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Spin Hall conductivity in three-dimensional topological insulator/normal insulator heterostructures

V. N. Men'shov[+*1)], *V. V. Tugushev*[+*×], *E. V. Chulkov*[*○∇]

[+]*National Research Centre "Kurchatov Institute", 123182 Moscow, Russia*

[*]*Tomsk State University, 634050 Tomsk, Russia*

[×]*Prokhorov General Physics Institute of the RAS, 119991 Moscow, Russia*

[○]*St. Petersburg State University, 198504 St. Petersburg, Russia*

[∇]*Departamento de Física de Materiales, Facultad de Ciencias Químicas, UPV/EHU and Centro de Física de Materiales CFM-MPC, Centro Mixto CSIC-UPV/EHU, 20080 San Sebastián, Basque Country, Spain*

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In the framework of an effective functional approach based on the $\mathbf{k}\cdot\mathbf{p}$ method, we study the combined effect of an interface potential and a thickness of a three-dimensional (3D) topological insulator (TI) thin film on the spin Hall conductivity in layered heterostructures comprising TI and normal insulator (NI) materials. We derive an effective two-dimensional (2D) Hamiltonian of a 3D TI thin film sandwiched between two NI slabs and define the applicability limits of approximations used. The energy gap and mass dispersion in the 2D Hamiltonian, originated from the hybridization between TI/NI interfacial bound electron states at the opposite boundaries of a TI film, are demonstrated to change sign with the TI film thickness and the interface potential strength. Finally, we argue that the spin Hall conductivity can efficiently be tuned varying the interface potential characteristics and TI film thickness.

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Introduction. Semiconductor heterostructures comprising a three-dimensional (3D) topological insulator thin films interfaced with 3D normal insulator (NI) materials are considered to be highly promising for spintronic device applications [1–3]. Indeed, a boundary between 3D topological insulator (TI) and 3D NI can host helical electron states with linear spectrum and spin-momentum locking [4–6] (see also discussion concerning this problem in Refs. [7, 8]). These remarkable properties are inherent to typical 3D TI materials which are tetradymite-like semiconductors with strong spin-orbit coupling such as Bi_2Te_3, Bi_2Se_3, Sb_2Te_3 and their alloys [4–6, 9]. They have a crystalline structure consisting of weakly coupled quintuple layers, which makes it relatively easy to grow high quality thin films using molecular beam epitaxy technology [10–12]. On the one hand, the NI/TI/NI trilayer can be considered as a fundamental building block of a layered TI/NI heterostructure. On the other hand, such the trilayer can serve as a basic model unit for an analytical and numerical study of the peculiar electronic properties of heterostructures. When the thickness of the TI film is comparable with the penetration length of the interfacial helical state into the film, the boundaries would significantly affect the electronic structure (energy spectrum and wave function) of the 3D TI film. This creates opportunities to design desirable transport and magneto-transport properties in TI/NI heterostructures.

The spin Hall (SH) effect in nonmagnetic solids refers to an edge spin polarization of carriers when an electric current is flowing through the sample. This amazing effect can be driven by impurity scattering ("extrinsic" effect) or by band structure ("intrinsic" effect) [13, 14]. The SH effect has extensively been studied in conventional semiconductors and metals [13, 14]. Recently, spin-sensitive transport measurements [15–18] have detected current-induced spin polarization of the edge states in epitaxially grown Bi_2Se_3, $(Bi_{0.53}Sb_{0.47})_2Te_3$, and $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ thin films. Owing to the topologically non-trivial nature of the Bloch band states in TIs, the intrinsic SH conductivity is theoretically predicted [4–6] to exhibit quantized (in units of e^2/h) behavior when the Fermi energy lies in the band gap of the system. To the best of our knowl-

1)e-mail: vnmenshov@mail.ru

edge, to date there are no experimental evidences for quantum SH effect in the 3D TI thin films.

A great advantage of 3D TIs is the tunability of topologically relevant electron states using various factors such as the film thickness, external fields, bringing into proximity to other materials. While numerous theoretical investigations have been focused on 3D TIs in the actual film geometry, an understanding of microscopic mechanisms for predicting and engineering their properties is far from being clear. In the most of previous approaches [19, 20], a drastic restriction in the form of the "open" (or "hard wall") boundary condition has been imposed upon the 3D TI wave function at the TI/NI interface. Thus an important subject of the NI substrate (or overlayer) influence on the 3D TI film properties has been merely ignored. Meanwhile, even for a particular case of the TI/vacuum interface the physical rationality of the "open" boundary condition has been called in question [21]. The effects of orbital intermixing and charge redistribution at the TI/NI interface on the spectral and spatial characteristics of the interfacial in-gap states were thoroughly explored within the framework of continual approach in a series of the works [22–25]. It was argued that these effects can correctly be taken into consideration via an effective interface potential (IP) which enters into the corresponding "natural" (or "zeroth flow") boundary condition at the TI/NI interface. It is understood that an important role of the interfaces becomes profoundly intricate in the TI/NI heterostructures where the 3D TI film thickness is comparable with the penetration length of the interfacial state.

In this Letter, we apply for the first time the IP concept [22–25] to study the low-energy electron states in the 3D TI film of the NI/TI/NI trilayer. To consider only the principal aspects of the problem we utilize an analytic procedure proposed in Refs. [19, 20] allowing to reduce the system under consideration to its formal counterpart described by an effective 2D Hamiltonian. We estimate the applicability limits of the used method and demonstrate that the parameters of the effective 2D Hamiltonian and, as consequence, the SH conductivity value of the NI/TI/NI trilayer depend strongly on both the 3D TI film thickness and the IP strength.

Model of the NI/TI/NI trilayer. We consider the heterostructure setup composed of a 3D TI film (for instance, few-quintuple layers of the Bi_2Se_3 crystal confined by the (111) planes) sandwiched between the slabs of 3D NI which is assumed to be a wide-gap nonmagnetic semiconductor. The 3D TI material is restricted along z-axis and occupies the finite region $|z| < l$. The TI/NI interfaces located at $z = \pm l$ are perfectly flat so that translational symmetry in the (x, y) plane remains. For simplicity, the heterostructure is regarded to be symmetric, i.e., the two TI/NI interfaces are identical.

We use the four band model proposed to describe the low energy and long wavelength bulk states near the Γ point of the narrow-gap semiconductor materials of Bi_2Se_3-type [26]. Within the $\mathbf{k}\cdot\mathbf{p}$ method, the minimal basis, $u_\Gamma = \{|+\uparrow\rangle, |-\uparrow\rangle, |+\downarrow\rangle, |-\downarrow\rangle\}$, is formed by four hybridized states of the Se and Bi p_z-orbitals, differing in parity (even or odd) and spin projection (up or down) onto the z quantization axis. The simplified version of the corresponding 4×4 Hamiltonian takes the form:

$$\mathbb{H}(\mathbf{k}) = \Xi(\mathbf{k})\tau_z \otimes \sigma_0 + A\tau_x \otimes (\boldsymbol{\sigma}\cdot\mathbf{k}), \tag{1}$$

where $\Xi(\mathbf{k}) = \Xi - \mathrm{B}k^2$, $\mathbf{k}$ is the wave vector measured from the Γ point ($\mathbf{k} = 0$), $k = |\mathbf{k}|$, σ_a and τ_β ($\alpha, \beta = 0, x, y, z$) denote the Pauli matrices in the spin and orbital space, respectively. The model has time-reversal symmetry and inversion symmetry. The expression (1) captures the remarkable feature of the 3D TI band structure: the inverted order in an energy of the basis states around $\mathbf{k} = 0$ under the condition $\Xi\mathrm{B} > 0$. The Hamiltonian (1) is particle-hole symmetric and isotropic, which helps us to simplify calculations.

The electron states of the contacting constituents – 3D TI and NI – intermix at the interface. Besides, there is charge density redistribution near the interface. We do not care how the wave-function behaves in the NI slabs (at $|z| > l$). Following Refs. [22–25], the effect of the TI/NI boundaries on the TI film is taken into account via an effective IP matrix, $\mathbb{U}(\mathbf{r})$. Then, in our continual approach, the electron energy of the 3D TI film reads:

$$\boldsymbol{\Omega} = \int\limits_{|z|\le l} d\mathbf{r}\Theta^+(\mathbf{r})[\mathbb{H}(-i\nabla) + \mathbb{U}(\mathbf{r})]\Theta(\mathbf{r}). \tag{2}$$

Here the operator $\mathbb{H}(-i\nabla)$ determined in Eq. (1) acts in the space of envelope functions (EFs) that are represented by spinor $\Theta(\mathbf{r})$ in the basis u_Γ. The EF spinor components $\theta_j(\mathbf{r})$ ($j = 1, 2, 3, 4$) are presumed to be smooth and continuous functions inside the film $|z| < l$. As long as the EF spatial variation in the z direction is sufficiently slow on the scale $\sim d$ of the order of a few lattice constants where potential $\mathrm{U}(\mathbf{r})$ is localized, one can adopt a local approximation for IP: $\mathrm{U}(\mathbf{r}) \to d\mathbb{U}\delta(|z| - l)$. Here IP is regarded being spin-independent, therefore it can be mapped by the diagonal matrix $\mathbb{U} = \mathrm{diag}\{U_1, U_2, U_1, U_2\}$, the components of which are associated with the relative energy offsets between the relevant band edges of the TI and NI materials [24].

In accordance with Refs. [22–25], we reformulate the IP approach as an eigenvalue problem with the "natural" boundary condition at the interfaces. The corresponding equations in the compact form are given by

$$[\mathbb{H}(\boldsymbol{\kappa}, -i\partial_z) - \mathbb{I}E]\Theta(\boldsymbol{\kappa}, z) = 0, \tag{3}$$

$$i\frac{\delta\mathbb{H}(\boldsymbol{\kappa}, -i\partial_z)}{\delta(-i\partial_z)}\Theta(\boldsymbol{\kappa}, z)\Big|_{z=\pm l} = 2d\mathbb{U}\Theta(\boldsymbol{\kappa}, \pm l), \tag{4}$$

where E is an energy of a sought electron state with EF $\Theta(\boldsymbol{\kappa}, z)$, $\boldsymbol{\kappa}$ being an in-plane wave-vector, $\partial_z = \partial/\partial z$, $\mathbb{I}$ is an unit matrix. Here we go beyond the frame of the "open" boundary condition, where the state has zero amplitude at the interfaces, $\Theta(\pm l) = 0$, which is rather unphysical.

Effective 2D Hamiltonian of the 3D TI film. We are interested in quest for the long-wavelength and low-energy states of the 3D TI film in NI/TI/NI trilayer. To this end the Hamiltonian (1) is expressed as

$$\mathbb{H}(\boldsymbol{\kappa}, -i\partial_z) = \mathbb{H}_0(0, -i\partial_z) + \mathbb{P}(\boldsymbol{\kappa}), \tag{5}$$

$$\mathbb{P}(\boldsymbol{\kappa}) = -\mathrm{B}\kappa^2\tau_z \otimes \sigma_0 + \mathrm{A}\tau_x \otimes (\boldsymbol{\sigma} \cdot \boldsymbol{\kappa}). \tag{6}$$

The Hamiltonian $\mathbb{H}_0(0, -i\partial_z)$ has a block-diagonal form, $\mathbb{H}_0 = \mathrm{h}^{(+)} \otimes \mathrm{h}^{(-)}$, where the superscript $\sigma = +/-$ means an up/down projection of electron spin onto the quantization axis. The lower block $\mathrm{h}^{(-)}$ is the time reversal of the upper block $\mathrm{h}^{(+)}$. The term $\mathbb{P}(\boldsymbol{\kappa})$ is regarded as a perturbation to $\mathbb{H}_0$ proportional to the deviation from the Γ point in the in-plane momentum.

It is not a principle matter to obtain a complete set of the discrete states for the Hamiltonian $\mathbb{H}_0(0, -i\partial_z)$ in the film geometry. Indeed one can implicitly find out the eigen energies, E_φ and E_χ, and the corresponding eigen functions, $\varphi^{(\pm)}(z)$ and $\chi^{(\pm)}(z)$, satisfying the boundary task:

$$\begin{aligned} &\mathrm{h}^{(\sigma)}(-i\partial_z)\varphi^{(\sigma)}(z) = \mathbb{I}E_\varphi\varphi^{(\sigma)}(z), \\ &\mathrm{h}^{(\sigma)}(-i\partial_z)\chi^{(\sigma)}(z) = \mathbb{I}E_\chi\chi^{(\sigma)}(z), \end{aligned} \tag{7}$$

$$\begin{aligned} &\mathrm{g}^{(\sigma)}(-i\partial_z, z)\varphi^{(\sigma)}(z)\big|_{z=\pm l} = 0, \\ &\mathrm{g}^{(\sigma)}(-i\partial_z, z)\chi^{(\sigma)}(z)\big|_{z=\pm l} = 0, \end{aligned} \tag{8}$$

where the operator $\mathrm{g}^{(\sigma)}$ is given by

$$\mathrm{g}^{(\sigma)}(-i\partial_z, z) = \\ = \begin{pmatrix} \mathrm{B}\partial_z + \mathrm{sgn}(z)dU_1 & i\sigma\,\mathrm{A}/2 \\ i\sigma\,\mathrm{A}/2 & -\mathrm{B}\partial_z - \mathrm{sgn}(z)dU_2 \end{pmatrix}. \tag{9}$$

The trial solutions of the task are the bispinors which components can be represented, due to the space symmetry of the system along the z-axis, as superpositions of the even functions $\cosh(q_{\varphi 1,2}z)$ and $\cosh(q_{\chi 1,2}z)$ or the odd functions $\sinh(q_{\varphi,2}z)$ and $\sinh(q_{\chi,2}z)$. The momenta $q_{\varphi 1,2} = q_{1,2}(E_\varphi)$ and $q_{\chi 1,2} = q_{1,2}(E_\chi)$, specifying a scale of the EF space variation, are connected with the energy via the relation $q_{1,2}^2(E) = (\mathrm{A}^2 - 2\Xi\mathrm{B} \pm \pm\sqrt{\mathrm{A}^4 - 4\mathrm{B}\Xi\mathrm{A}^2 + 4\mathrm{B}^2E^2})/2\mathrm{B}^2$. The φ-state and the χ-state have opposite space parities. Each of these states is two-fold degenerated in spin due to time-reversal symmetry. Inserting the trial solutions into Eqs. (7), (8), it is straightforward to determine the superposition coefficients as well as the energy values E_φ and E_χ.

In the spirit of the method [19, 20], we project the complete set of the states of the task (7), (8) onto a subspace spanned by a minimal basis. This orthogonal basis is composed of the four low-lying states, $\{\varphi^{(\pm)}; E_\varphi\}$, $\{\chi^{(\pm)}; E_\chi\}$ with $|E_{\varphi,\chi}| \ll \Xi$, that arise "genetically" from the nontrivial band structure of 3D TI. Within such the truncation approximation, the states with high energies, $|E| \approx \Xi$ and above, are excluded from the consideration. Arranging the sequence of the basis states in a relevant manner and then projecting the bulk Hamiltonian (5), (6) onto this subspace, we construct in the first order in $\mathbb{P}(\boldsymbol{\kappa})$ the effective 2D Hamiltonian for the sandwiched 3D TI film in a block-diagonal form: $\mathbb{H}_{\text{eff}}(\boldsymbol{\kappa}) = \varepsilon_0(\kappa)\mathbb{I} + \mathrm{f}^{(\Uparrow)}(\boldsymbol{\kappa}) \oplus \mathrm{f}^{(\Downarrow)}(\boldsymbol{\kappa})$, where

$$\mathrm{f}^{(\Uparrow)}(\boldsymbol{\kappa}) = \begin{pmatrix} \Delta(\kappa) & \mathrm{A}_{\varphi\chi}^{(+-)}k_- \\ \mathrm{A}_{\chi\varphi}^{(-+)}k_+ & -\Delta(\kappa) \end{pmatrix},$$

$$\mathrm{f}^{(\Downarrow)}(\boldsymbol{\kappa}) = \begin{pmatrix} -\Delta(\kappa) & \mathrm{A}_{\chi\varphi}^{(+-)}k_- \\ \mathrm{A}_{\varphi\chi}^{(-+)}k_+ & \Delta(\kappa) \end{pmatrix}. \tag{10}$$

The system is decoupled into two subsystems defied by $\mathrm{f}^{(\Uparrow)}$ and $\mathrm{f}^{(\Downarrow)}$ with opposite projections of the pseudospin degree of freedom (symbolized with $\Uparrow$ / $\Downarrow$) which here is a good quantum number [20]. We use the notations: $\varepsilon_0(\kappa) = E_0 - D\kappa^2$, $2E_0 = E_\varphi + E_\chi$, $2D = \mathrm{B}_\varphi + \mathrm{B}_\chi$, $\Delta(\kappa) = \Delta_0 - b\kappa^2$, $2\Delta_0 = E_\varphi - E_\chi$, $2b = \mathrm{B}_\varphi - \mathrm{B}_\chi$. These parameters are determined by the matrix elements between the basis states: $\mathrm{B}_\varphi = \mathrm{B}\int_{-l}^{l} dz\varphi^{(\sigma)+}\sigma_z\varphi^{(\sigma)}$, $\mathrm{B}_\chi = \mathrm{B}\int_{-l}^{l} dz\chi^{(\sigma)+}\sigma_z\chi^{(\sigma)}$, $\mathrm{A}_{\varphi\chi}^{(\sigma,-\sigma)} = \mathrm{A}\int_{-l}^{l} dz\varphi^{(\sigma)+}\sigma_x\chi^{(-\sigma)}$, $\mathrm{A}_{\chi\varphi}^{(\sigma,-\sigma)} = \mathrm{A}_{\varphi\chi}^{(-\sigma,\sigma)*}$ under the normalization stipulation $\int_{-l}^{l} dz\varphi^{(\sigma)+}\sigma_0\varphi^{(\sigma)} = \int_{-l}^{l} dz\chi^{(\sigma)+}\sigma_0\chi^{(\sigma)} = 1$. The edge energy positions E_φ and E_χ are involved above. Note that $|D|$ must be less than $|b|$, otherwise the gap disappears, and all discussions in the following are not valid.

Importantly, in our approach, the parameters specifying the Hamiltonian $\mathbb{H}_{\text{eff}}$ depend not only on the characteristics of the 3D TI bulk spectrum, Ξ, B, A, but also on the film thickness, $2l$, and the IP components, $U_{1,2}$. To capture the essential physics of the problem, we restrict ourselves to the relative thick film, $\mathrm{Re}(q_{1,2})l > 1$, and consider only two extreme cases for the IP strength: weak and strong. Under these restrictions, the energies of the relevant states are small, $|E_{\varphi,\chi}| \ll \Xi$, therefore the applied truncation procedure is surely justified. Besides, we focus on the most interesting situation $|E_{\varphi,\chi}/\Xi| < 4\lambda(1-\lambda) < 1$ ($\lambda = \mathrm{A}^2/4\mathrm{B}\Xi$, $0 < \lambda < 1$), when the characteristic momenta are complex, $q_{1,2} = p \pm iw$, p and w are real.

One keeps the first order in the direct/reverse potential, $|U_1^{\pm 1} + U_2^{\pm 1}|\Xi \ll 1$, and the leading asymptotic term in the overlap of the bound states coming from the opposite interfaces at $z = \pm l$, $\sim \exp(-2p_0 l) \ll 1$. Then, in the case of the strong IP, one arrives at:

$$E_0 = -|\mathrm{A}|\mathrm{B}(p_0^2 + w_0^2)d^{-1}(U_1^{-1} + U_2^{-1}),\ D = -\mathrm{B}E_0/\Xi, \tag{11}$$

$$\Delta_0 = -2|\mathrm{A}|(p_0^2 + w_0^2)w_0^{-1}\sin(2w_0 l)\exp(-2p_0 l), \tag{12}$$

$$b = 2|\mathrm{A}|(p_0^2 + w_0^2)w_0^{-2} l\cos(2w_0 l)\exp(-2p_0 l). \tag{13}$$

In turn, in the case of the weak IP, one obtains:

$$E_0 = 2p_0(p_0^2+w_0^2)(2p_0^2+w_0^2)^{-1}D(U_1+U_2),\ D = 0, \tag{14}$$

$$\Delta_0 = 2|\mathrm{A}|w_0(p_0^2+w_0^2)(2p_0^2+w_0^2)^{-1}\sin(2w_0 l)\exp(-2p_0 l), \tag{15}$$

$$b = -2|\mathrm{A}|(p_0^2 + w_0^2)(2p_0^2 + w_0^2)^{-1} l\cos(2w_0 l)\exp(-2p_0 l). \tag{16}$$

The variation scale of both Δ_0 and b is dominated by the bulk spectrum ingredients via $p_0 = |\mathrm{A}|/2\mathrm{B}$ and $w_0 = \sqrt{4\mathrm{B}\Xi - \mathrm{A}^2}/2\mathrm{B}$. The term $\varepsilon_0(\kappa)$ accounts for the particle-hole asymmetry generated by IP with the composition $U_1 \neq U_2$. As for the off-diagonal terms in Eq. (10), the magnitudes of $\mathrm{A}_{\varphi\chi}^{(\sigma,-\sigma)}$ and $\mathrm{A}_{\chi\varphi}^{(\sigma,-\sigma)}$ coincide with the bulk velocity value $|\mathrm{A}|$.

One needs to delineate the applicability domain of the approach. Actually, the $\boldsymbol{\kappa}$-dependence in the effective Hamiltonian $\mathbb{H}_{\mathrm{eff}}$ stems from term $\mathbb{P}(\boldsymbol{\kappa})$ averaged over the unperturbed state $\{\varphi^{(\pm)}; E_\varphi\}$, $\{\chi^{(\pm)}; E_\chi\}$. Correction to the basis function $\varphi^{(\pm)}$ or $\chi^{(\pm)}$ is small provided that the perturbation matrix elements are small with respect to an energy distance between the unperturbed levels, $|E_\varphi - E_\chi| = 2|\Delta_0|$ [27]. Taking into account Eqs. (12), (13) and (15), (16), this condition entails the restrictions for momentum related to a finite film size via the following inequalities: $\kappa \ll w_0\sin(2w_0 l)\exp(-2p_0 l)$ and $\kappa \ll \sqrt{w_0\tan(2w_0 l)/l}$. On the other hand, in the second order of the perturbation theory in $\mathbb{P}(\boldsymbol{\kappa})$, additional contribution of the second power in momentum, $\sim \mathrm{A}^2\kappa^2/|\Delta_0|$, would appear in the diagonal (or "mass") terms of $\mathbb{H}_{\mathrm{eff}}(\boldsymbol{\kappa})$. This contribution can be regarded as negligibly small if $\mathrm{A}^2 \ll |b\Delta_0|$ or $\exp(2p_0 l) \ll \sqrt{w_0 l\sin(4w_0 l)}$. On the basis of such the estimations we argue that, for relatively thick films and/or in the nearest region of the critical thickness at which $\Delta_0 = 0$ or $b = 0$, the momentum realm, where our approach is justified, is very narrow. Furthermore, the method to construct the effective 2D Hamiltonian for the 3D TI film is justified only at $\lambda \ll 1$.

We focus on the diagonal (or "mass") terms $\Delta(\kappa)$ in Eq. (10) which determine the topological properties of the 3D TI film in the present approach. It is worth to point out that the parameters of the effective 2D model of Eq. (10), which code all the information about the topological features of the film, cannot be viewed as independent from each other what has been assumed by many authors in the semi-phenomenological approaches (for example, see [28, 29]). Within the framework of the minimal model, we established that there is a rigid correlation between the hybridization gap $2\Delta_0$ and the parameter b (responsible for a dispersion of the "mass" term) with varying the confinement factors l and $U_{1,2}$ of Eqs. (12), (13), (15), and (16). Remarkably, both Δ_0 and b exhibit an oscillatory behavior as the functions of the film thickness. Furthermore, they switch sign with increasing the IP strength from the weak limit to the strong limit. This theoretical observation guesses us a possibility to tune the conductivity of the NI/TI/NI trilayer through the TI spacer thickness and (what is of partial interest) the NI slab material.

Peculiarities of the intrinsic SH effect in the NI/TI/NI trilayer. We have derived the effective 2D Hamiltonian (10) which is similar in form to that of the Chern insulator model [30]. In fact, as shown above, the applicability limitation of our approach is restricted to small momenta. Therefore, to describe the transport properties of the NI/TI/NI trilayer, we cannot directly adopt the results obtained within the Chern insulator model. The topological character of the system under consideration is featured by the intrinsic SH conductivity, $\sigma_{xy}^{(s)} = \sigma_{xy}^{(\Uparrow)} = -\sigma_{xy}^{(\Downarrow)}$, in a dependence on the film thickness and IP strength, where $\sigma_{xy}^{(\Uparrow)}$ and $\sigma_{xy}^{(\Downarrow)}$ are the conductivities of the upper, $\mathrm{f}^{(\Uparrow)}$, and lower, $\mathrm{f}^{(\Downarrow)}$, blocks of Eq. (10), respectively. Using the eigen energies and functions of the Hamiltonian (14) one can define the value $\sigma_{xy}^{(s)}$ by means of the Kubo formula at zero temperature and when the chemical potential lies inside the hybridization gap [20, 30]. In the continual approach, to estimate the conductivity we have to introduce the cut-off momentum, $\kappa_c(l)$, so that $\sigma_{xy}^{(s)} = Ce^2/h$, where the factor C is equal to

$$C = \frac{1}{2}\left[\mathrm{sgn}(\Delta_0) - \frac{\Delta(\kappa_c)}{\sqrt{\Delta^2(\kappa_c) + \mathrm{A}^2\kappa_c^2}}\right]. \tag{17}$$

Under the stipulation that $\lambda \ll 1$ and $|\Delta_0| > |b|\kappa_c^2$ (i.e. $l\kappa_c^2 \ll \sqrt{\Xi/\mathrm{B}}$), the SH conductivity expressed in the fundamental units of e^2/h, Eq. (17), turns out small and independent of the sgn(b), $C \approx \mathrm{sgn}(\Delta_0)(\mathrm{A}\kappa_c/2\Delta_0)^2$. At the same time, for utterly large κ_c (on the order of a reciprocal lattice constant) the model formally converges to the exactly quantized value of $C = [\mathrm{sgn}(\Delta_0) + \mathrm{sgn}(b)]/2$ being equal to 1 or -1, when b and Δ_0 have the same sign, $b\Delta_0 > 0$, and vanish otherwise, $b\Delta_0 < 0$. As pointed out above, our theory fails to work at large κ. Albeit, if the occupied states distant away from the middle of the Brillouin zone are considered from the topological point of view as inert, the power expansion around the Γ point up to second order in momentum can be sufficient to capture principal features of the low energy transport.

Bearing in mind the aforesaid comments, we can qualitatively characterize the SH phase in the NI/TI/NI trilayer. It then follows from the expressions (12), (13) for Δ_0 and (15), (16) for b that factor C is given by a simple formula

$$C = \pm\{\mathrm{sgn}[\cos(2w_0l)] - \mathrm{sgn}[\sin(2w_0l)]\}/2, \tag{18}$$

where the sign "$\pm$" is related to the case of the strong/weak IP, when $|U_1^{-1} + U_2^{-1}|\Xi \ll 1$ and $|U_1 + U_2|\Xi^{-1} \ll 1$, respectively. We unveil novel fine peculiarities of the finite size effect in the NI/TI/NI trilayer. As evident from Eq. (18), both the TI film thickness and the IP strength can drive the system through a quantum transition between phases with different SH conductivity specified by the factor C. Such the transition can occur in two different ways: either by closing/reopening the hybridization gap $\Delta_0 \sim \sin(2w_0l)$ or by changing the sign of the "mass" term dispersion $b \sim \cos(2w_0l)$. One can sketch out the main features of the generic phase diagram of the NI/TI/NI trilayer in the approximation $|U_1^{\pm 1} + U_2^{\pm 1}|\Xi^{\mp 1} \ll 1$ and $\exp(-2p_0l) \ll 1$. With varying the thickness $2l$, the factor C alternates in the sequence $\ldots, -1, 0, 1, 0, -1, 0, 1, \ldots$ with the period of $l_0 = \pi/w_0$, so that the topological phases with opposite direction of SH conductivity, $C = 1$ and -1, are separated from each other by trivial phase with zeroth SH conductivity, $C = 0$. In other words, augmenting the TI film thickness in the quarter-period, $l_0/4$, has to lead to the transition either from SH phase to trivial phase or vise versa. On the other hand, the TI/NI interfaces play a specific role in the topology of the film. Namely, with enlarging the effective IP strength from the weak to strong limit, the conductivity direction in the SH phase switches over (see the signs in Eq. (18)).

Conclusion. Within the framework of the NI/TI/NI trilayer model, we have revealed that both the TI film thickness and IP strength play a crucial role for the appearance of the SH phase and determine the SH conductivity value in the 3D TI/NI heterostructures. Here we restricted ourselves to the study of the model under the analytically solvable approximations. More detail analysis including the realm of the intermediate values of IP, ($|U_1 + U_2|\Xi^{-1} \approx 1$), and relatively thin films, $\exp(-2p_0l) \approx 1$, will be presented elsewhere. Note that the tuning effect related to the TI/NI interfaces demonstrated in the work is not similar to the effect of an applied external electric field [31–34] or the effect of a surface functionalization [35, 36] in which the electron states can be changed by breaking the spatial inversion symmetry of the 3D TI film.

We have succeeded in reducing the model of the NI/TI/NI trilayer based on the 3D $\boldsymbol{\kappa}\cdot\mathbf{p}$ Hamiltonian to the effective 2D Hamiltonian of helical electron states. However, it turns out that the utilized procedure has serious limitation in the TI film thickness, $\exp(2p_0l) \ll \sqrt{w_0l\sin(4w_0l)}$, which is valid just for a small band parameter, $\lambda \ll 1$. Therefore, within the framework of this approach it is impossible to provide a correct description of the crossover from the 3D regime to the 2D one in the NI/TI/NI trilayer with reducing the TI spacer thickness. Furthermore, the 2D Hamiltonian of Eq. (10) coincides with the Chern Hamiltonian only in the form. Yet, the expression for the factor C of Eq. (17) (that looks like a topological index) requires introducing the phenomenological cutoff momentum $\kappa_c(l)$. Hence, contrary to previous literature claims [4–6, 20, 28, 29], we assert that a prediction of a quantization of the spin Hall conductivity in 3D TIs should be taken with great care.

Our findings shed light on the possibility for achieving a control of electron properties in the TI/NI heterostructures. We demonstrate that the SH effect in the 3D TI thin films is more complicated and rich than it was thought before. So, experimental and theoretical explorations of the finite size and interface effects in the TI/NI heterostructures remain to be a challenging task.

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