Theoretical study of x-ray absorption of three-dimensional topological insulator Bi_2Se_3

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The x-ray absorption edge singularity which is usually relevant for metals is studied for the prototype topological insulator Bi_2Se_3. The generalized integral equation of the Nozières and Dominicis type for the x-ray edge singularity is derived and solved. The spin texture of surfaces states causes a component of singularity dependent on the helicity of the spin texture. It also yields another component for which the singularity from excitonic processes is absent.

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Introduction. The topological insulators (TIs) have been intensively studied recently.[1,2] TIs have a bulk energy gap but they have conducting (namely gapless) states at the boundary.[3] The quantum Hall state is an example of a 2-dimensional TI with broken time reversal symmetry, and the conducting states at the boundary are nothing but the well-known edge states.[3] There exist 3-dimensional TIs with time reversal invariance, and they have conducting surface states (SSs) which are protected by Z_2 topological invariants in the bulk.[4–6] The energy band of the SSs takes the form of a Dirac cone.[1,3] SSs were first observed in $Bi_{1-x}Sb_x$, but many of their important features were not clearly discerned due to the small bulk gap and disorder effect.[7] Stoichiometric TIs possessing the simplest SS structure, namely a single Dirac cone, have been proposed for Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3.[8,9] The single Dirac cone SS has been observed in ARPES experiments for Bi_2Se_3.[10] These materials can be realized as TIs owing to the band inversion mechanism driven by large spin-orbit coupling.[8] The spin texture which is a distinguishing feature of SSs has also been observed in the spin-resolved ARPES experiment.[11]

X-ray absorption (and emission) spectroscopy is a very important method in the study of the electronic structure of core electrons. An incident x-ray photon excites a deep core electron to an unoccupied state with higher energy, leaving behind a positively charged core hole which can be treated as being immobile in many cases.[12,13] If there exist conduction electrons (of metals), they react to this *suddenly* created potential by the deep core hole. The conduction electrons interact with the deep core hole in two distinctive ways: the excitonic process[14] which is essentially attraction between the hole and conduction electrons, and the orthogonality catastrophe[15] which means a vanishing overlap between the ground-state wave functions before and after the creation of the deep core hole. Both excitonic process and the orthogonality catastrophe are singular near the x-ray absorption edge for Fermi liquids, and they require nonperturbative treatments.[16–19] For TIs, partially filled SSs comprise the conduction electrons in spite of the energy gap in the bulk. Evidently, it is of interest to investigate how the above singular behaviors for the conventional Fermi liquids are modified for the conducting states realized by SSs of TIs.

However, there is a caveat. In x-ray absorption experiments with the incident photon perpendicular to the surface, x rays penetrate deep into the bulk of a sample, hence providing its bulk properties.[20] The SS of TIs reside near surface, so that in this experimental setup the contribution to the absorption from the SS is expected to be rather small. The decay length (along surface normal) of the SS of Bi_2Se_3 can be estimated to be in the range of $4 \sim 10$ Å using Eq. (32) and Table IV of Ref. 9. For the substantial amount of x-ray absorption to take place in conjunction with the SS the attenuation length of the x ray should be comparable to the decay length of the SS. The attenuation length of the x ray can be controlled by its energy and the incident angle (measured from the surface). Taking various factors mentioned above into account, we choose to focus on a core level $N_3 4p_{3/2}$ of Bi whose binding energy is 678.8 eV. At this energy the critical angle is 3.26° and the attenuation length at 3.4° is 40 Å which is indeed comparable to the decay length of the SS. We note that the attenuation length for the normal incidence is about 1000 Å.[20] Presently there seems to be no experimental report on the x-ray absorption in Bi_2Se_3.

In this Brief Report we report the results on the x-ray edge problem of Bi_2Se_3. The spin texture structure of the SS modifies the singular edge behavior compared to that of conventional Fermi liquids. The most salient differences are the appearance of a contribution depending on the helicity of spin texture and the other which is free of the singularity from excitonic process. The main result of this Brief Report is Eq. (34).

Setup. The Hamiltonian for the SS is given by [see Eq. (34) of Ref. 9, and $\alpha, \beta = \uparrow, \downarrow$ denote spin]

$$\begin{aligned} \mathsf{H}_{\mathrm{SS}} &= \sum_{\alpha,\beta=\uparrow,\downarrow} c^{\dagger}_{\mathbf{k}\alpha} \mathsf{h}_{\alpha\beta} c_{\mathbf{k}\beta}, \ \hat{\mathsf{h}} = (\mathsf{h}_{\alpha\beta}), \\ \hat{\mathsf{h}} &= \left[\tilde{C}_0 + \tilde{C}_2\left(k_x^2 + k_y^2\right)\right] \mathrm{I}_2 + \tilde{A}(\sigma_x k_y - \sigma_y k_x), \end{aligned} \tag{1}$$

where $\sigma_{x,y}$ are Pauli matrices acting on the spin space (I_2 is a unit matrix) and $c_{\mathbf{k}\alpha}$ is the destruction operator for the SS with wave number $\mathbf{k}$ and spin α. In Eq. (1) we have ignored the trigonal distortion terms proportional to $(k_x \pm i k_y)^3$. The numerical values of the parameters of Eq. (1) which are appropriate for Bi_2Se_3 are given by $\tilde{C}_0 = 3.37 \times 10^{-2}$ eV, $\tilde{C}_2 = 23.7\,\mathrm{eV\,Å}^2$, and $|\tilde{A}| = 3.30\,\mathrm{eV\,Å}$. Figure 4 of Ref. 9 suggests that the wave number cutoff should be $k_c \approx 0.1$ Å^{-1}. The energy eigenvalue is given by

$$E_{\pm}(\mathbf{k}) = \tilde{C}_0 + \tilde{C}_2 k_{\parallel}^2 \pm |\tilde{A}| k_{\parallel}, \ k_{\parallel} = \sqrt{k_x^2 + k_y^2}. \tag{2}$$

When the $\tilde{C}_2 k_\parallel^2$ is much smaller than $|\tilde{A}|k_\parallel$ the Dirac cone structure with apex at $\mathbf{k} = 0$ is manifest.

The noninteracting Matsubara Green's function of the SS can be expressed as (the hat denotes matrix and ϕ is the azimuth angle in the x-y plane)

$$\hat{g}(i\epsilon,\mathbf{k}) = \mathrm{I}_2\, g_d + [(+i)\hat{e}_{12}e^{-i\phi} + (-i)\hat{e}_{21}e^{i\phi}]\, g_o, \qquad (3)$$

where $\hat{e}_{ij}$ is a 2×2 matrix whose only nonvanishing element is 1 at (i,j) entry, and

$$g_d(i\epsilon,\mathbf{k}) = \frac{i\epsilon + \mu - \tilde{C}_0 - \tilde{C}_2 k_\parallel^2}{[i\epsilon + \mu - E_+(\mathbf{k})][i\epsilon + \mu - E_-(\mathbf{k})]},$$
$$g_o(i\epsilon,\mathbf{k}) = \frac{\tilde{A}k_\parallel}{[i\epsilon + \mu - E_+(\mathbf{k})][i\epsilon + \mu - E_-(\mathbf{k})]}, \qquad (4)$$

where μ is the chemical potential, and $\mu > \tilde{C}_0$ will be assumed (namely, the lower Dirac cone is completely occupied). The interrelation between the spin and the angle in Eq. (3) is nothing but the manifestation of the spin texture of the SS.[9] Note that the Green's functions of Eq. (4) are independent of the angle ϕ. The Green's functions summed over wave number in the long-time limit are given by (τ is imaginary time)

$$g_d(\tau) = -\frac{\rho}{\tau}, \quad g_o(\tau) = \mathrm{sgn}(\tilde{A})\, g_d(\tau), \qquad (5)$$

where $\rho = Ak_F/4\pi v_F$ is the density of states at Fermi energy (A is the area of unit cell), and v_F and k_F are the Fermi velocity and Fermi momentum, respectively, whose detailed form does not concern us here. Note the sign factor $\mathrm{sgn}(\tilde{A})$ in Eq. (5), which is the signature of the helicity of the spin texture of the SS.[9]

The core level $N_3 4p_{3/2}$ of Bi is labeled by the z component of the total angular momentum $J = 3/2$.

$$\mathsf{H}_{\mathrm{hole}} = E_h \sum_{m_J=\pm 3/2,\pm 1/2} b^\dagger_{m_J} b_{m_J}, \qquad (6)$$

where $b^\dagger_{m_J}$ is the creation operator of the hole. E_h is the core level energy, and $\mu + E_h$ is the (unrenormalized) threshold energy for x-ray absorption. The potential created by the deep core hole will be assumed to be spherically symmetric, and for simplicity we will consider the isotropic scattering only, so that the potential scattering matrix element for the SS is simplified to[18]

$$V_{\mathbf{k}\mathbf{k}'} = -V_0, \quad V_0 > 0 \ \text{ is constant.} \qquad (7)$$

Then the interaction Hamiltonian between the SS and the deep core hole is given by

$$\mathsf{H}_{\mathrm{int}} = \sum_{\mathbf{k},\mathbf{k}'}(-V_0)\left(\sum_\alpha c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}'\alpha}\right)\left(\sum_{m_J} b^\dagger_{m_J} b_{m_J}\right), \qquad (8)$$

where a suitable cutoff in the wave number sum is assumed implicitly. The total Hamiltonian consists of

$$\mathsf{H}_{\mathrm{tot}} = \mathsf{H}_{\mathrm{SS}} + \mathsf{H}_{\mathrm{hole}} + \mathsf{H}_{\mathrm{int}}. \qquad (9)$$

With the Hamiltonian Eq. (9) the hole quantum number m_J is conserved, and it implies that the deep core hole Green's function is given by

$$-\left\langle b_{m_J}(\tau) b^\dagger_{m'_J}(\tau')\right\rangle = \delta_{m_J,m'_J} D(\tau - \tau'), \qquad (10)$$

where the function $D(\tau)$ is independent of m_J. The x-ray absorption intensity $I(\omega)$ (ω is the frequency of the incident x ray) can be expressed in terms of the correlation function [using Eq. (10)] as follows:[21]

$$I(\omega) = \mathrm{Im}\int_0^\infty e^{i\omega\tau} F(\tau)\Big|_{i\omega\to\omega+i\delta},$$
$$F(\tau) = \sum_{\mathbf{k},\mathbf{k}',\alpha,\beta}\sum_{m_J} M_{\mathbf{q}\lambda}(\mathbf{k},\alpha|m_J) M^*_{\mathbf{q}\lambda}(\mathbf{k}',\beta|m_J) F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\tau),$$
$$F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\tau) = \langle c_{\mathbf{k}\alpha}(\tau) b_{m_J}(\tau) b^\dagger_{m_J}(0) c^\dagger_{\mathbf{k}'\beta}(0)\rangle, \qquad (11)$$

where $M_{\mathbf{q}\lambda}(\mathbf{k},\alpha|m_J)$ is the x-ray transition matrix element from the deep core state $|m_J\rangle$ to the SS (Bloch state) $|\mathbf{k},\alpha\rangle$, and $\mathbf{q}$ and λ are the wave number and the polarization of the incident x ray, respectively. In many cases of interest, the wave number $(\mathbf{q},\mathbf{k})$ dependence of the x-ray transition matrix element can be ignored. This is due to the localized nature of the wave function of the core electron. In the presence of the strong spin-orbit coupling such as the case of Bi, the electron-photon interaction receives an additional contribution from the spin-orbit coupling.[22] The explicit form of the transition matrix element including the spin-orbit contribution is

$$M_{\mathbf{q}\lambda}(\mathbf{k}\alpha|m_J) = \int d^3\vec{r}\, e^{i\mathbf{q}\cdot\vec{r}}\left\{\frac{(-e)}{m_e}\phi^\dagger_{\mathbf{k}}\left[-i\hbar\vec{e}_{\mathbf{q}\lambda}\cdot\nabla\Psi_{m_J}\right]\right.$$
$$+\frac{\hbar(-e)}{4m_e^2c^2}\phi^\dagger_{\mathbf{k}}\vec{\sigma}\cdot\left[-\hbar\omega\vec{e}_{\mathbf{q}\lambda}\times\nabla\Psi_{m_J}\right.$$
$$\left.\left.+\nabla V\times\vec{e}_{\mathbf{q}\lambda}\Psi_{m_J}\right]\right\}, \qquad (12)$$

where $\vec{e}_{\mathbf{q}\lambda}$ is the polarization vector of the x ray and $V(\vec{r})$ is the periodic crystal potential. $\phi_{\mathbf{k}}(\vec{r})$ and $\Psi_{m_J}(\vec{r})$ are the (spinor) Bloch wave function of the SS and the (spinor) wave function of the core electron, respectively. The dipole approximation $e^{i\mathbf{q}\cdot\vec{r}} \approx 1$ will be assumed below.

Correlation functions. The correlation function $F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\tau)$ of Eq. (11) can be obtained from

$$F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\xi,\xi'|\tau_1,\tau_2) = \langle T\, c_{\mathbf{k}\alpha}(\xi) b_{m_J}(\tau_1) b^\dagger_{m_J}(\tau_2) c^\dagger_{\mathbf{k}'\beta}(\xi')\rangle \qquad (13)$$

by the limiting procedure $\xi \to \tau_1 - \tau_c$ and $\xi' \to \tau_2 + \tau_c$ (τ_c is the short-time cutoff). T denotes time ordering. For the absorption we have to take $\tau_1 > \tau_2$. We employ the equation-of-motion method of Ref. 19 to derive the integral equation for $F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\xi,\xi'|\tau_1,\tau_2)$. The conservation of the hole number causes the equation of motion to close on itself,[19] and we find the integral equation

$$F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\xi,\xi'|\tau_1,\tau_2) = \delta_{\mathbf{k}\mathbf{k}'} g_{\alpha\beta}(\xi - \xi',\mathbf{k}) D(\tau_1 - \tau_2)$$
$$+\sum_{\mathbf{q}',\gamma}\int_{\tau_2}^{\tau_1} d\tau\, g_{\alpha\gamma}(\xi - \tau,\mathbf{k}) V_{\mathbf{k}\mathbf{q}'} F_{\mathbf{q}'\mathbf{k}'\gamma\beta|m_J}$$
$$\times(\tau,\xi'|\tau_1,\tau_2), \qquad (14)$$

where $g_{\alpha\beta}(\xi,\mathbf{k})$ is the Green's function Eq. (3) in the (imaginary) time domain. Decomposing $F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}$ as follows,

$$F_{\mathbf{k}\mathbf{k}'\alpha\beta|m_J}(\xi,\xi'|\tau_1,\tau_2) = G_{\mathbf{k}\mathbf{k}'\alpha\beta}(\xi,\xi'|\tau_1,\tau_2) D(\tau_1 - \tau_2), \qquad (15)$$

Eq. (14) becomes the following integral equation:

$$G_{\mathbf{k}\mathbf{k}'\alpha\beta}(\xi,\xi'|\tau_1,\tau_2) = \delta_{\mathbf{k}\mathbf{k}'}\, g_{\alpha\beta}(\xi-\xi',\mathbf{k}) + \sum_{\mathbf{q}',\gamma}\int_{\tau_2}^{\tau_1} d\tau\, g_{\alpha\gamma}(\xi-\tau,\mathbf{k}) \times V_{\mathbf{k}\mathbf{q}'}\, G_{\mathbf{q}'\mathbf{k}'\gamma\beta}(\tau,\xi'|\tau_1,\tau_2). \quad (16)$$

Equation (16) is the generalization of Eq. (17) a) in Ref. 18 to our case of the SS. $G_{\mathbf{k}\mathbf{k}'\alpha\beta}$ and $D(\tau_1-\tau_2)$ of Eq. (15) represent the excitonic processes and the orthogonality catastrophe, respectively.[18] It can be shown that the hole Green's function $D(\tau_1-\tau_2)$ can be obtained from the solution of Eq. (16) via the parametric integral [see Eq. (21) of Ref. 18 and Eq. (11) of Ref. 19]. Thus once Eq. (16) is solved, we can find the x-ray absorption intensity from Eqs. (11) and (15).

In fact, we need to find the Green's function $G_{\mathbf{k}\mathbf{k}'\alpha\beta}$ summed over wave number weighted by transition matrix element $M_{\mathbf{q}\lambda}(\mathbf{k}\alpha|m_J)$. In most cases of simple metals the wave number dependence of the transition matrix element is ignored. However, in our case such dependence is crucial because, as can be seen in Eq. (3), the spin texture structure is encoded in the angle dependence of the Green's function. In view of this we expand the transition matrix element in Fourier series of $e^{i\phi}$ but we will ignore the $k_\parallel = \sqrt{k_x^2+k_y^2}$ dependence:

$$M_{\mathbf{q}\lambda}(\mathbf{k}\alpha|m_J) \approx \sum_{n=0,\pm1} e^{in\phi} M^{(n)}_{\mathbf{q}\lambda}(\alpha|m_J), \quad (17)$$

where only $n=0,\pm1$ terms are kept since the higher order contributions will be smaller because they involve higher powers of $k_\parallel r$. Let us define (henceforth time arguments are suppressed for notational clarity)

$$\bar{G}_{\alpha\beta|n,n'} \equiv \sum_{\mathbf{k},\mathbf{k}'} e^{in\phi}(e^{in\phi'})^* G_{\mathbf{k}\mathbf{k}'\alpha\beta}, \quad (18)$$

where a cutoff in wave number sum is implicitly assumed. Applying the definition Eq. (18) to Eq. (3) we find

$$\begin{aligned} \bar{g}_{\alpha\beta|0,0} &= \bar{g}_{\alpha\beta|1,1} = \bar{g}_{\alpha\beta|-1,-1} = \delta_{\alpha\beta} g_d(\tau), \\ \bar{g}_{\alpha\beta|1,0} &= \bar{g}_{\alpha\beta|0,-1} = \delta_{\alpha\uparrow}\delta_{\beta\downarrow}(+i) g_o(\tau), \\ \bar{g}_{\alpha\beta|0,1} &= \bar{g}_{\alpha\beta|-1,0} = \delta_{\alpha\downarrow}\delta_{\beta\uparrow}(-i) g_o(\tau), \\ \bar{g}_{\alpha\beta|1,-1} &= \bar{g}_{\alpha\beta|-1,1} = 0. \end{aligned} \quad (19)$$

Now Eq. (16) can be recast into the following form [recall Eq. (7)]:

$$\bar{G}_{\alpha\beta|n,n'}(\xi,\xi'|\tau_1,\tau_2) = \bar{g}_{\alpha\beta|n,n'}(\xi-\xi') + (-V_0)\int_{\tau_2}^{\tau_1} d\tau\, \bar{g}_{\alpha\gamma|n,0}(\xi-\tau) \times \bar{G}_{\gamma\beta|0,n'}(\tau,\xi'|\tau_1,\tau_2), \quad (20)$$

which are coupled integral equations. Noting the factor $\bar{g}_{\alpha\gamma|n,0}$ and using Eq. (19), we find that the nontrivial solutions (with a nonvanishing second term) obtain only for $n=0,\pm1$.

Solution of integral equation. The well-known Nozières and Dominicis (ND) (asymptotic) solution in the long-time limit is [$g(\xi) = -\frac{\rho}{\xi}$ = noninteracting Green's function] [18]

$$G_{\mathrm{ND}}(\xi,\xi'|\tau_1,\tau_2) = \cos^2\delta\, g(\xi-\xi')\left[\frac{(\xi-\tau_2)(\tau_1-\xi')}{(\tau_1-\xi)(\xi'-\tau_2)}\right]^{\delta/\pi}, \quad (21)$$

which satisfies [compare with Eq. (20)]

$$G_{\mathrm{ND}}(\xi,\xi'|\tau_1,\tau_2) = g(\xi-\xi') + (-V_0)\int_{\tau_2}^{\tau_1} d\tau\, g(\xi-\tau) \times G_{\mathrm{ND}}(\tau,\xi'|\tau_1,\tau_2), \quad (22)$$

where δ is the s-wave scattering phase shift

$$\delta = \tan^{-1}[\pi V_0 \rho]. \quad (23)$$

For $n=n'=0$, using Eq. (19), Eq. (20) is found to reduce to Eq. (22). Hence (time arguments suppressed)

$$\bar{G}_{\alpha\beta|0,0} = \delta_{\alpha\beta} G_{\mathrm{ND}}. \quad (24)$$

Noting Eqs. (5) and (19) we also find the solutions for $n'=\pm1$:

$$\begin{aligned} \bar{G}_{\alpha\beta|0,1} &= \delta_{\alpha\downarrow}\delta_{\beta\uparrow}(-i)\mathrm{sgn}(\tilde{A}) G_{\mathrm{ND}}, \\ \bar{G}_{\alpha\beta|0,-1} &= \delta_{\alpha\uparrow}\delta_{\beta\downarrow}(+i)\mathrm{sgn}(\tilde{A}) G_{\mathrm{ND}}. \end{aligned} \quad (25)$$

For other values of n', $\bar{G}_{\alpha\beta|0n'} = 0$.

Next consider the case of $n=1$. From the property of $g_{\alpha\gamma|1,0}$ [see Eq. (19)] the nontrivial solutions obtain only for $\alpha = \uparrow$, so that

$$\bar{G}_{\downarrow\beta|1,n'} = \bar{g}_{\downarrow\beta|1,n'}. \quad (26)$$

Now take $\alpha = \uparrow$:

$$\bar{G}_{\uparrow\beta|1,n'}(\xi,\xi'|\tau_1,\tau_2) = \bar{g}_{\uparrow\beta|1,n'}(\xi-\xi') + (-V_0) \times \int_{\tau_2}^{\tau_1} d\tau\, \bar{g}_{\uparrow\downarrow|1,0}(\xi-\tau)\bar{G}_{\downarrow\beta|0,n'} \times (\tau,\xi'|\tau_1,\tau_2). \quad (27)$$

If $n'=-1$, then from $\bar{g}_{\uparrow\beta|1,-1}=0$ and $\bar{G}_{\downarrow\beta|0,-1}=0$ [see Eq. (25)], we conclude that

$$\bar{G}_{\uparrow\beta|1,-1} = 0. \quad (28)$$

For the case of $n'=0$ of Eq. (27), β should be $\downarrow$; otherwise both $\bar{g}$ and $\bar{G}$ vanish. Thus

$$\bar{G}_{\uparrow\uparrow|10} = 0 \quad (29)$$

and for $\beta = \downarrow$, multiplying both sides of Eq. (27) by $(-i)\mathrm{sgn}(\tilde{A})$, we find that the equation becomes exactly ND-type Eq. (22), so that

$$\bar{G}_{\uparrow\downarrow|10} = (+i)\mathrm{sgn}(\tilde{A}) G_{\mathrm{ND}}. \quad (30)$$

Repeating similar analyses for other cases, we obtain

$$\begin{aligned} &\bar{G}_{\alpha\beta|0,0} = \delta_{\alpha\beta} G_{\mathrm{ND}},\ \ \bar{G}_{\alpha\beta|1,-1} = \bar{G}_{\alpha\beta|-1,1} = 0, \\ &\bar{G}_{\alpha\beta|11} = \begin{pmatrix} G_{\mathrm{ND}} & 0 \\ 0 & g_d \end{pmatrix},\ \ \bar{G}_{\alpha\beta|-1-1} = \begin{pmatrix} g_d & 0 \\ 0 & G_{\mathrm{ND}} \end{pmatrix}, \\ &\bar{G}_{\alpha\beta|01} = \bar{G}_{\alpha\beta|-10} = \begin{pmatrix} 0 & 0 \\ -i\,\mathrm{sgn}(\tilde{A}) G_{\mathrm{ND}} & 0 \end{pmatrix}, \\ &\bar{G}_{\alpha\beta|10} = \bar{G}_{\alpha\beta|0-1} = \begin{pmatrix} 0 & i\,\mathrm{sgn}(\tilde{A}) G_{\mathrm{ND}} \\ 0 & 0 \end{pmatrix}. \end{aligned} \quad (31)$$

The leading behavior of the core-hole Green's function $D(\tau)$ can be obtained from the second-order linked-cluster expansion.[13] The important contribution turns out to be

$$V_0^2 \int_0^\tau d\xi \int_0^\tau d\xi' \mathrm{Tr}[g^{(0)}(\xi-\xi') g^{(0)}(\xi'-\xi)], \quad (32)$$

where $g^{(0)}(\xi-\xi') = \sum_{\mathbf{k}} g(\mathbf{k},\xi-\xi') = g_d(\xi-\xi')\mathrm{I}_2$. Thus the helicity of the spin texture of the SS does not affect the core-hole Green's function, so that the situation becomes essentially identical with that of the ND solution. The evaluation of the integral of Eq. (32) yields logarithms, which are to be exponentiated in the linked-cluster expansion. Comparing with the ND solution we find [$N_c = 2$, $(\uparrow,\downarrow)$]

$$D(\tau > 0) \sim e^{-\omega_T^* \tau} \frac{1}{(\tau/\tau_c)^{N_c(\delta/\pi)^2}}. \tag{33}$$

ω_T^* is the renormalized threshold for x-ray absorption.

Results. Combining the solutions Eqs. (31) and (33) with the transition matrix element Eq. (12) we can obtain the result for x-ray absorption intensity. Equation (12) has two components: one from the direct dipole transition and the other from spin-orbit coupling. The dipole transition conserves the spin, so that it is diagonal in spin (namely, $M_\alpha M_\beta^* \propto \delta_{\alpha\beta}$; this can be verified explicitly in our case). Then Eq. (31) tells us that only $\bar{G}_{\alpha\beta|(00),(11),(-1,-1)}$ contribute. Among these, G_{ND} includes the singularity from excitonic processes while g_d does not. The cross term of the dipole transition and the spin-orbit contribution allows spin off-diagonal configuration. From Eq. (31) we find that this contribution is proportional to the helicity $\mathrm{sgn}(\tilde{A})$. The above considerations give [$\Theta(x)$ is the step function]

$$I(\omega) \sim \Theta(\omega-\omega_T^*)\big[c_d'(\omega-\omega_T^*)^{N_c(\delta/\pi)^2} + [c_d + \mathrm{sgn}(\tilde{A})c_o](\omega-\omega_T^*)^{-2\delta/\pi+N_c(\delta/\pi)^2}\big], \tag{34}$$

where c_d', c_d, c_o are constants.

Summary and concluding remarks. We have studied the x-ray absorption edge singularity of the prototype TI, Bi_2Se_3. For the singularity to exist, gapless conducting states are necessary, and SSs provide those. Due to the spin texture of SSs, two interesting modifications compared to conventional metals arise: (1) the helicity-dependent contribution [$\mathrm{sgn}(\tilde{A})$ term of Eq. (34)] and (2) the contribution free of singularity from excitonic process [the first term of Eq. (34)]. These features can be verified experimentally by extracting the surface contributions using the angle and energy dependence of the penetration depth of the incident x ray, and we have also suggested a specific core level appropriate for experiments. The angle and energy dependence of the penetration depth can also be used in distinguishing the helicity effect of TI from that of the conventional Rashba spin-orbit energy bands since the latter reside in the bulk. We mention in comparison that the graphenes have *two* Dirac cones from the valley structure, so that their qualitative properties are different from those of TIs.[23] We also mention that when the Fermi energy crosses the apex of the Dirac cone, all of the singularities disappear.[23] However, this situation is not generic for TIs and is not elaborated in this Report.

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