaction gives rise to an effective action which is controlled by a "bond order" parameter defined between orbitals. The action of the interacting electrons and the path integral measure are invariant under an arbitrary chiral transformation [13]. The saddle point of the action has the γ^5 symmetry and determines the bond order parameter as well as fixes the coefficient of the chiral transformation. As a result one obtains an electromagnetic action which breaks the time reversal symmetry. The coefficient of the electromagnetic term is determined by the saddle point and the integration measure which fix the topological angle θ. Experimentally the topological angle is determined by the coupling constants and external perturbations such as stress [18]. The value of θ determines the Faraday rotation between two regions: the first region consists of an interacting *TI* and the second region represents a non-interacting insulator. The value of θ in turn is determined by the integration over the bond order parameter. At a particular interaction strength the value of θ is $\theta = \pm\pi$, time reversal symmetry is restored and the system is a *TI*. For $\theta = 0$ we have a regular insulator. Only for special values of the interaction, the values of $\theta = 0, \pm\pi$ are described by a second Chern number in three space dimensions. Since the second Chern number exists only for four space dimensions for non-interacting electrons, we conclude that the presence of electron–electron interaction in a three dimensional model with inverted bands has a second Chern topological invariant and behaves as a non-interacting *TI* in four space dimensions.

The contents of the Letter are as follows. In Section 2 we introduce the model for *TI* in the presence of a bond interaction which, with the help of the Hubbard–Stratonovich transformation, is represented as a chiral charge density wave field $\varphi(\vec{r})$. Section 3 represents the central part of this Letter, where we include the external electromagnetic field $\vec{A}^{ext}$ in the action. We perform a chiral transformation $e^{i\lambda(\vec{r})\gamma^5}$ for an arbitrary field $\lambda(\vec{r})$. Since the partition function is invariant under this transformation, the action and the integration measure are modified. The integration measure generates the term $\lambda(\vec{r})\vec{E}\cdot\vec{B}$ which breaks the time reversal symmetry. The fermionic action S contains a modified bond order parameter which depends on the field $\lambda(\vec{r})$. The value of $\lambda(\vec{r})$ can be fixed by demanding that the transformed bond order parameter vanishes. As a result, the term $\lambda(\vec{r})\vec{E}\cdot\vec{B}$ becomes a function of $\lambda(\varphi(\vec{r}))$. We perform a saddle point integration over the bond order parameter and obtain the electromagnetic response function $\theta(\frac{e^2}{2\pi h})\vec{E}\cdot\vec{B}$ (where θ is a function of the fluctuation fields around the saddle point). Section 4 contains our main conclusions.

2. Topological insulator in three space dimensions

We will compute the magnetoelectric response of the *TI* materials Bi_2Se_3 and Bi_2Te_3. The low energy bands consist of four projected states, the conduction and valence states $|P1^+_-,\pm\frac{1}{2}\rangle$ and $|P2^+_-,\pm\frac{1}{2}\rangle$ near the Fermi surface at the Γ point [17,19–23]. Due to the strong spin–orbit coupling the level $|P1^+_-,\pm\frac{1}{2}\rangle$ is pushed down while $|P2^+_-,\pm\frac{1}{2}\rangle$ is pushed up resulting in a band inversion. Using the notation $|orbital = \tau = 1\rangle \otimes |spin = \sigma = \uparrow,\downarrow\rangle \equiv |P1^+_-,\pm\frac{1}{2}\rangle$ and $|orbital = \tau = 2\rangle \otimes |spin = \sigma = \uparrow,\downarrow\rangle \equiv |P2^+_-,\pm\frac{1}{2}\rangle$ we obtain the effective Hamiltonian $\hat{h}^{3d}$ at the Γ point: $\hat{h}^{3d} = k_2(\sigma^1\otimes\tau^1) - k_1(\sigma^2\otimes\tau^1) + \eta k_3(\sigma^3\otimes\tau^1) + M(\vec{k})(I\otimes\tau^3)$, where $M(\vec{k}) = M(0) - Bk^2$ determines whether the insulator is trivial or topological. Here B is a parameter ("inverted" effective mass). For $\frac{M(0)}{B} > 0$ we have a *TI* (an insulator with an inverted gap) and a regular insulator for $\frac{M(0)}{B} < 0$ [6,8,23]. The band anisotropy in the z direction is given by $\eta \ll 1$. Due to the Nielsen–Ninomiya theorem [22] the total number of Dirac points must be even. The Dirac Hamiltonian linearized around the Γ point has been considered in Ref. [23] and contains additional non-relativistic terms. The eigenvalues in the vicinity of the Γ point are given by $E(\vec{k}) = \pm\sqrt{k_1^2 + k_2^2 + \eta^2 k_3^2 + M(\vec{k})^2}$. We extend the model (with a single Dirac point) to a torus and demand the momentum periodicity $-\pi \leqslant k_1 \leqslant \pi$, $-\pi \leqslant k_2 \leqslant \pi$, $-\pi \leqslant k_3 \leqslant \pi$. It is convenient to perform a unitary transformation $U = (e^{i\frac{\pi}{4}\sigma^3}\otimes I)$:

$$h^{3d} = U^{-1}\hat{h}^{3d}U = k_1\alpha^1 + k_2\alpha^2 + \eta k_3\alpha^3 + M(\vec{k})\beta, \tag{1}$$

where the matrices α and β are given by: $\alpha^i = (\sigma^i\otimes\tau_1)$, $i = 1,2,3$, and $\beta = (I\otimes\tau_3)$.

Next, we include the bond interactions in three space dimensions. We consider a particular type of bond interaction H_{int} in three space dimensions which we describe using the four component spinor $\Psi(\vec{r}) = [\Psi_{\tau=1}(\vec{r}), \Psi_{\tau=2}(\vec{r})]^T$, where $\Psi_\tau(\vec{r})$ is a two component spinor with $\sigma = \uparrow,\downarrow$, $\Psi_\tau(\vec{r}) = [\Psi_{\tau,\uparrow}(\vec{r}), \Psi_{\tau,\downarrow}(\vec{r})]^T$ and $n_{\tau,\sigma}(\vec{r}) = \Psi^\dagger_{\tau,\sigma}(\vec{r})\Psi_{\tau,\sigma}(\vec{r})$ represents the fermion number for the orbital τ and spin σ

$$\begin{aligned}
H_{int} &= \frac{-U_{eff}}{2}\int d^3r\Big[\sum_{\sigma=\uparrow,\downarrow}\big(\Psi^\dagger_{\tau=1,\sigma}(\vec{r})\Psi_{\tau=2,\sigma}(\vec{r}) \\
&\quad - \Psi^\dagger_{\tau=2,\sigma}(\vec{r})\Psi_{\tau=1,\sigma}(\vec{r})\big)\Big]^\dagger \\
&\quad \times\Big[\sum_{\sigma=\uparrow,\downarrow}\big(\Psi^\dagger_{\tau=1,\sigma}(\vec{r})\Psi_{\tau=2,\sigma}(\vec{r}) - \Psi^\dagger_{\tau=2,\sigma}(\vec{r})\Psi_{\tau=1,\sigma}(\vec{r})\big)\Big] \\
&= \frac{U_{eff}}{2}\int d^3r\Big[\sum_{\sigma=\uparrow,\downarrow}\Psi^\dagger_{\tau=1,\sigma}(\vec{r})\Psi_{\tau=2,\sigma}(\vec{r}) \\
&\quad - \sum_{\sigma=\uparrow,\downarrow}\Psi^\dagger_{\tau=2,\sigma}(\vec{r})\Psi_{\tau=1,\sigma}(\vec{r})\Big]^2 \\
&= \frac{-U_{eff}}{2}\int d^3r\big[\Psi^\dagger(\vec{r})\big(I\otimes\tau^2\big)\Psi^\dagger(\vec{r})\big]^2,
\end{aligned} \tag{2}$$

where $U_{eff} > 0$. The proposed interaction in Eq. (2) is related to the following "orbital Hartree–Fock" E_{H-F} interaction:

$$\begin{aligned}
E_{H-F} \equiv 2U_{eff}\int d^3r\big[&n_{1,\uparrow}(\vec{r})n_{2,\uparrow}(\vec{r}) + n_{1,\downarrow}(\vec{r})n_{2,\downarrow}(\vec{r}) \\
&+ n_{1,\uparrow}(\vec{r})n_{2,\downarrow}(\vec{r}) + n_{1,\downarrow}(\vec{r})n_{2,\uparrow}(\vec{r})\big].
\end{aligned} \tag{3}$$

The difference between E_{H-F} and H_{int} is given by the term: $-\frac{U_{eff}}{2}(n_{1,\uparrow}(\vec{r},t) + n_{2,\uparrow}(\vec{r},t) + n_{1,\downarrow}(\vec{r},t) + n_{2,\downarrow}(\vec{r},t))$. This term is taken into account in the calculation by using a modified chemical potential. Therefore the E_{H-F} Hamiltonian is a good approximation to the proposed bond interaction Hamiltonian H_{int}.

The action for the three dimensional *TI* Hamiltonian h^{3d} with the interaction H_{int} is given by:

$$\begin{aligned}
S = \int_{-\infty}^{\infty} dt\int d^3r\Big[&\Psi^\dagger(\vec{r},t)\Big[i\partial_t + i\alpha^1\partial_1 + i\alpha^2\partial_2 + i\eta\alpha^3\partial_3 \\
&- \beta\Big(M(0) - B\sum_{l=1,2}\partial_l^2\Big)\Big]\Psi(\vec{r},t) \\
&+ \frac{U_{eff}}{2}\big(\Psi^\dagger(\vec{r})\big(I\otimes\tau^2\big)\Psi^\dagger(\vec{r})\big)^2\Big].
\end{aligned} \tag{4}$$

Using the Hubbard–Stratonovich transformation we replace the interaction term by a chiral density wave field $\varphi(\vec{r},t)$. The interaction corresponds to a charge density wave order which acts between the bands (orbitals). The order parameter φ emerges from the ground state expectation value $\langle\sum_{\sigma=\uparrow,\downarrow}\Psi^\dagger_{\tau=1,\sigma}(\vec{r})\Psi_{\tau=2,\sigma}(\vec{r})\rangle = i\varphi$