Electron-phonon scattering in topological insulator thin films

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We present a theoretical study of electron-phonon scattering effects in thin films made of a strong topological insulator. Phonons are modelled by isotropic elastic continuum theory with stress-free boundary conditions, and the interaction with the helical surface Dirac fermions is mediated by the deformation potential. We determine the temperature-dependent electrical resistivity $\rho(T)$ and the quasiparticle decay rate $\Gamma(T)$ observable in photoemission. The low- and high-temperature power laws for both quantities are obtained analytically. Detailed estimates covering the full temperature range are provided for Bi$_2$Se$_3$.

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I. INTRODUCTION

The recently discovered state of matter called “topological insulator” (TI) currently represents one of the most active areas in condensed matter physics. TIs are characterized by an insulating gap in the bulk but at the same time have an odd number of gapless surface modes protected against all time-reversal invariant (and sufficiently weak) perturbations. In a three-dimensional (3D) TI, these surface modes correspond to massless two-dimensional (2D) Dirac fermions, where the spin direction is in the surface plane and perpendicular to momentum (“spin-momentum locking”). A typical reference material is Bi$_2$Se$_3$ with a bulk gap $\Delta_b \approx 0.3$ eV. The helical Dirac electron property of the TI surface state has been experimentally confirmed by spin- and angle-resolved photoemission spectroscopy (ARPES). The transport experiments are more difficult in that respect since the surface contribution is often masked by the residual conductivity due to impurities or defects in the bulk. In thin films made of TI materials, however, the bulk contribution is largely suppressed relative to the surface contribution, rendering the latter easier to observe.

In this paper, we provide a detailed theoretical analysis of both the temperature-dependent resistivity $\rho(T)$ and the quasiparticle lifetime $\Gamma(T)$ (observable in ARPES) for a thin TI film. The approach taken here generalizes previous work for the semi-infinite geometry (with only one surface) by two of us and significantly improves the earlier estimates for both quantities. Detailed estimates covering the full temperature range are provided for Bi$_2$Se$_3$.

In sufficiently thin films, the hybridization of the two surface states eventually causes insulating behavior, as has recently been observed experimentally from ARPES for Bi$_2$Se$_3$ films. For Bi$_2$Te$_3$, several calculations predicted a gap $\Delta(L)$ with (as a function of the width $L$) oscillations superimposed on an exponential decay. Similar calculations, however, found no oscillations, with a well-established TI phase already for $L \geq 3$ quintuple layers (QLs). Using the parameter set of Ref. 12, we also find no evidence for oscillations in $\Delta(L)$, see Sec. II A below. For large width, one then has (upper and lower) massless Dirac fermion surfaces.

Our working assumption below is that electron-phonon scattering is the dominant source of quasiparticle decay and backscattering. Electron-electron interactions are indeed expected to give only subleading corrections to the resistivity as long as $T \gtrsim 1$ mK. Disorder effects are more likely to compete with phonon-induced backscattering effects. However, for elevated temperatures, $T \gtrsim 100$ K, phonon effects dominate even for present-day samples, and anticipating higher purity films in the future, this crossover temperature may be lowered significantly. ARPES setups allowing to test our predictions for the quasiparticle decay rate are basically available. Other surface scattering techniques have also been applied to extract the phonon dispersions. Here we follow Ref. 11 and model the phonons using elastic continuum theory. Since even at room temperature, one effectively probes low energy scales, we keep only long-wavelength acoustic phonon modes. For these, previous work on related materials has shown that isotropic elastic continuum theory provides a reasonable approximation. The phonon eigenmodes in the thin film geometry and their coupling to electronic modes have previously been determined in the context of semiconductor quantum well structures. (Note that the semi-infinite case has been treated in Ref. 31.) We basically reproduce the phonon eigenmodes of Ref. 31 but the coupling to the helical electronic eigenstates in a TI film is different from the semiconductor case. Note that piezoelectric couplings are suppressed by symmetry here and spin-phonon type couplings are also expected to be subdominant to the deformation potential taken into account below.

Most TI experiments have so far addressed only optical phonons, cf. also the corresponding situation...
for Bi surfaces\textsuperscript{24}, but very recently ARPES studies reported phonon-induced broadening of the lineshape in Tl\textsubscript{3}\textsuperscript{25,26}. The observed Bi\textsubscript{2}Se\textsubscript{3} electron-phonon coupling strength,\textsuperscript{27} which has been extracted from the prefactor in the high-temperature quasiparticle decay rate $\Gamma \propto T$, is in good agreement with our theoretical estimates.\textsuperscript{21} This indicates that the low-energy approach indeed provides a reasonable starting point. To the best of our knowledge, no detailed measurements for the temperature dependence of the TI film resistivity have been reported so far. We mention in passing that for the related case of a 2D graphene monolayer, a similar comparison of theory\textsuperscript{25,26} to experiment\textsuperscript{22} has turned out to be successful. Remarkably, the electron-phonon coupling observed in experiment\textsuperscript{24} and independently estimated by us\textsuperscript{21} turns out to be quite large. Under room temperature conditions, the resulting lifetime of helical quasiparticles is therefore short, and the resistivity is rather large. This behavior is substantially different from what is found in graphene. We suspect that this is (partially) due to the different Debye temperatures in both materials.

The structure of the remainder of this paper is as follows. In Sec. II we discuss the model for the surface states in the thin film and their coupling to the quantized phonon modes. We then turn to the calculation of the electrical resistivity in Sec. III followed by the lifetime broadening in Sec. IV. The paper concludes with a brief discussion in Sec. V. Technical details of our calculations can be found in various appendices. Note that we use units with $\hbar = 1$.

II. MODEL

In this section we describe the model employed in our study of electron-phonon scattering in a TI film. The model parameters below are chosen for Bi\textsubscript{2}Se\textsubscript{3} as a concrete example. The film has infinite extension in the $xy$ plane and the width $L$, where $|z| < L/2$. We start by reviewing the construction of the effective surface Hamiltonian describing the (upper and lower) electronic surface states of a TI film.

A. Electronic surface states

Keeping all terms up to second order in the momentum around the $\Gamma$ point, $(k_x, k_y, k_z)$, the low-energy physics of 3D TI materials like Bi\textsubscript{2}Se\textsubscript{3} or Bi\textsubscript{2}Te\textsubscript{3} is well described by an effective four-band model.\textsuperscript{12} Using the basis states $\{|P1_+^z, \uparrow\rangle, |P2_+^z, \uparrow\rangle, |P1_+^z, \downarrow\rangle, |P2_+^z, \downarrow\rangle\}$, the low-energy bulk Hamiltonian reads\textsuperscript{12,14}

$$H = \begin{pmatrix} \epsilon_0 + M & -iA_1k_z & 0 & A_2k_- \\ iA_1k_z & \epsilon_0 - M & A_2k_- & 0 \\ 0 & A_2k_+ & \epsilon_0 + M & -iA_1k_z \\ A_2k_+ & 0 & iA_1k_z & \epsilon_0 - M \end{pmatrix}$$

(1)

with $\epsilon_0 = C + D_1k_z^2 + D_2(k_x^2 + k_y^2)$, $M = M_0 - B_1k_z^2 - B_2(k_x^2 + k_y^2)$ and $k_\pm = k_x \pm ik_y$. The model parameters for Bi\textsubscript{2}Se\textsubscript{3} have been determined from first principles.\textsuperscript{12}

$$M_0 = 0.28 \text{ eV}, \quad C = -0.0083 \text{ eV}, \quad A_1 = 2.26 \text{ eVÅ}, \quad A_2 = 3.33 \text{ eVÅ},$$
$$B_1 = 6.86 \text{ eVÅ}^2, \quad B_2 = 44.5 \text{ eV}^2, \quad D_1 = 5.74 \text{ eVÅ}, \quad D_2 = 30.4 \text{ eV}^2.$$

(2)

We may write the Hamiltonian (1) in the form $H = H_0 + H'$, where $H_0 = \begin{pmatrix} h_0(k_z) & 0 \\ 0 & h_0(k_z) \end{pmatrix}$ is the $2 \times 2$ block matrix obtained for $k_x = k_y = 0$, with

$$h_0(k_z) = \left( \begin{array}{cc} \epsilon_0(k_z) + M_0 - B_1k_z^2 & -iA_1k_z \\ iA_1k_z & \epsilon_0(k_z) + M_0 + B_1k_z^2 \end{array} \right).$$

(3)

Note that eigenstates of $H_0$ have conserved spin.

In order to find the surface states in the film geometry, we follow the usual strategy\textsuperscript{25,26} and first look for general spinor eigenstates of $h_0$,

$$h_0(k_z) \rightarrow -i\partial_z \Psi(z) = E_0 \Psi(z).$$

(4)

The general solution to Eq. (4) reads $(j = \pm, s = \pm)$

$$\Psi(z) = \sum_{js} c_{js} e^{-s\eta_j z} \left( E_0 - C + M_0 + (D_1 + B_1)\eta_j^2 \right) - sA_1\eta_j$$

(5)

with arbitrary $c_{js}$ and the inverse lengthscales

$$\eta_j = \left[ \left( -\tilde{B} \pm \sqrt{\tilde{B}^2 - 4\tilde{A}C} \right) / (2\tilde{A}) \right]^{1/2},$$

where $\tilde{A} = D_1^2 - B_1^2$, $\tilde{B} = A_1^2 - 2|M_0B_1 + D_1(C - E_0)|$, and $\tilde{C} = (E_0 - C)^2 - M_0^2$. The Dirichlet boundary conditions defining the film geometry, $\Psi(z = \pm L/2) = 0$, then imply the transcendental equation

$$\frac{E_0 - C + M_0 + (D_1 + B_1)\eta_j^2}{E_0 - C + M_0 + (D_1 + B_1)\eta_j^2} = \frac{\tanh(\eta_j L/2)}{\tanh(\eta_j L/2)},$$

or the same condition with $\eta_+ \leftrightarrow \eta_-$. on the right hand side. Numerical solution of these equations yields the $\Gamma$ point energies $E_0^{(\pm)}$. The corresponding eigenstates $\Psi_{\pm}(z)$ follow from Eq. (4).

$$\Psi_{\pm}(z) = \mathcal{N}_{\pm} \left( (D_1 + B_1)A_1F_{\mp}(z) \right) / A_1 F_{\mp}(z),$$

(6)

where the $\mathcal{N}_{\pm}$ are normalization constants and

$$A_{\pm} = \left[ \frac{\eta_+^2 - \eta_-^2}{\eta_+ \coth^2(\eta_j L/2) - \eta_- \coth^2(\eta_j L/2)} \right] E_0^{(\pm)}.$$

with $\coth^+(y) = \coth(y)$ and $\coth^-(y) = \tanh(y)$. Finally, the $F$ functions are

$$F_{\mp}(z) = \frac{cosh(\eta_j z)}{cosh(\eta_j L/2)} - \frac{cosh(\eta_j z)}{cosh(\eta_j L/2)} E_0^{(\pm)}.$$
where $E^{\pm}$ follows with $\cosh \to \sinh$. Note that the eigenstates $\Psi_{\pm}(z)$ describe both spin directions ($\sigma = \uparrow$ and $\sigma = \downarrow$).

We now project the full Hamiltonian $H$ to the basis spanned by the surface states [4]. We define Pauli matrices $\tau_{\alpha=x,y,z}$ switching between the two solutions $\Psi_{\pm}(z)$, Pauli matrices $\sigma_{\alpha}$ in spin space, and use $\tau_{0}$ and $\sigma_{0}$ as identities. With the energy scales

$$E_{0} = \frac{E_{0}^{(+)} + E_{0}^{(-)}}{2}, \quad \Delta = E_{0}^{(+)} - E_{0}^{(-)},$$

the low-energy ("surface") Hamiltonian resulting from this projection reads

$$H_{\text{eff}} = E_{0}\tau_{0}\sigma_{0} + \frac{\Delta}{2}\tau_{z}\sigma_{0} - A_{2}W\tau_{x}(k_{x}\sigma_{x} + k_{y}\sigma_{y}) + O(k^{2}),$$

where $W = \langle \Psi_{+}|\Psi_{-}\rangle$. The parameter $\Delta(L)$ is precisely the surface state gap described in the Introduction. For the parameters [2], $\eta_{-}$ is always real. However, $\eta_{+}$ is real for large $L$ but purely imaginary for small $L$. In any case, we find that $W$ is always real and positive.

Noting that $H_{\text{eff}}$ commutes with $\tau_{z}\sigma_{z}$, it can readily be diagonalized by the unitary transformation $U(\mathbf{k}) = \text{diag}(U_{+}, U_{-})$, where $\mathbf{k} = (k_{x}, k_{y})$ and the $U_{\pm}(\mathbf{k})$ are $2 \times 2$ matrices in spin space, with $\nu$ denoting the eigenvalue of $\tau_{z}\sigma_{z}$. With $\tan\alpha = 2A_{2}W|\mathbf{k}|/\Delta$ and $\tan\theta = k_{y}/k_{x}$, we find

$$U_{\pm} = \begin{pmatrix} e^{-i\theta/2}\cos(\alpha/2) & e^{-i\theta/2}\sin(\alpha/2) \\ -e^{i\theta/2}\sin(\alpha/2) & e^{i\theta/2}\cos(\alpha/2) \end{pmatrix}, \quad (9)$$

Switching to second-quantized notation, the eigenstates of $H_{\text{eff}}$ correspond to helical fermions with annihilation operator

$$\hat{c}_{\mathbf{k},\nu} = \sum_{\sigma}[U_{\nu}(\mathbf{k})]^{\dagger}_{\sigma\sigma}d_{\mathbf{k},\tau=\nu,\sigma}, \quad (10)$$

where $d_{\mathbf{k},\tau,\sigma}$ annihilates a spin-$\sigma$ electron with in-plane momentum $\mathbf{k}$ in the transversal state $\Psi_{\tau}(z)$. The low-energy electronic Hamiltonian (including the chemical potential $\mu$) then takes the final form

$$H_{\text{el}} = \sum_{\mathbf{k},\mathbf{q},\tau,\sigma}^{\dagger}c_{\mathbf{k},\nu}c_{\mathbf{k}_{\nu}^{\dagger}}c_{\mathbf{k}_{\nu}^{\dagger},\nu}^{\dagger},$$

where the dispersion relation is

$$\epsilon_{\mathbf{k},\pm} = E_{0} - E_{0}^{\infty} - \mu \pm \frac{\Delta}{2}\sqrt{1 + (2A_{2}W/\Delta)^{2}k_{z}^{2}.} \quad (12)$$

We here choose the zero of energy by setting $E_{0}^{\infty} = C + D_{1}M_{0}/B_{1} = \lim_{L \to \infty}E_{0}^{(+)}$. For the parameters [2], we find $E_{0}^{\infty} \approx 0.22$ eV. Moreover, for $L \to \infty$, the length-scales $\eta_{\pm}$ are given by $\eta_{+} \approx 12.3$ Å and $\eta_{-} \approx 1.9$ Å. For $kL \gg 1$, the dispersion relation [12] is linear, with

Fermi velocity $v_{F} \approx 2.77 \times 10^{5}$ m/s. Note that the index $s = \pm$ in Eq. [11] does not correspond to spin anymore.

Similarly, the particle density operator $\hat{n}(\mathbf{r}, z)$ with $\mathbf{r} = (x, y)$ is written in terms of the $d_{\mathbf{k},\tau,\sigma}$ operators,

$$\hat{n}(\mathbf{r}, z) = \sum_{\mathbf{k},\mathbf{q},\tau,\sigma}e^{-i\mathbf{q}\cdot\mathbf{r}}\rho_{\tau}(z)d_{\mathbf{k+q},\tau,\sigma}^{\dagger}d_{\mathbf{k},\tau,\sigma}. \quad (13)$$

Using Eq. [10], the density operator [13] can be transformed to the helical basis. We show the single-particle densities for the surface states [Eq. [9]],

$$\rho_{\tau}(z) = [\Psi_{\tau}^{\dagger}, \Psi_{\tau}](z), \quad (14)$$

in Fig. [1] for a film thickness of $L = 4$ QL, where 1 QL $\approx 9.5$ Å for Bi$_{2}$Se$_{3}$. This demonstrates that already for quite thin films, Eq. [6] describes surface states. Note that $\rho_{\tau}(z)$ is an even function of $z$. The inset of Fig. [1] shows the numerically obtained gap $\Delta(L)$, demonstrating the absence of oscillatory behavior for the parameters [2] as well as the exponential decay of $\Delta(L)$ due to the exponentially vanishing overlap of both surface states. We note in passing that for the parameters in Ref. [12], Eq. [7] instead predicts an oscillatory decay of $\Delta(L)$.

B. Phonon model

We now discuss the long-wavelength acoustic phonon modes in the TI film. We employ isotropic elastic continuum theory, where the longitudinal $(c_{l})$ and transverse $(c_{t})$ sound velocities correspond to the two Lamé constants. In Bi$_{2}$Se$_{3}$, they are given by $c_{i} \approx 2900$ m/s and $c_{i} \approx 1700$ m/s, respectively. Moreover, the mass density is $\rho_{M} \approx 7680$ kg/m$^{3}$. In order to model the film geometry, we impose stress-free boundary
follows from Eqs. (18) and (19) with
\begin{equation}
H_{ph} = \sum_{\Lambda} \Omega_{\Lambda} \left( b_{\Lambda}^{\dagger} b_{\Lambda} + 1/2 \right). \tag{16}
\end{equation}

The orthonormal eigenmodes $u_{\Lambda}(z)$ in Eq. (15) describe linear combinations of $e^{\pm ik_{t}z}$ waves, where
\begin{equation}
k_{t,t} = \sqrt{\left(\Omega_{\Lambda}/c_{t,t}\right)^{2} - q^{2}}; \tag{17}
\end{equation}

$k_{t,t} = i\kappa_{t,t}$ with $\kappa_{t,t} = \sqrt{q^{2} - \left(\Omega_{\Lambda}/c_{t,t}\right)^{2}}$ for $\Lambda < c_{t,t}q$. Writing $u_{\Lambda}(z)$ in the form
\begin{equation}
u(z) = \left( iq\phi_{t} - \frac{d\phi_{t}}{dz} \right) \hat{e}_{q} + \left( \frac{d\phi_{t}}{dz} + iq\phi_{t} \right) \hat{e}_{z}, \tag{18}
\end{equation}

where $\hat{e}_{q} = \mathbf{q}/|q|$ and
\begin{equation}
\phi_{t,t} = a_{t,t}\cos(k_{t,t}z) + b_{t,t}\sin(k_{t,t}z), \tag{19}
\end{equation}

the stress-free boundary conditions at $z = \pm L/2$ yield
\begin{equation}
2iq\frac{d\phi_{t}}{dz} - (q^{2} - k_{t}^{2})\phi_{t} = 0, \tag{20}
\end{equation}

\begin{equation}
2iq\frac{d\phi_{t}}{dz} + (q^{2} - k_{t}^{2})\phi_{t} = 0. \tag{21}
\end{equation}

Since both equations have to be fulfilled at $z = \pm L/2$, we have four linear equations for the four unknown parameters $(a_{t,t}, b_{t,t})$. Setting the corresponding determinant to zero, we obtain the following two possibilities. First, for symmetric modes ($\Lambda = S$), we have the condition
\begin{equation}
(q^{2} - k_{t}^{2})^{2}\cos(k_{t}L/2)\sin(k_{t}L/2) + 4q^{2}k_{t}\sin(k_{t}L/2)\cos(k_{t}L/2) = 0. \tag{22}
\end{equation}

Numerical solution of this transcendental equation obtains the quantized set of dilatational phonon frequencies $\Omega_{\Lambda=(q,S,n)}$. The corresponding eigenvector, $u_{\Lambda}(z)$, follows from Eqs. (18) and (19) with $a_{t} = b_{t} = 0$ and
\begin{equation}
\begin{align*}
a_{t} &= \frac{2N_{Ag}}{\cos(k_{t}L/2)}, \quad b_{t} = iN_{Si}(q^{2} - k_{t}^{2})/k_{t}\cos(k_{t}L/2) \tag{23}
\end{align*}
\end{equation}

Second, for antisymmetric modes ($\Lambda = A$), we arrive again at the condition in Eq. (21) but with the exchange $\cos \leftrightarrow \sin$. Solving that equation yields the set $\Omega_{\Lambda=(q,A,n)}$ of quantized flexural phonon modes. The eigenvector $u_{\Lambda}(z)$ follows again from Eqs. (18) and (19), where now $a_{t} = b_{t} = 0$ and
\begin{equation}
\begin{align*}
b_{t} &= \frac{2N_{Ag}}{\sin(k_{t}L/2)}, \quad a_{t} = -iN_{Ai}(q^{2} - k_{t}^{2})/k_{t}\sin(k_{t}L/2) \tag{24}
\end{align*}
\end{equation}

The normalization factors $N_{A=S,A}$ appearing in Eqs. (22) and (24) are given in Appendix A.

Numerical solution of Eq. (21) yields the spectrum, $\Omega_{\Lambda}$, for the symmetric mode ($\Lambda = S$). The result is shown in Fig. 2. We distinguish three different regions, namely a case where both $k_{t}$ and $k_{l}$ are purely imaginary (region I), when only $k_{l}$ is purely imaginary but $k_{t}$ is real (region II), and finally a case where both $k_{l}$ and $k_{l}$ are real (region III). We observe from Fig. 2 that the $n = 1$ mode is the finite-width analogue of the well-known Rayleigh surface mode. For the semi-infinite geometry, the Rayleigh mode is the lowest-lying phonon. It has the dispersion relation
\begin{equation}
\Omega = c_{R}q, \quad c_{R} \approx 0.92c_{t}. \tag{25}
\end{equation}

In fact, for $qL \gg 1$, both Eq. (21) and the corresponding equation for $\lambda = A$ reduce to
\begin{equation}
(q^{2} + k_{t}^{2})^{2} = 4q^{2}k_{t}k_{l}. \tag{26}
\end{equation}

As discussed in Ref. 27, this equation readily yields the sound velocity $c_{R}$ of the Rayleigh mode.
C. Electron-phonon coupling

The dominant coupling of the above phonon modes to the electronic surface states comes from the deformation potential \( n(r,z) \) [Eq. (13)] to the divergence of the displacement vector, \( \nabla \cdot \mathbf{U}(r,z) \), see Eq. (15). Since the surface state density \( \rho_z(z) \) in Eq. (14) is even in \( z \), the antisymmetric phonon mode (\( \lambda = A \)) does not couple to the surface states. We therefore keep only the symmetric phonon mode from now on (and omit the index \( \lambda = S \)). Transforming Eq. (13) to the helical basis, see Eq. (10), the second-quantized electron-phonon coupling Hamiltonian reads

\[
H_{e-\text{ph}} = \frac{\alpha}{\sqrt{A}} \sum_{\mathbf{q},k,n;\nu,s,s'} M_{k,\mathbf{q},n}^{(s,s')} b_{\mathbf{q},n}^{\dag} c_{\mathbf{k}+\mathbf{q},\nu,s'} c_{\mathbf{k},\nu,s'} + \text{H.c.,}
\]

where the \( M \) matrix elements involve the unitary matrices \( |U_v(k)|_{s\sigma} \) in Eq. (1).

\[
M_{k,\mathbf{q},n}^{(s,s')} = \frac{1}{\sqrt{2\rho_M \Omega_{q,n}}} \left( \frac{\Omega_{q,n}}{c_l} \right)^2 \sum_{\sigma} |U_v(k+q)|_{\nu,s}^* |U_v(k)|_{\nu,s'} \int_{-L/2}^{L/2} dz \rho_{\gamma=v,s}(z) \phi_l(z),
\]

with the phonon dispersion \( \Omega_{q,n} \) in Fig. 2 \( \phi_l \) is given by Eqs. (19) and (22). The deformation potential strength \( \alpha \) in Eq. (23) can be estimated as follows. The high-temperature behavior of the on-shell imaginary part of the electronic self-energy is (see Sec. IVV)

\[
\text{Im} \Sigma(k, T) = -\pi \lambda k B T,
\]

which allows to experimentally extract the dimensionless effective electron-phonon coupling constant \( \lambda \). The relation (27) has been observed for \( Bi_2Se_3 \) in ARPES experiments, and \( \lambda = 0.25 \pm 0.05 \) has been measured. In these experiments, the Fermi level was near the bottom of the conduction band, \( \mu \approx 0.28 \text{ eV} \), and \( k \) in Eq. (27) corresponds to energies \( \approx 50 \) to 100 meV above the Dirac point. Computing \( \lambda \) within our model, see Sec. IVV the observed value for \( \lambda \) corresponds to \( \alpha = (30 \pm 8) \text{ eV} \). We employ the value \( \alpha = 30 \text{ eV} \) below.

The total Hamiltonian employed in the following sections is then given by \( H = H_{\text{el}} + H_{\text{ph}} + H_{e-\text{ph}} \), see Eqs. (11), (16) and (25). We first address the phonon-induced resistivity \( \rho \) in Sec. III and then turn to the quasiparticle lifetime in Sec. IV.

III. RESISTIVITY

Here we discuss the \( T \)-dependent phonon contribution to the electrical resistivity, \( \rho \), in the TI film, using the Hamiltonian described in Sec. III. As explained in Sec. IV, only symmetric (dilatational) phonon modes can cause a finite resistivity for the low-energy surface states within the bulk gap. We compute \( \rho \) within the framework of the linearized Boltzmann equation, which has also been employed previously for the related graphene case. The resulting quasiclassical estimate for \( \rho \) is valid as long as \( \rho \) is small compared to the resistance quantum, \( \rho \ll h/e^2 \approx 25.8 \text{ k}\Omega \). We sketch the standard derivation for \( \rho \) in Appendix II. The result takes the form

\[
1 \rho = \frac{e^2}{2} \sum_{\nu,\pm} \int \frac{d\mathbf{k}}{(2\pi)^2} \epsilon_{k,\nu}^2 \tau_\nu(\epsilon_{k,\nu}) \left[ -\partial_\epsilon n_F(\epsilon_{k,\nu}) \right],
\]

where the dispersion relation for helical fermions [Eq. (12)] defines the group velocity, \( v_{k,\nu} = \mathbf{v}_k \cdot \nabla_k \epsilon_{k,\nu} \). Moreover, \( n_F(\epsilon) \) is the Fermi function, and the energy-dependent electron-phonon transport scattering rate (inverse time) is

\[
\frac{1}{\tau_\nu(\epsilon_{k,\nu})} = \sum_{\mathbf{q},s'} \left( 1 - \frac{v_{k+\mathbf{q},s'}}{v_{k,\nu}} \cos \theta_{k+\mathbf{q},\mathbf{q}} \right) \frac{1 - n_F(\epsilon_{k,\nu})}{1 - n_F(\epsilon_{k,\nu})} W_{(k,\nu,s') \rightarrow (k+\mathbf{q},\nu,s')},
\]
where $\theta_{k,q}$ is the angle between $k$ and $k + q$, and the transition probabilities are obtained from Fermi’s golden rule. Using Eq. (28), we find

$$ W_{(k,\nu,s)\rightarrow(k+q,\nu,s')} = \frac{2\pi\alpha^2}{A} \sum_{n;\nu=\pm} n_B(n\Omega_{q,n}) \left|M_{k,q,n}^{(s,s')}(\nu\Omega_{q,n})\right| \delta(\epsilon_{k,s} + n\Omega_{q,n} - \epsilon_{k+q,s'}). $$

(30)

where $n_B(e)$ is the Bose function. While the $M$ matrix elements (26) depend on the index $\nu = \pm$, we note that $|M|^2$ and therefore the transition probabilities $W$ are $\nu$-independent. This also implies that $\tau,\eta$ does actually not depend on $\nu.$

With the polar angle $\theta$ between $k$ and $q$, such that

$$ \cos \theta_{k,q} = \frac{k + q \cos \theta}{\sqrt{k^2 + q^2 + 2kq \cos \theta}}, $$

(31)

the angular integration in Eq. (29) can be encapsulated in the “transport Eliashberg function”, see also Ref. 11.

The $\theta$-integration in Eq. (32) can then be carried out analytically. We quote the (lengthy) result in Appendix C which is useful when computing $F$ numerically. For low temperatures, the quasi-elastic approximation, $\Omega_{q,n} \ll \sqrt{(\Delta/2)^2 + (A_2W k)^2}$, is applicable and allows to simplify the full result for $F$ to the $\nu$-independent form

$$ F_{k,n,s}(q) = \frac{\Theta(2k-q)}{\pi(2k/q)^2 - 1} \times \left[ -\frac{(\Delta/2)^2 + (A_2W k)^2}{(A_2W k)^2} |M_{k,q,n}^{(s,s')}| \right]_{\theta_0}, $$

(34)

where $\theta = \theta_0$ (see Appendix C) determines the polar angle between $k$ and $q$ appearing in the matrix element $M$, and the Heaviside function is denoted by $\Theta(y)$. Note that there is no contribution from interband transitions at low temperatures.

The crossover temperature from the low- to the high-temperature behavior in this system is set\textsuperscript{11} by the Bloch-Gr"{u}neisen temperature,

$$ T_{BG} = 2k_Fc_R/k_B, $$

(35)

with the Rayleigh velocity $c_R$ in Eq. (24). $k_F(L)$ is defined by $\epsilon_{k_F,s=\pm} = 0$ with the dispersion relation (12). For $T \ll T_{BG}$, the $F$ function can be approximated by the quasi-elastic expression [Eq. (34)]. It receives the dominant contribution from the $n = 1$ branch corresponding to the Rayleigh surface phonon. For small $q$, we find $\Omega_{q,n=1} = c_s q$ with $c_s = 2754$ m/s (which is slightly below $c_l$), see also Fig. 2. In addition, we have $\phi_t(z) = 2(c_l/c_s)^2/(q\sqrt{L})$ and $c_s \ll \min(|v_{kF}|, A_2W)$, leading to

$$ F_{k,F,1,\pm}(q) = \frac{(c_l/c_s)^4}{\pi\rho_M|v_{kF}|c_s k_F^2} \frac{q^2}{L}. $$

This allows us to perform all remaining integrations and yields a $T^4$ law for the resistivity at low temperatures,

$$ \rho(T \ll T_{BG}) = \frac{h}{e^2 A \left( \frac{T}{T_{BG}} \right)^4} \frac{4}{\pi\rho_M|v_{kF}|c_s k_F^2}, $$

(36)

where the dimensionless prefactor $A$ is

$$ A = \frac{8\gamma k_F^2 e^2 (c_l/c_s)^4}{\pi\rho_M v_{kF}^2 c_s} \frac{1}{L}, $$

(37)

$$ \gamma = \left[ \int_{-\infty}^{+\infty} dx \frac{2e^x}{(\pi^2 + x^2)(e^x + 1)^2} \right]^{-1} \approx 68.4925. $$

For $L \to \infty$, $A$ obviously vanishes. This suggests that for elevated temperatures (but still $T < T_{BG}$) and finite $L$, the $T^4$ law is replaced by the $L$-independent $\rho \propto T^5$Law found in Ref. 11. We can estimate the crossover
phonon branches indexed by \( n \) for very thin and clean TI films. We obtain the relaxation rate as a function of the energy. Since the linear term does not contribute to the resistivity \( \rho \) with the dimensionless prefactor \( C \) obtained numerically for a fixed width \( L = 4 \) QL and several values of the chemical potential \( \mu \), see Fig. 4.

In that case, when measured relative to \( E_g^\infty \), we have \( E_g^\infty \approx 16 \) meV and \( \Delta/2 \approx 13 \) meV. For the lowest \( \mu \) in Fig. 3 the Fermi level is thus located inside the surface gap and one has a very large resistivity, where the quasiparticle lifetime (inverse decay rate) for intermediate values of \( L \). Second, for \( L \to \infty \), \( \rho(L) \) approaches 1/4 of the single-surface value \( \rho_\infty(T) \) obtained for the semi-infinite geometry. Naively, we would expect \( \rho(L \to \infty) = \rho_\infty/2 \) because of the presence of two surfaces in the film geometry. This discrepancy indicates that the \( L \to \infty \) limit is singular, and it is not possible to really decouple both surfaces in such an interacting system; see also Ref. [21] for a related discussion.

### IV. LIFETIME BROADENING

Next we discuss the quasiparticle lifetime (inverse decay rate) for the surface fermions in the TI film due to their coupling to phonons, see \( H_{e-ph} \) in Eq. (25), which implies a finite linewidth of ARPES spectral features. The decay rate, \( \Gamma_k(T) = -2 \text{Im} \Sigma \), follows from the
imaginary part of the on-shell self-energy \( \Sigma_{s=\pm}(k, \omega = \epsilon_{k,n,s}) \).

Expanding up to second order in \( H_{e-\text{ph}} \), the “rainbow” diagram yields the self-energy

\[
\Sigma_s(k, \omega) = \alpha^2 \sum_{n,s'} \int \frac{dq}{(2\pi)^2} \left| M_{k,q,n}^{s,s'} \right|^2 \left( \frac{k}{q} \right)^2
\]

\[
\times \sum_{\nu,\nu'} \left[ n_B(\nu \Omega_{q,n}) + n_F(\epsilon_{k,q,n,s'} - \nu \Omega_{q,n} - \epsilon_{k,q,n,s}) \right].
\]

Introducing the Eliashberg function \( F_{k,n,s}(q) \) exactly as the transport Eliashberg function \( F \) in Eq. (32) but without the factor \( 1 - (\epsilon_{k,q,n,s}/\epsilon_{k,n,s}) \cos B(\theta) \), the quasiparticle decay rate follows as

\[
\Gamma_k(T) = \alpha^2 \sum_{n,s'} \int_0^\infty q dq F_{k,n,s}(q) q \Gamma_q k_B T,
\]

where \( \Gamma_q = \alpha^2 / 2 \pi \sum_{n,s'} \int_0^\infty q dq q F_{k,n,s}(q) q \). Expanding this result for high temperatures, \( T \gg T_{BG} \), as in Sec. III yields, see also Eq. (27), a linear \( T \)-dependence,

\[
\Gamma_k(T \gg T_{BG}) = 2\pi \lambda_k k_B T,
\]

\[
\lambda_k = \alpha^2 \sum_{n,s'} \int_0^\infty q dq q F_{k,n,s}(q) q \Omega_{q,n}.
\]

The \( L \)-dependence of \( \lambda_k \) is shown for \( k = k_F \) in Fig. 6. We observe an oscillatory dependence, with a saturation at one-half of the corresponding semi-infinite result.

For low temperatures and \( k = k_F \), the decay rate is dominated by the \( n = 1 \) phonon mode with \( q \rightarrow 0 \). After some algebra, we find that this implies a \( T^2 \) law,

\[
\Gamma_k(T \ll T_{BG}) = \frac{4\pi \alpha^4 (c_1/c_2)^4 (k_F c_R^2)^2}{\rho M} \frac{1}{L} \left( \frac{T}{T_{BG}} \right)^2.
\]

Again, when \( T \gg T_c \), the \( T^2 \) law (which scales \( \propto 1/L \)) competes with the \( L \)-independent \( T^3 \) law found in Ref. 11. Finally, when \( k \neq k_F \) and \( T \ll T_{BG} \), the quasiparticle decay rate saturates at the finite value

\[
\Gamma_{k\neq k_F} = \alpha^2 \sum_n \int_0^\infty q dq \Theta(|\epsilon_{k,+} - \epsilon_{k,n}|) F_{k,n,s}(q).
\]

with \( \nu = \text{sgn}(k_F - k) \).

Figure 6 shows that the \( L \rightarrow \infty \) limit of the decay rate always tends to \( \Gamma_\infty(T)/2 \), where \( \Gamma_\infty \) is the corresponding decay rate for the semi-infinite geometry. This discrepancy with the naive expectation \( \Gamma(L \rightarrow \infty) = \Gamma_\infty \) has the same origin as the anomalous factor 1/2 appearing in the large-\( L \) behavior of the resistivity discussed in Sec. III.

V. CONCLUSIONS

In this paper we have studied the effects of long-wavelength acoustic phonons on the topologically protected surface fermions in topological insulator films.
Our model employs the established low-energy electronic Hamiltonian and an isotropic elastic continuum approach for the phonons, with the deformation coupling providing the dominant interaction mechanism. The electron-phonon coupling turns out to be surprisingly strong, in accordance with recent ARPES results.\textsuperscript{24}

Using a quasiclassical approach, we have computed the temperature-dependent resistivity of the film due to phonon backscattering, and found a linear $T$ dependence above the Bloch-Gr"uneisen temperature. In this temperature regime, the phonon-induced resistivity can overcome the disorder-induced ($T$-independent) contribution and should be observable with present samples. Similarly, the linear $T$ dependence of the quasiparticle decay rate found here is observable\textsuperscript{24} in ARPES experiments. The low-temperature behaviors of the resistivity and of the quasiparticle decay rate are probably more difficult to observe.

An interesting extension of our work would be to include the effects of a magnetic field. Magnetotransport measurements in thin films were recently performed\textsuperscript{30} and found clear evidence for Landau level formation associated with the massless Dirac fermions forming on both surfaces. The observed broadening of the Landau levels was assigned to disorder and/or interaction effects, but at elevated temperatures, our analysis indicates that electron-phonon interactions may be relevant as well.

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\section*{Appendix A: Normalization constants}

Here we provide the normalization constants $N_{S,A}$ appearing in Eqs. (22) and (23) in Sec. II B. Specifically, we get these constants after some algebra from

\begin{equation}
N_{S}^{-2} = \frac{\Omega_s^2}{2c_s^4} \left[ \frac{c_s^2}{c_s} \frac{4q^2L}{\cos^2(k_{L}/2)} \left(1 + \frac{\sin(k_{L}/L)}{k_{L}}\right) + \frac{(q^2 - k_{L}^2)^2L}{k_{L}^2 \cos^2(k_{L}/2)} \left(1 - \frac{\sin(k_{L}/L)}{k_{L}}\right) - 8(q^2 - k_{L}^2) \frac{\tan(k_{L}/L/2)}{k_{L}} \right],
\end{equation}

\begin{equation}
N_{A}^{-2} = \frac{\Omega_A^2}{2c_A^4} \left[ \frac{c_A^2}{c_A} \frac{4q^2L}{\sin^2(k_{L}/2)} \left(1 - \frac{\sin(k_{L}/L)}{k_{L}}\right) + \frac{(q^2 - k_{L}^2)^2L}{k_{L}^2 \sin^2(k_{L}/2)} \left(1 + \frac{\sin(k_{L}/L)}{k_{L}}\right) + 8(q^2 - k_{L}^2) \frac{\cot(k_{L}/L/2)}{k_{L}} \right].
\end{equation}

\section*{Appendix B: Linearized Boltzmann equation}

The linearized Boltzmann equation has been derived for closely related problems before\textsuperscript{20,35,36,44} and we here follow those works and briefly sketch the derivation of Eq. (23). In the quasiclassical approximation, the quasiparticle distribution function $f_r(k,t)$ (for simplicity, we here omit the $v$ and $s$ indices) obeys the well-known Boltzmann equation. In the absence of a force $\mathbf{F} = -eE$ due to the external electric field, $f$ reduces to a Fermi function, $f = n_F(\epsilon_k)$, and the collision integral vanishes. In the presence of the force, $f$ is expanded in terms of Legendre polynomials $P_n(\cos(\alpha))$, where $\alpha$ is the angle between $\mathbf{k}$ and $\mathbf{F}$. Keeping only terms linear in $\mathbf{F}$, we have $f(k) = n_F(\epsilon_k) + \cos(\alpha)f_1(\epsilon_k)$. Using detailed balance, for given transition matrix elements $W_{k \rightarrow k'}$, we obtain the linearized Boltzmann equation (LBE),

\begin{equation}
\mathbf{F} \cdot \mathbf{v}_k \partial_t n_F(\epsilon_k) = \sum_{k'} W_{k \rightarrow k'} \left[ \frac{n_F(\epsilon_k)}{n_F(\epsilon_{k'})} \cos(\alpha')f_1(\epsilon_{k'}) - \frac{1 - n_F(\epsilon_{k'})}{1 - n_F(\epsilon_k)} \cos(\alpha)f_1(\epsilon_k) \right].
\end{equation}

Using the Ansatz $f_1(\epsilon_k) = -\tau(\epsilon_k)\mathbf{v}_k\mathbf{F}\partial_t n_F(\epsilon_k)$, after some algebra the LBE leads to the linear integral equation

\begin{equation}
\frac{1}{\tau(\epsilon_k)} = \sum_{k'} W_{k \rightarrow k'} \left[ 1 - \frac{\mathbf{v}_{k'} \tau(\epsilon_{k'})}{\mathbf{v}_k \tau(\epsilon_k)} \cos(\vartheta) \right] \frac{1 - n_F(\epsilon_{k'})}{1 - n_F(\epsilon_k)},
\end{equation}

where $\vartheta$ is the angle between $\mathbf{k}$ and $\mathbf{k}'$. The solution for $\tau(\epsilon_k)$ determines the electron momentum relaxation time. When the scattering of quasiparticles from long-wavelength acoustic phonons is quasielastic, $\Omega_{q,n} \ll |\mu|$, we can set $\tau(\epsilon_{k'}) = \tau(\epsilon_k)$ for the right-hand side of the above integral equation; this is equivalent to the “test particle approximation.”\textsuperscript{20} The current density,

\begin{equation}
j = -\frac{e}{A} \sum_k \mathbf{v}_k f(k),
\end{equation}

points parallel to the electric field direction and has the magnitude

\begin{equation}
j = -\frac{e^2F}{A} \sum_k \mathbf{v}_k^2 \cos^2(\alpha) \tau(\epsilon_k) \left[ -\partial_t n_F(\epsilon_k) \right].
\end{equation}

Using $\mathbf{v}_k = \mathbf{v}_k$ and performing the angular integration, we arrive at the phonon contribution to the resistivity quoted in Eqs. (28) and (29).

\section*{Appendix C: Transport Eliashberg function}

We here give the analytical result for the full transport Eliashberg function $F$ defined in Eq. (32). Some
straightforward yet tedious algebra allows to perform the \( \theta \)-integration. We find the (lengthy) result

\[
\mathcal{F}_{k,n,s}^{(v)}(q) = \frac{2 |A_{k,q,n,s}^{(v)}|}{\pi(A_2W)^2} \left( \Theta \left( Q_{k,q,n,s}^{(v)} + k - q \right) \Theta \left( q - \left| Q_{k,q,n,s}^{(v)} - k \right| \right) \right) \Theta \left( |A_{k,q,n,s}^{(v)}| - \Delta / 2 \right)
\]

\[
\times \sum_{s'} \Theta \left( s' A_{k,q,n,s}^{(v)} \right) \left( 1 - \left( \frac{\nu \Omega_{q,n}}{A_{k,q,n,s}^{(v)}} \right) \left( \frac{(Q_{k,q,n,s}^{(v)})^2 + k^2 q^2 - 2q^2 k^2}{2k^2} \right) \right) \left| M_{k,q,n}^{s',s} \right|^2 \theta_0,
\]

where we use the notations

\[
A_{k,q,n,s}^{(v)} = s \sqrt{\left( \Delta / 2 \right)^2 + (A_2Wk)^2 + \nu \Omega_{q,n}},
\]

\[
Q_{k,q,n,s}^{(v)} = \sqrt{\left( A_{k,q,n,s}^{(v)} \right)^2 - \left( \Delta / 2 \right)^2} / A_2W.
\]

and the polar angle \( \theta = \theta_0 \in [0, \pi] \) follows from

\[
\sqrt{k^2 + q^2 + 2kq \cos \theta_0} = Q_{k,q,n,s}^{(v)},
\]

fixing the polar angle between \( k \) and \( q \) in the matrix element \( M \).
We mention that Eq. (8) in Ref. 11 contains a mistake: in the denominator of the expression for $C^{-1}$, one should replace $\kappa_l^2 \kappa_t \to \kappa_l \kappa_t^2$. This implies $C \approx 0.78$ instead of the quoted value $C \approx 1.20$ in Ref. 11. Fortunately, this mistake has no consequences for the conclusions reached in Ref. 11.

In principle, the self-energy is off-diagonal in the $ss'$ indices, but for the rate $\Gamma$, only the diagonal element with $s = s'$ is needed. We also use the fact that $\Sigma$ then is $\nu$-independent.