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Ulrich Zülicke¹ ¹ School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria
University of Wellington, PO Box 600, Wellington 6140, New Zealand² Scuola Normale Superiore and NEST, Istituto Nanoscienze-CNR, I-56126 Pisa, Italy³ NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy⁴ Department of Quantum Matter, AdSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan⁵ Author to whom any correspondence should be addressed.E-mail: michele.governale@vuw.ac.nz**Keywords:** topological insulators, nanowires, optical transitions**Abstract**

We present a theoretical study of a nanowire made of a three-dimensional topological insulator. The bulk topological insulator is described by a continuum-model Hamiltonian, and the cylindrical-nanowire geometry is modelled by a hard-wall boundary condition. We provide the secular equation for the eigenenergies of the systems (both for bulk and surface states) and the analytical form of the energy eigenfunctions. We describe how the surface states of the cylinder are modified by finite-size effects. In particular, we provide a $1/R$ expansion for the energy of the surface states up to second order. The knowledge of the analytical form for the wavefunctions enables the computation of matrix elements of any single-particle operators. In particular, we compute the matrix elements of the optical dipole operator, which describe optical absorption and emission, treating intra- and inter-band transition on the same footing. Selection rules for optical transitions require conservation of linear momentum parallel to the nanowire axis, and a change of 0 or ± 1 in the total-angular-momentum projection parallel to the nanowire axis. The magnitude of the optical-transition matrix elements is strongly affected by the finite radius of the nanowire.

1. Introduction

Three-dimensional (3D) topological insulators (TI)s were predicted in 2007 [1] as electronic systems characterized by an insulating bulk and gapless conducting surface states (for a review, see references [2–5]). The states at the interface between the system and the vacuum are topologically protected against time-reversal invariant perturbations and consist, at low energy, of two-dimensional Dirac fermions [6–8]. Recent advances in nanofabrication techniques have enabled the realization of 3D-TI samples of reduced dimensionality, for example in the form of nanowires [9–26]. 3D-TI nanowires proximitised with an s-wave superconductor have been proposed as a possible platform for the realization of Majorana bound states [27, 28]. The availability of nanometer-scale samples is interesting also because it offers the opportunity to investigate the competition between the inverted bulk gap and the size-quantisation energy as well as the extent of the localization of surface states [29–38]. In reference [29], an approximate analytic model supplemented by a numerical scheme based on exact diagonalisation was introduced to study the quantum interference effects on the low-energy spectrum of Bi_2Se_3 nanowires.

In this paper we explore the properties of a finite-radius 3D-TI cylinder, using the envelope-function description of the TI bulk band structure developed in references [39, 40]. Our goal is to determine the dependence of its energy spectrum and eigenfunctions on the radius R . The central point of our analysis is the analytical expression of the eigenfunctions, which allow us to express cylindrical hard-wall boundary conditions in terms of secular equations that can be approximated in the limit of large radii: we obtain

Table 1. Values for parameters in the effective continuum-model Hamiltonian describing bulk-electronic states of currently available topological-insulator materials, from reference [41].

	Bi ₂ Se ₃	Bi ₂ Te ₃	Sb ₂ Te ₃
m_0 (eV)	−0.169	−0.296	−0.182
m_1 (eV Å ²)	3.353	9.258	22.136
m_2 (eV Å ²)	29.375	177.355	51.320
B (eV Å)	1.836	0.900	1.174
A (eV Å)	2.513	4.003	3.694

approximate expressions for the eigenenergies up to second order in $1/R$. The analytical functional form of the eigenfunctions, which is valid irrespective of the radius of the wire, enables the calculation of the matrix elements of any observable. As an example, we consider the dipole matrix elements for optical transitions. In particular, we find that the selection rules for absorption and emission are not modified by a finite radius, in contrast to the case of a spherical nanoparticle [36]. Numerical results are presented for three different materials, namely Bi₂Se₃, Bi₂Te₃, and Sb₂Te₃, which show qualitatively different behaviours. We compute eigenenergies as functions of the radius R and longitudinal momentum and compare them with approximate large-radius expressions. The eigenenergies are found to be oscillating for small values of R , especially in the case of Bi₂Te₃. Moreover, we characterize the behaviour of eigenfunctions by plotting the average radial coordinate and the corresponding variance as a function of the radius R . As expected, the average coordinate moves towards the centre of the nanowire for small values of R , more rapidly for Bi₂Te₃ than for Bi₂Se₃, while the variance increases in an oscillating fashion for increasing radii, reaching the asymptotic value more rapidly in the case of Bi₂Se₃ with respect to Bi₂Te₃. Finally, we calculate numerically the dependence of the optical dipole matrix elements on the radius finding quantitative important changes with respect to the bulk situation.

The paper is organized as follows. In section 2, we present an analytic treatment for a cylindrical 3D-TI nanowire with hard-wall confinement. We conclude section 2 with a complete analytic expression for the eigenfunction of the finite-radius 3D-TI. In section 3, we study the finite size effects on the topological properties of a cylindrical 3D-TI for two different materials. Specifically, we study the eigenenergies and characterise the eigenfunctions of the system as a function of the radius of the cylinder. Finally, in section 3.3, we calculate the optical dipole matrix elements of a cylindrical TI and study their dependence on the the radius of the cylinder.

2. Model

We consider an infinitely long cylinder of TI of radius R , whose axis is in the z -direction. The bulk TI is described by the Hamiltonian [39, 40]

$$H_0 = \begin{pmatrix} m(\mathbf{p}) & Bp_z & 0 & Ap_- \\ Bp_z & -m(\mathbf{p}) & Ap_- & 0 \\ 0 & Ap_+ & m(\mathbf{p}) & -Bp_z \\ Ap_+ & 0 & -Bp_z & -m(\mathbf{p}) \end{pmatrix}, \quad (1)$$

where $\mathbf{p} = (p_x, p_y, p_z)$ is the momentum operator, $m(\mathbf{p}) = m_0 + m_1 p_z^2 + m_2 (p_x^2 + p_y^2)$ is the mass term and $p_{\pm} = p_x \pm ip_y$. The effective Hamiltonian equation (1) is written in the basis of the four states closest to the Fermi energy at the Γ point, $\{|P1_z^+ \uparrow\rangle, |P2_z^- \uparrow\rangle, |P1_z^+ \downarrow\rangle, |P2_z^- \downarrow\rangle\}$, where the label $P1(2)_z$ indicates that they stem from atomic p_z orbitals of the two different atoms in the material and the superscript \pm refers to their parity [39, 40]. When the sign of m_0/m_2 is negative, the material is in the topological insulating phase, causing isolated boundaries to host surface states represented by gapless Dirac cones. The coefficients m_0 , m_1 and m_2 , as well as the coefficients A and B of the linear-momentum terms depend on the material [41]. The values of the parameters for the most common TIs are reported in table 1. As the system has cylindrical symmetry, it is convenient to express H_0 in cylindrical coordinates. Following Imura *et al* [42], we write the Hamiltonian as a sum of two terms

$$H_0 = H_{\perp} + H_{\parallel}, \quad (2)$$

where

$$H_{\perp} = \begin{pmatrix} m_{\perp} & 0 & 0 & -iAe^{-i\varphi}\partial_{\rho} \\ 0 & -m_{\perp} & -iAe^{-i\varphi}\partial_{\rho} & 0 \\ 0 & -iAe^{i\varphi}\partial_{\rho} & m_{\perp} & 0 \\ -iAe^{i\varphi}\partial_{\rho} & 0 & 0 & -m_{\perp} \end{pmatrix} \quad (3a)$$

$$H_{\parallel} = \begin{pmatrix} m_{\parallel} & Bp_z & 0 & -\frac{A}{\rho}e^{-i\varphi}\partial_{\varphi} \\ Bp_z & -m_{\parallel} & -\frac{A}{\rho}e^{-i\varphi}\partial_{\varphi} & 0 \\ 0 & \frac{A}{\rho}e^{i\varphi}\partial_{\varphi} & m_{\parallel} & -Bp_z \\ \frac{A}{\rho}e^{i\varphi}\partial_{\varphi} & 0 & -Bp_z & -m_{\parallel} \end{pmatrix} \quad (3b)$$

and with the mass terms given by the expressions

$$m_{\perp} = m_0 + m_2 \left(-\partial_{\rho}^2 - \frac{1}{\rho}\partial_{\rho} \right) \quad (4)$$

$$m_{\parallel} = -m_2 \frac{1}{\rho^2} \partial_{\varphi}^2 + m_1 p_z^2. \quad (5)$$

The Hamiltonian H_0 commutes both with p_z and with the z -component of the total angular momentum ($L_z + \frac{\hbar}{2}\sigma_z$) $\otimes \tau_0$, where τ_0 is the identity matrix in the orbital pseudo-spin subspace. In the following, to avoid cluttering the notation, we set $\hbar = 1$. The commutation relations of H_0 discussed above suggest the following *Ansatz* for the wave function:

$$\Psi(\rho, \varphi, z) = \frac{e^{ik_z z}}{\sqrt{2\pi}} \begin{pmatrix} \Phi_1(\rho)e^{i(j-\frac{1}{2})\varphi} \\ \Phi_2(\rho)e^{i(j-\frac{1}{2})\varphi} \\ \Phi_3(\rho)e^{i(j+\frac{1}{2})\varphi} \\ \Phi_4(\rho)e^{i(j+\frac{1}{2})\varphi} \end{pmatrix}, \quad (6)$$

where k_z is the eigenvalue of p_z and j (half integer) the eigenvalue of the z component of the total angular momentum. Solving the eigensystem requires applying the Hamiltonian equation (1) to the wavefunction in equation (6). The calculation is detailed in appendix A. In order to solve the radial part of the eigensystem, we make further *Ansätze* for the $\Phi_i(\rho)$ and rewrite equation (6) as

$$\Psi(\rho, \varphi, z) = \frac{e^{ik_z z}}{\sqrt{2\pi}} \begin{pmatrix} c_1 J_{j-\frac{1}{2}}(\kappa\rho)e^{i(j-\frac{1}{2})\varphi} \\ c_2 J_{j-\frac{1}{2}}(\kappa\rho)e^{i(j-\frac{1}{2})\varphi} \\ c_3 J_{j+\frac{1}{2}}(\kappa\rho)e^{i(j+\frac{1}{2})\varphi} \\ c_4 J_{j+\frac{1}{2}}(\kappa\rho)e^{i(j+\frac{1}{2})\varphi} \end{pmatrix}, \quad (7)$$

where $J_n(z)$ is a Bessel function of the first kind and κ and the coefficients c_1, \dots, c_4 need to be determined. In order for the *Ansatz* of equation (7) to be an eigenfunction of H_0 with energy E , the parameter κ needs to take one of the following two values

$$\kappa_{\pm} = \left[-\left(\frac{m_0}{m_2} + \frac{A^2}{2m_2^2} + \frac{m_1 k_z^2}{m_2} \right) \pm \sqrt{\frac{A^4}{4m_2^4} + \frac{E^2}{m_2^2} + \frac{A^2 m_0}{m_2^3} + \left(\frac{A^2 m_1}{m_2^2 m_2} - \frac{B^2}{m_2^2} \right) k_z^2} \right]^{1/2}. \quad (8)$$

For the coefficients $(c_1, c_2, c_3, c_4)^T$ there are four independent solutions (two for κ_+ and two for κ_-) given by

$$\left(\frac{iA\kappa_{\pm}}{\Delta_{\pm}}, 0, \frac{Bk_z}{\Delta_{\pm}}, 1 \right)^T, \quad \left(-\frac{Bk_z}{\Delta_{\pm}}, 1, -\frac{iA\kappa_{\pm}}{\Delta_{\pm}}, 0 \right)^T, \quad (9)$$

where $\Delta_{\pm} = m_2 \kappa_{\pm}^2 + m_1 k_z^2 + m_0 - E$. The general solution for the wavefunction with quantum numbers k_z, j and E is a linear combination of the four independent solutions obtained above:

$$\Psi(\rho, \varphi, z) = \frac{e^{ik_z z}}{\sqrt{2\pi}} \sum_{\eta=\pm} \left\{ \alpha_\eta \begin{pmatrix} \frac{iA\kappa_\eta}{\Delta_\eta} J_{j-\frac{1}{2}}(\kappa_\eta\rho) e^{i(j-\frac{1}{2})\varphi} \\ 0 \\ \frac{Bk_z}{\Delta_\eta} J_{j+\frac{1}{2}}(\kappa_\eta\rho) e^{i(j+\frac{1}{2})\varphi} \\ J_{j+\frac{1}{2}}(\kappa_\eta\rho) e^{i(j+\frac{1}{2})\varphi} \end{pmatrix} + \beta_\eta \begin{pmatrix} -\frac{Bk_z}{\Delta_\eta} J_{j-\frac{1}{2}}(\kappa_\eta\rho) e^{i(j-\frac{1}{2})\varphi} \\ J_{j-\frac{1}{2}}(\kappa_\eta\rho) e^{i(j-\frac{1}{2})\varphi} \\ -\frac{iA\kappa_\eta}{\Delta_\eta} J_{j+\frac{1}{2}}(\kappa_\eta\rho) e^{i(j+\frac{1}{2})\varphi} \\ 0 \end{pmatrix} \right\}. \quad (10)$$

We can now solve the confinement problem by assuming a hard-wall cylindrical confinement potential of radius R . We need to impose the boundary condition $\Psi(R, \varphi, z) = 0$. This leads to a system of equations for the coefficients α_η and β_η which has non-trivial solutions for energies obeying the secular equation

$$\frac{T_j(\kappa_+R)}{T_j(\kappa_-R)} + \frac{T_j(\kappa_-R)}{T_j(\kappa_+R)} = \frac{\kappa_+ \Delta_-}{\kappa_- \Delta_+} + \frac{\kappa_- \Delta_+}{\kappa_+ \Delta_-} + \frac{B^2}{A^2} k_z^2 \frac{(\Delta_+ - \Delta_-)^2}{\kappa_+ \kappa_- \Delta_+ \Delta_-}, \quad (11)$$

where we have defined the function $T_j(z) = \frac{J_{j+1/2}(z)}{J_{j-1/2}(z)}$. A detailed derivation of the secular equation is provided in appendix A. In the case $k_z = 0$, the problem decouples in two 2×2 problems and we have two independent secular equations

$$\frac{\kappa_+ \Delta_-}{\kappa_- \Delta_+} = \frac{T_j(\kappa_+R)}{T_j(\kappa_-R)}, \quad (12a)$$

$$\frac{\kappa_+ \Delta_-}{\kappa_- \Delta_+} = \frac{T_j(\kappa_-R)}{T_j(\kappa_+R)}, \quad (12b)$$

which are analogous to equation (28) of reference [36]. The $k_z = 0$ energy eigenstates associated with solutions of equation (12a) have $\beta_\eta = 0$ and therefore their only nonvanishing spinor components are the first and the fourth. Conversely, the eigenstates corresponding to solutions of equation (12b) have $\alpha_\eta = 0$ and therefore their only nonvanishing spinor components are the second and the third. Taking into account the transformation properties of the basis states under spatial inversion, it is straightforward to show that eigenstates associated with energy eigenvalues arising from the secular equation (12a) [(12b)] are also parity eigenstates with eigenvalue $(-1)^{j-\frac{1}{2}}$ [$(-1)^{j+\frac{1}{2}}$]. Even for finite k_z , the spinors multiplied by α_η [β_η] in the Ansatz (10) remain parity eigenstates with eigenvalue $(-1)^{j-\frac{1}{2}}$ [$(-1)^{j+\frac{1}{2}}$]. However, as the energy eigenstates for nonzero k_z are superpositions of these opposite-parity spinors, they are not eigenstates of parity.

Once we fix the quantum number j and k_z and solve the secular equation (11) we obtain a series of solutions both with positive and negative energies. Of these, we will only consider the two, one positive and one negative, with the smallest absolute value of the energy. We will indicate the positive(negative)-energy solution with $s = +(-)$.⁶ Furthermore, we will restrict our analysis to energies that lie within the bulk gap. The quantum numbers that we will use to label the states are $s = \pm, j, k_z$. The secular problem yields the full knowledge of the eigenfunctions. In order to simplify the notation, in the following we rewrite the eigenfunction equation (10) as

$$\Psi_{s,j,k_z}(\rho, \varphi, z) = \frac{e^{ik_z z}}{2\pi} \begin{pmatrix} \Phi_{1,s,j,k_z}(\rho) e^{i(j-\frac{1}{2})\varphi} \\ \Phi_{2,s,j,k_z}(\rho) e^{i(j-\frac{1}{2})\varphi} \\ \Phi_{3,s,j,k_z}(\rho) e^{i(j+\frac{1}{2})\varphi} \\ \Phi_{4,s,j,k_z}(\rho) e^{i(j+\frac{1}{2})\varphi} \end{pmatrix}, \quad (13)$$

where the wavefunction obeys the normalisation condition $\sum_{i=1}^4 \int_0^R d\rho \rho |\Phi_{i,s,j,k_z}(\rho)|^2 = 1$.

3. Results

In order to understand the effect of a finite radius of the cylinder and how it affects the topologically protected surface states, we start from the large-radius limit.

⁶ In principle, we could introduce another integer quantum number to label the different solutions as in the case of a particle in a box.

3.1. Large-radius expansion

A natural length scale in this context is the effective Compton length $R_0 = \left| \frac{A}{m_0} \right|$. In the following we perform an expansion in R_0/R and find corrections to the asymptotic (large R) results obtained by Imura *et al* [42]. To this aim, we make use of Hankel's asymptotic expansion for the Bessel function [43]

$$J_n(z) \approx \sqrt{\frac{2}{\pi z}} \left[P(n, z) \cos \left(z - \frac{1}{2}n\pi - \frac{1}{4}\pi \right) - Q(n, z) \sin \left(z - \frac{1}{2}n\pi - \frac{1}{4}\pi \right) \right]. \quad (14)$$

The functions $P(n, z)$ and $Q(n, z)$ are power series of $1/z$.

3.1.1. Zero axial momentum

We start by considering the case of zero axial momentum ($k_z = 0$), with the goal to understand the j -dependence of the surface states. We will consider only one of the two secular equations, namely equation (12a) which can be recast as

$$\kappa_+ \Delta_- J_{j-\frac{1}{2}}(\kappa_+ R) J_{j+\frac{1}{2}}(\kappa_- R) - \kappa_- \Delta_+ J_{j+\frac{1}{2}}(\kappa_+ R) J_{j-\frac{1}{2}}(\kappa_- R) = 0. \quad (15)$$

For realistic materials, see table 1, and small values of energies $E \ll |m_0|$, $\kappa_{\pm} = k \pm iq$ with $q > 0$. In the large-radius limit $qR \gg 1$, we keep only the terms proportional to $\exp(qR)$ in equation (14). The secular equation reduces to

$$\begin{aligned} & \kappa_+ \Delta_- \left[P \left(j - \frac{1}{2}, \kappa_+ R \right) - iQ \left(j - \frac{1}{2}, \kappa_+ R \right) \right] \left[P \left(j + \frac{1}{2}, \kappa_- R \right) + iQ \left(j + \frac{1}{2}, \kappa_- R \right) \right] = \\ & - \kappa_- \Delta_+ \left[P \left(j - \frac{1}{2}, \kappa_- R \right) + iQ \left(j - \frac{1}{2}, \kappa_- R \right) \right] \left[P \left(j + \frac{1}{2}, \kappa_+ R \right) - iQ \left(j + \frac{1}{2}, \kappa_+ R \right) \right]. \end{aligned} \quad (16)$$

Taking the zeroth order of the Hankel's expansion (i.e. $P(n, z) = 1$ and $Q(n, z) = 0$), the secular equation becomes

$$\kappa_+ \Delta_- + \kappa_- \Delta_+ = 0. \quad (17)$$

This equation has a zero-energy solution if $m_0/m_2 < 0$, i.e. when the system is in the topological phase.

Next, we consider the next two terms in the Hankel's expansion, that is $P(n, z) = 1 - (4n^2 - 1)(4n^2 - 9)/(128z^2)$ and $Q(n, z) = (4n^2 - 1)/(8z)$, and insert them into equation (16). After some tedious but otherwise standard algebra, we obtain the eigenenergies up to second-order in R_0/R

$$E = A \frac{j}{R} - \frac{A^2}{2m_0} \frac{j}{R^2}. \quad (18)$$

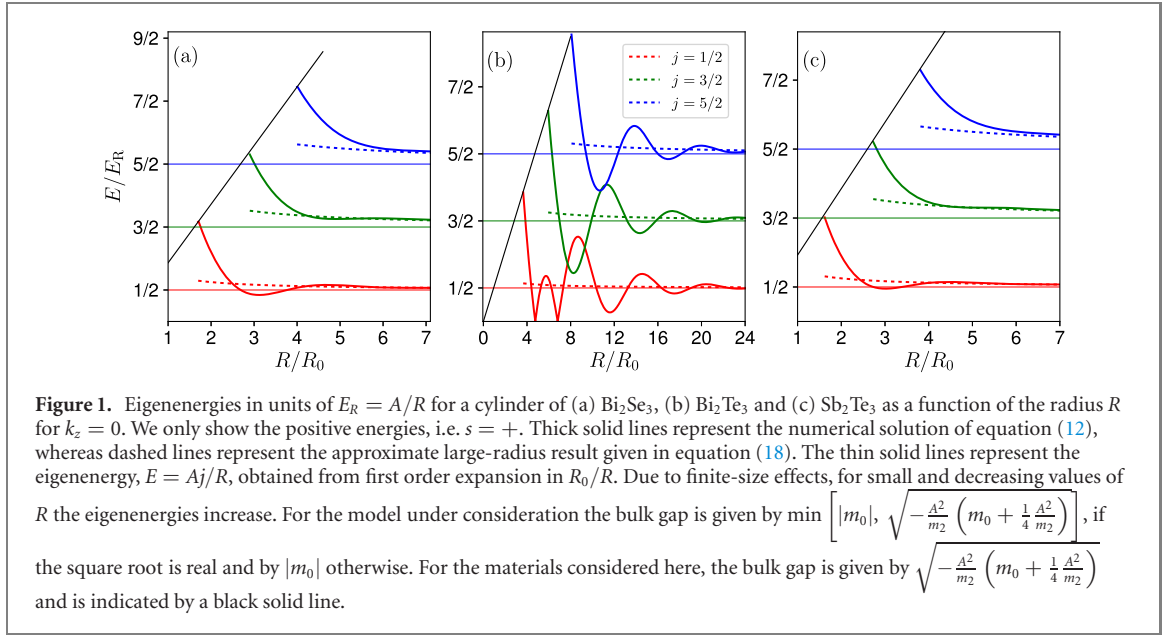
The first term is in agreement with reference [42], the second term gives the first correction to the asymptotic result. The other solution, with the opposite sign, $E = -Aj/R + \frac{A^2}{2m_0} \frac{j}{R^2}$ arises from solving equation (12b). The values of κ_{\pm} corresponding to the energies in equation (18) can be found by inserting equation (18) in equation (8) and setting $k_z = 0$.

3.1.2. Finite axial momentum

In this section we assume that $k_z R \gg 1$. Proceeding in the same way as for case $k_z = 0$, in zeroth-order in R_0/R the secular equation for the case of non-zero axial momentum reduces to

$$(\kappa_+ \Delta_- + \kappa_- \Delta_+)^2 + \frac{B^2}{A^2} k_z^2 (\Delta_+ - \Delta_-)^2 = 0. \quad (19)$$

This equation has the solutions



$$E = \pm Bk_z, \quad (20)$$

which represents the linear dispersion of the surface modes.

Considering the Hankel's expansion up to terms in $1/z^2$, that is $P(n, z) = 1 - (4n^2 - 1)(4n^2 - 9)/(128z^2)$ and $Q(n, z) = (4n^2 - 1)/(8z)$, we obtain the eigenenergies up to second order in R_0/R

$$E = \pm \left(Bk_z + \frac{1}{2} \frac{A^2 j^2}{Bk_z R^2} \right), \quad (21)$$

which corresponds to the Taylor expansion in second order in $1/(k_z R)$ of the result by Imura *et al* [42], $E = \pm \sqrt{B^2 k_z^2 + A^2 j^2 / R^2}$. Notice that we are not allowed to take the $k_z \rightarrow 0$ limit, as this result has been derived assuming $k_z \gg 1/R$. The values of κ_{\pm} corresponding to the energies in equation (21) can be found by inserting equation (21) in equation (8).

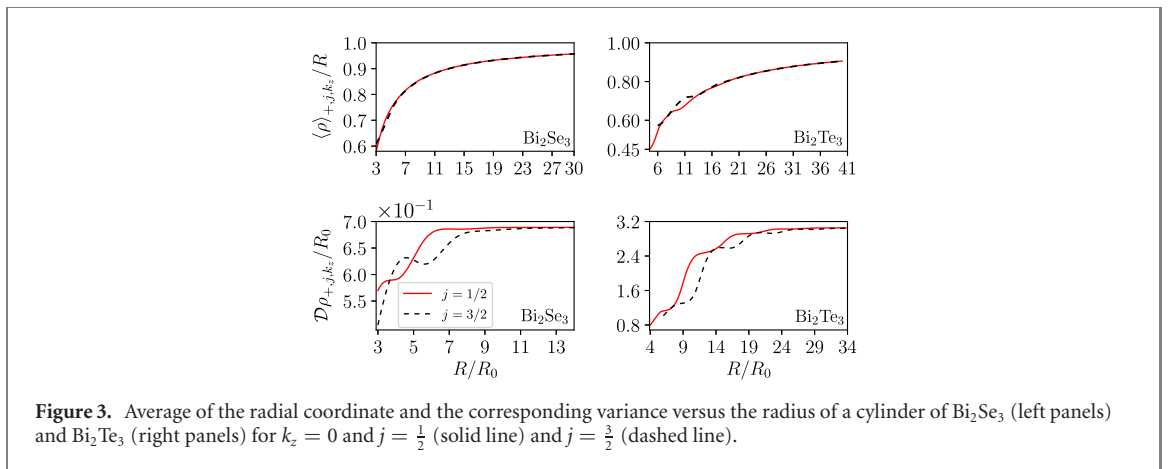
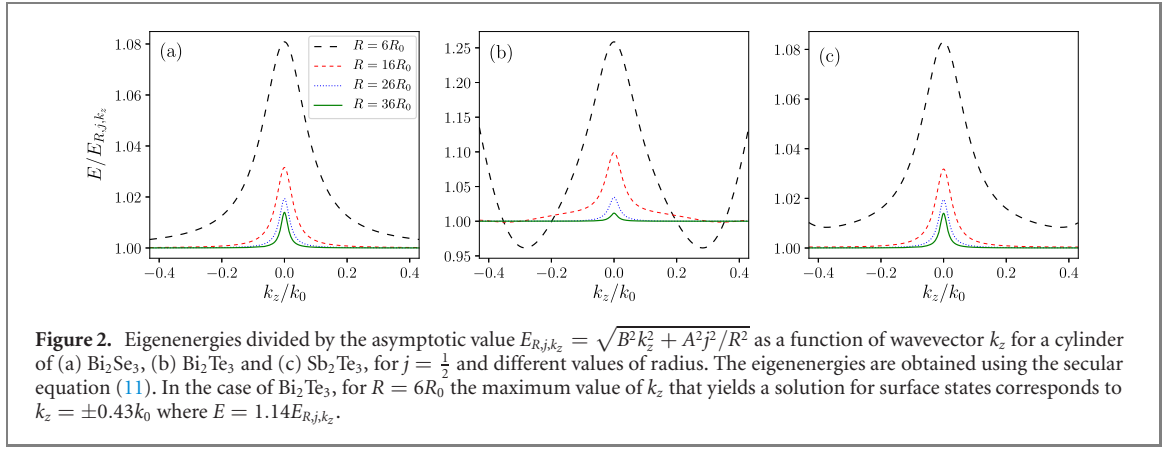
3.2. Numerical results

In this section we present numerical results for three different materials, namely Bi_2Se_3 , Bi_2Te_3 , and Sb_2Te_3 , using the parameters of table 1. We use the following units for length and momentum, respectively,

$$R_0 = \left| \frac{A}{m_0} \right| \quad \text{and} \quad k_0 = \left| \frac{m_0}{B} \right|,$$

where $R_0 = 1.49$ nm for Bi_2Se_3 , 1.35 nm for Bi_2Te_3 , and 2.03 nm for Sb_2Te_3 .

Figure 1 shows how the eigenenergies in units of $E_R = A/R$ depend on the radius of the cylinder for the three materials and for three different values of j . Here we show only the positive energies, that is $s = +$. Solid curves refer to the exact result obtained by solving equation (12), while the dashed curves refer to the large-radius analytic expression equation (18). We observe that the latter solutions approximate well the numerical results when $R \gtrsim 6R_0$ for Bi_2Se_3 and Sb_2Te_3 , and when $R \gtrsim 20R_0$ for Bi_2Te_3 , respectively. For Bi_2Se_3 and Sb_2Te_3 it is worthwhile noticing that at $R = 6R_0$, especially for $j = 3/2$ and $5/2$, the normalized eigenenergies have not yet reached the asymptotic ($R \gg R_0$) value (represented by the thin solid lines, see equation (18)). On the other hand, when the radius of the cylinder is small, figure 1 shows an oscillatory behaviour, especially in the case of Bi_2Te_3 , that is more pronounced for smaller values of j , similarly to a spherical nanoparticle [36]. For Bi_2Te_3 , the effect of these oscillations are so large that, for some values of the radius, the surface-state energy goes to zero. For these values of the radius the two states $s = \pm$ become degenerate, the degeneracy is preserved by the fact that they have opposite parity. This oscillatory behaviour is a consequence of the fact that the wavefunction is no longer localized on



the surface of the cylinder. We conclude that Bi_2Te_3 is the ideal candidate material to observe finite size effects in TI nanowires. The oscillations are consistent with the results of reference [29] (see also appendix B). The similarity between the results presented here and the corresponding results for a spherical nanoparticle is not surprising, as for $k_z = 0$ the system is equivalent to a disk, i.e., the twodimensional sphere, and the basic structure of the secular equation mirrors that for a sphere in three dimensions. In particular, energy eigenstates are also parity eigenstates as for the spherical nanoparticle. This ceases to be the case for $k_z \neq 0$.

In figure 2 we show the positive eigenenergies, divided by the asymptotic value $E_{R,j,k_z} = \sqrt{B^2 k_z^2 + A^2 j^2 / R^2}$, as a function of wavevector k_z . Finite-size effects appear in this plot as deviations from unity of the normalized eigenenergies and are more pronounced from small values of k_z .

Since we have the full knowledge of the eigenfunctions, we can calculate the expectation values of any single-particle operator. The average of the radial coordinate in the state Ψ_{s,j,k_z} is simply given by

$$\langle \rho \rangle_{s,j,k_z} = \sum_{i=1}^4 \int_0^R d\rho \rho^2 |\Phi_{i,s,j,k_z}(\rho)|^2, \quad (22)$$

and its variance by

$$\mathcal{D}\rho_{s,j,k_z} = \sqrt{\langle \rho^2 \rangle_{s,j,k_z} - \langle \rho \rangle_{s,j,k_z}^2}. \quad (23)$$

Figure 3 (top panels) shows that the average of the radial coordinate, $\langle \rho \rangle_{s,j,k_z}$, approaches R for large values of the radius as expected for topologically-protected surface states. The average of the radial position for both materials increases monotonically with the radius of the cylinder, showing weak oscillations only for the case of Bi_2Te_3 . As shown in figure 3 (bottom panels), the variance in itself approaches, in an

oscillatory fashion, a constant value of the order of R_0 for large values of radius (the variance varies very little for $R \gtrsim 8R_0$ for Bi_2Se_3 and $R \gtrsim 24R_0$ for Bi_2Te_3). Since the value of R_0 is similar for the two materials ($R_0 = 1.5$ nm for Bi_2Se_3 and $R_0 = 1.35$ nm for Bi_2Te_3), we can conclude that in Bi_2Se_3 the asymptotic form of the surface states is reached for smaller values of the radius compared to Bi_2Te_3 .

3.3. Optical transitions in cylindrical topological insulators

In typical semiconductor nanostructures, optical transitions between size-quantized levels can be neatly categorized as being either intra-band or inter-band transitions [44]. In the narrow-gap materials of interest for our present work, however, these two types of transitions are not well-separated in energy and need to be treated on the same footing. A versatile formalism for calculating all optical-transition matrix elements in such systems using the envelope part of the confined-charge-carrier wave functions was developed in reference [36]. Here we recall the basic features of this approach before applying it to the case of cylindrical TI nanowires.

Optical transitions are mediated by matrix elements of the electric-dipole operator \mathbf{d} , which can be written as the sum of intra- and inter-band contributions [36, 44]

$$\mathbf{d} = \mathbf{d}^{(\text{intra})} + \mathbf{d}^{(\text{inter})} \quad . \quad (24)$$

The intra-band part $\mathbf{d}^{(\text{intra})} \equiv e\mathbf{r} \mathbb{1}$ pertains to transitions between size-quantized states within the same band, i.e., envelope wave functions multiplying the same basis state in $\mathbf{k} \cdot \mathbf{p}$ space. In contrast, the inter-band part $\mathbf{d}^{(\text{inter})}$ accounts for optical transitions between different bands, i.e., different $\mathbf{k} \cdot \mathbf{p}$ basis states, whose magnitude is renormalized by the overlap of associated envelope wave-function components. Calculation of $\mathbf{d}^{(\text{inter})}$ within the envelope-function formalism is aided by a fundamental relationship of the electric-dipole matrix elements between $\mathbf{k} \cdot \mathbf{p}$ basis states with coefficients of the linear-in- \mathbf{k} terms appearing in the multi-band envelope-function Hamiltonian H_0 . More specifically, writing H_0 from equation (1) as

$$H_0 = [m_0 + m_1 k_z^2 + m_2 (k_x^2 + k_y^2)] \tau_z \otimes \sigma_0 + B k_z \tau_x \otimes \sigma_z + A k_x \tau_x \otimes \sigma_x + A k_y \tau_x \otimes \sigma_y, \quad (25)$$

where σ_i and τ_i are Pauli matrices in spin and orbital-pseudo-spin space, respectively, we have [44]

$$\langle \tau' \sigma' | e\mathbf{r} | \tau \sigma \rangle = \tau \frac{ie}{2m_0} \langle \tau' \sigma' | (\partial H_0 / \partial \mathbf{k})_{\mathbf{k}=0} | \tau \sigma \rangle \quad . \quad (26)$$

Here $|\tau \sigma\rangle$ represents the basis functions in the orbital and spin space of the Hamiltonian H_0 defined in equation (1), and τ is the eigenvalue of τ_z associated with the eigenstate $|\tau \sigma\rangle$. Taking the derivative $\partial H_0 / \partial \mathbf{k}$ of H_0 in equation (25) and setting $\mathbf{k} = 0$, we find

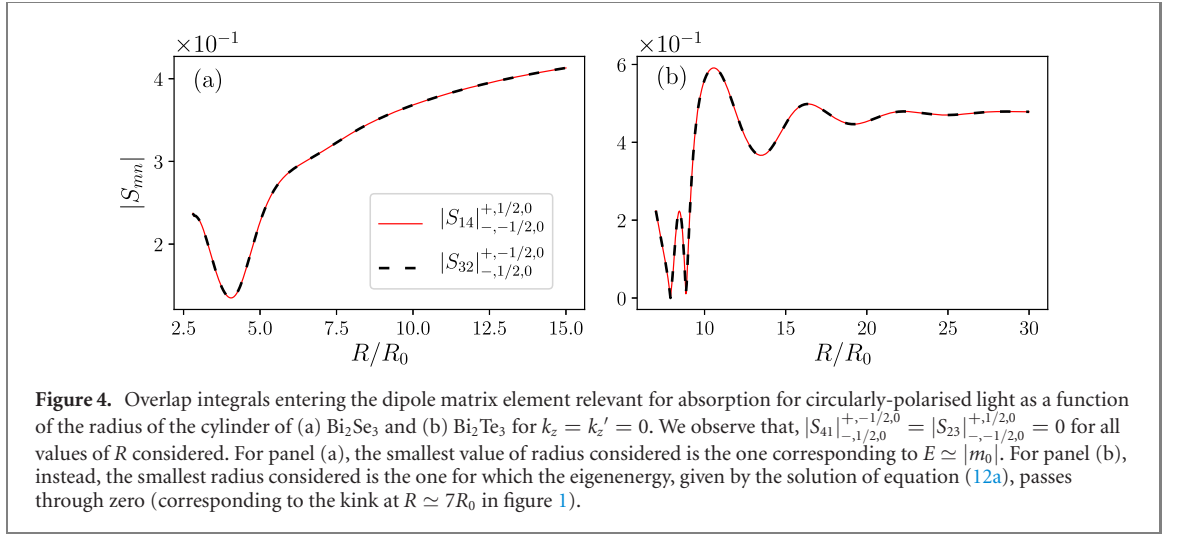
$$\mathbf{d}^{(\text{inter})} = \frac{eB}{2m_0} \tau_y \otimes \sigma_z \hat{z} + \frac{eA}{2m_0} \tau_y \otimes \sigma_y \hat{y} + \frac{eA}{2m_0} \tau_y \otimes \sigma_x \hat{x} \quad . \quad (27)$$

Using the general formalism discussed in the previous paragraph, the optical-dipole matrix elements between confined TI-nanowire states is obtained as

$$\mathbf{d}_{s_j, k_z}^{s'_j, k'_z} = \int dz \int_0^R \rho d\rho \int_0^{2\pi} d\varphi \Psi_{s'_j, k'_z}^\dagger(\rho, \varphi, z) \mathbf{d}(\rho, \varphi, z) \Psi_{s_j, k_z}(\rho, \varphi, z) \quad . \quad (28)$$

Here $\mathbf{d}(\rho, \varphi, z) \equiv e(\rho \cos \varphi \hat{x} + \rho \sin \varphi \hat{y} + z \hat{z}) \mathbb{1} + \mathbf{d}^{(\text{inter})}$, with $\mathbf{d}^{(\text{inter})}$ given in equation (27). Using equation (10) and performing the integrals over φ and z , we obtain

$$(d_x + id_y)_{s_j, k_z}^{s'_j, k'_z} = \delta_{k_z, k'_z} \delta_{j', j+1} \left[e \sum_{i=1}^4 (\mathcal{R}_{ii})_{s_j, k_z}^{s'_j, j+1, k_z} - \frac{ieA}{m_0} \left((\mathcal{S}_{14})_{s_j, k_z}^{s'_j, j+1, k_z} - (\mathcal{S}_{23})_{s_j, k_z}^{s'_j, j+1, k_z} \right) \right], \quad (29)$$



and

$$(d_x - id_y)_{s,j,k_z}^{s',j',k'_z} = \delta_{k_z,k'_z} \delta_{j',j-1} \left[e \sum_{i=1}^4 (\mathcal{R}_{ii})_{s,j,k_z}^{s',j-1,k_z} - \frac{ieA}{m_0} \left((\mathcal{S}_{32})_{s,j,k_z}^{s',j-1,k_z} - (\mathcal{S}_{41})_{s,j,k_z}^{s',j-1,k_z} \right) \right], \quad (30)$$

where we have defined the overlap integrals

$$(\mathcal{S}_{mn})_{s,j,k_z}^{s',j',k'_z} = \int_0^R d\rho \rho \Phi_{m,s',j',k'_z}^*(\rho) \Phi_{n,s,j,k_z}(\rho) \quad (31)$$

and the matrix elements of radial position

$$(\mathcal{R}_{mn})_{s,j,k_z}^{s',j',k'_z} = \int_0^R d\rho \rho^2 \Phi_{m,s',j',k'_z}^*(\rho) \Phi_{n,s,j,k_z}(\rho). \quad (32)$$

For circular polarization in the plane perpendicular to the nanowire axis, we find the conventional selection rule $j' = j \pm 1$, which is mandated by the conservation of total-angular-momentum projection (including the photon's) parallel to the nanowire axis. In addition, linear momentum k_z parallel to the nanowire axis is conserved in any optical transition. The energy threshold for absorption is associated with transitions between $(s' = +, j = \pm 1/2, k'_z = 0)$ and $(s = -, j \mp 1/2, k_z = 0)$. At the subband edge ($k_z = 0$ and $k'_z = 0$) for $d_x + id_y$ only the overlap integral $(\mathcal{S}_{14})_{-,-1/2,0}^{+,1/2,0}$ is non-vanishing for absorption, while for emission the only non-vanishing overlap integral is $(\mathcal{S}_{23})_{+,-1/2,0}^{-,1/2,0}$. For the opposite polarization, namely $d_x - id_y$, the non-vanishing overlap integrals at the band edge are: $(\mathcal{S}_{32})_{-,-1/2,0}^{+,1/2,0}$ for absorption and $(\mathcal{S}_{41})_{+,-1/2,0}^{-,1/2,0}$ for emission, respectively. The overlap integrals relevant for the absorption threshold are shown in figure 4 as a function of the radius of the wire. It needs to be noticed that also the matrix elements of the radial position $(\mathcal{R}_{mn})_{s,j,k_z}^{s',j',k'_z}$ contribute both to absorption and emission. The sum of these matrix elements for the case of absorption is shown in figure 5 as a function of the radius of the wire. The finite radius of the nanowire does not affect the selection rules but leads to significant quantitative changes of the dipole matrix elements.

Matrix elements of the optical-dipole component parallel to the nanowire axis are given by

$$(d_z)_{s,j,k_z}^{s',j',k'_z} = \left\{ e \sum_{i=1}^4 (\mathcal{S}_{ii})_{s,j,k_z}^{s',j',k'_z} \int dz z \frac{e^{i(k_z - k'_z)z}}{2\pi} + \delta_{k_z,k'_z} \frac{ieB}{2m_0} \right. \\ \left. \times \left[(\mathcal{S}_{21})_{s,j,k_z}^{s',j',k'_z} - (\mathcal{S}_{12})_{s,j,k_z}^{s',j',k'_z} + (\mathcal{S}_{34})_{s,j,k_z}^{s',j',k'_z} - (\mathcal{S}_{43})_{s,j,k_z}^{s',j',k'_z} \right] \right\} \delta_{j',j}. \quad (33)$$

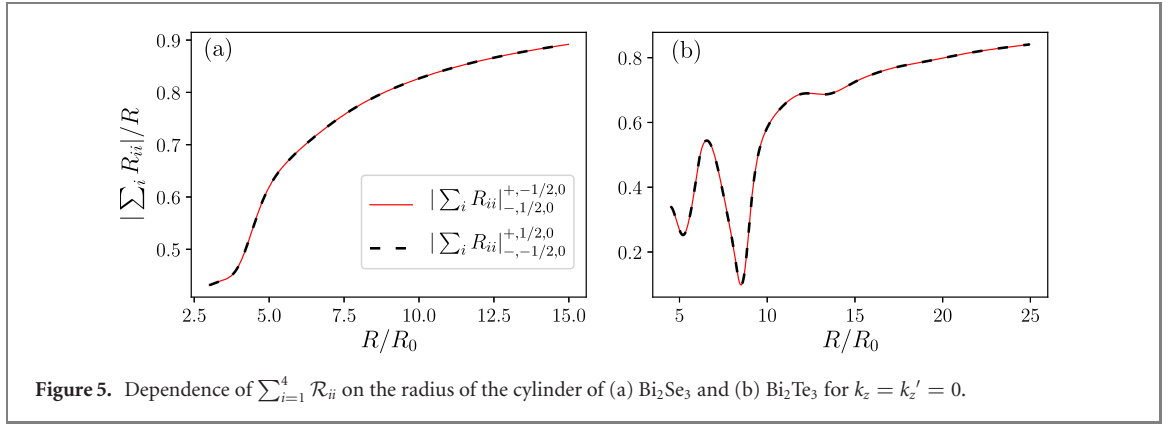


Figure 5. Dependence of $\sum_{i=1}^4 \mathcal{R}_{ii}$ on the radius of the cylinder of (a) Bi_2Se_3 and (b) Bi_2Te_3 for $k_z = k_z' = 0$.

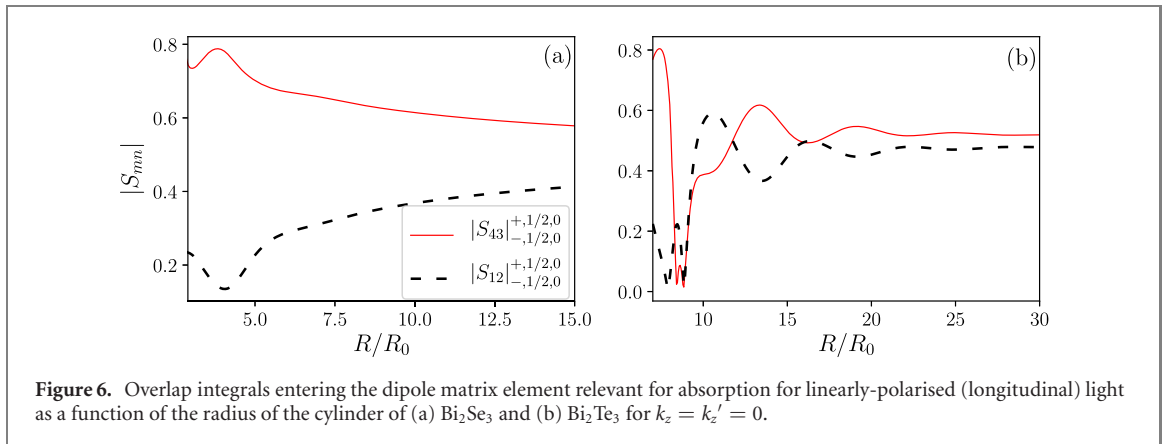


Figure 6. Overlap integrals entering the dipole matrix element relevant for absorption for linearly-polarised (longitudinal) light as a function of the radius of the cylinder of (a) Bi_2Se_3 and (b) Bi_2Te_3 for $k_z = k_z' = 0$.

The first term on the r.h.s. of equation (33) is ill-defined because the envelope functions are not localized in their dependence on the z coordinate and, hence, the dipole approximation is not valid. However, the remaining basis-function-mediated contributions describe valid optical transitions. For these, both linear momentum k_z and the total-angular-momentum projection j parallel to the nanowire axis are the same for initial and final states involved in optical transitions. For states at the energy threshold of absorption, we find that the only non vanishing overlap integrals are $(\mathcal{S}_{12})_{-, \pm 1/2, 0}^{+, \pm 1/2, 0}$ and $(\mathcal{S}_{43})_{-, \pm 1/2, 0}^{+, \pm 1/2, 0}$, while for emission the non vanishing overlap integrals are $(\mathcal{S}_{21})_{+, \pm 1/2, 0}^{-, \pm 1/2, 0}$ and $(\mathcal{S}_{34})_{+, \pm 1/2, 0}^{-, \pm 1/2, 0}$. The overlap integrals relevant for absorption are shown in figure 6. Again, the selection rules for optical transitions are consistent with the basic symmetries associated with a cylindrical-nanowire geometry, and finite-size effects are manifested as significant quantitative changes in the magnitude of dipole matrix elements.

4. Conclusions

In this paper we have studied a nanowire made of TI. In particular, we have provided the analytical form of the energy eigenfunctions, which is central to the derivation of an analytical secular equation for the eigenenergies. This secular equation, on one hand, enables an analytical expansion for large radii and, on the other hand, is amenable to straightforward numerical solution. We study the dependence of the eigenenergies on the radius of the wire and we find oscillations as a function of the radius, which are very pronounced for Bi_2Te_3 . The analytical form of the energy eigenfunctions enables the computation of the matrix elements of any single-particle operator. We have considered the optical dipole matrix elements. While we find the usual selection rules for absorption/emission, the value of the matrix elements is strongly dependent on the radius of the cylinder.

Our work can inform further detailed exploration of physical properties exhibited by TI nanowires. For example, the implications of cylindrical symmetry on the topological magnetoelectric effect have previously

been studied within the framework of macroscopic continuum-electromagnetic theory [45]. To gain insight about the materials-size dependence of unconventional electromagnetic responses, the formalism of reference [45] could be generalized to treat the magnetoelectric effect in TI nanowires by adopting appropriate boundary conditions that reflect the surface-electromagnetic response [46]. Calculation of the relevant parameters entering amended boundary conditions for the electromagnetic fields could be facilitated by the explicit form of surface- and bound-state wave functions provided in our present work. Recent studies [47, 48] have revealed interesting topological-electromagnetic responses of spherical nanoparticles, and we expect a future investigation of the TI-nanowire electromagnetic response to be equally fruitful.

Appendix A. Secular equation for confined states

In this appendix we provide the detailed derivation of the secular equation for the state of the TI cylinder. Acting with the Hamiltonian (2) on the wave function equation (6) and looking for eigenfunctions with energy E , we obtain

$$\begin{pmatrix} m_{\perp} + m_{-}(j, k_z) - E & Bk_z & 0 & -iA \left[\partial_{\rho} + \frac{1}{\rho} \left(j + \frac{1}{2} \right) \right] \\ Bk_z & -[m_{\perp} + m_{-}(j, k_z) + E] & -iA \left[\partial_{\rho} + \frac{1}{\rho} \left(j + \frac{1}{2} \right) \right] & 0 \\ 0 & -iA \left[\partial_{\rho} - \frac{1}{\rho} \left(j - \frac{1}{2} \right) \right] & m_{\perp} + m_{+}(j, k_z) - E & -Bk_z \\ -iA \left[\partial_{\rho} - \frac{1}{\rho} \left(j - \frac{1}{2} \right) \right] & 0 & -Bk_z & -[m_{\perp} + m_{+}(j, k_z) + E] \end{pmatrix} \begin{pmatrix} \Phi_1(\rho) \\ \Phi_2(\rho) \\ \Phi_3(\rho) \\ \Phi_4(\rho) \end{pmatrix} = 0, \quad (\text{A.1})$$

where we have defined $m_{\pm}(j, k_z) = m_2 \frac{1}{\rho^2} (j \pm \frac{1}{2})^2 + m_1 k_z^2$. To solve the eigensystem equation (A.1) we make the *Ansatz*

$$\begin{pmatrix} \Phi_1(\rho) \\ \Phi_2(\rho) \\ \Phi_3(\rho) \\ \Phi_4(\rho) \end{pmatrix} = \begin{pmatrix} c_1 J_{j-\frac{1}{2}}(\kappa\rho) \\ c_2 J_{j-\frac{1}{2}}(\kappa\rho) \\ c_3 J_{j+\frac{1}{2}}(\kappa\rho) \\ c_4 J_{j+\frac{1}{2}}(\kappa\rho) \end{pmatrix}, \quad (\text{A.2})$$

where $J_n(z)$ is a Bessel function of the first kind and κ and the coefficients c_1, \dots, c_4 need to be determined. Substituting the *Ansatz* equation (A.2) in (A.1), we obtain the following equation for the coefficients

$$\begin{pmatrix} -\left(\kappa^2 + \frac{m_1 k_z^2 + m_0 - E}{m_2} \right) & -\frac{Bk_z}{m_2} & 0 & i\frac{A\kappa}{m_2} \\ \frac{Bk_z}{m_2} & -\left(\kappa^2 + \frac{m_1 k_z^2 + m_0 + E}{m_2} \right) & -i\frac{A\kappa}{m_2} & 0 \\ 0 & -i\frac{A\kappa}{m_2} & -\left(\kappa^2 + \frac{m_1 k_z^2 + m_0 - E}{m_2} \right) & \frac{Bk_z}{m_2} \\ i\frac{A\kappa}{m_2} & 0 & -\frac{Bk_z}{m_2} & -\left(\kappa^2 + \frac{m_1 k_z^2 + m_0 + E}{m_2} \right) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = 0. \quad (\text{A.3})$$

Equation (A.3) has non-trivial solutions for

$$\left(\kappa^2 + \frac{m_1 k_z^2 + m_0}{m_2} \right)^2 + \frac{A^2}{m_2^2} \kappa^2 + \frac{B^2}{m_2^2} k_z^2 - \frac{E^2}{m_2^2} = 0 \quad (\text{A.4})$$

which yields⁷

$$\kappa = \kappa_{\pm} = \sqrt{-\left(\frac{m_0}{m_2} + \frac{A^2}{2m_2^2} + \frac{m_1 k_z^2}{m_2} \right) \pm \sqrt{\frac{A^4}{4m_2^4} + \frac{E^2}{m_2^2} + \frac{A^2 m_0}{m_2^3} + \left(\frac{A^2 m_1}{m_2^2 m_2} - \frac{B^2}{m_2^2} \right) k_z^2}}. \quad (\text{A.5})$$

There are four independent solutions for $(c_1, c_2, c_3, c_4)^T$ and are given by

⁷ The negative sign for the outer square root does not give a different solution and therefore should not be considered due to the property of the Bessel's functions: $J_n(z) = (-1)^n J_n(-z)$ for integer n .

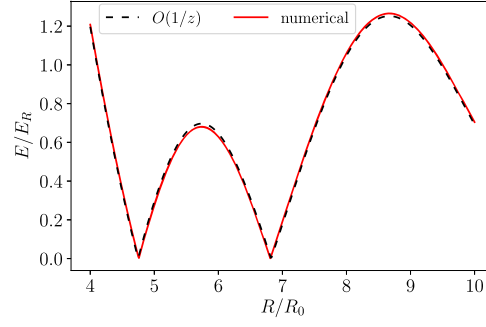


Figure B1. Eigenenergies with $j = \frac{1}{2}$ and $s = +$ for a cylinder of Bi_2Te_3 as a function of radius for $k_z = 0$. The solid red curve is the exact numerical solution of equation (11) while the dashed black curves is obtained by means of the Hankel's expansion at first order in $1/z$.

$$\left(\frac{iA\kappa_{\pm}}{\Delta_{\pm}}, 0, \frac{Bk_z}{\Delta_{\pm}}, 1 \right)^T, \quad (\text{A.6})$$

$$\left(-\frac{Bk_z}{\Delta_{\pm}}, 1, -\frac{iA\kappa_{\pm}}{\Delta_{\pm}}, 0 \right)^T, \quad (\text{A.7})$$

where we have introduced the following abbreviation $\Delta_{\pm} = m_2\kappa_{\pm}^2 + m_1k_z^2 + m_0 - E$. The general solution with quantum numbers k_z, j and E can therefore be written as

$$\Psi(\rho, \varphi, z) = \frac{e^{ik_z z}}{\sqrt{2\pi}} \sum_{\eta=\pm} \left\{ \alpha_{\eta} \begin{pmatrix} \frac{iA\kappa_{\eta}}{\Delta_{\eta}} J_{j-\frac{1}{2}}(\kappa_{\eta}\rho) e^{i(j-\frac{1}{2})\varphi} \\ 0 \\ \frac{Bk_z}{\Delta_{\eta}} J_{j+\frac{1}{2}}(\kappa_{\eta}\rho) e^{i(j+\frac{1}{2})\varphi} \\ J_{j+\frac{1}{2}}(\kappa_{\eta}\rho) e^{i(j+\frac{1}{2})\varphi} \end{pmatrix} + \beta_{\eta} \begin{pmatrix} -\frac{Bk_z}{\Delta_{\eta}} J_{j-\frac{1}{2}}(\kappa_{\eta}\rho) e^{i(j-\frac{1}{2})\varphi} \\ J_{j-\frac{1}{2}}(\kappa_{\eta}\rho) e^{i(j-\frac{1}{2})\varphi} \\ -\frac{iA\kappa_{\eta}}{\Delta_{\eta}} J_{j+\frac{1}{2}}(\kappa_{\eta}\rho) e^{i(j+\frac{1}{2})\varphi} \\ 0 \end{pmatrix} \right\}. \quad (\text{A.8})$$

Assuming a hard-wall cylindrical confinement potential of radius R , we need to impose the boundary condition $\Psi(R, \varphi, z) = 0$ which leads to the following system of equations:

$$\begin{pmatrix} \frac{iA\kappa_+}{\Delta_+} J_{j-\frac{1}{2}}(\kappa_+R) & -\frac{Bk_z}{\Delta_+} J_{j-\frac{1}{2}}(\kappa_+R) & \frac{iA\kappa_-}{\Delta_-} J_{j-\frac{1}{2}}(\kappa_-R) & -\frac{Bk_z}{\Delta_-} J_{j-\frac{1}{2}}(\kappa_-R) \\ 0 & J_{j-\frac{1}{2}}(\kappa_+R) & 0 & J_{j-\frac{1}{2}}(\kappa_-R) \\ \frac{Bk_z}{\Delta_+} J_{j+\frac{1}{2}}(\kappa_+R) & -\frac{iA\kappa_+}{\Delta_+} J_{j+\frac{1}{2}}(\kappa_+R) & \frac{Bk_z}{\Delta_-} J_{j+\frac{1}{2}}(\kappa_-R) & -\frac{iA\kappa_-}{\Delta_-} J_{j+\frac{1}{2}}(\kappa_-R) \\ J_{j+\frac{1}{2}}(\kappa_+R) & 0 & J_{j+\frac{1}{2}}(\kappa_-R) & 0 \end{pmatrix} \begin{pmatrix} \alpha_+ \\ \beta_+ \\ \alpha_- \\ \beta_- \end{pmatrix} = 0. \quad (\text{A.9})$$

We then obtain the secular equation

$$\begin{aligned} & \left[\kappa_+ \Delta_- J_{j-\frac{1}{2}}(\kappa_-R) J_{j+\frac{1}{2}}(\kappa_+R) - \kappa_- \Delta_+ J_{j-\frac{1}{2}}(\kappa_+R) J_{j+\frac{1}{2}}(\kappa_-R) \right] \\ & \times \left[\kappa_+ \Delta_- J_{j-\frac{1}{2}}(\kappa_+R) J_{j+\frac{1}{2}}(\kappa_-R) - \kappa_- \Delta_+ J_{j-\frac{1}{2}}(\kappa_-R) J_{j+\frac{1}{2}}(\kappa_+R) \right] \\ & + \frac{B^2}{A^2} k_z^2 (\Delta_+ - \Delta_-)^2 J_{j-\frac{1}{2}}(\kappa_-R) J_{j-\frac{1}{2}}(\kappa_+R) J_{j+\frac{1}{2}}(\kappa_-R) J_{j+\frac{1}{2}}(\kappa_+R) = 0. \end{aligned} \quad (\text{A.10})$$

Notice that the term in the third line of equation (A.10) vanishes for $k_z = 0$. By simple algebraic manipulations, equation (A.10) can be cast in the form of equation (11).

Appendix B. Small-radius limit

In section 3.2 we found interesting finite-size effects for small values of the radius R , such as the oscillatory behaviour of the eigenenergies. In order to understand the origin of the oscillations in figure 1, here we use

the Hankel's asymptotic expansion (equation (14)), but without approximating the trigonometric functions, and solve the secular equation at each given order. The plot of the eigenenergy as a function of R , obtained by taking into account only the first order in $1/z$ [$P(n, z) = 1$ and $Q(n, z) = (4n^2 - 1)/(8z)$], is shown in figure B1 as a dashed black curve: it is found to agree remarkably well with the full numerical results (solid red curve). The expansion up to second order in $1/z$ (not shown) [$P(n, z) = 1 - (4n^2 - 1)(4n^2 - 9)/(128z^2)$ and $Q(n, z) = (4n^2 - 1)/(8z)$] is practically indistinguishable from the full numerical results.

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