Substrate-limited helical edge states

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We derived analytical results for the gapless edge states of two-dimensional topological insulators in the presence of electron-surface optical (SO) phonon interaction due to substrates. We followed an analytical algorithm, called Lee-Low-Pines variational approximation in the conventional polaron theory, to examine the substrate induced effects on both bulk and edge states of a two dimensional topological insulator within the frame work of Bernevig-Hughes-Zhang (BHZ) model. By implementing this algorithm, we propose a novel phonon-dressed BHZ Hamiltonian which allows one to investigate the effects of various substrates not only on bulk states but also on the associated gapless helical edge states (HESs). We found that both the bulk and HESs are significantly renormalized in the momentum space due to the substrate-related polaronic effects. The model we developed here clarifies which substrates favor the HESs of quantum spin Hall system and which are not. Correspondingly, our work demonstrates that the substrate related polaronic effects have significant role on the emergence of HESs. In other words, we show that SO phonons due to substrates modify the electronic band topology of topological insulators together with the associated HESs and therefore they can be used to tune quantum phase transitions between topological insulators and non-topological ones.

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I. INTRODUCTION

Following the first model for quantum Hall effect in the absence of an external magnetic field suggested by Haldane, the quantum spin Hall (QSH) phase was proposed as a new state of matter by Kane and Mele for graphene system. This QSH system shows an energy gap in the bulk, while it has gapless helical edge states (HESs) with different spins moving in opposite directions. These gapless HESs are topologically protected by time-reversal symmetry, and they are robust to any perturbations. Their first realistic theoretical model were predicted by Bernevig et al., and soon after they were observed in semiconductor HgTe/CdTe quantum wells (QWs) by König et al. Later, similar effect arising in Type-II semiconductor QWs made from InAs/GaSb/AlSb was predicted by Liu et al. Following these pioneering works, there has been a significant interest in studying the exotic properties of QSH effect. However, up till now, apart from the experimental realizations of this effect in these QW systems, its achievement on an appropriate substrate has not been experimentally realized.

It is expected that, when a QSH system is situated on a polar substrate, interaction of the carries of the QSH system with the field induced by surface modes of the dielectric substrate leads to inevitable effects. In particular, the formation of the HESs of the QSH system is affected by these interactions taken place at the interface of the substrate and the QSH system. Such a kind of interaction strongly modifies the single particle properties of the system under consideration, leading to many-body renormalization of the relevant parameters. In fact, the interaction of electrons with the surface optical (SO) phonons of the substrate is a well-established many body problem since the works of Sak, Wang and Mahan. It is also well-known that, for instance, in graphene, it is responsible for the modification of many physical properties such as the renormalization of Fermi velocity, enhanced intra- and inter-band magneto-optical absorption peaks. Thus, to understand their effects on a QSH system, we develop here an analytical method within the frame work of Lee-Low-Pines (LLP) approximation in the polaron theory to propose a novel phonon-dressed BHZ model which comprises the substrate induced effects on both bulk and edge states.

Although the QSH phase depends on the universal topological characteristics of the system, its emergence in a topological material depends crucially on material specific parameters, particularly, on the symmetries of the substrate system upon which topological materials are grown. Indeed, very recently, it is demonstrated that, to control the relevant orbitals in a two-dimensional (2D) QSH insulators, and thus to create large-gap QSH systems in monolayer-substrate composites, substrates play decisive roles in the engineering of such materials. As a matter of fact, it is theoretically shown that, in room temperature, bismuthene on SiC substrate is one of the most probable candidates for QSH materials. Our model developed here not only clarifies why SiC substrate favors the edge states of QSH system, but also makes some predictions on which substrates are most suitable for the QSH system and which are not. Correspondingly, we show that SO phonons due to substrates modify the electronic band topology of topological insulators together with the associated HESs and therefore they can be used to tune quantum phase transitions between topological insulators and non-topological ones. Our claims are also compatible with the predictions of Garate.
insulators. To date, there have been already numerous theoretical studies to deal with the effects of deformation potential coupling to longitudinal acoustic phonons on band topology of 3D topological insulators, topological insulator thin films and HgTe/CdTe quantum wells (including coupling to nonpolar optical phonons).

The paper is organized as follows. In Section II and Section III, we present our main results for both bulk and edge state dispersions, respectively, and discuss them in detail. Section IV ends with a brief conclusion.

II. PHONON-DRESSED BHZ MODEL

In the presence of electron-SO phonon interaction, the effective four-band Hamiltonian which was proposed by Bernevig et al. in order to QSH effect for HgTe/CdTe QWs can be written as

$$\mathcal{H}_{2D}(k) = \mathcal{H}_{BHZ}(k) + \mathcal{H}(k)I_4. \quad (1)$$

Here, $\mathcal{H}_{BHZ}$ is a $4 \times 4$ Hamiltonian for QSH effect, and is given by

$$\mathcal{H}_{BHZ}(k) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix}, \quad (2)$$

where $H(k) = \epsilon_k I_2 + d^\dagger(k)\sigma_z$ is a $2 \times 2$ Hamiltonian with $I_2$ and $\sigma_z$ being $2 \times 2$ unit matrix and Pauli matrices, respectively. For small $k$’s, $\epsilon_k = C - D(k_x^2 + k_y^2)$, $d^1 = Ak_x$, $d^2 = Ak_y$, and $d^3 = M - B(k_x^2 + k_y^2)$ together with the material parameters $A$, $B$, $C$, $D$ and $M$, that all depend on the QW geometry. For the QW thickness $d = 7.0\text{nm}$, they are given as $A = 3.645\text{eVÅ}$ ($h \nu_{F}$), $B = -68.6\text{eVÅ}^2$, $D = -51.2\text{eVÅ}^2$, and $M = -0.010\text{eVÅ}^3$. It should be noted that, the upper-left block of Eq. (1), i.e., $H(k)$, which is for spin up, and is related to the lower-right one which is for spin down, by time-reversal symmetry, so it is convenient to focus on the $H(k)$ for the rest of the paper.

The Hamiltonian in Eq. (1), $\mathcal{H}(k)$, is the sum of Hamiltonians of the free SO-phonons and their coupling to the electron, respectively, and it is taken into account diagonal in the helicity of the Dirac electrons due to the high symmetry of the $\Gamma$ point. It can be written as

$$\mathcal{H}(k) = \sum_q \hbar \omega b_q^\dagger b_q + \sum_q [M_q(z) e^{iq \cdot r} b_q + \text{H.C.}] \quad (3)$$

where $r$ is the 2D position vector of the electron in $xy$-plane, $b_q^\dagger(b_q)$ is the creation (annihilation) operators for a SO phonon of frequency $\omega$ and wave vector $q$. $M_q(z)$ is the interaction amplitude of electrons with SO phonons of the substrate, and its spatial dependence is given by

$$M_q(z) = i\sqrt{g} e^{-qz} \sqrt{q}$$

where $g$ is the coupling parameter defined by $g = 2\pi\hbar \omega e^2/\beta S$ and $z$ is the distance of the electron from the surface of the substrate. Here, $S$ is the area of the surface, $e$ is the free electron charge together with $\beta = (\epsilon_0 - \epsilon_{\infty})/(\epsilon_0 + 1)(\epsilon_{\infty} + 1)$ where $\epsilon_0$ and $\epsilon_{\infty}$ are low- and high-frequency dielectric constants of the substrate subsystem. Our Fröhlich type Hamiltonian for 2D topological insulators given by Eqs. (1-3) describes the electrons trapped at the interface between topological material and the substrate due to SO phonons of the substrates. The last term in Eq. (3) contains phonon creation (annihilation) operators $b_q^\dagger(b_q)$ linearly, and thus it needs to be diagonalized.

This can be realized by two successive transformations within the framework of LLP theory. The first unitary transformation

$$U_1 = \exp\left(-i\mathbf{r} \cdot \sum_q \hbar \mathbf{q} b_q^\dagger b_q\right)$$

eliminates the electron coordinates $\mathbf{r}$ from the interaction Hamiltonian. Applying the transformation $U_1$ on $b_q$ and $\mathbf{p}$ yields $U_1^{-1}b_q U_1 = b_q \exp(-i\mathbf{q} \cdot \mathbf{r})$ and $\mathbf{p} = U_1^{-1}\mathbf{p} U_1 = \mathbf{p} - \hbar \sum_q \mathbf{q} b_q^\dagger b_q$, respectively, so we can write the transformed Hamiltonian $\tilde{\mathcal{H}}(k) = U_1^{-1}\mathcal{H}(k) U_1$ as

$$\tilde{\mathcal{H}}(k) = \begin{pmatrix} M - B \left( k - \sum_q \mathbf{q} b_q^\dagger b_q \right)^2 \sigma_z + A\sigma \cdot \left( k - \sum_q \mathbf{q} b_q^\dagger b_q \right) \\
C - D \left( k - \sum_q \mathbf{q} b_q^\dagger b_q \right)^2 + \sum_q \hbar \omega b_q^\dagger b_q + \sum_q [M_q(z) b_q + \text{H.C.}] \end{pmatrix} I_2. \quad (4)$$

where $\sigma = (\sigma_x, \sigma_y)$. Since, the electron-SO phonon interaction part of the Hamiltonian given by Eq. (4) is still non-diagonal in phonon coordinates, we impose the second LLP transformation, to generate coherent boson
states from the phonon vacuum $|0\rangle_{PH}$, given by

$$U_2 = \exp \left[ \sum_q (f_q b_q - f_q^* b_q^*) \right]$$

which shifts the phonon coordinates by an amount of $f_q$, i.e., $U_2^{-1} b_q U_2 = b_q + f_q$. Here, $f_q(f_q^*)$ is the variational function to be determined. In terms of the transformed operators, Eq. (4) can be written as

$$\tilde{H} = U_2^{-1} H(k) U_2 = H^{(0)} + H^{(1)} + H^{(2)}.$$ 

While $H^{(1)}$ and $H^{(2)}$ contains terms with single creation and annihilation terms as well as bilinear ones such as $b_q^* b_q$ which all disappear when they are applied to vacuum $|0\rangle_{PH}$. The explicit forms of $H^{(1)}$ and $H^{(2)}$ are given in Appendix A. $H^{(0)}$ consists of only the terms free from phonon operators whose diagonal matrix components are given as

$$H^{(0)}_{11} = C + M - (B + D) \left[ k^2 + \sum_q q^2 |f_q|^2 - 2k \cdot \sum_q q f_q^2 + \left( \sum_q q^2 |f_q|^2 \right) \right]$$

$$+ \sum_q [\hbar \omega |f_q|^2 + M_q(z) f_q + M_q^*(z) f_q^*],$$

$$H^{(0)}_{22} = C - M + (B - D) \left[ k^2 + \sum_q q^2 |f_q|^2 - 2k \cdot \sum_q q f_q^2 + \left( \sum_q q^2 |f_q|^2 \right) \right]$$

$$+ \sum_q [\hbar \omega |f_q|^2 + M_q(z) f_q + M_q^*(z) f_q^*],$$

which can be easily done by following the conventional procedure of the selfconsistent equation for $\eta$ in Eq. (9) may be written as

$$f_q = - \frac{M_q^*(z)}{\hbar \omega + |B_+| |q^2 - 2k \cdot q(1 - \eta)|}$$

$$\eta \mathbf{k} = \frac{1}{4\pi} \hbar \omega e^{2qz} \int d^2 \mathbf{q} \frac{e^{-2qz}}{q} \frac{q}{|\hbar \omega + |B_+| |q^2 - 2k \cdot q(1 - \eta)|^2}. $$

The integral over $\mathbf{q}$ in Eq. (11) can be analytically evaluated for slow electrons, $k \ll q_p = \sqrt{\hbar \omega / B_+}$. It should be noted that our small $k$ approximation is compatible with the BHZ model which describes well only the states for small $k$’s, particularly for the valence bands. After, by multiplying both sides of Eq. (11) with $\mathbf{k}$, we first expand the integrand as power series of $\mathbf{k}$, and then keep only the terms up to order $k^2$, it is straightforward to show that the resultant equation

$$\eta = \frac{1}{4\sqrt{\pi}} \alpha_0 (1 - \eta) G^{1,1}_{1,1} \left( \begin{array}{c} \sqrt{2} \\vspace{0.5cm} \alpha \end{array} \right)$$

solves $\eta$ as $\eta = \alpha / (1 + \alpha)$. This is formally equivalent to the one obtained from conventional LLP theory for the bulk polaron, but with different $\alpha$ composition

$$\alpha = \frac{1}{4\sqrt{\pi}} \alpha_0 G^{1,1}_{1,1} \left( \begin{array}{c} \sqrt{2} \\vspace{0.5cm} 1 \end{array} \right).$$
with \( \alpha_0 = \frac{\varepsilon^2 \beta}{\sqrt{\hbar \omega |B_z|}}, \) and \( G^{3,1}_{1,3} \) is the Meijer G-function. The \( \alpha \) in Eq. (12) can be regarded as a position dependent electron-SO phonon coupling parameter in analogy to the bulk polaron theory. Consequently, the diagonal and non-diagonal matrix elements of \( H(0) \) defined by Eqs. (13-14) can be rewritten as

\[
H_{11}^{(0)} = C + M - B (1 - \eta)^2 k^2 - C^{01} - (D - D^{01}) (1 - \eta)^2 k^2 \\
H_{22}^{(0)} = C - M + B (1 - \eta)^2 k^2 - C^{02} - (D + D^{02}) (1 - \eta)^2 k^2,
\]

as material parameters of the topological insulator, and their explicit expressions are given in Appendix B. Thus, by rearranging the matrix elements of \( H(0) \) in Eqs. (13-14), we arrive at our new phonon-dressed BHZ Hamiltonian for the upper-left block as

\[
H^{(0)}(k) = \begin{bmatrix}
C^1 - D^1 k^2 + M - B^1 k^2 \\
A^1 k_-
\end{bmatrix} \begin{bmatrix}
A^1 k_+ \\
C^2 - D^2 k^2 - M + B^1 k
\end{bmatrix}
\]

with the new phonon-dressed material parameters \( A^1 = A (1 - \eta), C^i = C - D_i, D^i = (D \mp D_0^i) (1 - \eta)^2 \) (where plus sign is for \( i = 2 \), and minus sign for \( i = 1 \), respectively), and \( B^1 = B (1 - \eta)^2 \). Subsequently, the bulk energy spectrum of our new phonon-dressed BHZ model, i.e., \( E = E(k) \), can then be found by solving the eigenvalue equation for the upper-left block \( H^{(0)} \psi_\uparrow(k) = E(k) \psi_\uparrow(k) \) as

\[
E_{\pm} = C - Dk^2 \pm [M^2 + (A^2 - 2MB)k^2 + B^2k^4]^{1/2}
\]

where our new phonon-dressed material parameters are given by

\[
A = A (1 - \eta), \\
B = \left[ B - \frac{1}{2} (D^{01} + D^{02}) \right] (1 - \eta)^2, \\
C = C - \frac{1}{2} (C^{01} + C^{02}), \\
D = \left[ D + \frac{1}{2} (D^{02} - D^{01}) \right] (1 - \eta)^2, \\
M = M + \frac{1}{2} (C^{02} - C^{01}).
\]

Eq. (16) is the key result of this section, and includes phonon-dressed material parameters given by Eq. (17). They are all the functions of substrate parameters \( \beta \) and \( \hbar \omega \) as well as \( z \) through Eqs. (B1-B5) in Appendix B, including material parameters of the topological insulator. Therefore, both bulk and edge state solutions of Eq. (15) can obtained in the standard way but with modified or phonon-dressed material parameters defined by Eq. (17).

### III. HELICAL EDGE STATES

In this section, the edge states from the phonon-dressed BHZ Hamiltonian derived above will be reconsidered for the open boundary conditions. For the edge states, we deal with a semi-infinite plane, \( y < 0 \), so as only an edge solution of the form

\[
\psi_\uparrow(k_x, y) = \phi_{\lambda}(k_x) e^{\lambda y}
\]

is allowed (\( \text{Re} \lambda > 0 \)). The spatial dependence in the \( y \)-direction can be taken into account by applying Peierls substitution: \( k_y \to -i \partial_y \) to \( k_y \) in \( H^{(0)}(k) \). The solution \( \psi_\uparrow(k_x, y) \) can easily be found by virtue of the time reversal operator \( \Theta = -i \sigma_y K \) in Eq. (18) as \( \psi_\uparrow(k_x, y) = \Theta \psi_{\uparrow}(k_x, y) \) where \( K \) is the complex conjugation operator.

Consequently, the secular equation gives two allowed values for \( \lambda \) :

\[
\lambda_{1, 2}^2 = k_x^2 + F \pm \sqrt{F^2 - \frac{M^2 - E^2}{B_+ B_-}}
\]

with

\[
F = \frac{1}{2B_+ B_-} [A^2 - 2(MB + ED)].
\]

To find an edge state solution, the wave function must decay to zero when deviating from the boundary. Thus, we adopt the Dirichlet boundary condition \( \psi_\uparrow(k_x, y = 0) = \psi_{\uparrow}(k_x, y = -\infty) = 0 \), then the general solution in the presence of boundary is

\[
\psi_\uparrow = \left( \frac{c(k_x)}{d(k_x)} \right) (e^{\lambda_1 y} - e^{\lambda_2 y})
\]

(19)
with $k_x$-dependent spinor coefficients $\vec{c}(k_x)$ and $\vec{d}(k_x)$. Since it is required that $\lambda$ should be positive to fulfill necessity of exponentially damping solution in Eq. (19), one can follow the usual method to handle the energy dependence of $\lambda_{1,2}$, and obtains

$$\lambda_{1,2} = \frac{1}{\sqrt{B_+B_-}} \left[ \frac{|A|}{2} \mp \sqrt{Z_{k_x}} \right]$$

with

$$Z_{k_x} = \left( \frac{A^2}{4} - \frac{M}{B} B_+ B_- \right) - \frac{D |A| \sqrt{B_+ B_-}}{B} k_x + B_+ B_- k_x^2$$

which satisfies the conditions

$$\lambda_1 \lambda_2 = \frac{BM + DE}{B_+ B_-} - k_x^2,$$

$$\lambda_1 + \lambda_2 = \frac{DM + BE}{k_x^2 B_+ B_-}.$$  

TABLE I. Surface-optical phonon modes for different substrates SiO$_2$, AlN, Al$_2$O$_3$, HfO$_2$ (taken from Ref. (38)), CdTe (taken from Ref. (37)), 6H - SiC (taken from Refs. (35,39)), and h-BN (taken from Ref. (40)).

| Substrate | $\epsilon_0$ | $\epsilon_\infty$ | $\omega_{SO,1}$ | $\omega_{SO,2}$ | $\beta$ |
|-----------|--------------|------------------|----------------|----------------|--------|
| SiO$_2$   | 3.9          | 9.14             | 12.53          | 22.0           | 0.08   |
| AlN       | 6.0          | 12.0             | 25.0           | 40.0           | 0.07   |
| Al$_2$O$_3$ | 8.0         | 14.0             | 30.0           | 50.0           | 0.16   |
| HfO$_2$   | 10.0         | 16.0             | 35.0           | 55.0           | 0.12   |
| CdTe      | 12.0         | 18.0             | 50.0           | 70.0           | 0.03   |
| 6H - SiC  | 14.0         | 20.0             | 55.0           | 80.0           | 0.04   |
| h-BN      | 16.0         | 22.0             | 60.0           | 90.0           | 0.03   |

The energy spectrum of our phonon-dressed effective BHZ Hamiltonian is given in FIG. 1 for a SiC substrate. The bare material parameters we use here are from Ref. (32), $A = 364.5$ meV nm, $B = -686$ meV nm, $M = -10$ meV, $D = -512$ meV nm$^2$, and the surface optical phonon modes and the related dielectric constants of substrates we used in this paper are summarized in Table II. In the left panel, bulk and edge state dispersions are given by using our phonon-dressed BHZ Hamiltonian, Eq. (16) and Eq. (17), for the parameters of SiC. In the right panel, all are given in wide scale to see where the HESs dive into the bulk. In the figure, while the undressed bulk and edge states, i.e., states without electron-phonon interaction are given by dashed lines, dressed ones are represented by solid lines. The edge states are displayed by using red (blue) curves for the spin-up (spin-down) case. Although we choose the energy offset $C$ to be equal to zero, it is easily seen from the figure that both valence and conduction bands move down to deeper negative values, but asymmetrically, just like an expected electronic behavior of graphene carriers in the presence of electron-phonon interaction. Moreover, in this process, insulator-like behavior of the bulk and the metallic massless Dirac-like dispersion of the HESs are both preserved. However, the slope of HESs is changed at the expense of decreasing gap term. It should be noticed that the enhancement in the massive $D$ term due to the electron-SO phonon interaction that breaks the particle-hole symmetry gives rise to asymmetry between conduction and valence bands. Therefore, the diving points of the HESs to the bulk are modified depending on the parameters of the substrate. As clearly seen from the right panel of the FIG. 1, the region where the edge states exist is reduced in $k$ space compared with that found in the absence of electron-SO phonon interaction. Hence, the penetration depth of the edge states becomes longer in the presence of electron-SO phonon interaction. This means that penetration depth of the edge states into the bulk is not only the function of material parameters but also the function of substrate parameters. Although the HESs are expected to be localized at the edge or at least near the edge, but in reality they are not,
they penetrate to the bulk. So their penetration depth length, \( \ell \) which is expected to be of order of the lattice constant, and its control is recognized as an important issue in QSH systems to be able to observe HESs.

By assuming \( \lambda_1 > \lambda_2 \), we plot behavior of inverse of the penetration depth length \( \ell^{-1} = \lambda_2 \) in FIG. 2 for different substrates. Its zeros, i.e., \( k^\pm = D N \left[ 1 \pm \sqrt{1 + (BM/D^2N^2)} \right] / B \), correspond to the points where HESs dive into the bulk in \( k \) space with 

\[ N = A / 2 \sqrt{B + B -} \]

In the absence of electron-SO phonon interaction the minimum of the penetration depth length occurs at \( (k^+_z + k^-_z) / 2 = 0.30 \, \text{nm}^{-1} \) with \( \ell^{-1}_{\text{min}} \sim 6.2 \, \text{nm} \) which is compatible with that found in Ref. 34. The presence of electron-SO phonon interaction shifts the position of this minimum to a little bit smaller \( k \) values, due to the asymmetry between conduction and valence bands caused by the massive character of parameter \( D \). Then \( \ell_{\text{min}} \) occurs over 10 nm, except that of SiC and h-BN substrates. This shows that the most suitable substrates are SiC and h-BN substrates with these material parameters to be able to observe HESs.

In the BHZ model, for real \( \lambda \)'s, HESs in the topological insulator regime exists only where \( A^2/4B^2 \geq M/B \geq 0 \). In other words, \( M < 0 \) corresponds to QSH regime, otherwise, i.e., \( M > 0 \) for a trivial state. To make a comparison of this region for a standard BHZ model and with that obtained by our approach based on the phonon-dressed BHZ model, we plot \( 4MB/A^2 \) as a function of \( z \) for different substrates in FIG. 3. This is just a number for a conventional HgTe quantum well, i.e., \( 4MB/A^2 = 0.207 \), and shown by gray horizontal dashed line in FIG. 3. Strikingly, this region is getting smaller and smaller for substrates with high \( \beta \) values that indicate high polarizability of the associated substrate, especially for experimentally accessible region of \( z \), i.e., around \( 3 - 10 \, \text{Å} \).

Substrate induced effects make the quantity \( 4MB/A^2 \) \( z \)-dependent and critical \( z > z_c \) occurs to fulfill the HESs criteria for substrates SiO\(_2\), AlN, Al\(_2\)O\(_3\) and HfO\(_2\). For values of \( 4MB/A^2 \) close to zero, it is impossible to observe HESs. On the contrary, substrates like SiC, h-BN and CdTe cover whole region without constraints on \( z \) parameter.

These phonon-dressed material parameters can also be extended to derive an effective model for an ultrathin film...
FIG. 4. (Left panel) Bulk and edge state dispersion in the absence (dashed lines) and in the presence (solid lines) of electron-SO phonon interaction for a H – SiC substrate for the parameters of BiSe, BiTe films, \( M = -0.021 \text{eV} \), \( D = 7.5\text{eV} \text{Å}^2 \), \( B = -12.5\text{eV} \text{Å}^2 \) and \( v_F = 6.16 \times 10^5 \text{m/s} \). (Right Panel) same as the left one, but to see where the HESs dive into the bulk, it is given in large scales.

FIG. 5. Penetration depth of the edge states for different substrates Bi$_2$Se$_3$ and Bi$_3$Te$_3$ thin films for \( z = 0.3 \text{ nm} \), \( M = -0.021 \text{eV} \), \( D = 7.5\text{eV} \text{Å}^2 \), \( B = -12.5\text{eV} \text{Å}^2 \) and \( v_F = 6.16 \times 10^5 \text{m/s} \). (BZ). This can be clearly seen from FIG. 5 for different substrates. In FIG. 5 We plot the behavior of inverse of the penetration depth length \( \ell^{-1} = \lambda_2 \) in this figure for different substrates by using the material parameters of Ref. [35]. We notice that (i) the position of the minimum of the penetration depth length shifts to a little bit smaller \( k \) values, due to the asymmetry between conduction and valence bands caused by the massive character of parameter \( D \), and (ii) it occurs over 5 nm, except that of SiC and h-BN substrates. In other words, HESs are well localized around 3 nm in SiC and h-BN substrates with these material parameters.

IV. CONCLUSION

In this work, we show that the formation of HESs critically depends on the dielectric properties of substrates. Furthermore, observation of these states on a given substrate depends on the distance between the topological insulator and the substrate, as well as the parameters of the substrate. Our results indicate that electron-SO...
phonon interactions have weak effects on the emergence of HESs in the case of h – BN and 6H – SiC due to their weak polarizability and high SO phonon frequencies. This can be understood from the $\beta$ and $\hbar\omega$ dependence of the strength of the position dependent electron-phonon coupling parameter, i.e., $\alpha_q = e^2/\sqrt{|\hbar\omega| B_+}$. It is directly proportional to difference of the dielectric parameters of the material through $\beta$ and inverse square root of $\hbar\omega$. This quantity in the case of h – BN and 6H – SiC is less than that of other substrates considered here. So, these substrates favor the emergence of HESs. From our calculations, we also see that, for BiSe and BiTe thin films, HESs survive in a wide range of $k$ in BZ for, in particular, h – BN and 6H – SiC substrates. These compounds provide more realistic model for observing HESs in SiC and h-BN substrates which give rise to well-localized states around 3 nm. Because of the fact that SO phonons induced by surface modes of the dielectric substrate may drastically modify the electronic band topology of topological insulators together with the associated HESs, they can be used to tune the band gap and its sign of 2D topological insulators, and hence they can play a critical role to drive the system from non-topological state into a QSH phase.

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Appendix A: The matrix elements of $H^{(1)}$ and $H^{(2)}$ Hamiltonians

The diagonal matrix elements of the transformed Hamiltonian $H^{(1)}$ can be written as

$$H_{11}^{(1)} = \sum_q \{ [M_q^*(z) + \Omega^- f_q] b_q^\dagger + \text{H.C.} \}$$

$$H_{22}^{(1)} = \sum_q \{ [M_q^*(z) + \Omega^+ f_q] b_q^\dagger + \text{H.C.} \}$$  \hspace{1cm} (A1)

together with non-diagonal ones

$$H_{12}^{(1)} = -A \sum_q (b_q^\dagger f_q + b_q f_q^\dagger)$$

$$H_{21}^{(1)} = -A \sum_q (b_q^\dagger f_q + b_q f_q^\dagger)$$  \hspace{1cm} (A2)

where $\Omega^\pm = \hbar\omega \pm (B \mp D) [q^2 - 2k \cdot q (1 - \eta)]$ and finally the diagonal matrix elements of the transformed Hamiltonian of $H^{(2)}$ are

$$H_{11}^{(2)} = \sum_q \left[ \Omega^- b_q^\dagger b_q - (B + D) f_q q \cdot \sum_{q'} q' f_q^* b_{q'}^\dagger b_{q'} \right]$$

$$+ (B - D) \sum_{q} q \cdot q' \left[ b_{q'}^\dagger b_{q'} b_{q} b_{q}^\dagger + f_q q f_q^* b_{q'}^\dagger b_{q'} + 2 f_q q b_{q'}^\dagger b_{q'} b_q + \text{H.C.} \right]$$

$$H_{22}^{(2)} = \sum_q \left[ \Omega^+ b_q^\dagger b_q + (B - D) f_q q \cdot \sum_{q'} q' f_q^* b_{q'}^\dagger b_{q'} \right]$$

$$+ (B - D) \sum_{q} q \cdot q' \left[ b_{q'}^\dagger b_{q'} b_{q} b_{q}^\dagger + f_q q b_{q'}^\dagger b_{q'} + 2 f_q q b_{q'}^\dagger b_{q'} b_q + \text{H.C.} \right]$$  \hspace{1cm} (A3)

together with non-diagonal ones

$$H_{12}^{(2)} = -A \sum_q q_+ b_q^\dagger b_q$$

$$H_{21}^{(2)} = -A \sum_q q_- b_q^\dagger b_q.$$  \hspace{1cm} (A4)

Appendix B: Substrate dependent parameters

In this appendix, we give all phonon-dressed material parameters in Eq. (17) which are essential for Eq. (10) as

$$C^{01} = \frac{1}{2} \alpha_0 \hbar \omega \left[ \text{Ci} (2\pi) \sin (2\pi) + \frac{1}{2} \cos (2\pi) (\pi - 2\text{Si} (2\pi)) \right]$$  \hspace{1cm} (B1)

$$C^{02} = -C^{01} + \frac{1}{4\sqrt{\pi}} \alpha_0 (1 + \xi) \hbar \omega C^{3,1}_{1,3} (\pi^2 \left| 0 \right. - \frac{1}{2}, \frac{1}{2})$$  \hspace{1cm} (B2)
where $\text{Ci}(x)$ is the cosine integral function $\text{Ci}(x) = \int_0^x \frac{\cos t}{t} \, dt$, and similarly $\text{Si}(x)$ is the sine integral function. Here, we have defined $D^{02}$ in terms of $D_1^{02}$ and $D_2^{02}$ as $D^{02} = (2 + 3\xi)D_1^{02} - D_2^{02}$, together with $\xi = |B_-|/|B_+|$. 

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\[ D^{01} = \frac{1}{4\sqrt{\pi}} \alpha_0 |B_+| |G^{3,1}_{1,3}| \left( z^2 \right) \left[ -\frac{1}{2} \bar{z} \left( \frac{1}{2} \right) \right] \] (B3) 
\[ D^{12} = \frac{1}{12\sqrt{\pi}} \alpha_0 |B_+| |G^{3,1}_{1,3}| \left( z^2 \right) \left[ -\frac{1}{2} \bar{z} \left( \frac{1}{2} \right) \right] \] (B4) 
\[ D^{22} = \frac{1}{12\sqrt{\pi}} \alpha_0 |B_+| |G^{3,1}_{1,3}| \left( z^2 \right) \left[ -\frac{1}{2} \bar{z} \left( \frac{1}{2} \right) \right] \] (B5)