Photon dressed electronic states in topological insulators: tunneling and conductance

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Abstract

We have obtained analytic results for the surface states of three-dimensional topological insulators in the presence of circularly polarized light. This electron–photon interaction results in an energy gap as well as a novel energy dispersion of the dressed electron–photon states, different from both graphene and the standard two-dimensional electron gas (2DEG). Additionally, we made calculations of the ballistic conductance and Klein tunneling in both two- and three-dimensional topological insulators as well as investigating how these phenomena are affected in the presence of circularly polarized light. We have found a critical energy for an incoming particle, separating two substantially different types of tunneling.

(Some figures may appear in colour only in the online journal)

1. Introduction

The unusual energy band structure of topological insulators (TIs), as a novel class of quantum spin materials, has received a considerable amount of theoretical attention in the last few years [1]. The energy dispersion is characterized by an insulating gap in the three-dimensional (3D) bulk states as well as by topologically protected conducting states localized either around the two-dimensional (2D) surface for 3DTIs or around the edge for 2DTIs [2]. In this paper, we adopt the conventional classification (2D/3D) for TIs based on their geometry.

Quantum spin Hall (QSH) topological states were discovered in HgTe/CdTe quantum wells (QWs). The existence of these QSH states is determined by the QW thickness greater than a critical value. For films thicker than 6 nm, such QWs are exemplary 2DTIs but become conventional insulators otherwise [3]. Typical examples of 3DTIs include half-space Bi\textsubscript{1−x}Sb\textsubscript{x} alloys as well as Bi\textsubscript{2}Se\textsubscript{3}, Bi\textsubscript{2}Te\textsubscript{3} and Sb\textsubscript{2}Te\textsubscript{3} binary crystals. The surfaces of these 3DTIs support spin-polarized Dirac cones analogous to graphene [4, 5].

It has been shown that topological states may acquire an energy gap [6, 7]. Since it is usually produced as a geometrical gap, it requires a finite size along a given direction. The energy gap depends on either the ribbon width for a QW in a 2DTI or the separation between two surfaces of a 3DTI. In this paper, we propose another approach for generating an energy gap by coupling the topological surface states to circularly polarized light. This type of dynamic gap was predicted in graphene based on both a semiclassical approach [8] and a quantum mechanical formalism [9–11]. Some relevant properties of TIs interacting with light were addressed in [12, 13]. Discussion of the appearance of an energy gap induced by electron–photon interaction has been given in [14].

The creation of an energy gap may lead to a metal–insulator phase transition. The conical dispersion of metallic graphene provides unimpeded electron tunneling...
through a p–n junctions (Klein paradox) \[4, 5\]. On the other hand, Klein-like total reflection has been predicted for bilayer metallic graphene with its massive but still chiral electrons \[15\]. Chirality is shown to be the key property for total reflection. However, perfect tunneling may still be expected for certain values of the longitudinal momentum of electrons in the barrier region because these transmission resonances are not affected by the chirality.

The light-induced energy gap is able to break the chirality \[16\] and suppresses the Klein effect in graphene. In this paper, we would expect that a similar effect may occur in TIs because the helicity of the topological states is also broken by an energy gap. Our numerical results demonstrate a cross-over behavior from Klein-like tunneling in a TI to tunneling of a conventional two-dimensional electron gas (2DEG). Here, by Klein-like we mean that the energy dispersion of topological states deviates from the Dirac cone. For instance, in a 3DTI, there exists an inherent mass term in the effective surface Hamiltonian, which affects the Klein effect in TIs. The interplay between the induced and inherent mass terms, as well as their competing effects on the electron transmission, are the main subjects of our investigation. In \[17\], tunneling and transport problems in the presence of tilted uniform magnetic and electric fields were studied, and we will briefly discuss the effect of the dynamic gap for these cases.

The rest of our presentation is organized as follows. In section 2, we first discuss the dressed topological states and obtain their energy dispersion and wavefunctions for surface states and present an effective surface Hamiltonian derived from the Dirac cone. For instance, in a 3DTI, there exists an inherent mass term in the effective surface Hamiltonian, which affects the Klein effect in TIs. The interplay between the induced and inherent mass terms, as well as their competing effects on the electron transmission, are the main subjects of our investigation. In \[17\], tunneling and transport problems in the presence of tilted uniform magnetic and electric fields were studied, and we will briefly discuss the effect of the dynamic gap for these cases.

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2. Electron–photon interaction and dressed states

In this section, by including electron–photon coupling, we derive an effective Hamiltonian for the surface states of TIs based on quantum field theory. Both the single-mode and double-mode optical fields are considered and their energy dispersions for dressed electron states are compared. Analogously to graphene-like massless particles, the effect of massive particles in TIs on electron states and tunneling is studied.

Let us now consider electron–photon interaction on the surface of a 3DTI. We obtain the dressed electronic states analytically and investigate the tunneling properties of these states. We first assume that the surface of the 3DTI is irradiated by circularly polarized light with its quantized vector potential given by

$$\hat{A} = F_0 \left( e_+ \hat{a} + e_- \hat{a}^\dagger \right), \quad (1)$$

where the left and right circular polarization unit vectors are denoted by \(e_\pm = (e_x, \mp i e_y) / \sqrt{2}\), and \(e_x, e_y\) is the unit vector in the \(x, y\) direction. The amplitude of the circularly polarized light is related to the photon angular frequency \(\omega_0\) by \(F_0 \sim \sqrt{1/\omega_0}\). Here, we consider a weak field (energy \(\sim F_0^2\)) compared to the photon energy \(\hbar \omega_0\). Additionally, the total number \(N_0\) of photons is fixed for the optical mode represented by equation (1), corresponding to the case with focused light incident on a portion of an optical lattice modeled by Floquet theory \[8\].

The non-interacting Hamiltonian of a 3DTI was derived in \[18\] and we write it as

$$H_{em}^{3D} = D k_\perp^2 \bar{I}_{[2]} + A \bar{\sigma} \cdot \mathbf{k} = \begin{pmatrix} D k_\perp^2 & A k_- \\ A k_+ & D k_\perp^2 \end{pmatrix}, \quad (2)$$

where \(\bar{I}_{[2]} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\) is a 2 × 2 unit matrix, \(\bar{\sigma}\) stands for the usual Pauli matrices, \(\mathbf{k} = (k_x, k_y)\) is the in-plane surface wavevector with respect to the \(\Gamma\)-point and \(k_\perp = k_z \pm i k_y\). For the 3DTI considered here, the group velocity is of the same order of magnitude as graphene, i.e., \(\bar{V} \sim h v_F \sim 10^{-29} J m\). It was shown that the leading quadratic term in equation (2) is necessary although the higher-order terms with respect to \(O(k^3)\) may be neglected. The massless form of the Hamiltonian in equation (2) with no quadratic term, \(D = 0\), formally coincides with graphene Dirac cones and retains all graphene electronic properties. Specifically, for electron tunneling, these properties include the absence of back-scattering for head-on collisions (Klein paradox) as well as distinct tunneling resonances in the electron energy distribution.

The energy dispersion relation associated with equation (2) is \(E_{em}^{3D} = D k_\perp^2 + A |\mathbf{k}|\), where \(\beta = \pm 1\) is analogous to the pseudo-spin in graphene. Both \(A\) and \(D\) are independent of the wavevector \(k\). This dispersion relation shows that the particle–hole symmetry is broken by virtue of the massive \(D\)-term. For completeness, the transmission amplitude of the massless topological states (with \(D = 0\)) is presented in figure 1. Comparing figures 1(a) and (b), we clearly see a significant difference although the thickness of a potential barrier is only 50 nm. The effect of coupled dressed states on the tunneling is much stronger for a \(\delta\)-function barrier. At the same time, the tunneling resonant peaks are broadened significantly compared with graphene. From figures 1(c) and (d), we also find that the angular distribution of transmission side peaks at larger angles displays a non-monotonic dependence on the barrier width \(W\) for the higher scaled electron energy \(\varepsilon / V_0 = 5\). In addition, the broadening of resonant peaks at small angles is also significant in comparison with graphene.

The interaction with the optical mode may be introduced into the Hamiltonian in equation (2) via a standard transformation of \(k \rightarrow k + e \hat{A} / \hbar\). In appendix A, we have
shown that this transformation leads to the following effective Hamiltonian, after the field correction has been neglected:

\[
\hat{H} = \hbar \omega_0 \hat{a}^\dagger \hat{a} + D \hat{k}^2 \hat{a}^\dagger \hat{a} + 2 \zeta D (\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger),
\]

where we have introduced a small parameter \( \zeta = e F_0 / (\sqrt{2} \hbar) \) to describe the light–matter interaction. We assume that the optical mode accommodates a large number \( N_0 \) of photons with \( N_0 \gg 1 \). Consequently, all the terms of order \( \zeta^2 \sim O(1/N_0) \) may be neglected. Under these conditions, the energy dispersion associated with equation (3) becomes

\[
\varepsilon_{\text{surf}}(\Delta) = N_0 \hbar \omega_0 + D \hat{k}^2 + \beta \sqrt{\Delta^2 + (A \hat{k})^2}
\]

with \( \beta = \pm 1 \) and the induced energy gap defined by

\[
\Delta = \sqrt{\omega_0^2 + (\hbar \omega_0)^2} - \hbar \omega_0 \sim \hbar \omega_0 \left( \frac{\alpha^2}{2} \right),
\]

where \( \alpha = \omega_0 / (\hbar \omega_0) \) and \( \omega_0 \) is the electron–photon interaction energy. For the upper subband with \( \beta = 1 \) in equation (4), the energy gap is related to the effective mass around \( \hat{k} = 0 \) through \( 2m^*_e = \hbar^2 / [\hat{A}^2 / (2 \Delta) + D] \), where the photon dressing decreases the effective mass. This is in contrast with single-layer graphene, where electron–photon interaction leads to an effective mass. A similar phenomenon on the effective mass reduction is also found in bilayer graphene under the influence of circularly polarized light. We will consider the biggest possible value for \( \omega_0 \) to maximize the light-coupling effect, although the condition \( \omega_0 < \hbar \omega_0 \) must be maintained to ensure the validity of the approximations made in this paper. Here, as an example, we will just use the leading-order Dirac cone term \( \hat{A} \hat{\sigma} \cdot \hat{k} \) to estimate the light-induced energy gap. The small correction from the parabolic \( D \) term can be neglected for not very large \( \hat{k} \) values.

The dressed state wavefunction corresponding to equation (4) is given by

\[
\phi_{\beta}^{\hat{k}}(x, y) = \frac{1}{\sqrt{1 + \gamma^2(\beta)}} \left( \gamma(\beta) e^{i \hat{\varphi}} \right) e^{i \hat{k}_x x + i \hat{k}_y y},
\]

where \( \gamma(\beta) = \Delta k / (\Delta + \beta \sqrt{\Delta^2 + (A \hat{k})^2}) \) and \( \phi = \tan^{-1}(k_y / k_x) \). The energy dispersions associated with the Hamiltonian in equation (3) (see also equation (A.17)) for two-mode light interaction with electrons are given by

\[
\varepsilon_{[N_0, N_0 + 1, N_0 + 1]}(k, \Delta) = (N_0 + \frac{1}{2}) \hbar \omega_0 + D \hat{k}^2 \pm \sqrt{C_1(k, \Delta) \pm \sqrt{C_2(k, \Delta)}},
\]

where a doubled state space is used for spanning the Hamiltonian,

\[
C_1(k, \Delta) = \hbar \omega_0^2 + \frac{3}{2} \nu \Delta A \hat{k}^2 + \frac{1}{2} \nu^2 \Delta^2 + \frac{3}{2} \nu \Delta \hat{A}^2 \hat{k}^2 + \frac{3}{2} \nu \Delta \hat{A} \hat{k}^2 + \frac{3}{2} \nu \Delta \hat{k}^2
\]

with \( \nu = \alpha / 2 \).

As \( \hat{\varphi} \Delta \rightarrow 0 \) and \( \nu \Delta \rightarrow 0 \), the two-mode dressed states become decoupled and are simply given by

\[
\varepsilon_{[N_0, N_0 + 1]}(k, \Delta) = (N_0 + \frac{1}{2}) \hbar \omega_0 + D \hat{k}^2 \pm \sqrt{\Delta^2 + (A \hat{k})^2},
\]

where \( \gamma(\beta) = \Delta k / (\Delta + \beta \sqrt{\Delta^2 + (A \hat{k})^2}) \) and \( \phi = \tan^{-1}(k_y / k_x) \). The energy dispersions associated with the Hamiltonian in equation (3) (see also equation (A.17)) for two-mode light interaction with electrons are given by

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\]
In this section, we compare the surface states of a 3DTI with bilayer graphene in order to find out how the quadratic term in their energy dispersions influences tunneling. The electron tunneling behaves like massless Dirac fermions for high incident energies above a critical value; this has been compared with electrons in a graphene layer. On the other hand, the electron tunneling behaves like Schrödinger massive particles at lower incident energies below this critical value; this is similar to the 2DEG. Additionally, the modification from a dressed state energy gap to electron tunneling is investigated for both low and high incident energies.

Let us first turn to the tunneling problem associated with the Hamiltonian in equation (2) in the absence of electron–photon coupling. The main input of the p–n junction tunneling is the electron wavefunction [15, 21]

$$\Psi_k(x, y) = \frac{1}{\sqrt{2}} \left( \frac{i}{\beta} e^{i\phi} \right) e^{i(k_x x + k_y y)}, \quad (15)$$

where $\beta = \pm 1$, as before, and $\phi = \tan^{-1}(k_y/k_x)$. This wavefunction is simple and chiral, and is an eigenstate of the projection of the electron momentum operator along the pseudo-spin direction (chirality/helicity operator) given by $\hat{h} = \hat{\sigma} \cdot \hat{p} / (2\hbar)$. For the tunneling process along the $x$ direction, the transverse momentum $\hbar k_y$ is conserved, whereas the...
The physical meaning of equation (19) is decrease of the incidence. There exists a case, we have $A$ 3DTI Hamiltonian were studied in [22]. In the present $k$ value are transmitted like normal Schrödinger electrons in However, particles with incoming energies below this critical the transmission behaves like Dirac electrons in graphene. Equation (16) yields not only propagating but also evanescent modes in the barrier region. Moreover, because of the quadratic energy dispersion, both the wavefunctions and their derivatives need to be matched at boundaries, similarly to the evanescent contributions. By neglecting the higher-order terms, equation (16) is simplified to

$$k_{x,2} = \sqrt{\frac{(\varepsilon - V_0)^2}{2D(\varepsilon - V_0) + A^2} - k^2_y}. \quad (17)$$

The result for the special case of massless Dirac fermions of graphene may be directly obtained from the above equation after setting $D \rightarrow 0$.

Clearly, from equation (17), the electron transmission varies with the incoming particle energy as well as the angle of incidence. There exists a critical energy $\varepsilon_{cr} \ll V_0$ above which the transmission behaves like Dirac electrons in graphene. However, particles with incoming energies below this critical value are transmitted like normal Schrödinger electrons in 2DEG. For head-on collisions with $k_y = 0$, the critical energy is calculated to be

$$\varepsilon_{cr} = V_0 - \frac{A^2}{2D}. \quad (18)$$

The dimensionless two-terminal tunneling conductance, $g(\varepsilon)$, may be calculated from [23]

$$g(\varepsilon) = \frac{G(\varepsilon)}{2G_0} = \frac{1}{2} \int_{-\pi/2}^{\pi/2} T(\phi, \varepsilon) \cos(\phi) d\phi. \quad (19)$$

The physical meaning of equation (19) is decrease of the electron conductance in the presence of the barrier due to $T(\phi, \varepsilon) \leq 1$, where $T(\phi, \varepsilon)$ is the transmission probability.

According to [24], $G_0$ in the case of $D = 0$ may be estimated using

$$G_0 = \left( \frac{\varepsilon^2}{h} \right) \frac{L_y}{2\pi} \int_{-k_y}^{k_y} \frac{dk_y}{\cosh^2(k_y L_y/2)}, \quad (20)$$

where $k_F$ is the Fermi wavenumber and $L_y$ and $L_x$ are the normalization length and width of the sample. When $k_F L_y \ll 1$, we have $\tanh(k_F L_y/2) \approx k_F L_y/2$ and obtain in a straightforward way that $G_0 = (2\varepsilon^2/h)(L_y/2\pi)(\varepsilon_F/A)$ for the Dirac cone with $\varepsilon_F = A k_F$. In the presence of a small energy gap $\Delta \ll A k_F$, on the other hand, $G_0$ is modified to

$$G_0 = \left( \frac{2\varepsilon^2}{h} \right) \frac{L_y^2 \sqrt{\varepsilon_F^2 - \Delta^2}}{2\pi A}. \quad (21)$$

where $\varepsilon_F$ is the Fermi energy at $k = k_F$.

The calculated results based on equation (19) are presented in figure 3. Comparing figures 3(a) and (b), we find that the existence of the critical energy in (b) plays a crucial role in the electron tunneling. A series of resonant peaks occur above the critical energy $\varepsilon_{cr}$ in (b) and above the barrier height $V_0$ in (a) although these two values are quite different. The former is unique to surface states of a massive particle in a 3DTI while the latter is related to the transition from Klein tunneling to regular tunneling for massless fermions in graphene. It is more interesting to notice that the electrons tunneling below $V_0$ in (a) and below the critical energy in (b) are also qualitatively different, in that the electrons behave like Dirac fermions for Klein tunneling in (a) and like Schrödinger particles for evanescent wave tunneling in (b). The transition when $\varepsilon = \varepsilon_{cr}$ is extremely sharp in (b).

It is very helpful to compare the results obtained in this section with bilayer graphene having quadratic dispersion. For bilayer graphene, its lowest energy states are described by the Hamiltonian [15]

$$\hat{H}_{bgl} = \frac{\hbar^2}{2m_b} \left( k_x^2 \sigma_+ + k_y^2 \sigma_- \right), \quad (22)$$

where $m_b$ is the effective mass of electrons in the barrier region. In this case, the longitudinal wavevector component in the barrier region is given by

$$k_{x,2}^b = \beta' \sqrt{2m_b \beta (\varepsilon - V_0) - k_y^2}, \quad (23)$$

![Figure 3](image-url) Two-terminal tunneling conductance for the effective surface model of a 3DTI with different barrier widths. In panels (a) and (b), we present numerical results for tunneling conductance as a function of the incident particle energy for the case of the Dirac cone and a 3DTI with $Dk_F/A = 0.4$. 

longitudinal wavevector component $k_{x,2}$ in the barrier region with $V(x) = V_0$ is determined by

$$k_{x,2} = \sqrt{\frac{(\varepsilon - V_0)^2}{2D(\varepsilon - V_0) + A^2} - k^2_y}. \quad (16)$$


where $\beta', \beta = \pm 1$. An evanescent wave having a decay rate $\kappa_b$ can coexist with a propagating wave having wave vector $k_{x,2}$ such that $k_{x,2}^2 + k_{y,2}^2 = k_0^2 - \kappa_b^2 = 2n_b \beta (\varepsilon - V_0)$. This implies that the evanescent modes should be taken into account simultaneously. For bilayer graphene, both wavefunctions and their derivatives must be continuous at the interfaces. Consequently, the Klein paradox persists in bilayer graphene for chiral but massive particles. However, one finds complete reflection, instead of complete transmission, in this case. This effect has direct links with the specific electron–hole conjugation, i.e. $k_{x,2} \rightarrow i k_b$, in the barrier region [15].

To understand the physics for electron tunneling in bilayer graphene, we first present analytical results for single-layer graphene, i.e. $D = 0$. By taking into account all four modes from equation (16), for a $\delta$-potential barrier, we obtain the transmission probability as [23]

$$T_{b,g} = \frac{1}{1 + \sin^2(\lambda) \tan^2(\phi)},$$

(24)

which reproduces the Klein paradox for the head-on collision corresponding to $\phi = 0$. However, the periodic dependence of the transmission on the scaled barrier strength $\lambda$ in equation (24) is non-trivial. Such perfect tunneling with $T_{b,g} = 1$ also exists for a set of $\lambda$ values when $\sin(\lambda) = 0$ is satisfied. Furthermore, this prediction is consistent with finite-width barrier tunneling (see figure 1(c)). In fact, the expression in equation (24) may be derived directly from the general result for electron transmission through a very high potential barrier with $V_0 \gg \varepsilon$, that is,

$$T_b = \frac{\cos^2(\phi)}{1 - \cos^2(k_{x,2} W) \sin^2(\phi)} = \frac{1}{1 + \sin^2(k_{x,2} W) \tan^2(\phi)},$$

(25)

where $k_{x,2} \sim -V_0/A$ is used for $V_0 \gg \varepsilon$. It is clear that $\lambda$ in equation (24) plays the role of $k_{x,2} W$ for a finite barrier width $W$.

For a conventional 2DEG with a $\delta$-function potential barrier [25], the transmission amplitude is given by $T_\delta = 2\hbar^2 \varepsilon/(2\hbar^2 + m^* \lambda^2 W^2)$. Here, we consider a head-on collision with $k_x = \sqrt{2m^* \varepsilon / \hbar^2}$ and $m^*$ is the electron effective mass. One may easily see that for $\lambda \rightarrow 0$ (or a very thin barrier layer) complete transmission ($T_\delta \rightarrow 1$) can be obtained. When $\lambda \rightarrow \infty$, on the other hand, one gets complete reflection.

Figure 4 presents our numerical results for the transmission amplitude $T(\phi, \varepsilon)$ for several values of the barrier width in the absence of photon dressing or when the coefficient $\Delta = 0$ in the energy dispersion relation. From this figure, we find that the coupling between dressed states with different pseudo-spins is very strong for a double-mode optical field, similar in nature to the result in figure 2(c). Here, Dirac-like tunneling above a critical energy may be seen for a thick barrier layer, as described by equation (25). Schrödinger-like tunneling below the critical energy, on the other hand, may only be observed for a relatively thin barrier layer under the normal-incidence condition, as discussed for 2DEG with $\lambda \rightarrow 0$. With decreased $W$, electron tunneling below the critical energy is gradually enhanced as $\phi \rightarrow 0$. From direct comparison between figures 4 and 1(a) we know that the major effect of the massive $D$-term on the electron tunneling is associated with the occurrence of a critical energy below which no significant electron tunneling is expected for a thick barrier layer. In addition, the critical energy shifts up with decreasing $W$ and the contribution from the evanescent mode to the transmission is found to be finite as long as the barrier width $W$ meets the condition $W |\operatorname{Im}(k_{x,2})| < 1$.

According to [26], $-k^3$ terms could become an important correction. Now, let us briefly discuss how the electron transmission is affected after the $-k^3$ term in the energy spectrum has been taken into account. For simplicity, we do not consider electron–photon dressed states, but only the transmission probability for non-interacting electrons. The inclusion of light–electron coupling will not change the conclusion presented below qualitatively. Here, we will consider two different situations, i.e., the case of small corrections $\pm B k^3$ to the energy dispersions and the case when the cubic terms make equal or even prevailing modifications to the energy eigenvalues. The first case only gives rise to a small correction to the critical energy in equation (18) as well as to the longitudinal wavenumber $k_{x,2}$. The main difference for the second case comes from the fact that the significant cubical terms lead to another mode of electron propagation in the barrier region, similar to an evanescent mode in bilayer graphene with quadratic energy dispersion. Under a cubical term, the electron modes in the barrier region can be propagating, evanescent or both, depending on the material property and the electron incoming energy. In short, if the cubical corrections become small, which is the case...
considered in this paper for small $k$ values, the additional modes become either fast-oscillating or extremely decayed and can be neglected in a leading-order approximation.

We now turn to the model for the 3DTI surface with $\Delta \neq 0$. For this, the longitudinal momentum of the electron dressed states may be approximated by

$$k^\Delta_{\perp} = \sqrt{\frac{(\varepsilon - V_0)^2 - \Delta^2}{2D(\varepsilon - V_0) + A^2} - k_y^2}. \quad (26)$$

Numerical results for the transmission amplitudes based on equation (26) are presented in figure 5, where the same parameters were chosen as those in figure 4. Comparing figure 5(a) with 1(a) for $D = 0$, we find that the effect of a photon-induced energy gap is to produce additional side peaks in the angle distribution of $T(\phi, \varepsilon)$.

### 4. Electron tunneling in 2DTIs and ZNRs

According to the Kane model for a HgTe/CdTe semiconductor quantum well [2, 7], the 2DTI system may be effectively described by the following $4 \times 4$ matrix Hamiltonian:

$$\mathcal{H}_{2D}(k_x, y) = \begin{pmatrix} h_B(k_x, y) & 0 & -i & 0 \\ 0 & h_B^{-1}(k_x, y) & 0 & 0 \\ 0 & 0 & h_B^{-1}(k_x, y) & 0 \\ -i & 0 & 0 & h_B(k_x, y) \end{pmatrix}, \quad (27)$$

where

$$h_B(k_x, y) = \left( C + \mathcal{M} - (D + B)k^2 - B, A(k_x + i\sigma_y) \right) \frac{A(k_x - i\sigma_y)}{C - \mathcal{M} - (D + B)k^2 - B^*}. \quad (28)$$

and $k_x$ is assumed small. Additionally, we assumed translational invariance along the $z$-axis so that $k_x \rightarrow -i\sigma_x$.

The coefficients $A, B, C, D$ and $\mathcal{M}$ are expansion parameters within the Kane model. Their role in the energy dispersion is such that $\mathcal{M}$ is usually referred to as the Dirac mass and $B$ is called the Newtonian mass. We note that $\mathcal{M}$ changes sign at the critical thickness $d_{cr} \approx 6.1$ nm. For a layer with $d > d_c$, $\mathcal{M}$ is negative; this is referred to as an *inverted*-type TI.

The Hamiltonian (27) leads to the following energy dispersion relations [7]:

$$\varepsilon_B + \frac{AMD}{B} = \beta \sqrt{\Delta_z^2 + \left[ \frac{A}{B^2}(B^2 - D^2)k_x \right]^2 + O(k_y^2)}, \quad (29)$$

showing the existence of an energy gap. $\Delta_z$ is defined as

$$\Delta_z = \frac{4\mathcal{M}M(B^2 - D^2)}{B^3[4MB - 4\mathcal{M}(B^2 - D^2)]}. \quad (30)$$

We note that the Hamiltonian in equation (27) is block diagonal, for which we expect two independent wavefunctions, $\Psi_+$ and $\Psi_-\equiv \Psi_+^*$. Corresponding to different directions of the electron spin projection. It is straightforward to show that $\Psi_+$ and $\Psi_-$ are related to each other by a time-reversal operator [7], i.e. $\Psi_- = -i\sigma_z\Psi_+^*$. This implies that any transmission associated with $\Psi_+$ must accompany another transmission of $\Psi_-$ in the opposite direction along the same edge of the 2DTI. For that reason, the eigenstates $\Psi_{\pm}$ are usually referred to as helical edge states [2]. For all the calculations which follow, we made use of the fact that $C$ only appears along the diagonal of the matrix in equation (28). By making the replacement $\varepsilon \rightarrow - \varepsilon - C$, one may show in a straightforward way that the $C$-term is irrelevant to electron transmission.

Before solving the eigenvalue problem, we estimate [27] all quantities and coefficients in the Hamiltonian in equations (27) and (28) at $d = 5$ nm ($<d_{cr}$). The range of considered wavevectors is chosen as $k \approx 10^{-2}$ Å$^{-1} \ll k_F$. In this range, the parameters appearing in the Hamiltonian are [2] $C \approx 10^{-2}$ eV, $AK \approx Bk^2 \approx DK^2 \approx 10^{-2}$ eV. Consequently, each term in the Hamiltonian in equation (28) has the same order of magnitude and none of them should be neglected. Since $B \approx D$, we get $B_+ \equiv B + D \approx 2B$ and $B_- \equiv B - D \ll B$.

In the limiting semi-infinite geometry for a 2DTI, we obtain the following exact 1D effective edge model along the $y$-direction [2]:

$$\mathcal{H}^{1D}_\text{em} = Ak_y \sigma_z \epsilon. \quad (31)$$

whose corresponding dispersion relations are $\epsilon^{1D}_\text{em} = \pm Ak_y$ with corresponding wavefunctions which are the
Figure 6. Zigzag nanoribbon wavefunctions and tunneling conductance. Panel (a) demonstrates transverse decay rates $\lambda_{x,n}$ depending on the longitudinal momentum $k_x$ for various nanoribbon widths. Panel (b) shows the $y$-dependence of the edge-state wavefunctions inside the barrier region ($\lambda_b$) and outside the barrier region ($\lambda_0$), as well as contour plots of wavefunctions. Panel (c) presents a density plot for the dependence of the two-terminal conductance $g(e)$ on $\lambda_0$ and $\lambda_b$.

eigenfunctions of $\sigma_z$, i.e., $\Psi_T = [0,1]$ and $\Psi_T = [1,0]$, which yield a transmission amplitude $T_{\text{sem}} = 1$ through a barrier of any height analogous to the Klein paradox for head-on collisions in graphene. In contrast to the 2D model in equation (27), we find that the electron transmission for edge states with a finite width is substantially suppressed.

Taking the limit $L_y \to \infty$, we can also consider bulk states which are located far away from either edge. In this case, we make the substitution $k_y = -i\delta y$. By retaining terms up to order $O(k^3)$, calculation leads to a new energy dispersion for $A \gg B k$,

$$\varepsilon_{\text{bulk}}^L = -Dk^2 \pm \sqrt{\mathcal{M}^2 + (A^2 - 2MB)k^2}. \tag{32}$$

The Hamiltonian in equation (28) assumes the simple form $\pm \mathcal{M} \hat{\sigma}_z$ at $k = 0$, where the gap parameter $\mathcal{M}$ strongly depends on the thickness $d$ of the quantum well and can be arbitrarily small or even set equal to zero. The energy dispersion relations in equation (32) formally reduce to those of gapped graphene or graphene irradiated with circularly polarized light. The tunneling problems for this case were addressed in [23, 16]. The most significant effect of radiation on electron tunneling is the breaking of chiral symmetry on the order of $O(\mathcal{M}^2)$. Consequently, significantly different behavior in the electron transmission at small incident angles ($|k_y| \ll |k_x|$) is expected compared to infinite graphene in the absence of light illumination [15].

One can conclude that the electronic states and tunneling properties of a 2DTI have a lot of similar features to zigzag nanoribbons (ZNRs) [28], which are also quasi-1D edge states. The boundary conditions are such that each of the wavefunction components vanishes at one of the two ribbon edges. Real solutions for the transverse decay coefficients $\lambda_{x,n}$ exist only if both the conditions $k_y > \lambda_{y,n}$ and $L_y \lambda_{y,n} > 1$ are satisfied. We will assume that the ribbon is sufficiently wide so that $k_y L_y > 1$ for $k_x$ in the range of interest. For real $\lambda_{y,n}$, the edge states decay exponentially with decay length $1/\lambda_{y,n}$. This situation is similar to the case of a 2DTI discussed earlier in this section. However, the traverse wavefunction distribution is drastically different from a graphene armchair nanoribbon (ANR) which has a plane-wave-type wavefunction $\Psi_{\text{ANR}}(y) \sim e^{i\lambda_b y}$. We also note that for large $k_y$, one gets $\lambda_{y,n} \approx 0$, i.e., fast moving electrons with large longitudinal momenta have a negligible decay rate. Therefore, the wavefunction in this case extends far away from the ribbon edges. For a chosen ribbon width, there exists a maximum value for the decay rate.

The energy dispersion for a ZNR is given by $\varepsilon_{\text{ZNR}} = \beta \sqrt{k_x^2 - \lambda_{y,n}^2}$. We confine our attention to low potential barriers, such that $\lambda_{y,n}$ is real within a barrier region. Unimpeded tunneling in ZNRs was investigated in [29].

From figure 6(a), we find that a wavefunction’s transverse decay length $\lambda_{y,n}^{-1}$ decreases with increasing width of a zigzag nanoribbon. Figure 6(b) shows us that the minima of the edge-state wavefunctions in the transverse direction are at the center ($y = 0$) for regions both inside and outside the barrier. Furthermore, the wavefunctions are symmetric with respect to $y = 0$. Our numerical results are presented in figure 6(c). The diagonal line in figure 6(c) reflects the fact that $T(e, y) \equiv 1$ (or $g(e) \equiv 1$) for the same decay rates $\lambda_0 = \lambda_b$. The periodic resonant peaks with respect to $\lambda_b$ can be clearly seen in figure 6(c) similarly to the prediction by equation (24).

5. Concluding remarks

In summary, we have analytically obtained the energy dispersion relations as well as the wavefunctions of electron dressed states in TIs irradiated by circularly polarized light. A number of helical systems, such as graphene, nanoribbons and topological insulators, are compared. Similarly to graphene, the electron–photon coupling in a TI leads to an energy gap in the electron energy dispersion relations and eigenstates with the broken chirality symmetry. The tunneling over a square potential barrier is modified significantly if there exists a gap in the energy dispersion of the electrons. The combination of Schrödinger-like (massive) and Dirac-like (massless) electron tunneling below and above a critical energy gives rise to very novel properties. We have further found that some lower energy subbands become nearly dispersionless with increasing light intensity, which results in unusual electronic properties.
As shown in [9] for graphene, a laser power of $10^2$ W may produce an energy gap $\Delta \sim 10-100$ meV required to make the effect noticeable for THz light frequencies at room temperature. Since the linear-term coefficient (group velocity) of the 3DTI Hamiltonian has the same order of magnitude as graphene, we expect that an experimental verification will be possible. Indeed, for a circular-polarized CO$_2$ laser beam of power $P \sim 10^2$ W, wavelength $\lambda \sim 10^{-5}$ m and beam size of the order of $\sim \lambda$, from the field energy density $w \sim F(\lambda^2c)$ we find the electric field amplitude $E_0 \sim \sqrt{P/(\epsilon_0 \lambda^2 c)} = 10^5$ V cm$^{-1}$. This leads to the light-coupling energy $W_0 \sim 10^{-20}$ J and the light-induced energy gap $\Delta \sim 0.01-0.1$ eV for Bi$_2$Se$_3$ with $A = 10^{-29}$ J m.

Although the linear term in the energy dispersion of 3DTIs gives spin-polarized Dirac cones with the chirality of the corresponding eigenstates, the appearance of a quadratic term introduces additional effects on the electron tunneling. Our calculations for electron tunneling through a square potential barrier indicate that electrons may be transmitted either like chiral particles as they are in graphene or like conventional 2DEG electrons, depending on whether the incident particle energy is above or below a critical energy.

We have also investigated the tunneling properties of edge states for massive particles in 2DTIs, such as HgTe/CdTe quantum wells, where an energy gap is introduced by the finite width of the samples [7]. From the analysis of the dressed edge-state wavefunction in the presence of circularly polarized light, we have found that particles can always freely propagate along the ribbon edges, which is similar to zigzag graphene nanoribbons but different from semi-infinite 2DTIs where either perfect transmission or complete reflection is obtained for electron–electron and electron–hole transitions, respectively. Although the wavefunctions in both 2DTIs and zigzag ribbons are localized around the edges, the decay rate of the edge-state wavefunctions of a 2DTI does not depend on the longitudinal wavenumber, in contrast to the decay rate in a zigzag ribbon.

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Appendix A. Model of a 3DTI surface irradiated with circularly polarized light

The Hamiltonian describing the surface states (at $\z = 0$) of a 3DTI to order $O(k^2)$ is given by

$$\hat{\mathcal{H}}_{\text{surf}}^{3D} = Dk^2 + \vec{A} \cdot \vec{\sigma} \cdot \vec{k} = \begin{pmatrix} Dk^2 & Ak_- \\ Ak_+ & Dk^2 \end{pmatrix},$$  \hspace{0.5cm} (A.1)

where $\vec{k} = (k_x, k_y)$ is the in-plane surface wavevector and $k_z = k_x \pm ik_y$. The energy dispersion associated with this Hamiltonian is given by $E_{\text{surf}}^{3D} = Dk^2 + \beta Ak$ with $\beta = \pm 1$.

We now turn to the case when the surface of the 3DTI is irradiated by circularly polarized light with vector potential

$$\hat{A} = \mathcal{F}_0 \left( e_x \hat{a} + e_y \hat{a}^\dagger \right),$$  \hspace{0.5cm} (A.2)

where $e_x = (e_x \pm ie_y) / \sqrt{2}$, $e_x$ and $e_y$ are unit vectors in the $x$ and $y$ directions, respectively. Consequently, the in-plane components of the vector potential may be expressed as

$$\hat{A}_x = \mathcal{F}_0 \sqrt{2} (\hat{a} + \hat{a}^\dagger), \quad \hat{A}_y = i \mathcal{F}_0 \sqrt{2} (\hat{a} - \hat{a}^\dagger).$$  \hspace{0.5cm} (A.3)

In order to include electron–photon coupling, we make the following substitutions for the electron wavevector:

$$k_x \rightarrow k_x + e \hat{A}_x / h = k_x + e \mathcal{F}_0 \sqrt{2} (\hat{a} + \hat{a}^\dagger),$$

$$k_y \rightarrow k_y + e \hat{A}_y / h = k_y + e \mathcal{F}_0 \sqrt{2} (\hat{a} - \hat{a}^\dagger),$$

$$k_+ \rightarrow k_+ + \sqrt{2} e \mathcal{F}_0 / h \hat{a}^\dagger,$$

$$k_- \rightarrow k_- + \sqrt{2} e \mathcal{F}_0 / h \hat{a},$$

$$k^2 = k_+ k_- \rightarrow k^2 + \frac{2e \mathcal{F}_0}{h} \left( k_+ \hat{a} + k_- \hat{a}^\dagger \right) + \left( \frac{\sqrt{2} e \mathcal{F}_0}{h} \right)^2 \hat{a}^\dagger \hat{a}.$$  \hspace{0.5cm} (A.4)

In our investigation, we consider high-intensity light with $N_0 = (\hat{a}^\dagger \hat{a}) \gg 1$, and then $\hat{a} \hat{a}^\dagger \sim \hat{a}^\dagger \hat{a}$ due to $\hat{a} \hat{a}^\dagger = \hat{a}^\dagger \hat{a} + 1$ for bosonic operators. We adopt this simplification only for the second-order terms $\sim(\sqrt{2} e \mathcal{F}_0 / h)^2$ but not for the principal ones containing $\h_0$. With the aid of these substitutions, the Dirac-like contribution to the Hamiltonian in equation (A.1) becomes

$$\hat{\mathcal{H}}_{\text{Dirac}} = A \sqrt{\alpha} \cdot \vec{k} = A \begin{pmatrix} \sigma_- k_+ + \sigma_+ k_- \\ \sigma_+ k_+ + \sigma_- k_- \end{pmatrix} + \frac{\sqrt{2} e \mathcal{F}_0}{h} A \begin{pmatrix} \sigma_- \hat{a}^\dagger + \sigma_+ \hat{a} \end{pmatrix}.$$  \hspace{0.5cm} (A.5)

where $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$. To describe a full electron–photon coupled system, we also need to take into account the photon energy term $\h_0 \hat{a}^\dagger \hat{a}$. This yields

$$\hat{\mathcal{H}} = (\h_0 + 4D \xi^2) \hat{a}^\dagger \hat{a} + Dk^2 \sqrt{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + 2\xi D \left( k_+ \hat{a} + k_- \hat{a}^\dagger \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + A \begin{pmatrix} \sigma_- k_- + \sigma_+ k_+ \\ \sigma_+ k_- + \sigma_- k_+ \end{pmatrix} + 2\xi A \begin{pmatrix} \sigma_- \hat{a}^\dagger + \sigma_+ \hat{a} \end{pmatrix}.$$  \hspace{0.5cm} (A.6)
where $\zeta = \epsilon_F a_0/(\sqrt{2}h)$. We may also rewrite the Hamiltonian in equation (A.6) in matrix form as

$$\hat{H} = \left(\hbar \omega_0 + 4 D \zeta^2\right) \hat{a}^\dagger \hat{a} + \frac{1}{2} + \frac{3}{2}$$

$$= \left(\hbar \omega_0 + 4 D \zeta^2\right) \hat{a}^\dagger \hat{a} + \left(D k^2 + A k_+ + A k_+ \right)$$

$$+ 2 \zeta D \left(\begin{array}{ccc} (k_+ \hat{a}^\dagger + k_+ \hat{a}) & 0 \\ 0 & (k_- \hat{a} + k_+ \hat{a}) \end{array}\right)$$

$$+ 2 \zeta A \left(\begin{array}{ccc} 0 & \hat{a}^\dagger \\ \hat{a} & 0 \end{array}\right),$$  

(A.7)

where $1 \equiv \hat{H}_{\text{surf}}^{0}$ denotes the initial surface Hamiltonian with no electron–photon interaction, $2$ gives the principal effect due to light coupled to electrons (the only non-zero term at $k = 0$) and $3$ is the leading term demonstrating the difference between dressed states in graphene and a 3DTI.

We know from equation (A.7) that the Hamiltonian at $k = 0$ reduces to the exactly solvable Jaynes–Cummings model, after we neglect the field correction of the order of $\mathcal{O}(\zeta^2)$. We obtain

$$\hat{H}_{k=0} = \hbar \omega_0 \hat{a}^\dagger \hat{a} + 2 \zeta A \left(\begin{array}{ccc} \hat{a}^\dagger \hat{a} + \hat{\sigma}^- \hat{\sigma}^+ \\ \hat{a} \hat{a}^\dagger \end{array}\right).$$

(A.8)

Following the method adopted in [9, 16], we expand the eigenfunctions of equation (A.8) as

$$|\Psi_{\uparrow,0}^0, N_0\rangle = |\mu_{\uparrow, N_0} \uparrow \downarrow, N_0 + 1\rangle + |v_{\uparrow, N_0} \downarrow \uparrow, N_0 + 1\rangle,$$

$$|\Psi_{\downarrow,0}^0, N_0\rangle = |\mu_{\downarrow, N_0} \downarrow \uparrow, N_0 - 1\rangle - |v_{\downarrow, N_0} \uparrow \downarrow, N_0 - 1\rangle.$$  

(A.9)

By using the properties

$$\hat{a}^\dagger \hat{a} \downarrow \uparrow, N_0 = \sqrt{N_0 + 1} \downarrow \uparrow, N_0 + 1\rangle,$$

$$\hat{a} \hat{a}^\dagger \uparrow \downarrow, N_0 = \sqrt{N_0 - 1} \uparrow \downarrow, N_0 - 1\rangle,$$

$$\hat{\sigma}^+ \downarrow \uparrow, N_0 = (1 - \mathcal{D} + \mathcal{D}) \uparrow \downarrow, N_0\rangle,$$

(A.10)

we obtain the energy eigenvalues

$$\frac{\epsilon_{\pm \uparrow, N_0}}{\hbar \omega_0} = N_0 \pm \frac{1}{2} \pm \frac{1}{2} \sqrt{\frac{\alpha^2}{N_0} + \frac{1}{2} \pm \frac{1}{2}}$$

$$\simeq N_0 \pm \frac{1}{2} \pm \sqrt{\frac{1}{4} + \frac{1}{4} \alpha^2} = N_0 \pm \frac{\alpha^2}{4}. \quad (A.11)$$

(A.12)

where $\Delta \approx \Delta^0$ is the energy gap at $k \neq 0$ and we have employed the relations for $N = N_0$ or $N_0 + 1$,

$$\vec{\sigma} \cdot \mathbf{k} |\Psi_{\uparrow,0}^0\rangle = \vec{\sigma} \cdot \mathbf{k} (|\mu\uparrow, N_0 + 1\rangle + |v\downarrow, N_0 + 1\rangle) \approx \mu_{\uparrow, N_0 + 1} \uparrow \downarrow, N_0 + 1\rangle$$

$$\approx \mu_{\downarrow, N_0 - 1} \downarrow \uparrow, N_0 - 1\rangle + v_{\downarrow, N_0 - 1} \uparrow \downarrow, N_0 - 1\rangle.$$  

(A.13)

(A.14)

Consequently, we only need to keep one pair of index-free coefficients $[\mu, \nu]$ such that $\mu = \cos(\Phi)$, $\nu = \sin(\Phi)$, with $\Phi = \tan^{-1}(a/2)$. Furthermore, from the first equality in equation (A.11), it follows that the energy gap still depends on $N_0$ in general. However, the difference $\Delta N_0 + 1 - \Delta N_0 \approx \Delta^0 \nu/N_0$ is so small that we neglect it for $N_0 \gg 1$.

Generalizing equation (A.9), we still expand the wavefunction $\Psi_k$ over the eigenstates of the Hamiltonian in equation (A.8) for $k \neq 0$, i.e.

$$|\Psi_k\rangle = \sum_{j=0}^{N_0+1} \left(\begin{array}{c} \varepsilon_k^{-j} \Psi_{j+1,0}^0 \Psi_{j+1,1}^0 \Psi_{j,0}^0 \Psi_{j+1,1}^0 \Psi_{j+1,0}^0 \Psi_{j+1,1}^0 \end{array}\right)$$

$$= \varepsilon_k^0 \Psi_{j+1,0}^0 + \varepsilon_k^1 \Psi_{j+1,1}^0 \langle \Psi_{j,0}^0 \Psi_{j+1,1}^0 \rangle$$

$$+ \varepsilon_k^0 \Psi_{j+1,0}^0 \Psi_{j+1,1}^0$$

$$+ \langle \varepsilon_k^0 \Psi_{j+1,0}^0 + \varepsilon_k^1 \Psi_{j+1,0}^0 \rangle \langle\Psi_{j+1,1}^0 \Psi_{j+1,1}^0 \rangle.$$  

(A.15)

(A.16)

Using equation (A.16) we project the full Hamiltonian in equation (A.6) onto the representation $\{\varepsilon_k^0 \Psi_{j+1,0}^0, \varepsilon_k^1 \Psi_{j+1,1}^0, \varepsilon_k^0 \Psi_{j+1,1}^0\}$. This yields

$$\left(\begin{array}{ccc} \hbar \omega_0 + 4 D \zeta^2 & \mu^2 A k_+ & 0 \\ \mu^2 A k_- & D k + D k_+ & \mu \omega - 2 D \zeta \omega \\ 0 & \mu \omega - 2 D \zeta \omega & D k + D k_- \end{array}\right).$$

(A.17)

where $\Delta \approx \Delta^0$ is the energy gap at $k \neq 0$ and we have employed the relations for $N = N_0$ or $N_0 + 1$,

$$\vec{\sigma} \cdot \mathbf{k} |\Psi_{\uparrow,0}^0\rangle = \vec{\sigma} \cdot \mathbf{k} (|\mu\uparrow, N_0 + 1\rangle + |v\downarrow, N_0 + 1\rangle) \approx \mu_{\uparrow, N_0 + 1} \uparrow \downarrow, N_0 + 1\rangle$$

$$\approx \mu_{\downarrow, N_0 - 1} \downarrow \uparrow, N_0 - 1\rangle + v_{\downarrow, N_0 - 1} \uparrow \downarrow, N_0 - 1\rangle.$$  

(A.18)

(A.19)

After calculating the eigenvalues for the Hamiltonian in equation (A.17), we obtain closed form analytic expressions with energy dispersion

$$\varepsilon_{[N_0 \uparrow, N_0 \downarrow, \Delta]} (k, \Delta) = \left(\begin{array}{c} N_0 + \frac{1}{2} \end{array}\right) + \text{DK}^2$$

$$\pm \sqrt{C_1 (k, \Delta) \pm \sqrt{C_2 (k, \Delta)}}.$$  

(A.20)

(A.21)
\[ C_1(k, \Delta) = (\hbar \omega_0/2)^2 + \kappa v A D k^2 \]
\[ + \left[ \kappa^2 D^2 + A^2 (1 + 5/2 \nu^2) \right] k^2, \quad (A.22) \]
\[ C_2(k, \Delta) = \kappa^2 A^2 D^2 k^4 (1 + v^2) + 4v(\kappa v D + A) A^3 k^4 \]
\[ - 3v(2\kappa D + v A) A \hbar \omega_0 k^2 + 4\hbar^2 \omega_0^2 (\Delta^2 + A^2 k^2). \quad (A.23) \]

Taking the limits \( \kappa D \to 0 \) and \( v k \to 0 \), we are left with two uncoupled energy subbands
\[ \varepsilon_{(N_0, N_0)}(k, \Delta) = N_0 \hbar \omega_0 + D k^2 \]
\[ \pm \sqrt{\Delta^2 + A^2 k^2}, \quad (A.24) \]
\[ \varepsilon_{(N_0+1, N_0+1)}(k, \Delta) = (N_0 + 1) \hbar \omega_0 + D k^2 \]
\[ \pm \sqrt{\Delta^2 + A^2 k^2}. \quad (A.25) \]

Therefore, we conclude that the effect of electron–phonon interaction is quite similar to that in graphene as far as one photon number \( N_0 \) is concerned. The main difference is that the energy gap in the 3DTI is of order \( O(\zeta^2) \), which may be neglected for low-intensity light. Consequently, the energy dispersion relation becomes
\[ \varepsilon_{\beta}(k, \Delta_0) = N_0 \hbar \omega_0 + D k^2 \]
\[ + \beta \sqrt{[\Delta_0 + O(\zeta^2)]^2 + (\Delta k)^2}, \quad (A.26) \]
where \( \beta = \pm 1 \) and \( \Delta_0 \) is the photon-induced energy gap as in graphene.

### Appendix B. Dressed 3DTI electron surface states

It follows from Appendix A that the effect due to \( \sim \hat{A}^2 \)-terms would play a role only if two optical modes are considered. This effect is of order \( O(\zeta^2) \) and may be neglected in our calculations. When a surface of the 3DTI is irradiated with circularly polarized light, the light will penetrate into the sample and decay exponentially away from the surface, similarly to the wavefunction for a surface electronic state. Therefore, by including this decay effect, the vector potential in equation (A.2) is generalized as
\[ \hat{A} = \hat{A}_0 \left( \hat{e}_+ \hat{a} + \hat{e}_- \hat{a}^\dagger \right) e^{-\frac{\Delta z}{\xi}}, \quad (B.1) \]
where \( 1/\xi \) is the decay length. By including the \( \epsilon \) dependence, the Hamiltonian of the electron system is found to be
\[ \hat{H}_{3D}(k, z) = \hat{H}_{3D}^{(1)}(z) + \hat{H}_{3D}^{(2)}(k), \quad (B.2) \]
where
\[ \hat{H}_{3D}^{(1)}(z) = \left( \begin{array}{cc} \mathcal{C} & \mathcal{M} + \hat{B}_0 \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 \hat{B}_0 \hat{a}^\dagger \hat{\sigma}_1 \hat{\sigma}_1 & \hat{A}_0 \hat{B}_0 \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 \hat{B}_0 \hat{a}^\dagger \hat{\sigma}_1 \hat{\sigma}_1 \\ (\mathcal{M} + \hat{B}_0 \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 & \hat{A}_0 \hat{B}_0 \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 \hat{B}_0 \hat{a}^\dagger \hat{\sigma}_1 \hat{\sigma}_1 & 0 \end{array} \right) \]
\[ \hat{H}_{3D}^{(2)}(k) = \left( \begin{array}{cc} \mathcal{D}_k \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 & \hat{B}_0 \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 \hat{B}_0 \hat{a}^\dagger \hat{\sigma}_1 \hat{\sigma}_1 \hat{B}_0 \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 \hat{B}_0 \hat{a}^\dagger \hat{\sigma}_1 \hat{\sigma}_1 \\ (\mathcal{D}_k & \hat{B}_0 \hat{a} \hat{\sigma}_1 \hat{\sigma}_1 \hat{B}_0 \hat{a}^\dagger \hat{\sigma}_1 \hat{\sigma}_1 & 0 \end{array} \right). \quad (B.3) \]

The Hamiltonian in equation (B.5) may be rewritten compactly as
\[ \hat{H}_{3D}(k, z) = \hat{H}_{3D}^{(1)}(z) + \hat{H}_{3D}^{(2)}(k, z), \quad (B.7) \]

In analogy with equation (A.9), we construct a basis set containing four states, i.e., \( |++\rangle = [1, 0, 0, 0] \), \( |-+\rangle = [0, 1, 0, 0] \), \( |+\rangle = [0, 0, 1, 0] \), \( |-\rangle = [0, 0, 0, 1] \). For this basis set, the Hamiltonian in equation (B.5) may be written as
\[ \hat{H}_{3D}(k, z) = \left( \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right). \]

We may also expand the dressed electronic states at \( k = 0 \) over this basis set, leading to
\[ |\Psi_{++\,+}^{0\,+}\rangle = \mu_{++\,+} |++\rangle + \nu_{++\,+} |-+\rangle + \kappa_{++\,+} |+\rangle + \lambda_{++\,+} |-\rangle, \]
\[ |\Psi_{+-\,+}^{0\,+}\rangle = \mu_{+-\,+} |++\rangle + \nu_{+-\,+} |-+\rangle + \kappa_{+-\,+} |+\rangle + \lambda_{+-\,+} |-\rangle \]
For $N \gg 1$ and $\alpha' \ll 1$, calculation shows that

$$\mu_{N,+} \simeq \mu_{N,-} \simeq \mu_{N+1,+} \simeq \mu_{N+1,-} \simeq 1 - \left( \frac{\alpha'}{2} \right)^2,$$

and

$$\nu_{\perp} \simeq \nu_{\perp+} \simeq \nu_{\perp+1} \simeq \nu_{\perp+1,-} \simeq \alpha'. \tag{B.9}$$

Introducing the pair of operators

$$\vec{\gamma}_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{B.10}$$

$$\vec{\gamma}_{34} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{B.11}$$

we obtain

$$\vec{\gamma}_{12} \ket{N, -+} = \ket{N, ++},$$

$$\vec{\gamma}_{34} \ket{N, ++} = \ket{N, -+}, \tag{B.12}$$

$$\vec{\gamma}_{34} \ket{N, -+} = \ket{N, ++},$$

$$\vec{\gamma}_{12} \ket{N, ++} = \ket{N, -+}. \tag{B.13}$$

For the Hamiltonian in equation (A.7) within the $2 \times 2$ subspace, as a special case, we introduce

$$\vec{\sigma}_{+} = \vec{\gamma}_{12}, \quad \vec{\sigma}_{-} = \vec{\gamma}_{34}. \tag{B.14}$$

Finally, we can rewrite the full Hamiltonian in equation (B.2) for $k \neq 0$, using the basis set $|N_0, \pm\rangle$, as

$$\tilde{H}_{3D}(k, z) = N_0 \hbar v_0 \left( \begin{array}{cc} c_{\downarrow} - D_\downarrow z - D_\uparrow z^+ & A_{\downarrow 0} \\ -A_{\downarrow 0} & c_{\uparrow} - D_\uparrow z - D_\downarrow z^+ \end{array} \right) \begin{pmatrix} 0 & A_{\downarrow \uparrow} \\ A_{\uparrow \downarrow} & 0 \end{pmatrix} \begin{pmatrix} c_{\downarrow} - D_\downarrow z - D_\uparrow z^+ & A_{\downarrow 0} \\ -A_{\downarrow 0} & c_{\uparrow} - D_\uparrow z - D_\downarrow z^+ \end{pmatrix}, \tag{B.15}$$

where the $\pm$ signs correspond to opposite pseudo-spins in the basis set. Making use of equation (B.15), we obtain the secular equation for the energy dispersion relations when $\Delta = 0$, that is,

$$\varepsilon^2 - A_{\perp}^2 k^2 + N_1 N_1 + A_{\parallel}^2 \xi^2 + D_\perp N_1 \xi^2 + D_\parallel N_2 \xi^2 + D_\perp D_\parallel N_2 \xi^2 + D_\perp D_\parallel \xi^4 - (N_1 + N_2 + 2D_\parallel^2) \varepsilon = 0, \tag{B.16}$$

where we have introduced the notation

$$N_{1,2}(k) = C \pm M \pm (D_\perp \mp B_\perp) k^2, \tag{B.17}$$

$$D_\perp = D_2 \pm B_2. \tag{B.18}$$

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