Continuum theory of edge states of topological insulators: variational principle and boundary conditions

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Abstract
We develop a continuum theory to model low energy excitations of a generic four-band time reversal invariant electronic system with boundaries. We propose a variational energy functional for the wavefunctions which allows us to derive natural boundary conditions valid for such systems. Our formulation is particularly suited for developing a continuum theory of the protected edge/surface excitations of topological insulators both in two and three dimensions. By a detailed comparison of our analytical formulation with tight binding calculations of ribbons of topological insulators modelled by the Bernevig–Hughes–Zhang (BHZ) Hamiltonian, we show that the continuum theory with a natural boundary condition provides an appropriate description of the low energy physics.

1. Introduction
One of the physically observable phenomena in topological insulators (TIs) is the existence of the linearly dispersing gapless edge (in two dimensions (2D)) or surface (in three dimensions (3D)) states which are topologically protected against moderate electronic interactions or nonmagnetic disorder [1–5]. The fact that these conducting edge states can host spin current without dissipation makes TIs a promising candidate for technological applications [6, 7]. Understanding the nature of the edge states has been an aspect of interest in theoretical studies of TIs [8–15].

Properties of edge states can be studied by constructing appropriate tight binding model Hamiltonians of TIs and examining their eigenstates for lattices with boundaries. An alternative route is to construct a low energy continuum theory [3, 9, 16] that allows for analytical treatment that aids the development of field theoretic description in the presence of interactions [17, 18]. Such approaches have already been gainfully employed in studies of graphene [19–23]. In the analytic calculation, the edge states are obtained by subjecting the wavefunction to appropriate boundary conditions (BCs). Here one usually [8–15] imposes a fixed BC (also called the essential or Dirichlet BC in the mathematical literature [24]) where the wavefunction is assumed to be zero at the boundaries or at a fictitious layer of atoms just outside the boundaries. Such a choice of BC constrains the nature of the wavefunction in that the maximum weight of the edge state does not occur in the edge layers but in bulk layers that are near the edge layer. In the presence of interactions, the edge states and bulk states mix and the ensuing physics is determined crucially by this mixing. In a recent study [25], it was shown that the Mott transition in topological insulator ribbons can occur in two different routes—the synchronous and asynchronous routes—depending on the nature of the edge states. A continuum field theoretic analysis of such a phenomenon, therefore, requires careful treatment of the edge states so that their profile correctly captures the mixing with the bulk states. Another problem which requires the correct calculation of the profile of the edge state wavefunction is the prediction of the tunnelling current in surface probe experiments.

With this motivation, in this paper we develop a continuum theory of time reversal invariant four-band model Hamiltonians that have been extensively used in the analysis of topological insulators in two and three dimensions. We
construct an energy functional of the wavefunctions; the
wavefunction that renders this energy functional extremum
is shown to satisfy a stationary Schrödinger equation that
matches the four-band lattice theory at long wavelengths. As
a key outcome of this approach, we derive a new BC, the
natural BC [24]. This BC is valid for any four-band time
reversal invariant system in two and three dimensions. We use
the Bernevig–Hughes–Zhang (BHZ) model [3] that has been
studied earlier [8, 9, 13, 14] to show that within a regime
of parameters of this model, the natural BC provides an excellent
description of the edge states. For example, the energy gap
calculated using the natural BC matches the tight binding
result to within 10%, whereas that given by the fixed BC is
off by more than 40%. In the process of this study, we
show that the gap that arises from the hybridization of the
topological edge states localized on the opposite edges of a ribbon is
a non-monotonic function of the ribbon width. Such physics
was mooted in [10] and shown explicitly in the case of Bi$_2$Se$_3$,
a 3D topological insulator. Here we show that there exists
a parameter regime in which the BHZ model also shows
similar behaviour. This could potentially be useful in many
applications such as design of thermoelectric devices [26, 27].

In the following section (section 2) we introduce a general
four-band lattice Hamiltonian that is time reversal invariant.
Section 3 contains the continuum theory of these systems,
the formulation of a variational principle and derivation of the
BCs. A detailed comparison of the numerical tight binding
calculations and the analytical continuum theory is carried
out in section 4 using the BHZ model [3], in its topological
regime. The paper is concluded in section 5 which contains a
discussion of the significance of the results and a summary.

2. Four-band time reversal invariant systems

Consider a Bravais lattice in 2D or 3D whose sites are labelled by $I$.
Each lattice site has two orbitals (or ‘basis’ sites such as the
A–B sites in the graphene lattice, sometimes also referred
to as ‘flavours’) labelled by $\alpha$. The operator $C_{\alpha I}^I$ creates an
electron of spin $\sigma$ (quantized along some convenient axis)
in the orbital $\alpha$ at site $I$. The Hamiltonian of the system is given by

$$H = - \sum_{Ib} t_{\alpha\beta, \sigma\sigma'}(b) (b) C_{(I+b)\alpha\sigma}^I C_{I\beta\sigma'}$$

(1)

where $b$ runs over lattice vectors; summation over repeated
orbital and spin indices is implied. The hopping matrix
elements $t_{\alpha\beta, \sigma\sigma'}(b)$ are such that the Hamiltonian equation (1)
is time reversal invariant. Hamiltonians discussed in the
literature on topological insulators [4, 5] are of this type.

With the aim of developing a long wavelength continuum theory
of such systems, we cast the Hamiltonian in the reciprocal space:

$$\mathcal{H} = \sum_{k \in B} H_{ab}(k) C_{k\alpha}^I C_{kb}$$

(2)

where $a$ (and $b$) is an index that represents the composite $\alpha \sigma$.
Repeated $a$ and $b$ indices are summed over and $k$ runs over
$B$, the Brillouin zone which is a torus for 2D systems and a
3-torus in 3D systems. Following [28, 29, 1], we now write the
matrix $H(k)$ in a basis of $16 \times 4 \times 4$ matrices, broken up into
two groups $H^m(m=0-5)$ and $A^m(n=1-10)$, i.e.

$$H(k) = \sum_{n=0}^5 d_n(k) + 10 e_n(k) A^m$$

(3)

where $d_n(k)$ and $e_n(k)$ are smooth functions of $k$. The matrices
$\Gamma$ and $\Lambda$ are defined using $\sigma$ and $\alpha$, the $2 \times 2$ Pauli matrices
associated with the orbital and spin degrees of freedom, and
$1$, the $2 \times 2$ identity matrix. We have ($\Gamma^0 = 1 \otimes 1$).

$$\Gamma^{1,2,3,4,5} = \{\tau^x \otimes 1, \tau^y \otimes 1, \tau^z \otimes \sigma^1, \tau^x \otimes \sigma^2, \tau^y \otimes \sigma^3 \}.$$ (4)

The 10 elements $\Lambda^m$, $m = 1, \ldots, 10$ can be obtained from
the commutators $[\Gamma^n, \Gamma^m]/(2i)$, $n, m = 1, \ldots, 5, n' > n$. The grouping of these matrices into $\Gamma$s and $\Lambda$s is motivated by
the fact that under the action of the time reversal operator
$\Theta = -i(1 \otimes \sigma^3)K$, where $K$ is the complex conjugation
operator [30], $\Theta^{-1} \Gamma^m \Theta = \Gamma^{m'}$ while $\Theta^{-1} \Lambda^m \Theta = -\Lambda^m$.
From the fact that the Hamiltonian in equation (2) is time
reversal invariant, and from the properties of the $\Gamma$ and $\Lambda$
mats just mentioned, we get from equation (3) that [1]

$$d_n(-k) = d_n(k)$$

$$e_n(-k) = -e_n(k).$$

(5)

Equation (2) along with equations (3) and (5) describes a
general four-band Hamiltonian with time reversal symmetry.
The systems of interest are those which possess a gap in
their energy dispersion—two bands separated from the other
by an energy gap; the chemical potential lies in this gap.
The nature of this insulating state (topological or trivial)
is determined by the topological properties of the occupied
bands and is characterized by the $Z_2$ index [1–3, 31–33].
While our formulation is applicable to any four-band system
with time reversal symmetry, we shall focus on topological
insulators which possess protected edge/surface states.

3. Continuum theory, variational principle and BCs

The continuum theory is developed by focusing on a region of the
Brillouin zone, i.e. specifically around the $k$-points which
support low energy excitations. In the case of topological
insulators with a bounding edge (or surface), the low energy
excitations (i.e. excitations close to the chemical potential)
usually occur near a time reversal invariant momentum
(TRIM) [4]. TRIMs occur at the origin of the Brillouin zone,
at the zone edges, etc. In what follows, we shall develop the
continuum theory focusing on the $k = 0$ TRIM; generalization
to any other TRIM of interest is straightforward.

We discuss the continuum theory in the first quantized form.
For our four-band model, the wavefunction is a four-
component vector function $\psi_{\alpha}(x)$ of the position $x$.
We look to determine a Hamiltonian operator $\mathbb{H}$ that dictates
the time evolution of $\psi_{\alpha}(x)$, i.e.

$$i\frac{\partial}{\partial t} \psi_{\alpha}(x) = \mathbb{H}_{ab} \psi_{\beta}(x)$$

(6)

where the dot represents the time derivative and the repeated
index $b$ is summed over. We have set $\hbar = 1$. To determine $\mathbb{H},$
we expand the function $d_n(k)$ and $e_m(k)$ about $k = 0$ up to quadratic order, which upon using equation (5) gives

$$
\begin{align*}
    d_n(k) &= d_n^0 + k_i S^n_{ij} k_i \\
    e_m(k) &= 2\Lambda^m_{ab} k_i 
\end{align*}
$$

where the constants $d_n^0$, tensors $S^n_{ij}$ and vectors $\Lambda^m_{ab}$ are properties of the four-band system that characterize the dispersion near $k = 0$. We thus have

$$
H_{ab}(k) \approx (d_n^0 + S^n_{ij} k_i) \Gamma^n_{ab} + 2\Lambda^m_{ab} k_i \Lambda^m_{ab}
$$

where repeated $n$ and $m$ indices are summed over the ranges indicated in equation (3). $H_{ab}$ can now be obtained as $H_{ab} = H_{ab}(k_i \rightarrow -i\partial_i)$, where $\partial_i \equiv \partial/\partial x_i$, i.e.

$$
H_{ab} = (d_n^0 - S^n_{ij} \partial_i \partial_j) \Gamma^n_{ab} - 2i\Lambda^m_{ab} \partial_i \Lambda^m_{ab}
$$

which completes the discussion of equation (6).

Consider now a region of space (in 2D or 3D) $\Omega$ bounded by a boundary $\partial \Omega$ (which may be an edge or a surface). The stationary states at low energy are eigenstates of the continuum Hamiltonian $H$, i.e.

$$
H_{ab} \Psi_a(x) = E \Psi_a(x)
$$

where $E$ is the energy eigenvalue, with appropriate BCs for the four-component wavefunction $\Psi_a(x)$ on $\partial \Omega$.

To aid the determination of the BCs, here we propose an energy functional associated with a four-component wavefunction $\Psi_a(x)$:

$$
\mathcal{E}[\Psi^*(r), \Psi(r)] = \int_\Omega d^3r \left[ \Psi^*_a \Gamma^n_{ab} \Psi_b - (\partial_i \Psi^*_a)(S^n_{ij} \partial_j \Psi_b) - i \left[ (\partial_i \Psi^*_a) \Lambda^m_{ab} \partial_j \Psi_b + (\partial_i \Psi^*_a) \Lambda^m_{ab} \Lambda^m_{ab} \Psi_b \right] - E \Psi^*_a \Psi_a \right]
$$

where $E$ is a Lagrange multiplier that ensures that the wavefunction $\Psi_a$ is fixed (usually to zero), or

$$
\delta \Psi^*_a = 0
$$

which corresponds to the fixed BC where the values of the wavefunction $\Psi_a$ is fixed (usually to zero), or

$$
n_i (S^n_{ij} \partial_j \Psi_b + i\Lambda^m_{ab} \Lambda^m_{ab} \Psi_b) = 0
$$

which is the natural BC (note, again, that all the repeated indices are summed). We emphasize that this BC is applicable to any time reversal invariant four-band system in 2D or 3D. In particular, the formulation is tailored for the study of edge (surface) states of topological insulators. In section 4, we illustrate this framework by calculating (analytically) the edge states of a topological insulator described by the well known BHZ model [3].

4. BHZ model: comparison of continuum theory and tight binding results

The BHZ model [3] describes 2D topological insulators realized in HgTe/CdTe quantum wells. The tight binding version of the model is obtained by considering four spin–orbit coupled orbitals, $|s\uparrow\rangle$, $|p\uparrow\rangle$, $|s\downarrow\rangle$, and $|p\downarrow\rangle = (|p_+ - i p_\downarrow\rangle)$, per site on a square lattice whose lattice spacing $a$ is taken as unity. The model can be written as

$$
H = \sum_{i and \sigma} \epsilon^s_i C^s_i \sigma C^s_i + \sum_{i and \sigma} t_{sp} (\delta^s \sigma) C^s_i (\uparrow \pm \delta \sigma) C^s_i
$$

where $\delta^s \sigma = \pm$, and $\sigma$ denote the orbital energies. $\sigma = \uparrow, \downarrow$ and $\delta$ is a nearest neighbour vector. The hopping matrix elements $t_{sp} (\delta^s \sigma)$ are given by

$$
t(\pm \delta \sigma) = \begin{pmatrix} t_{ss} & \pm \sigma & \pm t_{sp} \\ \pm \sigma & t_{pp} & t_{pp} \\ \pm t_{sp} & t_{pp} & t_{pp} \end{pmatrix}
$$

where $t_{ss}$, $t_{sp}$ and $t_{pp}$ are overlap integrals and $\sigma = +1 (-1)$ for spin $\uparrow (\downarrow)$. In the reciprocal space, as in equation (2), this Hamiltonian is described by a matrix

$$
H(k) = \begin{pmatrix} \hbar(k) & 0 \\ 0 & \hbar^*(\mathbf{-k}) \end{pmatrix}
$$

where

$$
\hbar(k) = \begin{pmatrix} \epsilon_s - 2t_4 (\cos k_x + \cos k_y) \\ 2t_4 (\sin k_x - i \sin k_y) \\ 2t_4 (\sin k_x + i \sin k_y) \\ \epsilon_p + 2t_4 (\cos k_x + \cos k_y) \end{pmatrix}
$$

where we have set $t_{ss} = t_{pp} = t_s$. Further defining $\epsilon_0$ such that $\epsilon_s = -(\epsilon_0 - 4t_s)$ and $\epsilon_p = (\epsilon_0 - 4t_s)$ we have

$$
H(k) = -d_2(k) \Gamma^2 + e_1(k) \Lambda^1 + e_2(k) \Lambda^2
$$
in the form of equation (3), with $\Gamma^2 = \mathbf{r}^2 \otimes 1$, $\Lambda^1 = \mathbf{r}^1 \otimes \mathbf{o}$; $\Lambda^2 = \mathbf{r}^2 \otimes 1$ and

$$d_2(k) = -\epsilon_0 + 2t_s(2 - (\cos k_x + \cos k_y))$$
$$e_1(k) = 2t_{sp} \sin k_x$$
$$e_2(k) = 2t_{sp} \sin k_y.$$  \hspace{1cm} (21)

All other $d(k)$ and $e(k)$ are zero. Note that here we have relabelled the $m$ index in equation (3) for convenience. With this, focusing on the TRIM at $k = 0$, we get the continuum Hamiltonian operator as

$$e(k) \cdot \sigma = H(k)$$

which gives four solutions for $q$. $q_{1,2} = \pm q_1$, $q_{3,4} = \pm q_2$, given by

$$q_{1,2}^2 = k^2 + \frac{(a_0 \delta_k + 2t_{sp}^2)}{\epsilon_0^2 + \frac{4t_{sp}^2(t_{sp}^2 - \epsilon_0 \delta_k) + t_s^2 E^2}{t_s^2}}.$$  \hspace{1cm} (27)

Therefore the general solutions for $\Phi$ and $\Psi$ are given by

$$\Psi(y) = \frac{1}{E + 2t_{sp}k} \{ G(D) + H(D) \} \Phi(y)$$  \hspace{1cm} (29)

where $A_{1,2,3}$ are four constants. The complete solution for the wavefunction is given by

$$\Psi_{\phi}(x, y) = \frac{\psi_s}{\psi_p} e^{ik_y} = \frac{1}{2} \left( \frac{\phi + \psi}{\phi - \psi} \right) e^{ik_x}.$$  \hspace{1cm} (30)

The determination of the energy eigenvalue $E$ and the constants $A_{1,2,3}$ requires the BCs. The fixed BC [9] equation (14) reads

$$\begin{align*}
\Psi_s(0) &= \psi_p(0) = 0 \\
\Psi_s(L) &= \psi_p(L) = 0
\end{align*}$$  \hspace{1cm} (31)

while the natural BC derived in equation (15) provides

$$\begin{align*}
t_s \frac{d\psi_s}{dy} + t_{sp} \psi_p &= 0 \\
t_s \frac{d\psi_p}{dy} + t_{sp} \psi_s &= 0
\end{align*}$$  \hspace{1cm} (32)

on $\partial \Omega$, i.e. at $y = 0$ and $L$.

In the remainder of the discussion $t_s$ is set to unity. It is useful to discuss the nature of the solution of $q$ before proceeding to compare the analytical results with the numerical tight binding calculations. Note that the value of $q$ depends on the energy eigenvalue $E$ (equation (27)). Since $k = 0$ corresponds to a TRIM, we expect a pair (time reversal related) of topologically protected edge states at $k = 0$, and by the symmetry of the problem we expect $E = 0$ to be their energy eigenvalue. The values of $q$ with $E = 0$ are then determined by the parameters $\epsilon_0$ and $t_{sp}$, i.e. they are characterized by the same parameters that determine the ‘topology’ of the system. Figure 1 shows a plot of the $q$ as a function of the parameter $\epsilon_0$. We find that there are two regimes of $\epsilon_0$. $\epsilon_0 < t_{sp}^2$, where there are four distinct real roots for $q$-s and $\epsilon_0 > t_{sp}^2$ where the $q$ are complex and appear in conjugate pairs. In the former regime, magnitudes of $q_1$ and $q_2$ increase with increasing $\epsilon_0$, while that of $q_3$ and $q_4$ decrease with increasing $\epsilon_0$. In the latter regime, the real parts of $q$ are unaffected, while their imaginary parts increase in magnitude. Clearly, the nature of the edge states for $\epsilon_0 < t_{sp}^2$ is different from that for $\epsilon_0 > t_{sp}^2$. In the former case, the edge state wavefunction is non-oscillating and falls exponentially with distance from the edge. In the latter case, the wavefunction also has an oscillatory part, and as we shall show later, this leads to quite interesting physics and possibilities.
Let us first consider a semi-infinite plane with its boundary at $y = 0$. Then the bounded solution for $\phi$ is given by

$$\phi(y) = A_2 e^{-q_2 y} + A_4 e^{-q_4 y}. \quad (33)$$

The energy eigenvalues and the wavefunctions can be determined by imposing either the fixed BC equation (31) or the natural BC equation (32). After some simple algebra, it can be shown that for small $k$

$$E(k) = 2t_{SP} k. \quad (34)$$

a linear dispersion for the edge states, that is, remarkably, independent of which BC is chosen.

This value of $E(k)$ can be now used to determine the constant coefficients $A_{2,4}$ and hence $\Psi_{SP}$. The profile of the wavefunction, of course, depends strongly on the BCs. Figure 2 shows a comparison of the results of the analytical formulation presented above with the two different BCs and the wavefunction obtained from numerical calculations with the full tight binding model. Figure 2 corresponds to values of $t_{0} = 0.25$ and $t_{SP} = 0.5$ which corresponds to the parameter regime considered in [9]. The wavefunction with the fixed BC (agreeing with that of [9]) differs significantly from that of the tight binding results for points close to the edge (near $y = 0$). The wavefunction with the natural BC does not vanish at the boundary and has the expected exponential decay into the bulk. At large distances from the boundary, the tight binding result for the wavefunction falls between the analytical results of the fixed and natural BCs. This can be understood by noting that the fixed BC kills the weight of the edge state near the boundary, and hence overestimates the weight of the wavefunction in the bulk. The effect is the opposite with the natural BC, where the weight in the bulk is underestimated compared to the tight binding result. We now consider figure 2(b), which shows the comparison of the edge state wavefunction with $t_{SP} = 2$, but still with $t_{0} = 0.25$. In this case we see that the wavefunction determined by the natural BC not only closely reproduces the qualitative aspects of the tight binding solution, but is also in excellent quantitative agreement with it at large distance from the edge. Finally, in figure 2 we show the comparison of the wavefunctions in the regime of parameters with $t_{0} = t_{SP}^2$. We see, again, that the analytical wavefunction obtained with the natural BC more closely matches the results of tight binding calculation. Parameter regimes shown in figures 2(b) and (c) have not been reported in [9].

4.2. Ribbons

We now consider ribbons of finite width $L$. In this case, the edge states emanating from the edges at $y = 0$ and $y = L$ overlap and hybridize, rendering the system gapped (see figure 3). A stronger test of the validity of the continuum formulation and the correctness of the BC can be achieved by comparing the gap calculated using the analytical formulation with that obtained from the tight binding numerics. Figure 4(a) shows a comparison of the calculated gaps as a function of the ribbon width $L$. In this regime of parameters the gap falls exponentially with the ribbon width as it is determined by the overlap matrix element of the two edge states emanating from the opposite edges. Again, we see that in this parameter regime, the tight binding gap lies between the fixed BC result which is the largest, and the natural BC value which is the smallest. This can be understood based on the result of section 4.1. The weight of the edge state wavefunction in the bulk is overestimated by the use of the fixed BC, and hence this gives rise to a larger gap owing to a larger overlap of the wavefunctions emanating from the opposite edges. For the same reason, the natural BC underestimates the gap. For a larger value of $t_{SP}$, the natural BC is in better quantitative agreement with the tight binding results. This is because the wavefunction is better estimated by the natural BC.

Our final result pertains to the energy gap in ribbons with parameters in the regime $t_{0} > t_{SP}^2$. Figure 5 shows a plot of the gap as a function of the ribbon width in such a regime; we see that the gap is non-monotonic. Although the gap follows an exponential fall with increasing ribbon width, there are ‘magic widths’ at which the gap is very small; indeed our analytical results with the natural BCs do reproduce these features. The physics behind this phenomenon can be traced to the oscillatory nature of the edge state wavefunction in this parameter regime; for some particular widths of the ribbon, there is a 'near destructive interference' of the wavefunctions emanating from the opposite edges that renders their overlap matrix element small, resulting in a smaller gap. To the best of our knowledge, this is the first report of such physics in the BHZ model which has been demonstrated [10] in models.
Figure 2. Comparison of the edge state wavefunctions obtained analytically by using the two different BCs with the corresponding result from the tight binding calculation. The wavefunctions plotted are for $k = 0$; only the $\Psi_s$ component is shown.

Figure 3. Energy dispersion of edge states of a BHZ ribbon of width $L = 20$. For the parameter values shown, the continuum theory with the natural BC (equation (15)) reproduces the tight binding result more accurately.

Figure 4. Comparison of the energy gap obtained analytically by using the two different BCs with the corresponding result from the tight binding calculation.

4.3. Discussion

To understand the physical underpinnings of the natural BC consider a general wavefunction $\Psi_n(x)$—this, in general, is a four-component object in our context. The particle current density associated with this wavefunction, after a brief calculation, is found to be

$$J_i(x) = \frac{1}{i} \left[ -S_{ij}^{(n)} \frac{\partial}{\partial x} \Psi_n(x) \partial_j \Psi_n(x) - \partial_j \Psi_n(x) \partial_i \Psi_n(x) \right] - 2iA^{i}A_{ab}^{m} \Psi_n^{*}(x) \Psi_n(x) \right]$$

(35)
where, again, all repeated indices are summed. We immediately see that the current is a sum of many terms over different flavours. Note, also, that the current is made of two parts, the first is the usual term relating the gradient of the wavefunction, and second is the ‘mixing term’ that is arises from the mixing of the different flavours in the Hamiltonian.

The condition equation (15) ensures that the total particle current normal to the boundary vanishes. An important point to be noted now is that equation (15) does not require the wavefunction of all the flavours to vanish at the boundary. For example, for the BHZ model this leads to equation (32), where it is seen that the derivative of one component normal to the boundary is proportional to the other component. The proportionality is determined by the ‘component mixing’ \( t_{sp} \) of the two components. When such mixing is large, a wave of one flavour can be reflected off the boundary as another flavour, ensuring that the total particle current normal to the boundary is zero. As is evident from our results, a continuum field theory with a natural BC provides an excellent description of systems with strong ‘component mixing’. In the case of the BHZ model, in this regime, the wavefunction of each flavour is complex, and hence current carrying the particle flux brought in to the boundary in one favour channel is reflected back in another flavour channel.

This may be contrasted with systems with a single component wavefunction such as in a simple ‘one component’ tight binding model where the appropriate continuum BC is the vanishing of the wavefunction at the boundary, i.e. the fixed BC. In such cases, the appropriate wavefunctions (such as \( \Psi(y) \) in equation (23) or \( \phi(y) \) in equation (33)) are all real and non-current carrying, as in a simple square lattice ribbon where no eigenstate carries current along \( y \) (direction perpendicular to the ribbon edges). On the other hand, topological insulators that are ‘deep’ in their topological phase (such as a large \( \epsilon_0 \) and \( t_{sp} \)) are strongly ‘multi-component’ in nature, with complex current carrying wavefunctions for each of their flavours. For such systems the natural BC is more appropriate.

5. Summary

In this paper we have developed a continuum theory that is applicable to the study of four-band time reversal invariant systems. We formulate a variational energy functional and show that the Schrödinger equation in the bulk is the Euler–Lagrange equation of this functional. This formulation allows us to obtain the natural BC of the system. We have compared our analytical results with full tight binding calculation for the BHZ model for the half space and finite ribbons. We show that in the interesting topological regime, the natural BC derived in this paper is more appropriate. We believe that our continuum formulation and BCs will be useful in developing the theory of devices and applications of topological insulators, and continuum theory modelling of experiments such as tunnelling from surface states. The non-monotonic dependence of the gap on the width of a BHZ ribbon is of interest; we believe such features are generic and can have numerous applications.

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\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5.png}
\caption{Non-monotonic dependence of the energy gap with ribbon width \( L \) in the parameter regime \( \epsilon_0 > \epsilon_{sp} \). The dashed line is a guide to the eye to show an overall exponential dependence on the ribbon width.}
\end{figure}
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