Reverse Stark effect, anomalous optical transitions, and control of spin in topological insulator quantum dots

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Formed through a closed domain magnetic heterostructure on the surface of a three-dimensional topological insulator, a quantum dot permits a class of quantized interfacial states of topological origin. We find that these states exhibit a remarkable reverse Stark effect in response to an applied electric field. In particular, those topological states whose energies are within the gap exhibit peculiar electrical alignments that are opposite to those associated with the conventional quantum-confined Stark effect in that the positive- (negative-) energy states tend to align with (against) the direction of the field. The phenomenon has unusual implications for the associated optical transitions. Furthermore, the exotic topological states exhibit polarized spin textures that can be effectively controlled electrically or optically, opening an avenue for potential applications in Dirac-material-based spintronics.

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I. INTRODUCTION

In systems exhibiting the conventional quantum-confined Stark effect (QCSE), e.g., a semiconducting quantum well, an external electrical field shifts the electronic states in the conduction band to lower energies and the hole states in the valence band to higher energies [1]. As a result, the energy differences between the electronic and hole states are narrowed, reducing the frequencies of the permitted photon absorption or emission. In this paper, we report the intriguing phenomenon of reverse Stark effect: in topological Dirac materials an applied electrical field tends to widen the energy differences and consequently increase the light absorption or emission frequencies.

Uncovering, understanding, and exploiting exotic quantum phases are frontier problems in physics [2]. Recent years have witnessed a great deal of effort in phase phenomena of certain topological origin [3,4]. For example, two-dimensional (2D) gapless topological phases were predicted and realized at the interface between bulk Bi2Se3 crystal and the vacuum [5], where a change in the Z2 invariant from the former to the latter occurs. Inducing an energy gap by breaking the time-reversal symmetry in the vicinity of a magnetic material can lead to exotic phases of broken symmetry with dramatic physical consequences [4,6] such as the zero-field half-integer quantum Hall effect [3], topological magnetoelectric effect [7], and magnetic monopole [8]. Topological effects in gapped Dirac materials are thus quite intriguing, where topologically protected chiral interfacial states carrying dissipationless currents, which share the same mechanism as that for the Jackiw-Rebbi modes [9], can arise. More recently, it was demonstrated that tuning the topological behaviors through an electric field can lead to the quantum spin Hall effect, bringing field-effect topological transistors closer to reality [10].

We investigate the response of the topological states in a confined geometry, e.g., a quantum dot formed on the surface of a three-dimensional (3D) topological insulator via a closed magnetic domain heterostructure, to an applied electric field. The system can be described by the Dirac equation subject to proper mass confinement. With an inverted mass profile, a branch of quantized topological edge states can emerge [11]. We find that, when an external electric field is applied, the under-gap topological states exhibit quite unusual alignments: the positive- (negative-) energy electronic states follow (align against) the direction of the field. As a result, a reverse QCSE occurs in that the frequencies of the permitted light absorption or emission increase. Remarkably, these states possess spin textures of ringlike in-plane polarization, which can be effectively controlled electrically or optically. We provide an analysis based on solutions of the Dirac equation to explain these counterintuitive phenomena. The findings can have potential applications in Dirac material based optoelectronics and spintronics.

This paper is organized as follows. In Sec. II, we formulate the theoretical model and demonstrate the emergence of quantized topological edge states. In Sec. III, we investigate the response of the topological edge states to an external electric field and present the phenomena of reverse electric alignments, electrically controllable spin, and optical transitions. To elaborate on the practical significance of these phenomena, in Sec. IV, we discuss feasible experimental schemes and potential applications.

II. HAMILTONIAN AND QUANTIZED TOPOLOGICAL STATES

Consider a dot geometry formed on the surface of a 3D topological insulator (TI) through a nanoscale magnetic heterostructure, as schematically shown in Fig. 1(a). For low energies, the system is described by the following 2D Dirac Hamiltonian [4,12]:

\[ \hat{H} = v_F \hat{\sigma} \cdot \hat{p} - e \varphi + M(r) \hat{\sigma}_z, \]  

where \( v_F \) is the Fermi velocity, \( \hat{\sigma} \) is the vector of Pauli matrices, \( \hat{p} = (p_x, p_y, 0) \), \( r = (x, y, 0) \), the potential \( \varphi \) comes from the applied electric field \( \mathbf{E} = -\nabla \varphi \), and \( -e < 0 \) is the charge of an electron. The position-dependent “mass” term \( M \) is responsible for the confinement through a time-reversal symmetry-breaking mechanism. For simplicity, we assume...
that the confined region is circularly symmetric with potential jumps at the boundary:

\[ \mathcal{M}(r) = \mathcal{M}_1 \Theta(R - r) + \mathcal{M}_2 \Theta(r - R), \]

where \( R \) is the dot radius, as shown in Fig. 1(b), the corresponding energy diagram for the confinement. A constant electric field is applied in the \( x \) direction: \( \mathcal{E} = \mathcal{E}_0 \sigma_x \). In the polar coordinates, the Hamiltonian can be written as \( \hat{H} = \hat{H}_0 + \hat{H}_1 \), where

\[ \hat{H}_0 = \left( \frac{\mathcal{M}}{\hat{L}^2} \right), \quad \hat{H}_1 = e \mathcal{E}_0 r \cos \theta, \]

and

\[ \hat{L}_\pm = -i \hbar v_F e^{\pm i\theta} \left( \sigma_\theta \pm i \frac{\partial}{\partial r} \right). \]

For zero field (\( \mathcal{E}_0 = 0 \)), the \( z \) component of the total angular momentum, \( \hat{J}_z = -i \hbar \partial_\theta + (\hbar/2) \sigma_z \), commutes with \( \hat{H} \). As a result, the eigenstates take on the following general form [13]:

\[ |r, \tau, n, \nu \rangle = \frac{1}{\sqrt{N_\nu}} \exp(i\theta) \left( \frac{f_1(\kappa, r)}{\xi_\nu} f_{1+1}(\kappa, r) e^{i\varphi} \right), \]

where

\[ \xi_\nu = \hbar v_F \kappa \nu/(\epsilon_\nu + \mathcal{M}), \]

\[ \kappa_\nu = \sqrt{\epsilon_\nu^2 - \mathcal{M}_1^2 / \hbar v_F}, \]

and the radial distribution function is \( f_1(\kappa, r) = J_1(\kappa, r) \) for \( r < R \) and \( f_1 = C H^{(1)}_1(\mathcal{M}) \) otherwise (\( J_1 \) and \( H^{(1)}_1 \) are, respectively, the Bessel and the Hankel functions of the first kind). Introducing the compact index \( \nu = [r, \tau, n] \), we can use the integers \( l \) and \( n \) to specify the orbital angular momentum and the discrete bound states due to the radial confinement, respectively, and \( \tau = \pm 1 \) to denote the sign of the bound-state energies. The eigenvalues \( \epsilon_\nu = \epsilon_\nu \hbar v_F / R \) can be determined by imposing the continuity of the wave function \( \psi_\nu(r, \theta) \) at \( r = R \), and the associated unknown coefficients can be calculated using

\[ C = \frac{1}{\sqrt{\epsilon_\nu^2 - \mathcal{M}_1^2 (1) \hbar v_F}}, \]

\[ N_\nu = 2\pi \int_0^\infty r |f_1(\kappa, r)|^2 + |\xi_\nu f_{1+1}(\kappa, r)|^2 dr = \mathcal{R}_{\nu}^2. \]

Figure 1(c) shows, for the zero-field case, the dependence of the eigenenergies on the inner-region mass (in units of energy) \( \mathcal{M}_1 = \mathcal{M}_1 \hbar v_F / R \) for one fixed value of the outer-region mass \( \mathcal{M}_2 = 10 \hbar v_F / R \). As \( \mathcal{M}_1 \) changes from positive to negative (in the sense that a sign change in the mass occurs between the inner and outer domains, i.e., \( \mathcal{M}_1 \mathcal{M}_2 < 0 \)), a class of new electronic states arises, localized at the dot edge. The mechanism behind the formation of these edge states is the Jackiw-Rebbi modes, which are protected by topological changes due to a sign change in the band masses between the two sides of a boundary. The edge states are a quantized version of the modes (henceforth quantized Jackiw-Rebbi states). For the configuration shown in Fig. 1(a, it is thus possible to engineer quantum (electronic) states topologically by tuning the sign of \( \mathcal{M}_1 \) for a fixed \( \mathcal{M}_2 \) value, as demonstrated in Fig. 1(c). It is remarkable that the emergent topological states have special spin polarization and carry a dissipationless current. Along with the definition of the spin operator \( \hat{S} = \hbar/2(\sigma_y - \sigma_z, \sigma_z) \), we show in Fig. 1(d) the density distribution and the spin textures of a representative topological state [one marked by the red dot in Fig. 1(c)]. For comparison, we also display a normal state marked by the blue dot in Fig. 1(c), which is localized within the inner dot domain and exhibits conventional spin polarization due to the given inner-region mass. Our goal is to study and understand the response of these quantized topological states to an external electric field.

**III. RESULTS**

Say the external electric field is along the \( x \) direction. Due to the lack of a circular symmetry in \( \hat{H} \), the eigenstates and eigenenergies can be calculated numerically through an expansion of the state vector: \( |\tau, n, c_v |v \rangle = \sum_c c_v |v \rangle \), in terms of the eigenstates \( |v \rangle \) of the circularly symmetric case (\( \mathcal{E}_0 = 0 \)), where \( c_v \) are the expanding coefficients. Note that the particle-hole symmetry (i.e., symmetry between the positive and negative energies) is preserved even in the presence of an external electric field [14]. This can be seen by transforming \( \hat{H} \) in the Hamiltonian with \( \varphi = -\mathcal{E}_0 x \) to \( \hat{H}' = U \hat{H} U^\dagger = \)

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$-\hat{H}$ through the unitary transformation $\hat{U} = \delta_x \mathcal{R}_x$, with $\mathcal{R}_x$ denoting the reflection operation with respect to $x = 0$, provided that the confinement potential $\mathcal{M}(r)$ is an even function of $x$. For the disk geometry considered, the resulting bounded energies occur in symmetric pairs with respect to the zero-energy line. For simplicity, we adopt the hard-wall confinement to explicitly generate a set of complete orthogonal states $\{E_n, \{n, \tau, \rho\}\}$ for a given electric field $\mathcal{E}_0$ through numerical diagonalization of the matrix Hamiltonian $[H_{\mu\nu}]$ of elements

$$H_{\mu\nu} = \delta_{\mu\nu}E_v + \langle \mu | \hat{H}_1 | \nu \rangle.$$

For convenience, we use the dimensionless parameter $\lambda = E_0 R e/(h v_F / R)$ to characterize the applied electric field strength and set $\mathcal{M}_2$ to be $+\infty$. The mass potential inside is set as $\mathcal{M}_1 = \pm 2h v_F / R$, which characterizes the normal and topological quantum dot systems, respectively. We use a basis of size about 800 to calculate approximately 50 pairs of bound states with a maximum convergence accuracy of $10^{-6}$ for any $\lambda$ within the range of $[-5, 5]$.

### A. Reverse electric alignments

The bound-state energies as a function of the dimensionless electric field strength $\lambda$ are shown in Figs. 2(a) and 2(b) for the normal ($\mathcal{M}_1 = 2h v_F / R$) and the topological ($\mathcal{M}_1 = -2h v_F / R$) cases, respectively. As expected, for both cases, the spectra exhibit particle-hole symmetry. In addition, there is a Stark shift between levels that have approximately equal energies (quasidegeneracy), and a stronger field generates a larger shift. A striking phenomenon is that, as $\lambda$ is increased, the dependence of the under-gap topological bound-state energies on $\lambda$ (the red curves) exhibits a pattern that is strictly opposite those for the normal bound states [blue curves, Figs. 2(a) and 2(b)] and for the over-gap topological bound states [green curves, Fig. 2(b)]. We note that the under-gap topological states are in fact the quantized anomalous Hall effect (QAH) states with absolute values of energies less than $|\mathcal{M}_1|$ that defines a basic insulating gap for the inner region of the dot. Despite the fact that these states originate from the same topological mechanism as and share similar edge-localized density distributions with other topological bound states, the effects of an applied electric field can be quite different. This can be further seen from Figs. 2(c)–2(h), where the responses of the corresponding electronic states to the external electric field are shown. For the normal bound states [thick solid lines, Figs. 2(c)–2(e)] and over-gap topological bound states [dashed green lines, Figs. 2(f)–2(h)], we observe the usual alignment behavior: the positive-energy electronic states move against the direction of the applied field, while the negative-energy states move towards the direction of the field. The under-gap topological bound states [thick solid black lines, Figs. 2(0)–2(h)], however, follow the opposite pattern, which is consistent with the behavior observed from the energy spectrum.

To understand the abnormal electric response behavior exhibited by the under-gap topological bound states, we develop a perturbation analysis by treating $\lambda$ as a small parameter. From the standard time-independent nondegenerate perturbation theory [15], we can calculate the perturbed energy for a given unperturbed bound state $|\nu\rangle$ up to second order in $\lambda$ through the expansion $E_{\nu} = E_{\nu}^{(0)} + \lambda E_{\nu}^{(1)} + \lambda^2 E_{\nu}^{(2)}$. We obtain the corresponding corrections (expressed in dimensionless form): $E_{\nu}^{(0)} = \langle \nu | \hat{H}_0 | \nu \rangle = E_v, \lambda E_{\nu}^{(1)} = H_{1}^{\nu\nu}$, and

$$\lambda E_{\nu}^{(2)} = \sum_{\mu \neq \nu} \frac{|H_{1}^{\nu\mu}|^2}{E_v - E_\mu}, \quad (4)$$

where the matrix element $H_{1}^{\nu\mu}$ is given by

$$H_{1}^{\nu\mu} = \lambda \langle \mu | \rho \cos \theta | \nu \rangle = \lambda \pi [\delta_{\mu, \nu} + \delta_{\mu, \nu + 1}] A_{\mu}^{-1} A_{\nu}^{-1} \times \int_0^1 \rho^2 J^*_\mu (k_\rho \rho) J_\nu (k_\rho \rho) + \xi^*_\mu \xi_{\nu + 1} (k_\rho \rho) J_{\nu + 1} (k_\rho \rho) d\rho$$

and $\rho \equiv r/R, \ k_\rho \equiv Rk_\rho$. We see that $H_{1}^{\nu\nu} = 0$, and hence, the first-order energy correction $E_{\nu}^{(1)}$ vanishes. To analyze the second-order effect and relate it to the numerical results, we focus on the lowest (highest) positive (negative) unperturbed electronic state, i.e., $[0, 01)$ (1, 1, 11]). From

$$E_{\nu}^{(2)} = \sum_{\mu \neq \nu} \frac{|\langle \mu | \rho \cos \theta | \nu \rangle|^2}{E_v - E_\mu},$$

we can conclude that the leading term is restricted to two nearest-neighbor states in the energy domain with the angular momentum difference $\pm 1$ relative to the given state $|\nu\rangle$, e.g., for $|\nu\rangle = [0, 01)$, $|\mu\rangle \in \{-1, -11\}, [1, 11\}$; $\nu < \epsilon_0 < \epsilon_{1, \pm 11}$, and $\mu < \epsilon_0 < \epsilon_{1, \pm 11}$.
Finally, we have
\[ E_{v}^{(2)} = \pi \left[ \frac{\left| \mathcal{I}_{\mu_{1}v} \right|^{2}}{\epsilon_{v} - \epsilon_{\mu_{1}}} - \frac{\left| \mathcal{I}_{\mu_{2}v} \right|^{2}}{\epsilon_{v} - \epsilon_{\mu_{2}}} \right], \]
where
\[ \mathcal{I}_{\mu_{1}v} = \frac{1}{\mathcal{A}_{\mu_{1}}A_{v}} \int_{0}^{1} \rho^{2} \mathcal{F}_{1}(\rho) d\rho, \]
\[ \mathcal{I}_{\mu_{2}v} = \frac{1}{\mathcal{A}_{\mu_{2}}A_{v}} \int_{0}^{1} \rho^{2} \mathcal{F}_{2}(\rho) d\rho, \]
\[ \mathcal{F}_{1}(x) = \mathcal{J}_{x}^{*}(k_{\mu_{1}}x)\mathcal{J}_{0}(k_{\nu}x) + \xi_{\mu}^{*} \xi_{\nu} \mathcal{J}_{x}^{*}(k_{\mu_{1}}x)\mathcal{J}_{1}(k_{\nu}x), \]
\[ \mathcal{F}_{2}(x) = \mathcal{J}_{x}^{*}(k_{\mu_{2}}x)\mathcal{J}_{0}(k_{\nu}x) + \xi_{\mu}^{*} \xi_{\nu} \mathcal{J}_{x}^{*}(k_{\mu_{2}}x)\mathcal{J}_{1}(k_{\nu}x), \]
the subindices \( \mu_{1} = [-1, -1], \nu = [1, 0, 1], \) and \( \mu_{2} = [1, \pm 1] \) denote the relevant states, and the corresponding energies satisfy the relation \( \epsilon_{\mu_{1}} = -\epsilon_{v} < 0 < \epsilon_{v} < \epsilon_{\mu_{2}}. \)
Specifically, for the normal case (\( \mathcal{M}_{1} = 2\hbar v_{F}/R \)), we have \( \mu_{2} = [1, 1], \mathcal{M}_{1} < \epsilon_{v} = -\epsilon_{\mu_{1}} \ll \epsilon_{\mu_{2}}, \) and hence,
\[ (\epsilon_{\mu_{2}} - \epsilon_{v}) \ll (\epsilon_{v} - \epsilon_{\mu_{1}}) = 2\epsilon_{v}, \]
\[ \xi_{\mu_{2}}^{*} \xi_{\nu} = -1, \]
\[ \xi_{\mu_{1}}^{*} \xi_{\nu} \ll 1. \]
Using these relations, we obtain
\[ |\mathcal{I}_{\mu_{2}v}| \sim 2|\mathcal{I}_{\mu_{1}v}|. \]
It is thus straightforward to conclude \( E_{v}^{(2)} < 0, \) and consequently, a decreasing energy-field strength relation. For the topological case of \( \mathcal{M}_{1} = -2\hbar v_{F}/R, \) we see that the states \( |\mu_{1}\rangle \) and \( |\nu\rangle \) are the highest negative and the lowest positive under-gap topological states, respectively, while the state \( |\mu_{2}\rangle = [1, -1] \) is an adjacent positive over-gap normal state. Finally, we have
\[ (\epsilon_{\mu_{2}} - \epsilon_{v}) > (\epsilon_{v} - \epsilon_{\mu_{1}}), \]
\[ |\mathcal{I}_{\mu_{2}v}| \sim |\mathcal{I}_{\mu_{1}v}|/3, \]
leading to \( E_{v}^{(2)} > 0 \) and hence a reverse dependence of the energies on the strength of the applied field.

**B. Optical transition and spin control**

The phenomenon of reverse electric field alignments for the under-gap topological bound states and our perturbation analysis suggest the occurrence of abnormal QCSE in our mass-confined Dirac system, with potential applications in Dirac material-based optoelectronic and spintronic devices. As a concrete demonstration, we calculate the electric-field-dependent optical absorption intensity \( \alpha \) between the highest negative \( |g\rangle \) and the lowest positive \( |f\rangle \) energy states, which is determined by dipole matrix element \( d_{gf} \) as
\[ \alpha \propto |\mathbf{v} \cdot \mathbf{d}_{gf}|^{2}, \]
where
\[ d_{gf} = \frac{i\epsilon_{e} \hbar v_{F}}{E_{f} - E_{g}} \langle g|\hat{\sigma}|f \rangle \]
and \( \mathbf{v} = (\epsilon_{e} + \epsilon_{y})/\sqrt{2} \) is the polarization vector of the incident light [16,17].

Figure 3 shows the calculated absorption spectra for the normal (blue dots) and topological (red dots) cases, where the sizes of the dots are scaled by the values of the corresponding optical absorption intensity. We see that, in contrast to the normal case where increasing the electric field strength reduces the transition energies and hence the optical absorption frequencies as with conventional QCSE [18], the under-gap topological states generate a small electric-field-modulated optical absorption rate but, within a certain range of the field strength, lead to an opposite dependence of the transition energy on the field strength.

A remarkable phenomenon is that the spin texture of the topological states [see Fig. 1(d)] renders possible control of spin (and hence the associated magnetic properties) through modulation of the electrical field. To demonstrate this, we calculate the expectation values of the in-plane spin for the topological states,
\[ \langle S_{x,y} \rangle = \pm \hbar/2\langle j|\hat{\sigma}_{y,x}|j \rangle \]
for \( j = g, f. \) Figure 4(a) shows the dependence of \( \langle S_{x,y} \rangle \) on the electric field strength \( \lambda, \) where the dashed and solid lines are for states \( |g\rangle \) and \( |f\rangle, \) respectively, and the results for the normal states are included in the inset. Compared with the normal states, the topological states have the intriguing feature that the applied in-plane polarized electric field can modulate the in-plane spins effectively, which is highly desired in spintronics applications. This feature can be further seen
To discuss the experimental scheme, it is convenient to use the actual physical units of the related dimensionless quantities with specific material parameters. We obtain $\hbar v_F \sim 400$ meV nm for typical TI materials [5], say, Bi$_2$Se$_3$ or Pb$_x$Sn$_{1-x}$Te. To compare with existing results on the conventional InAs/GaAs self-assembled [18] and HgTe quantum dots [25], we consider a similar dot size, e.g., $R = 10$ nm, where the relevant bound-state energies lie within the range of $[-120, 120]$ meV for the mass potential magnitude $|\mathcal{M}_1| \sim 80$ meV. The applied electric field is $E_0 \sim 400$ kV/cm, i.e., ranging from $-200$ to $200$ kV/cm for $\lambda \in [-5, 5]$. Correspondingly, we obtain the transition energy $\Delta E \sim 40\delta$ meV with the associated wavelength $\sim h c/(40\delta) = 30.996/\delta \mu m$. For clarity, we also include these quantities with the related physical units in Figs. 3 and 4(a). We see that the electric-field-dependent optical transitions for both the conventional and topological cases occur at the mid-infrared (mid-IR) regime in our system, which can be promising for developing reversal QCSE mid-IR optical modulators. Interestingly, for the topological states, the in-plane spin texture can be effectively controlled when varying the applied electric field, thanks to the unusual ringlike spin orientation of the associated topological modes. We remark that the electric field strength analyzed here is actually on the same order of magnitude as that used for the conventional quantum dot systems [18]. Since the bulk band gap of typical materials such as Bi$_2$Se$_3$ of about 300 meV [4,5] is indeed much larger than the energy scales of our system, the phenomena uncovered in this paper are potentially experimentally realizable.

V. CONCLUSION

To summarize, we uncovered a striking reverse Stark effect in TI-based quantum dot systems that permits a class of quantized topological states. With an in-plane electric field, the under-gap topological states exhibit reverse electric alignments, leading to a reverse QCSE phenomenon. We show that the counterintuitive phenomenon can be fully explained by using a second-order perturbation theory. The phenomenon is not only fundamental to relativistic quantum mechanics of Dirac materials but also practically significant. For example, the reverse Stark effect leads to an inverted optical absorption spectrum, and this anomalous feature can be exploited to develop Dirac-material-based optoelectronic devices, e.g., reverse QCSE mid-IR optical modulators. In addition, due to their special spin textures, the in-plane spin degree of freedom of the under-gap topological states can deposited on the surface of a 3D topological insulator. Depending on the local exchange coupling of the topological insulator and ferromagnetic insulator as well as the interface quality between them, the magnitude of the induced mass potential can be several to a hundred meV [19,21,23]. Interestingly, the sign of the induced mass is tunable by changing the direction of the magnetization in the topological insulator capper layer, which can be achieved by means of the anisotropic feature of the materials [6,22]. The gate electrode can be attached to the topological insulator through which an external electric field can be applied [24].

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be effectively controlled electrically or optically, opening an avenue for spintronics applications. We further discuss feasible experimental validation schemes and potential applications. Interesting issues to be explored include the effects of symmetry breaking and impurity scattering.

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