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A Bipartite Kronig-Penney Model with Dirac-delta Potential Scatterers

Abstract. Here we present a simple extension to the age-old Kronig-Penney model, which is made to be bipartite by varying either the scatterer separations or the potential heights. In doing so, chiral (sublattice) symmetry can be introduced. When such a symmetry is present, topological chiral symmetry protected edge states are seen to exist in correspondence with the standard quantised Zak phase bulk invariant. This quantisation behaviour may also be observed within a ‘gauge’-invariant on-diagonal matrix element of a unit eigenvalue equation. The solution proceeds through the conventional scattering formalism used to study the Kronig-Penney model, which does not require further tight-binding approximations or mapping into a Su-Schrieffer-Heeger model. The cases in which chiral symmetry is absent are then seen to not host topologically protected edge states, as verified by zero bulk invariants.

Kronig-Penney, one-dimensional, topological symmetry protection, edge states

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1. Introduction

For many years now, the subjects of topological protection and topological order have been hot topics within the theoretical condensed matter physics community. Ever since the seminal papers of Thouless et al. [1], Thouless [2] wherein the quantisation of Hall conductance was shown to be of topological origin, the quest has been on to discover and delve all systems in which the topological character of the bulk system manifests itself within some observable of the finite bounded system;[3–10] a phenomenon termed bulk-boundary correspondence.

Within this paper we take inspiration from the one-dimensional Su-Schrieffer-Heeger (SSH) model[11–13] that is known to host zero-energy topologically protected edge states.[14, 15] We thus consider an extended, closed Kronig-Penney model[16, 17] with Dirac-delta potentials that is allowed to become bipartite (or dimerised) by the suitable variation of certain physical variables; namely the scatterer separations or the scatterer potential heights.

The significance of topologically protected edge states lies in their resistance and robustness against adiabatic lattice deformations and perturbations, to say nothing about their fundamental theoretical interest. Provided that a system is in a topologically non-trivial phase then any adiabatic deformation that respects certain symmetries will not affect the existence of the symmetry-protected edge states.[14, 15]

As such, it is expected that this behaviour should be present in the bipartite Kronig-Penney model where the widths between the scatterers act in the same way as the hopping parameters within the SSH model.

In relation to the Kronig-Penney model, there has been much study undertaken into the finite system that possesses open boundary conditions. In such cases, charge quanta may be pumped through the chain by a suitable adiabatic deformation of parameters and the quantisation is of a topological origin.[18, 19]

In the present case, we impose hard wall boundary conditions such that all states must exist within the chain itself and dimerise the system, i.e. make it bipartite. Then, through Bloch’s theorem in the bulk, the parameter space is the first Brillouin zone.

This paper is divided into five parts. Firstly, the general bulk system is solved by considering a periodic geometry of the chain. A pseudo scattering matrix for the unit cell is found in terms of a unit eigenvalue problem involving the wavefunction coefficients.

Secondly, the general finite system is presented and explained. Due to the non-exact nature of the energies within both the bulk and finite models, the final calculations must be performed numerically.

Thirdly and fourthly, we consider systems in which we fix the potential heights to a constant and vary the separations between the potential scatterers. The two separate and distinct cases in which the potential heights are either negative or positive are considered. In these cases, we seek (respectively) negative and positive energy solutions to the Schrödinger equation.

Finally, conclusions are drawn and the results are discussed in the context of physical systems for which this theory may be applied. Within the appendices are shown the non-topological cases wherein the potential heights are varied in the presence of constant widths.

2. The Bulk Solution

We solve the one-dimensional time-independent Schrödinger equation as given by:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \Psi_k(x) = E(k)\Psi_k(x),$$

(1)

for the system as shown in Figure 1 with potential scatterers that have Dirac-delta profiles. The potential $V(x)$ within the unit cell is then given by:

$$V(x) = V_1 \delta(x - x_1) + V_2 \delta(x - x_2).$$

(2)

However, rather than either mapping this differential equation into an effective Hamiltonian or using a tight-binding approximation, we solve the system in the standard scattering paradigm. From now on, we assume natural units such that $\hbar = m = 1$.

In passing, we note that the topological features of edge states have been also studied, with a similar scattering matrix approach, by Fulga et al. [20]. There, the focus is on lattice (i.e. tight-binding) models. Here we adopt instead a “wave-mechanics” description that captures all the physics of the problem without making parameter-dependent assumptions, e.g., ignoring next-nearest neighbour interactions in tight-binding models.

Following the conventional scattering paradigm, we solve the problem posed by (1) in the regions in which the potential vanishes. We then match such solutions by using the standard boundary conditions for delta potentials. These are that, at the position of
each scatterer, the wavefunction is continuous and that
the difference of the derivatives of the wavefunction
yields the product of the delta potential height and
the difference of the derivatives of the wavefunction
each scatterer, the wavefunction is continuous and that
may be realised by varying \( v \) and \( w \) or by varying \( V_1 \) and \( V_2 \).

The standard solution to this problem, both
within the bulk and in the finite chain, is that the
wavefunction within each unit cell is simply the linear
combination of right and left moving waves with
coefficients that differ between wells. In other words:

\[
\Psi_k(x) = \mathcal{N}_c(k) \sum_{n=1}^{M} \Theta_n(x) \psi_{n,k}(x),
\]

where \( \Theta_n(x) = \theta(x - x_{n-1}) \theta(x - x_n) \), \( \psi_{n,q_k}(x) = C_n e^{iq_k x} + D_n e^{-iq_k x} \) and the wavevector \( q_k \) is related
to the energy of the wavefunction by \( E(k) = q_k^2/2 \).
The number of regions, \( M \), is 3 in the bulk and \( N + 1 \)
in the finite chain, with \( N \) as the number of scatterers.
The normalisation constant is found in the standard
way through the inner product \( \langle \Psi | \Psi \rangle = 1 \).

The boundary conditions for the scatterers are
then formulated within the unit cell with the first and
second scatterers located at \( x_1 \) and \( x_2 \) respectively with
the edges of the unit cell as \( x_0 = -d/2 \) and \( x_3 = d/2 \).
Thus we have, for \( n \in \{1,2\} \) here, that:

\[
\psi_{n,q_k}(x_n) = \psi_{n+1,q_k}(x_n),
\]

\[
V_n[\psi_{n,q_k}(x_n) + \psi_{n+1,q_k}(x_n)] = \psi'_{n+1,q_k}(x_n) - \psi'_{n,q_k}(x_n),
\]

and \( \psi_{3,q_k}(x_n) = \psi_{1,q_k}(x_n - d) e^{ikd} \).

Keeping within the scattering paradigm, we build
a real eigenvalue equation in terms of an unitary (non-
Hermitian) matrix in the case of real (imaginary)
wavevector and positive (negative) potential heights.
In the positive-potential case, such a matrix is a
scattering matrix. This is not strictly true in the
negative-potential case, but we will continue to call
it as such to simplify the discussion. The scatterings
across the two potentials within the unit cell are solved

and the following real eigenvalue equation is found:

\[
\begin{pmatrix}
D_1(k) \\
C_2(k)
\end{pmatrix} = \begin{pmatrix}
\mathcal{R}(k) & -t^*(k) e^{i\phi_k} \\
-t(k) e^{i\phi_k} & \mathcal{R}^*(k)
\end{pmatrix} \begin{pmatrix}
D_1(k) \\
C_2(k)
\end{pmatrix},
\]

(6)
the details of which are laid out in Appendix A, where
the matrix will be notated as \( S(k) \).

The quantities \( \mathcal{R}(k) \) and \( t(k) \) are pseudo reflection
and transmission coefficients for the entire unit cell
whilst \( \phi_k \) is the phase of the scattering matrix, where
\( \det S(k) = \phi_k \) since \( |r|^2 + |t|^2 = 1 \), and are given by:

\[
r(k) = e^{i\phi_k} \frac{V_1 V_2 e^{iq_k d}[e^{2i(q_k d + 2(x_1 - x_2))} - q_k^2 e^{i k d}]}{(V_1 - i q_k)(V_2 - i q_k)},
\]

(7)

\[
t(k) = i q_k \frac{V_1 e^{iq_k d} e^{-ikd} + V_2 e^{iq_k d} e^{ikd}}{(V_1 - i q_k)(V_2 - i q_k)},
\]

(8)

\[
e^{i\phi_k} = e^{2iq_k d} \left[ (V_1 + i q_k)(V_2 + i q_k) \right]^{-1} \frac{(V_1 - i q_k)(V_2 - i q_k)}{(V_1 - i q_k)(V_2 - i q_k)}.
\]

(9)

The transcendental equation that defines the
energy bands of any states within the system is found
by solving the eigenvalue problem as given in (6).
When done so, it is found that:

\[
q_k^2 \cos(kd) = V_1 V_2 \cos \{q_k [d + 2(x_1 - x_2)] \}
+ \{q_k^2 - V_1 V_2\} \cos(q_k d) + q_k (V_1 + V_2) \sin(q_k d),
\]

(10)
a result that conforms with that found elsewhere.[21]
When the right-hand side has a value greater (lesser)
than +1 (-1) there are no real solutions and thus the
band gaps are defined. Since this equation relates \( k \)
to \( q_k \) with \( q_k \propto \sqrt{E(k)} \) it may only be solved using
numerical root finding methods.

The topological invariant in one-dimensional
Schrödinger systems is the sum of the Zak phases of
all occupied bands:[14, 22–25]

\[
\theta_Z = \sum_m \theta_Z^m = i \sum_m \int_{-\frac{\pi}{d}}^{\frac{\pi}{d}} \text{d}k \langle u_k^m| \partial_k u_k^m \rangle,
\]

(11)

where \( \theta_Z^m \) is the Zak phase of the \( m \)th band and the inner product signifies to integrate over the entire unit-cell in \( x \).

As such, for this system, the Zak phase of the \( m \)th band
is calculated explicitly as:

\[
\theta_Z^m = i \int_{-\frac{\pi}{d}}^{\frac{\pi}{d}} \text{d}k |N_c^m(k)|^2 \sum_{n=1}^{3} \int_{x_{n-1}}^{x_n} \text{d}x
\]

\[
\times \left[ -ix + \partial_k \frac{N_c^m(k)}{N_c(k)} \right] \left\{ |\psi_{n,h,k}^m(x)|^2 + \psi_{n,h,k}^m(x) \partial_k \psi_{n,h,k}^m(x) \right\}.
\]

(12)

As will be seen in Section 4, the mid-gap energy of the
bands is an arbitrary energy shift. As such, it may be
safely ignored and so assumed that only the lower band
is occupied. Thus, $\theta_Z$ is that of the lowest energy band only. This will in fact make no matter to the bands of Section 5 as their phases are all found to be zero.

As made clear by Zak [24], $\theta_Z$ is well-defined and quantised into units of $\pi$ if, and only if, the unit-cell density, $|\Psi_k(x)|^2$, is centro-symmetric. As such, the unit cells in each case must be constructed in such a way that this condition is met.

The result of choosing a symmetric $|\Psi_k(x)|^2$ is that the contribution to the Zak phase of the polarisation term (proportional to $x$) vanishes. Furthermore, the normalisation contribution must also vanish as it is symmetric over the Brillouin zone. Thus, the Zak phase is given only in terms of the curvature contribution of the wavefunctions:

$$\theta_Z = i \int_{-\pi/d}^{+\pi/d} dk |N^m_c(k)|^2 \times \sum_{n=1}^3 \int_{x_n}^{x_1} dx [\psi^*_{n,k}(x) \partial_k \psi_{n,k}(x)]. \quad (13)$$

Then $\theta_Z$ takes the distinct values of 0 and $\pi$ when within the topologically trivial and non-trivial phases.

The solution of (6) yields $D_1 = t$ and $C_2 = 1 - r$ from which the other coefficients may be found using the matrix $S_2(k)$ as shown in Appendix A. Furthermore, the integral over $x$ of the Zak phase in (13) may be operated analytically and the result is shown in Appendix A. However, the integral over the Brillouin zone can only be calculated numerically since $q_k$ is non-analytic and may only be found through (10).

The coefficient $r(k)$ can be seen to be proportional to $x_1 - x_2$, which is always equal to $v$ regardless of the positioning of the unit-cell. Furthermore, it self-consistently relates $D_1$ to itself, i.e., $D_1 = r D_1 + t C_2$, so its phase cannot be changed trivially by redefining $D_1$, unlike $t$. Thus it is a ‘gauge’-invariant quantity where the gauge here is the unit-cell detail. As a result it shows distinct winding behaviours akin to $\theta_Z$ within each topological region of the phase space and the winding number may be calculated through:

$$W_c = \frac{1}{2\pi i} \int_{-\pi/d}^{+\pi/d} dk \left( \frac{d}{dk} \{\ln|r(k)|\} \right). \quad (14)$$

3. The Finite Solution

The analysis of the finite system differs since periodic boundary conditions no longer apply. Instead, closed boundary conditions are imposed such that the wavefunction vanishes outside of the chain of scatterers. In other words, we terminate the chain with hard walls that possess infinite potential heights.

The wavefunction is identical to the bulk case as in (3) with the only differences being the number of regions $M = N + 1$ and the fact that the wavevector, $q_k$, no longer depends on $k$. We will now denote the finite wavevector with $q$. The boundary conditions are identical to those in (4).

The ends of the chain are defined as $x_0 = -L/2$ and $x_{N+1} = +L/2$ (see figure 2) and the hard walls impose that the wavefunction vanishes when $x < -L/2$ and $x > L/2$, i.e., $C_0 = C_1 = C_{N+2} = D_{N+2} = 0$.

The method of solution then proceeds similarly to the bulk case. However, rather than build an eigenvalue matrix equation we now use the boundary conditions in (4) to generate a zero-eigenvalue equation:

$$M \cdot v = 0, \quad (15)$$

where $M$ is a 2Nx2N square matrix and $v = (C_1, D_1, \ldots, C_{N+1}, D_{N+1})^T$ is the vector of wavefunction coefficients. The non-trivial solution ($v \neq 0$) occurs when the determinant of the matrix is equal to zero: $\det M = 0$. From this condition, the energy eigenvalues are found numerically using the RootSearch.m Mathematica package developed by Ted Ersek and the non-trivial vector $v$ is determined using singular value decomposition (SVD).[26]

4. Negative Potentials

So, firstly, we investigate the case of negative potentials of constant height. In this case we have that $q_k \rightarrow i\tilde{q}_k$, $q \rightarrow \tilde{q}$ and $V_{1,2} \rightarrow -V$ so that $E(k) = -\tilde{q}_k^2/2$ and $E = -\tilde{q}^2/2$. This causes the trigonometric functions in the transcendental equation in (10) to become hyperbolic and so it possesses only two roots for $q_k$.

It must be noted that the choice of $q_k \rightarrow i\tilde{q}_k$ over $q_k \rightarrow -i\tilde{q}_k$ is a trivial one. Taking $q_k \rightarrow i\tilde{q}_k$ yields the bulk well wavefunctions as $C_n e^{-i\tilde{q}_k x} + D_n e^{i\tilde{q}_k x}$ whilst taking $q_k \rightarrow -i\tilde{q}_k$ yields $C_n e^{i\tilde{q}_k x} + D_n e^{-i\tilde{q}_k x}$. In other

\[ \text{https://library.wolfram.com/infocenter/Demos/4482/} \]
words, $C_n$ and $D_n$ swap roles, which makes no matter to $\theta_2^\tau$ since it is a manifestly gauge-invariant quantity.

In figure 3(a) is shown the energy spectrum for one of these very cases for which $|V| = 10$. The bands may be seen to be symmetric, exactly akin to the SSH model, about the mid-gap point of $E(0) = -|V|^2$. The Zak phase of the lowest occupied band may be calculated and the phase diagram is shown in figure 3(b). Further, the invariant $W_v$ may also be calculated and be found to be quantised in a similar way to the Zak phase. Then there is another invariant, which conforms with $W_Z = \theta_Z / \pi$, that can be found, without the need of calculating the wavefunction, as $W = |1 - W_v|$. This fact is the novel aspect of this paper as the calculation of $W$ is much less demanding numerically than the calculation of $\theta_Z$.

To establish the necessary bulk-boundary correspondence, the finite system must be solved and shown to host flat mid-gap energy states within the topologically non-trivial regime for both an odd and an even number of scatterers.

The finite chain energy band spectra are plotted in figures 3(e,f). As may be seen, there are clear ‘zero’ (meaning flat) energy mid-gap states of clearly similar nature as one would find in the SSH model. Indeed, if one were to solve the SSH model with hoppings of $\tau$, $\tau' = 1 - \tau$ and a constant potential $V = 10$, as is done in Appendix B, one would see energy bands strikingly similar to those as shown here.

Comparing these plots in figures 3(c,d) with figures B2(a,b) in Appendix B, one sees that, in the even case, the topological transition and coming together of the bulk bands to form a degenerate edge state is a sharp one. By which it is meant that there is very little overlap between the edges of the chain that would cause these bands to remain non-degenerate even within the non-trivial region. Thus the even edge state(s) are very well-defined and localised strongly over the vast majority of the non-trivial region $v > d / 2$.

All this conjecture may be seen in the plots of the edge states for the cases of $N = 19$ and $N = 20$ in figure 3(e-h). In the odd case, panels (e,f), the edge state migrates from one side of the chain to the other upon the transition. In the even case, panels (g,h), it only exists when $v > w$. For $v \sim w$, this edge state is shared between the two ends of the chain, as seen in figure 3(h), however as $v$ and $w$ diverge in value they are attenuated and amplified at either end thereby becoming like figures 3(e,f). Crucially, the edge state band remains degenerate indicating the presence of chiral symmetry, even though it ceases to be mid-gap indicating a lack of sublattice symmetry. This is an effect that occurs in non-Hermitian $PT$-symmetric systems wherein chiral and sublattice symmetry become distinct but the states remain topologically chiral symmetry protected.\cite{27,28}

The degenerate nature of the even case edge state indicates the absence of sublattice-dependent on-site potentials that would otherwise differentiate the two sublattices non-trivially. Thus they are topologically protected by the presence of chiral symmetry. In other words, the edge states are chiral pairs precisely because they are degenerate. They are not mid-gap, however, due to the breaking of sublattice symmetry as $v$ is made significantly different from $w$. Furthermore, the states within the chain localise strongly to the potential scatterers, which all have the same strength. So there can be no chiral symmetry breaking term within the Hamiltonian, neither from long-range interactions nor on-site potentials. As such, even though there is no low-energy two-level effective Hamiltonian that commutes with the chiral operator, the symmetry is still seen to exist. Then, the presence of a quantised
bulk invariant protects the existence of the edge states within the non-trivial region of the phase space.

These two points would motivate the development of a tight-binding model for this negative potential case to elucidate the problem, which is currently a work-in-progress.

As a final note, the observed behaviour would appear to be opposite to the SSH model in that the topologically non-trivial region is defined for \( v > w \) rather than for \( v < w \), as is standard. However, this is because the hopping integral between neighbouring sites is \textit{larger} when the separations between the potentials is \textit{smaller}. As such, when \( v > w \) then \( \tau < \tau' \) whilst when \( v < w \) then \( \tau > \tau' \).

5. Positive Potentials

We turn now to the case in which the potentials have positive strengths and so search for solutions with positive energy. In this case we have that \( V_{1,2} \rightarrow V \) and real wavevector, \( q_k \), so we expect to find infinitely many bands due to the sinusoidal functions in the transcendental equation. Indeed, this is the case, as may be seen in the plots in figures 4(a,b).

Interestingly here, decreasing the height acts to not only lower the energies of the bands but to also effectively close any band gaps. This is because the higher energy bands will simply ignore the effects of the potentials if the heights are much smaller. This is evident in panel (a) too since the band gaps that occur for \( k = 0 \) decrease in size as \( E(k) \) increases.

However, an interesting feature emerges as seen in the right-hand plot. At \( k = 0 \), the fourth and fifth bands appear to be close to touching as opposed to the second and third bands, which are far apart. At some certain value of \( v \) the bands do indeed cross and reopen as \( v \) is increased once again. This would appear to be the same mechanism of a topological transition through band closing and reopening as in the negative scatterer case. However, it is not, as the Zak phases of all the bands, regardless of whether they are occupied or not, is zero for all \( v \) and so \( \theta_Z = 0 \). The windings of \( r(k) \) may also be calculated and seen to conform with the Zak phase. Thus, they are instead trivial band closings and so the edge states of the system will not be symmetry protected.

This is confirmed when the finite solution is solved. The spectra for two chains consisting of \( N = 19 \) and \( N = 20 \) scatterers are shown in figures 4(c,d) wherein edge states can be seen that vary in energy with \( v \). In the odd case, a single edge state exists within each of the band gaps but not at a constant mid-gap energy. Indeed they are seen to move in \( E \) as \( v \) is varied and to track the bulk states quite closely. In the even case, states detach from an upper band and come together to form a degenerate edge state that again tracks the bulk closely before joining the lower band.

These edge states are indeed degenerate, however their energies are \( v \)-dependent indicating a lack of sublattice symmetry, as was the case previously. The lack of chiral symmetry is observed within the behaviour of the states themselves. As shown in figure 4(e-h), the states can be seen to exponentially localise to the edges however they are not solely confined to a single sublattice, in this case the wells, which indicates the lack of chiral symmetry. This is because, when chiral symmetry is present, the topologically protected edge states of the SSH model are confined to exist solely on a single sublattice due to being eigenstates of the chiral operator.[14]

This degeneracy of the edge states occurs within
the SSH model if chiral symmetry is absent in the presence of inversion symmetry.\cite{23} This is indeed the case here, as the change of seeking positive energy solutions in the presence of positive potentials does not change the inversion symmetry of the unit-cell.

The reason for not only the breaking of chiral symmetry but also the maintenance of inversion symmetry is as a result of the difference in widths of the neighbouring wells, \( v \) and \( w \). In this positive potentials case, the states exist within the wells and so the differing widths affect their on-site energies non-trivially (the energy of a lone quantum well is \( E \propto a^{-2} \) where \( a \) is the width of the well). Thus an on-site, chiral symmetry breaking, potential is introduced here that, crucially, is inversion-symmetric about the centre of the unit-cell. This is the same logic used in the discussion of the Zak phase and its quantisation.

6. Discussion

Within the context of tight-binding models, the time-independent Schrödinger equation is solved as an Hermitian matrix eigenvalue equation. There, the topological character of the matrix Hamiltonians may be categorised by the symmetries that they possess. In order that topologically protected edge states exist, the Hamiltonian must possess at least chiral symmetry but may also possess any of particle-hole, time-reversal and inversion symmetries.\cite{29}

In the present case, we solve the time-independent Schrödinger equation through the scattering formalism whereby the boundary conditions at the potentials are solved. This generates an unit eigenvalue equation involving an unitary/non-Hermitian matrix (corresponding to positive/negative energy solutions) that, nevertheless, encodes the topological character of the system through the wavefunction.

Since a two-level matrix Hamiltonian may not be readily generated in this problem without obscuring assumptions, the presence of chiral symmetry may not be observed \textit{a priori} but instead must be inferred upon the solution of the problem. Then, through the wavefunction, the known topological invariant shows quantised behaviour that maps to the number of edge modes. Ergo, a bulk-boundary correspondence is seen between these two invariants thereby showing the states to be symmetry protected.

7. Summary and Conclusions

In summary, the simplified Kronig-Penney model with Dirac-delta potentials has been extended so as to become bipartite. This may be done by alternately modulating the distances between the potentials or, as shown in Appendix C and Appendix D, the potential strengths. The cases of negative and positive potential heights were investigated wherein the wavevector was imaginary and real respectively.

The solution proceeded within the scattering, rather than tight-binding, formalism wherein the boundary conditions at each Dirac scatterer were solved to obtain a unit cell scattering matrix. Such a formalism is different from the lattice-scattering-matrix approach of \cite{20}, which relies on an underlying tight-binding model.

Topologically protected states were seen to be present in the case involving negative energies only. A bulk-boundary correspondence was established between the number of these edge states and the Zak phase invariant \( \theta_Z \) as found from the sum of the Zak phases of the occupied bands. In addition another topological invariant was found: the number \( \mathcal{W} = |1 - \mathcal{W}_r| \) where \( \mathcal{W}_r \) was the winding of the on-diagonal matrix element, \( r(k) \), of the unit-cell scattering matrix \( S(k) \), which was seen to be ‘gauge’-invariant and does not require the calculation of the wavefunction, unlike the Zak phase.

The second case was seen to lack such protected states, however was not wholly uninteresting as a result. It was seen to possess strikingly similar characteristics to the negative heights and varying widths case. Namely that edge states of almost identical character exist between the bands. They were, however, seen to not possess topological protection due to the lack of a bulk quantised invariant that would establish the necessary bulk-boundary correspondence.

Having established the result for a chain of Dirac scatterers, which is a simplified Kronig-Penney model, this analysis may be readily applied to a system of finite barriers or wells. Indeed, the present system is simply the finite-well Kronig-Penney model in the limit of infinitely deep and infinitely narrow wells.

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Appendix A. Calculation of the Bulk Scattering Matrix and the Integrand of the Zak Phase

Taking the boundary conditions that apply for the localised wavefunction within the unit cell as specified in (4) with the wavefunctions as defined in (3), the scattering equations across each Dirac potential may be found as:

\[
\begin{pmatrix}
D_1(k) \\ C_2(k)
\end{pmatrix} = S_1(k) \begin{pmatrix}
C_1(k) \\ D_2(k)
\end{pmatrix}, \quad (A.1)
\]

\[
\begin{pmatrix}
D_2(k) \\ C_3(k)
\end{pmatrix} = S_2(k) \begin{pmatrix}
C_2(k) \\ D_3(k)
\end{pmatrix}, \quad (A.2)
\]

where the matrices \(S_i(k)\) are found as:

\[
S_i(k) = \frac{1}{V_i + iq_k} \begin{pmatrix}
-V_i e^{2iq_k x}, & iq_k \\ iq_k e^{-2iq_k x}, & -V_i
\end{pmatrix}. \quad (A.3)
\]

Then, using \(\psi_{3,k}(x + d) = \psi_{1,k}(x) e^{ik d}\) to see that \(\{C_3, D_3\} = \{C_1 e^{-i q_k}, D_1 e^{i q_k}\} e^{ik d}\) the second scattering equation may be manipulated to become:

\[
\begin{pmatrix}
C_1(k) \\ D_2(k)
\end{pmatrix} = \tilde{S}_2(k) \begin{pmatrix}
D_1(k) \\ C_2(k)
\end{pmatrix}, \quad (A.4)
\]

where:

\[
\tilde{S}_2(k) = \frac{1}{V_2 + iq_k} \begin{pmatrix}
-V_2 e^{2iq_k (d - x_2)}, & iq_k e^{i q_k (d - x_2)} \\ iq_k e^{i q_k x_2}, & -V_2 e^{2iq_k x_2}
\end{pmatrix}. \quad (A.5)
\]

Thus, the scattering matrix equation is found simply by substituting (A.4) into (A.1) and so achieving:

\[
\begin{pmatrix}
D_1(k) \\ C_3(k)
\end{pmatrix} = S(k) \begin{pmatrix}
D_1(k) \\ C_2(k)
\end{pmatrix}, \quad (A.6)
\]

where \(S(k) = S_1(k) \tilde{S}_2(k)\) is the matrix as quoted in (6) whose entries are as in (7, 8, 9).

As was mentioned in the text, once this scattering matrix equation is solved for \(D_1(k)\) and \(C_2(k)\), these may be substituted into (A.4) in order to find \(C_1(k)\) and \(D_2(k)\) whilst \(C_3(k)\) and \(D_3(k)\) are found using the Bloch condition. These are:

\[
C_1 = \tilde{r}_2 t + \tilde{t}_2 (1 - r), \quad D_1 = t, \quad (A.7)
\]

\[
C_2 = 1 - r, \quad D_2 = -\tilde{r}_2^* e^{i \tilde{\phi}_2} t + \tilde{t}_2^* e^{i \tilde{\phi}_2} (1 - r), \quad (A.8)
\]

\[
C_3 = [\tilde{r}_2 t + \tilde{t}_2 (1 - r)] e^{i (q_k - k)d}, \quad D_3 = t e^{i (k + q_k)d}. \quad (A.9)
\]

Thus, the unit cell wavefunction is entirely determined through the unit-cell and internal scattering matrices.

Recalling that the integrand of the Zak phase reduces to the curvature contributions of the wavefunction as in (13), we take the wavefunctions as \(\psi_{n,k}(x) = C_n e^{i q_k x} + D_n e^{-i q_k x}\) and are then able to show that we may operate the inner product \(\langle \psi_{n,k} | \partial_k \psi_{n,k} \rangle\), where we have dropped the band index \(m\) for clarity. However, the result is different depending on whether \(q_k\) is real or imaginary. When \(q_k = i \tilde{q}_k\) we have that:

\[
\int_{x_{n-1}}^{x_n} dx \left[ \psi_{n,k}^* (x) \partial_k \psi_{n,k}(x) \right] =
\]

\[
(C_n^* \partial_k C_n + D_n^* \partial_k D_n)(x_n - x_{n-1})
\]

\[
+ \frac{i}{2} (C_n^* D_n - D_n^* C_n) \partial_k \tilde{q}_k (x_n^2 - x_{n-1}^2)
\]

\[
+ \frac{1}{2 \tilde{q}_k} D_n^* \partial_k D_n (e^{2iq_k x_n} - e^{-2iq_k x_{n-1}} - 1)
\]

\[
- \frac{1}{2 \tilde{q}_k} C_n^* \partial_k C_n (e^{-2iq_k x_n} - e^{-2iq_k x_{n-1}} + 1)
\]

\[
- 4 \tilde{q}_k \partial_k \tilde{q}_k \left[ (e^{2iq_k x_n} - e^{-2iq_k x_{n-1}}) + 1 \right]
\]

\[
\int_{x_{n-1}}^{x_n} dx \left[ \psi_{n,k}^* (x) \partial_k \psi_{n,k}(x) \right] =
\]

\[
(C_n^* \partial_k C_n + D_n^* \partial_k D_n)(x_n - x_{n-1})
\]

\[
+ \frac{i}{2} (C_n^* D_n - D_n^* C_n) \partial_k \tilde{q}_k (x_n^2 - x_{n-1}^2)
\]

\[
- \frac{i}{2 \tilde{q}_k} D_n^* \partial_k D_n (e^{2iq_k x_n} - e^{-2iq_k x_{n-1}} - 1)
\]

\[
- \frac{i}{2 \tilde{q}_k} C_n^* \partial_k C_n (e^{-2iq_k x_n} - e^{2iq_k x_{n-1}} + 1)
\]

\[
- 4 \tilde{q}_k \partial_k \tilde{q}_k \left[ (e^{2iq_k x_n} - e^{-2iq_k x_{n-1}}) + 1 \right]. \quad (A.10)
\]
Appendix B. Relevant Solutions to the SSH Model

In the SSH model, the time-independent Schrödinger equation is solved as \( H |\psi\rangle = E |\psi\rangle \) in the basis of lattice sites. A general finite SSH model Hamiltonian, with the first (left-hand side) lattice site belonging to the A sublattice, takes the following form:[14]

\[
H = \sum_{i=1}^{N} \left[ V_i \hat{a}^\dagger_i \hat{a}_i + W_i \hat{b}^\dagger_i \hat{b}_i + \tau_i (\hat{a}^\dagger_i \hat{b}_i + \hat{b}^\dagger_i \hat{a}_i) \right] + \sum_{i=1}^{N-1} \tau'_i (\hat{a}^\dagger_{i+1} \hat{b}_i + \hat{b}^\dagger_i \hat{a}_{i+1}),
\]

where \( H.C. \) signifies to take the Hermitian conjugate and the summations are over the unit cells. The first sum involves hoppings within the unit cell whilst the second sum involves hoppings between unit cells. As a simple example, for a system of 2 unit cells, and thus 4 lattice sites for the even case and 5 lattice sites for the odd case, the following single-particle matrix Hamiltonians are generated:

\[
H_{\sigma} = \begin{pmatrix}
V_1 & v_1 & 0 & 0 \\
v_1 & W_1 & w_1 & 0 \\
0 & w_1 & V_2 & v_2 \\
0 & 0 & v_2 & W_2
\end{pmatrix},
\]

\[
H_{\sigma} = \begin{pmatrix}
V_1 & \tau_1 & 0 & 0 \\
\tau_1 & W_1 & \tau'_1 & 0 \\
0 & \tau'_1 & V_2 & \tau_2 \\
0 & 0 & \tau_2 & W_2
\end{pmatrix}.
\]

To emulate the first system considered within this paper, we take \( \tau_i = \tau, \tau'_i = 1 - \tau \), \( V_i = W_i = 10, \forall i \), whilst for the second system, we take \( v_i = w_i = 0.5, V_i = T, W_i = 10 - T, \forall i \).

In the thermodynamic limit, \( N \rightarrow \infty \), wherein periodic boundary conditions may be imposed, the Hamiltonian becomes two-dimensional in the unit cell basis. Then, it takes the form below:

\[
\mathcal{H}(k) = \begin{pmatrix}
V & \tau + \tau' e^{-ik} \\
\tau + \tau' e^{ik} & W
\end{pmatrix},
\]

where \( h(k) = \tau + \tau' e^{-ik} \) is the quantity that exhibits the appropriate topological winding. When \( \tau < \tau' \) then \( h(k) \) encloses the origin in its winding through the Brillouin zone whilst when \( \tau > \tau' \) it does not.

When \( V = W \), the resultant \( V\sigma_0 \) term is an arbitrary energy shift since it does not enter as a \( \sigma_z \) term. This is not the case when \( V \neq W \) since we may always say that \( V = X + Y \) and \( W = X - Y \) with appropriate \( X \) and \( Y \). Then chiral symmetry is broken by the entering of a \( \sigma_z \) term, which is seen in the finite band spectra. The migratory state is due to the mirror/reflection symmetry inherent in the odd finite chain.

One can also observe the invariant within the Zak phase as found from the wavefunction. The solution to \( \mathcal{H}(k) |\psi\rangle = E |\psi\rangle \) with \( V = W = 0 \) is \( |\psi\rangle = (1, \pm e^{-i\theta(k)})^T \) where \( e^{-i\theta(k)} = h(k) |h(k)|^{-1} \). Then, the Zak phase is:

\[
\theta_z = i \int_{-\pi}^{+\pi} dk \langle \psi | \partial_k \psi \rangle = \theta(\pi) - \theta(-\pi) = \begin{cases}
\pi, & \tau < \tau', \\
0, & \tau > \tau'.
\end{cases}
\]

Appendix C. Negative Potentials with Varying Heights

We now consider the case in which the distances between the potential scatterers are fixed to be equivalent and equal to \( d/2 \) whilst varying the potential heights. Again, the wavevector is made to be imaginary \( q_k \rightarrow iq_k \) however the potentials are varied as \( V_1 \rightarrow -W \) and \( V_2 \rightarrow -U + W \). The trigonometric functions within the transcendental equation become hyperbolic once more and so two roots for \( q_k \) are expected again.

The bulk energy spectra for two cases are shown in figures C1(a,b). The left has \( U = 20 \) and \( W = 9.9 \) whilst the right has \( U = 10 \) and \( W = 4.9 \). Interestingly, the bands have identical forms to the case of varying widths with the lowest point of the upper band at \( \max(V_1^2, V_2^2) \) and the highest point of the lower band at \( \min(V_1^2, V_2^2) \).

This comes as no surprise however since both are bipartite unit cells of bound states. The difference then comes as a result of the different physical origin and character of the bipartite-ness and the total absence of chiral symmetry. Indeed, the differing potential heights act as on-site potential terms, which in the SSH model destroys chiral symmetry, and the specification that \( v = w = d/2 \) causes the hopping probabilities to be...
identical. As such not only is the topological behaviour destroyed but also the very edge states themselves.

The finite system is solved and spectra are shown in figures C1(c,d). The potential heights are chosen as $|V_0| = W$ and $|V_2| = U - W$ with $U = 10$ and the widths of each well are set to $v = w = d/2$. As may be seen, a state is seen to migrate from the lower band to the upper band in the odd scatterer case, panel (c), as $W$ is increased across the transition point of $W = U/2$. As in the previous case, this is exactly the same result as one would find in the SSH model of the same configuration as is shown in Appendix B. Therefore, there is no topological protection here and in fact no edge states at all.

This can be explained physically by the following mirror symmetry argument. For an even number of scatterers there are equal numbers of small and large potentials. In this $N = 10$ case we have five small and five large for all $V_1$ and $V_2$. However, when $N$ is odd, this is not the case and there is a mismatch. For $N = 9$ there are five small and four large scatterers when $V_1 < V_2$. Thus, when $V_1$ becomes greater than $V_2$ this switches such that we have four small and five large. Thus, one of the five states that existed in the lower band with lower energy corresponding to one of the five small potentials is ejected to join the upper band, which now has higher energy, that also now corresponds to the five large potentials.

Appendix D. Positive Potentials with Varying Heights

Now we turn to, what would initially appear to be, the strongest candidate of all the considered systems for the hosting of topological edge states. In the positive heights case, the wavevector is real and so the local wavefunctions exist within the wells. All the wells are identical in this case since $V_0 = 0$ and $v = w = d/2$.

Thus, with analogy to the SSH model, the scatterer heights $V_1 = W$ and $V_2 = U - W$ would take the place of the hopping integrals $v, w$.

The bulk solution is solved and the band spectra are shown in figures D1(a,b). They may be seen to be almost identical to the previous positive case. The difference, however, is that the band gaps situated along $k = 0$ never close as a result of the modulation of $W$ as opposed to the previous case. As a result, the finite solution will show band closings and potential band crossings only when $V_1 = V_2$, i.e. $W = U/2$, which now has higher energy, that also now corresponds to the five large potentials.
whereat the gaps at $k = \pm \pi/d$ close.

The finite system is solved and the spectra are shown in figures D1(c,d). As may be seen, the only band crossings occur when $W = U/2$. A state may be seen to migrate between bands to the upper band only in the odd number of scatterer case by the same mirror symmetry argument as used throughout the previous cases.

The striking characteristic of these band spectra is the appearance of entirely flat bands. As it turns out, these are the $mN + 1$ bands where $m$ is an integer and their characters over the chain are shown in figure D2. As may be seen, they are effectively entirely localised with equal weight within each well with zero overlap between the wells. Indeed, this is the very reason for their flatness. Since they do not occur within a band-gap, wherein the wavevector must be imaginary, they are not themselves edge states.