Shift charge and spin photocurrents in Dirac surface states of topological insulator

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The generation of photocurrent in condensed matter is of main interest for photovoltaic and optoelectronic applications. Shift current, a nonlinear photoresponse, has attracted recent intensive attention as a dominant player of bulk photovoltaic effect in ferroelectric materials. In three-dimensional topological insulators Bi_2X_3 (X = Te, Se), we find that Dirac surface states with a hexagonal warping term support shift current by linearly polarized light. Moreover, we study "shift spin current" that arises in Dirac surface states by introducing time-reversal symmetry breaking perturbation. The estimate for the magnitudes of the shift charge and spin current densities are $0.13I_0$ and $0.40I_0$ (nA/m) for Bi_2Te_3 with the intensity of light I_0 measured in (W/m^2), respectively, which can offer a useful method to generate these currents efficiently.

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Introduction and background. Interaction of light with topological matters has drawn keen attention in the condensed matter community. Not only the characterization of topological matter has been done by light-assisted experimental tools that probe electronic bands [1–3] and its spin textures [4,5], optical conductivities, Kerr rotation [6–10], Faraday effect [8–11], etc., but also light plays active roles to dynamically induce topological phase transitions [12–18] and generates a new type of topological excitations [19–21].

Among them, photocurrent generation in condensed matters is an active research field closely related to light-harvesting energy research [22–26] and optoelectronic device applications [27–32]. In particular, shift current is the nonlinear optical responses, where the dc current is produced by light irradiation without the external electric field or potential gradient, whose direction is determined by the crystal structure or the direction of the electric polarization. The shift current is considered to play a dominant role in bulk photovoltaic effect of ferroelectric materials including hybrid perovskite materials [23,24]. Further optimal engineering of materials that support shift current is investigated [32] to enhance photovoltaic efficiency.

The shift current has a geometrical origin that is described by the Berry phase connection $\boldsymbol{a}_n(\boldsymbol{k})$ of Bloch wave functions (n: band index; $\boldsymbol{k}$: crystal momentum), and is nonvanishing only in noncentrosymmetric crystals. Namely, the real space position $\boldsymbol{r}_n$ of the wave packet made from the Bloch wave functions of band n is given by the expression

$$\boldsymbol{r}_n = i\frac{\partial}{\partial \boldsymbol{k}} + \boldsymbol{a}_n(\boldsymbol{k}). \quad (1)$$

The first term comes from the canonical conjugate relation between the real space coordinate $\boldsymbol{r}$ and the wave vector $\boldsymbol{k}$, and the second term named "intracell coordinates" originates from the constraint that the wave functions are confined in a manifold, i.e., subset of the Hilbert space spanned by the Bloch states of band n [33,34]. The covariant derivative with the "connection" $\boldsymbol{a}_n(\boldsymbol{k})$ is the physical operator for this curved manifold. From the symmetry point of view, Berry phase is allowed in noncentrosymmetric systems when the time-reversal symmetry is not broken. This is because the Berry curvature $\boldsymbol{b}_n(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} \times \boldsymbol{a}_n(\boldsymbol{k})$ satisfies $\boldsymbol{b}_n(\boldsymbol{k}) = -\boldsymbol{b}_n(-\boldsymbol{k})$ due to the time-reversal symmetry $\mathcal{T}$. The inversion symmetry $\mathcal{I}$ further gives the constraint $\boldsymbol{b}_n(\boldsymbol{k}) = -\boldsymbol{b}_n(\boldsymbol{k})$, which concludes $\boldsymbol{b}_n(\boldsymbol{k}) = \boldsymbol{0}$ and one can choose the gauge $\boldsymbol{a}_n(\boldsymbol{k}) = \boldsymbol{0}$. Therefore, it is essential to break either $\mathcal{T}$ or $\mathcal{I}$ for the nonzero $\boldsymbol{a}_n(\boldsymbol{k})$. As the Berry connection is "intracell coordinates," it is related to the electric polarization $\boldsymbol{P}$ in ferroelectrics [35,36]. Also, the difference between $\boldsymbol{a}_{n=c}(\boldsymbol{k})$ and $\boldsymbol{a}_{n=v}(\boldsymbol{k})$ represents the shift in the intracell coordinates of electrons accompanied with the optical transitions from the valence band v to the conduction band c as schematically shown in Fig. 1. Under steady optical pumping, the constantly induced shift described above results in the dc current, which is the shift current. Furthermore, when the shift differs between the up and down spins, the shift spin current is induced as shown in Fig. 1(c).

Topological surface states are good candidates to support shift currents as the inversion symmetry $\mathcal{I}$ is always broken at the surface of materials. We show in this paper that linearly polarized light can generate shift currents on warped topological surface states [37,38] in Bi_2X_3-type topological insulators. Here the warping term breaks the mirror symmetry in one direction, and this determines unique combination of current and electric field directions to have nonzero shift currents. Furthermore, in this paper we introduce a new notion of "the shift spin current," which is also of geometrical origin described by Berry phase connection. As for the surface states of topological insulators, we propose that pure shift spin current (without shift charge current) is induced by breaking the time-reversal symmetry $\mathcal{T}$ with magnetic doping. Shift charge and spin current production on Dirac surface states discussed here will give a basis for optoelectronic and optospintronic devices by topological insulators.

Model and formalism for shift charge and spin currents. The shift current can be understood in several ways as explained below. Sipe and Shkrebtii [39] studied the photocurrent $J_j^{\text{shift}} = \sum_{i=x,y} \chi_j^{ii} E_i E_i$ by using the standard perturbation theory. In

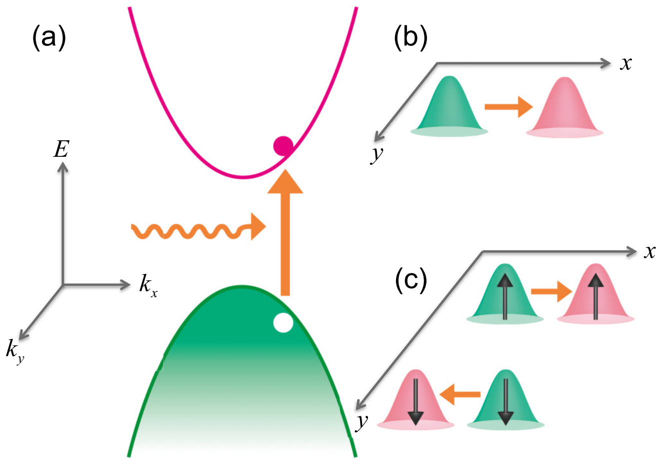

FIG. 1. Generation of shift charge current and shift spin current are pictorially described. (a) An electronic excitation induced by light from valence band to conduction band is schematically shown. (b) When the center of charge of Bloch state is shifted upon interband transition, from the green to the red wave packet, the shift charge current is generated. (c) Two wave packets consisting of opposite spins can exhibit different shifts upon optical transition, which results in the shift spin current.

the case of a linearly polarized light, they obtained a compact formula given by

$$\chi_j^{ii} = \frac{\pi}{\Omega^2}\int \frac{d^d\boldsymbol{k}}{(2\pi)^d}\delta(\omega_{cv}-\Omega)\left|v_{vc}^i\right|^2\left(\partial_{k_j}\varphi_{cv}^i + a_c^j - a_v^j\right), \tag{2}$$

where i and j are Cartesian coordinates, and Berry connection $a_c^j = -i\langle\psi_c|\partial_{k_j}\psi_c\rangle$ and $a_v^j = -i\langle\psi_v|\partial_{k_j}\psi_v\rangle$ for conduction and valence band, respectively. The contributions are from the states satisfying the resonant condition: $\omega_{cv} - \Omega = \epsilon_c - \epsilon_v - \Omega$. The bracket on the right side is called a shift vector as the Berry connection a_c^j indicates a shifting in real space of conduction band Bloch wave function along j_{th} direction. $(a_c^j - a_v^j)$ is a difference of shifting between conduction and valence band as discussed for Fig. 1, and $\partial_{k_j}\varphi_{cv}^i$ maintains the gauge invariance.

An alternative derivation of the photocurrent expression was obtained by two of the authors previously [40,41] by using Floquet formalism with Keldysh Green's function. They rederived the second-order photocurrents in an easier manner compared to previous approaches [39,42,43], which we briefly review to facilitate understanding of the following discussions. First we consider, for simplicity, a two-band system under a periodic time-dependent electric field with frequency Ω, $\boldsymbol{E}(t) = -\partial_t\boldsymbol{A}(t) = -i\Omega(\boldsymbol{A}e^{i\Omega t} + \text{c.c.})$. Treating the external field classically, we can write a Floquet Hamiltonian in the basis of valence and conduction bands [12,14,40,44] (hereafter, $\hbar = 1$ and $e = 1$ is used):

$$H_F = \begin{pmatrix} \epsilon_v + \Omega & i\boldsymbol{A}^*\cdot\boldsymbol{v}_{vc} \\ -i\boldsymbol{A}\cdot\boldsymbol{v}_{cv} & \epsilon_c \end{pmatrix}, \tag{3}$$

where we concentrate on one valence band with a single photon absorbed and one conduction band. $\epsilon_{c,v}$ are eigenvalues of original Hamiltonian H. Two bands in the Floquet Hamiltonian are coupled by time-dependent terms, $\langle u_v|\frac{1}{T}\int_0^T H(\boldsymbol{k}-\boldsymbol{A}^*(t))e^{i\Omega t}dt|u_c\rangle$. By taking the linear order of external field only, the coupling can be expressed in terms of Fermi velocity: $i\boldsymbol{A}^*\cdot\boldsymbol{v}_{vc} = i\sum_j A_j^* v_{vc}^j$ with $v_{vc}^j = \langle\psi_v|\partial_{k_j}H|\psi_c\rangle = |v_{vc}^j|e^{i\varphi_{vc}^j}$. By the proper transformation, the monochromatic time dependence of the off-diagonal matrix elements is eliminated and instead the shift of the energy by Ω appears in the diagonal component in Eq. (3) [12,14,44]. By using this Floquet Hamiltonian, the current in the steady state (shift current) is written as

$$J_j = \int \frac{d^d k}{(2\pi)^d}\text{Im}\left[\delta(\omega_{cv}-\Omega)(\boldsymbol{A}^*\cdot\boldsymbol{v}_{vc})\left(\boldsymbol{A}\cdot\partial_{k_j}\boldsymbol{v}\right)_{cv}\right], \tag{4}$$

with the vector potential $\boldsymbol{A}$ of electromagnetic field and

$$\left(\boldsymbol{A}\cdot\partial_{k_j}\boldsymbol{v}\right)_{cv} = \sum_i A_i\langle u_c|\partial_{k_j}v^i|u_v\rangle. \tag{5}$$

Provided that [40] $(\partial_{k_j}v^i)_{cv} = \partial_{k_j}v_{cv}^i - \langle\partial_{k_j}u_c|v^i|u_v\rangle - \langle u_c|v^i|\partial_{k_j}u_v\rangle$, one can recover the shift current expression found by Sipe and Shkrebtii [39] in terms of Berry connections. Expressed in terms of v_{vc}^i and $(\partial_{k_j}v^l)_{cv}$, Eq. (4) just looks like a correlation function between paramagnetic current and diamagnetic current. A Kubo conductivity in the linear response theory is obtained by taking a correlation function between two paramagnetic currents, $j_{\text{para}}^i = \frac{\partial H(\boldsymbol{k}-\boldsymbol{A}(t))}{\partial A_i}\big|_{\boldsymbol{A}=0} = -v^i$. Equation (4) is also a current-current correlation function. Since a diamagnetic current contains the vector potential as $j_{j,\text{dia}}^l = \frac{\partial^2 H(\boldsymbol{k}-\boldsymbol{A}(t))}{\partial A_l\partial A_j}\big|_{\boldsymbol{A}=0}A_l = (\partial_{k_j}v^l)A_l$, the photocurrent J is proportional to the square of electric field. Namely, the susceptibility of current $J_j = \sum_{il}\chi_j^{il}E_iE_l$ in Eq. (4) can be computed by the one-loop integration similar to the linear response function. (See Supplemental Material S1 [45] for details.) Note that Eq. (4) does not contain the dissipation due to the coupling to other degrees of freedom or the electron-electron scattering. These effects can be treated by the self-energy of Keldysh Green's function, and does not change the results essentially when the spectrum of incident light has a width larger than the relaxation rate. (See Ref. [40] for more details.)

Lastly, we introduce a shift spin current, which is an extension of a shift charge current discussed so far. In a similar manner to the shift of charge center upon optical transition, one can also think of the shifting of spin center that leads to a shift spin current as shown in Fig. 1(c). This can be most conveniently obtained by generalizing the formula for the shift charge current in Eq. (4), where the diamagnetic current is replaced by the diamagnetic spin current, i.e., the anticommutator between diamagnetic current and spin operator $\hat{s}_\alpha = \sigma_\alpha/2$ for α component. (See Supplemental Material S1 [45] for details.) Young and Rappe [46] first discussed the spin bulk-photovoltaic effect in antiferromagnets by computing shift current for spin up and spin down, independently. Our formalism is applicable to more general cases with spin orbit couplings.

In the following, we show that the breaking of the inversion symmetry $\mathcal{I}$ is required to have a shift charge current, and the breaking of the time-reversal symmetry $\mathcal{T}$ is additionally required to have a shift spin current. To demonstrate, we consider two examples in $3d$ topological insulators: warped Dirac surface states that carry shift charge currents, and massive Dirac surface states with band-bending that carry shift spin currents.

Shift charge current in Dirac surface states of topological insulators. A system with the inversion symmetry supports a zero shift current. We first review this fact. This is intuitively understood, because a state $|\boldsymbol{k}\rangle$ and its inversion symmetric partner $\mathcal{I}|\boldsymbol{k}\rangle$ will be shifted in opposite direction after being excited to a conduction band. (More formal discussion is given in Supplemental Material S2 [45].) Note that, since the spin is invariant under the inversion symmetry operation, $\mathcal{I}:\hat{s}_\alpha \to \hat{s}_\alpha$, the susceptibility of shift spin current is also exactly canceled between inversion symmetry partners.

Now we study Dirac surface states in $3d$ topological insulators that are localized near open surfaces. Its low energy effective Hamiltonian is $H_0 = -v_F k_y \sigma_x + v_F k_x \sigma_y$, for which the inversion symmetry is absent. But, $H_0(\boldsymbol{k} - \boldsymbol{A}(t))$ does not contain diamagnetic terms ($\sim A_i A_l$), hence no shift current. Instead, we find that shift charge currents are nonzero by including warping effects which is allowed with C_{3v} crystalline symmetry and is found to be present in $3d$ topological insulators of $\mathrm{Bi}_2 X_3$ (where $X = \mathrm{Te, Se}$) type [37]. The warped Dirac surface state Hamiltonian is [38]

$$H = -v_F k_y \sigma_x + v_F k_x \sigma_y + \lambda\left(k_x^3 - 3k_x k_y^2\right)\sigma_z. \tag{6}$$

The energy dispersion of Eq. (6) is shown in Fig. 2(a), where the light with frequency Ω induces transition between the lower and upper branches satisfying the energy conservation. This Hamiltonian is mirror symmetric along x, but not along y. As a result, the susceptibility χ_j^{il} $(j,i,l = x,y)$ can be nonzero when the index y appears the odd number of times so that its mirror symmetric partner does not cancel the shift current. Indeed, a straightforward calculation of current-current correlation function shows that nonzero components are (see Supplemental Material S4 [45]) $\chi_y^{xx} = \chi_x^{yx} = -\chi_y^{yy} = \frac{3\lambda}{16 v_F^2}$. Figures 2(b), 2(c), and 2(d) show the momentum distributions of the matrix elements appearing in the integrals for the y component of the shift current for the incident light polarized along y direction. For a linearly polarized light $\boldsymbol{E}(t) = E_0(\cos\phi\hat{x} + \sin\phi\hat{y})\cos\Omega t = E_0\hat{x}'\cos\Omega t$ in the general direction, an induced shift current is

$$\begin{aligned}\boldsymbol{J}_{\text{warp}} &= -\frac{3\lambda}{16v_F^2}\left[E_y^2\hat{y} - E_x^2\hat{y} - E_xE_y\hat{x} - E_yE_x\hat{x}\right]\\ &= \frac{3\lambda E_0^2}{16v_F^2}[\sin(3\phi)\hat{x}' + \cos(3\phi)\hat{y}'],\end{aligned} \tag{7}$$

where $\hat{x}$ and $\hat{y}$ are unit vectors corresponding to the crystal axes, and $\hat{x}'$ and $\hat{y}'$ are those for the coordinates where $\hat{x}'$ is along the applied electric field. It is clear in this coordinate that the shift current is in accordance with C_{3v} crystalline symmetry. Interestingly, the shift charge photocurrent found here is photon-frequency independent. This is remarkable since the effect of warping is expected to be reduced as the frequency Ω approaches to zero because the corresponding wave number k becomes small and higher order warping term becomes irrelevant. The derivative with respect to k in the expression of the shift current enhances the effect of the warping term, and results in the frequency independent contribution.

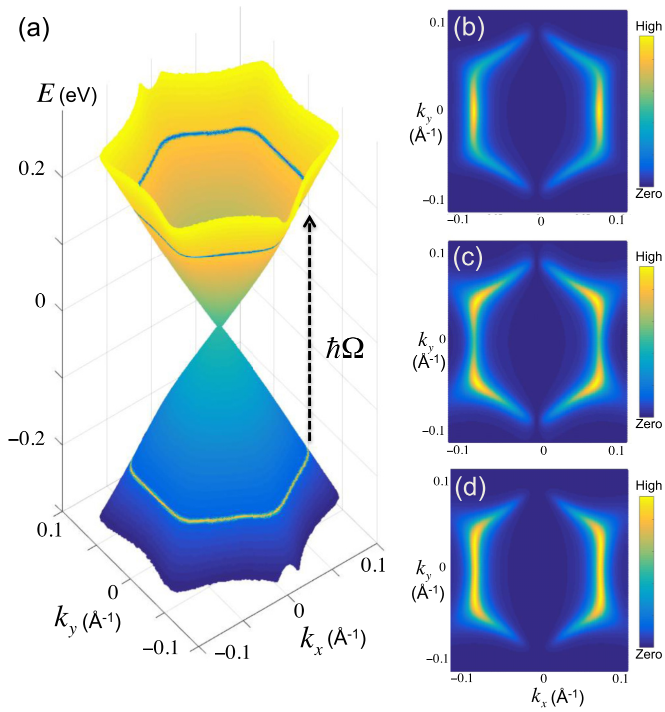

FIG. 2. Warped Dirac surface state carries the shift charge current. The Fermi velocity $v_F = 2.55\hbar^{-1}(\mathrm{eV\,\AA})$ and the warping strength $\lambda = 250(\mathrm{eV\,\AA}^3)$ are used [38]. We show the matrix elements that contribute to the nonlinear susceptibility χ_y^{yy}. (a) The energy dispersion is drawn with electronic states satisfying the resonant condition, $\epsilon_c - \epsilon_v = \Omega$, in distinct colors. (b) The coupling strength of Bloch states in the resonant condition to diamagnetic current response, $|(\partial_{k_y} v^y)_{cv}|$, is shown in color. (c) The coupling strength of Bloch states in the resonant condition to a linearly polarized light, $|(v^y)_{vc}|$, is shown in color. (d) The contribution of Bloch states to the shift charge current, $|(v^y)_{vc}(\partial_{k_y} v^y)_{cv}|$, is shown in color.

We give an estimate of the shift current in Dirac surface states with warping effect by using the microscopic parameter obtained from experiments [38,47,48]. The estimate is given by $J_{\text{warp}} = 19 I_0 - 130 I_0 (\mathrm{pA/m})$, where I_0 is the intensity of light in the unit of $(\mathrm{W/m^2})$ (see Supplemental Material S6 [45].) In recent experiments [49–51], photocurrents are measured in Dirac surface states using oblique incident light, which effectively breaks the in-plane rotational symmetry. Assuming the sample size of $1(\mathrm{mm}^2)$, the photocurrent density is of the order of $1 I_0 (\mathrm{pA/m})$. Compared to this value, the shift current is expected to be two orders of magnitude larger and should be feasible to measure experimentally.

Theoretical proposals and recent experiments on photocurrent generation in topological insulators are all based on the circular photogalvanic effect (CPGE), which relies on the selective interband excitations of Bloch states by introducing various perturbations that break the rotational symmetry and the time-reversal symmetry. For example, magnetic superlattices [52], external in-plane magnetic field or strains [53,54], orbital and Zeeman coupling [54], the dielectric ferromagnetic proximity effect [55], and photon-drag effect [49,50,53,54] are employed. See Supplemental Material S6 [45] for their numerical comparisons with the shift currents. We emphasize that the mechanism of the shift currents is clearly distinct from that of the CPGE, which can be computed from the three point paramagnetic current correlation [53] or equivalently from Fermi's Golden rule [52,54,55].

Note that the relaxation of hot electrons in Dirac surface states has been intensively studied in experiments [56–61]. The expression of shift currents in Eq. (4) does not take into account the dephasing and relaxation effects explicitly. However, as the reported lifetime of photoexcited electrons in Dirac surface states is in order of μsec in bulk-insulating topological insulator [61], which is much larger than the typical time scale of photoexcitation ($\sim p$sec), shift currents should be measurable. See Supplemental Material S7 [45] for further discussion.

Shift spin current in Dirac surface states of topological insulator with magnetic ordering. A shift spin current generated by one state is exactly canceled by its time-reversal partner state. Thus the absence of both inversion and time-reversal symmetries is required for a system to support shift spin currents. (See Supplemental Material S2 [45] for details.)

A simple example of a Dirac surface state with perturbations that generate a shift spin current with zero charge current is described by

$$H = -v_F k_y \sigma_x + v_F k_x \sigma_y + m\sigma_z + g\left(k_x^2 + k_y^2\right)\sigma_0. \quad (8)$$

The third term on the right hand side corresponds to the magnetic ordering on the surface of $3d$ topological insulator that breaks the time-reversal symmetry. A band bending, the last term, is commonly observed in discovered topological insulators [47,48,62]. It provides diamagnetic terms ($\sim A_i A_l$). The resultant energy dispersion is shown in Fig. 3(a). Computing the susceptibilities for different combinations of indices, we obtain the following nonzero components: $-\chi^{xx}_{x,\hat{s}_x} = \chi^{yx}_{x,\hat{s}_y} = -\chi^{xy}_{y,\hat{s}_x} = \chi^{yy}_{y,\hat{s}_y} = \frac{gm}{2v_F\Omega^2}$ for $\Omega > m$. Figures 3(b), 3(c), and 3(d) show the momentum distribution of the matrix elements appearing in the integral for the spin shift current. We note that the susceptibilities obtained here are exact results for Hamiltonian Eq. (8), in contrast to the expression for the shift charge current for the warped Dirac surface state where we only keep the leading order of warping strength λ. For a linearly polarized light in the general direction, $\boldsymbol{E}(t) = E_0(\cos\phi\hat{x} + \sin\phi\hat{y})\cos\Omega t = E_0\hat{x}'\cos\Omega t$, the shift spin current is given by (see Supplemental Material S5 [45])

$$\boldsymbol{J}_{\text{spin}} = -\frac{gmE_0^2}{2v_F\Omega^2}\hat{x}'(\cos\phi\hat{s}_x + \sin\phi\hat{s}_y). \quad (9)$$

The direction of shift spin current is parallel to that of electric field. Note that in linearly polarized light, ϕ and $\phi+\pi$ is equivalent. This is also seen above that when $\hat{x}'$ is rotated by π, the spin direction is reversed so that the spin photocurrent remains the same. In contrast to the shift charge current in warped Dirac surface states, we have more flexibility to control the strength of m with different magnetic dopants. With typical values of magnetic TIs, $m = 30$(meV), $\Omega = 100$(meV), along with experimentally observed Fermi

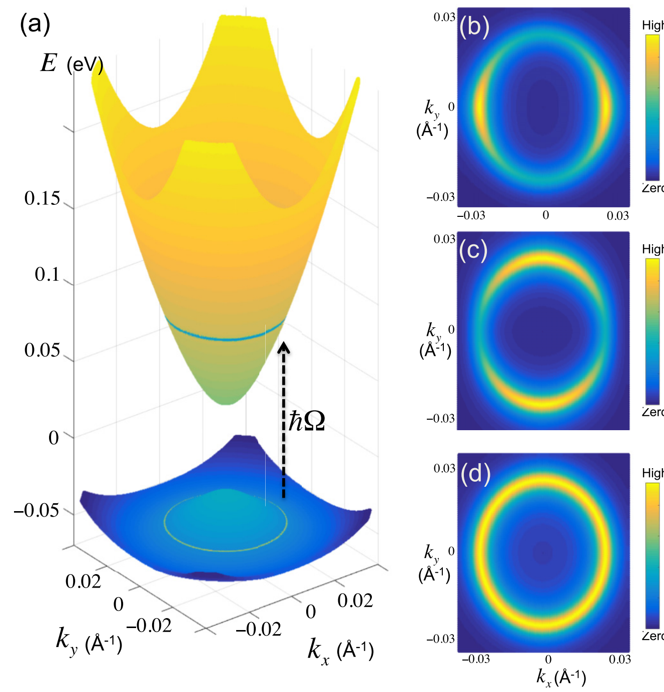

FIG. 3. Massive Dirac surface state with band-bending carries the shift spin current. The Fermi velocity $v_F = 2.84\hbar^{-1}$(eV Å), Zeeman term $m = 0.03$(eV), and band-bending strength $g = 41.1\hbar^{-2}$(eV Å^2) are used [47] for Bi_2Te_3. We show the matrix elements that contribute to the nonlinear susceptibility $\chi^{xx}_{x,\hat{s}_x}$. (a) The energy dispersion is drawn with electronic states satisfying the resonant condition, $\epsilon_c - \epsilon_v = \Omega$, in distinct colors. (b) The coupling strength of Bloch states in the resonant condition to diamagnetic spin current response, $|(\{\hat{s}_x, \partial_{k_x} v^x\})_{cv}|$, is shown in color. (c) The coupling strength of Bloch states in the resonant condition to a linearly polarized light, $|(v^x)_{vc}|$, is shown in color. (d) The contribution of Bloch states to the shift charge current, $|(v^x)_{vc}(\{\hat{s}_x, \partial_{k_x} v^x\})_{cv}|$, is shown in color.

velocity and band bending parameters [47], we obtain shift spin current density $0.40I_0$(nA/m) [I_0 is in the unit of (W/m^2)], which is larger the shift charge current estimated previously. The shift spin current of massive Dirac surface state is large enough to be measured in experiments, as CPGE spin currents observed in topological insulator [49,50] and quantum wells [63] are 1–100 (pAW^{-1}cm^2), which is equivalent to photocurrent density $0.1I_0 - 10I_0$(pA/m) assuming beam size is 1 (mm^2). (See Supplemental Material S6 [45] for details.)

To summarize, we showed that shift charge and spin currents can be formulated as two point correlation functions of paramagnetic and diamagnetic currents. We discussed two examples that support shift charge and spin currents, which are both realized in the Dirac surface states of TIs by incorporating suitable perturbations. Detection of those photocurrents is shown to be experimentally feasible.

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[1] D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. Cava, and M. Z. Hasan, Nature (London) **452**, 970 (2008).
[2] D. Hsieh, Y. Xia, D. Qian, L. Wray, F. Meier, J. Dil, J. Osterwalder, L. Patthey, A. Fedorov, H. Lin *et al.*, Phys. Rev. Lett. **103**, 146401 (2009).
[3] Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. Hor, R. Cava *et al.*, Nat. Phys. **5**, 398 (2009).
[4] D. Hsieh, Y. Xia, L. Wray, D. Qian, A. Pal, J. Dil, J. Osterwalder, F. Meier, G. Bihlmayer, C. Kane *et al.*, Science **323**, 919 (2009).
[5] D. Hsieh, Y. Xia, D. Qian, L. Wray, J. H. Dil, F. Meier, J. Osterwalder, L. Patthey, J. G. Checkelsky, N. P. Ong, A. V. Fedorov, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature (London) **460**, 1101 (2009).
[6] R. ValdésAguilar, A. Stier, W. Liu, L. Bilbro, D. George, N. Bansal, L. Wu, J. Cerne, A. Markelz, S. Oh *et al.*, Phys. Rev. Lett. **108**, 087403 (2012).
[7] G. S. Jenkins, A. B. Sushkov, D. C. Schmadel, N. P. Butch, P. Syers, J. Paglione, and H. D. Drew, Phys. Rev. B **82**, 125120 (2010).
[8] W.-K. Tse and A. H. MacDonald, Phys. Rev. Lett. **105**, 057401 (2010).
[9] W.-K. Tse and A. H. MacDonald, Phys. Rev. B **84**, 205327 (2011).
[10] R. Shimano, G. Yumoto, J. Yoo, R. Matsunaga, S. Tanabe, H. Hibino, T. Morimoto, and H. Aoki, Nat. Commun. **4**, 1841 (2013).
[11] A. B. Sushkov, G. S. Jenkins, D. C. Schmadel, N. P. Butch, J. Paglione, and H. D. Drew, Phys. Rev. B **82**, 125110 (2010).
[12] T. Kitagawa, E. Berg, M. Rudner, and E. Demler, Phys. Rev. B **82**, 235114 (2010).
[13] T. Kitagawa, T. Oka, A. Brataas, L. Fu, and E. Demler, Phys. Rev. B **84**, 235108 (2011).
[14] N. H. Lindner, G. Refael, and V. Galitski, Nat. Phys. **7**, 490 (2011).
[15] M. C. Rechtsman, J. M. Zeuner, Y. Plotnik, Y. Lumer, D. Podolsky, F. Dreisow, S. Nolte, M. Segev, and A. Szameit, Nature (London) **496**, 196 (2013).
[16] G. Usaj, P. M. Perez-Piskunow, L. E. F. FoaTorres, and C. A. Balseiro, Phys. Rev. B **90**, 115423 (2014).
[17] Y. T. Katan and D. Podolsky, Phys. Rev. Lett. **110**, 016802 (2013).
[18] H. Dehghani, T. Oka, and A. Mitra, Phys. Rev. B **90**, 195429 (2014).
[19] T. Karzig, C.-E. Bardyn, N. H. Lindner, and G. Refael, Phys. Rev. X **5**, 031001 (2015).
[20] C.-E. Bardyn, T. Karzig, G. Refael, and T. C. H. Liew, Phys. Rev. B **91**, 161413 (2015).
[21] A. V. Nalitov, D. D. Solnyshkov, and G. Malpuech, Phys. Rev. Lett. **114**, 116401 (2015).
[22] T. Choi, S. Lee, Y. Choi, V. Kiryukhin, and S.-W. Cheong, Science **324**, 63 (2009).
[23] S. M. Young and A. M. Rappe, Phys. Rev. Lett. **109**, 116601 (2012).
[24] S. M. Young, F. Zheng, and A. M. Rappe, Phys. Rev. Lett. **109**, 236601 (2012).
[25] J. H. Heo, S. H. Im, J. H. Noh, T. N. Mandal, C.-S. Lim, J. A. Chang, Y. H. Lee, H.-j. Kim, A. Sarkar, M. K. Nazeeruddin *et al.*, Nat. Photon. **7**, 486 (2013).
[26] N. H. Lindner, G. Refael, and F. von Oppen, arXiv:1403.0010.
[27] J. Wunderlich, B.-G. Park, A. C. Irvine, L. P. Zârbo, E. Rozkotová, P. Nemec, V. Novák, J. Sinova, and T. Jungwirth, Science **330**, 1801 (2010).
[28] F. Bonaccorso, Z. Sun, T. Hasan, and A. Ferrari, Nat. Photon. **4**, 611 (2010).
[29] Q. H. Wang, K. Kalantar-Zadeh, A. Kis, J. N. Coleman, and M. S. Strano, Nat. Nanotechnol. **7**, 699 (2012).
[30] H. Yu, H. Zhang, Y. Wang, C. Zhao, B. Wang, S. Wen, H. Zhang, and J. Wang, Laser Photon. Rev. **7**, L77 (2013).
[31] J. Sánchez-Barriga, A. Varykhalov, J. Braun, S.-Y. Xu, N. Alidoust, O. Kornilov, J. Minár, K. Hummer, G. Springholz, G. Bauer *et al.*, Phys. Rev. X **4**, 011046 (2014).
[32] A. M. Cook, B. M. Fregoso, F. de Juan, and J. E. Moore, arXiv:1507.08677.
[33] E. Adams and E. Blount, J. Phys. Chem. Solids **10**, 286 (1959).
[34] N. Nagaosa, J. Sinova, S. Onoda, A. MacDonald, and N. Ong, Rev. Mod. Phys. **82**, 1539 (2010).
[35] R. Resta, Rev. Mod. Phys. **66**, 899 (1994).
[36] R. Resta and D. Vanderbilt, *Physics of Ferroelectrics* (Springer, New York, 2007), pp. 31–68.
[37] Y. Chen, J. Analytis, J.-H. Chu, Z. Liu, S.-K. Mo, X.-L. Qi, H. Zhang, D. Lu, X. Dai, Z. Fang *et al.*, Science **325**, 178 (2009).
[38] L. Fu, Phys. Rev. Lett. **103**, 266801 (2009).
[39] J. E. Sipe and A. I. Shkrebtii, Phys. Rev. B **61**, 5337 (2000).
[40] T. Morimoto and N. Nagaosa, Sci. Adv. **2**, e1501524 (2016).
[41] T. Morimoto and N. Nagaosa, Phys. Rev. B **94**, 035117 (2016).
[42] P. Král and J. E. Sipe, Phys. Rev. B **61**, 5381 (2000).
[43] P. Král, J. Phys.: Condens. Matter **12**, 4851 (2000).
[44] J. H. Shirley, Phys. Rev. **138**, B979 (1965).
[45] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.95.035134 for details of shift charge and spin currents including their symmetry properties, derivation for Dirac surface states, and numerical estimates.
[46] S. M. Young, F. Zheng, and A. M. Rappe, Phys. Rev. Lett. **110**, 057201 (2013).
[47] C.-X. Liu, X.-L. Qi, H. J. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Phys. Rev. B **82**, 045122 (2010).
[48] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nat. Phys. **5**, 438 (2009).
[49] K. N. Okada, N. Ogawa, R. Yoshimi, A. Tsukazaki, K. S. Takahashi, M. Kawasaki, and Y. Tokura, Phys. Rev. B **93**, 081403 (2016).
[50] J. McIver, D. Hsieh, H. Steinberg, P. Jarillo-Herrero, and N. Gedik, Nat. Nanotechnol. **7**, 96 (2012).
[51] P. Olbrich, L. Golub, T. Herrmann, S. Danilov, H. Plank, V. Bel'kov, G. Mussler, C. Weyrich, C. Schneider, J. Kampmeier *et al.*, Phys. Rev. Lett. **113**, 096601 (2014).
[52] N. H. Lindner, G. Refael, and F. von Oppen, arXiv:1403.0010 [cond-mat].
[53] P. Hosur, Phys. Rev. B **83**, 035309 (2011).
[54] A. Junck, G. Refael, and F. von Oppen, Phys. Rev. B **88**, 075144 (2013).
[55] Y. G. Semenov, X. Li, and K. W. Kim, Phys. Rev. B **86**, 201401 (2012).
[56] Y. H. Wang, D. Hsieh, E. J. Sie, H. Steinberg, D. R. Gardner, Y. S. Lee, P. Jarillo-Herrero, and N. Gedik, Phys. Rev. Lett. **109**, 127401 (2012).
[57] J. A. Sobota, S. Yang, J. G. Analytis, Y. L. Chen, I. R. Fisher, P. S. Kirchmann, and Z.-X. Shen, Phys. Rev. Lett. **108**, 117403 (2012).

[58] M. Hajlaoui, E. Papalazarou, J. Mauchain, L. Perfetti, A. Taleb-Ibrahimi, F. Navarin, M. Monteverde, P. Auban-Senzier, C. Pasquier, N. Moisan *et al.*, Nat. Commun. **5**, 3003 (2014).

[59] M. Hajlaoui, E. Papalazarou, J. Mauchain, G. Lantz, N. Moisan, D. Boschetto, Z. Jiang, I. Miotkowski, Y. Chen, A. Taleb-Ibrahimi *et al.*, Nano Lett. **12**, 3532 (2012).

[60] C. Kastl, C. Karnetzky, H. Karl, and A. W. Holleitner, Nat. Commun. **6**, 6617 (2015).

[61] M. Neupane, S.-Y. Xu, Y. Ishida, S. Jia, B. M. Fregoso, C. Liu, I. Belopolski, G. Bian, N. Alidoust, T. Durakiewicz *et al.*, Phys. Rev. Lett. **115**, 116801 (2015).

[62] Y. Zhang, K. He, C.-Z. Chang, C.-L. Song, L.-L. Wang, X. Chen, J.-F. Jia, Z. Fang, X. Dai, W.-Y. Shan, S.-Q. Shen, Q. Niu, X.-L. Qi, S.-C. Zhang, X.-C. Ma, and Q.-K. Xue, Nat. Phys. **6**, 584 (2010).

[63] S. D. Ganichev and W. Prettl, J. Phys.: Condens. Matter **15**, R935 (2003).