Emergent Non-Hermitian Effects in an Hermitian Tight-binding Model

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An analytical tight-binding calculation is implemented for the bipartite Kronig-Penney model in the presence of negative Dirac-delta potentials. Due to the non-negligible influence of the overlap between neighbouring sites, the resulting tight-binding eigenvalue problem is non-Hermitian and the bulk Hamiltonian is $PT$-symmetric. As a result, the energy eigenvalues are real, the topological invariant is given by a bulk winding number of $Z$-type yet the edge states display the non-Hermitian anomalous skin-effect of attenuation and amplification at either end of the finite chain.

I. INTRODUCTION

The field of topological protection in non-Hermitian systems continues to grow at pace\textsuperscript{1–11}. The study of non-Hermitian systems in general has historically been eschewed on the basis of non-physicality\textsuperscript{12–14}. Indeed, in paradigmatical quantum mechanical Hamiltonian eigenvalue problems, the Hermiticity of said Hamiltonians i) guarantees the reality of the resultant energy eigenvalues, ii) enforces the required unitarity of the time-evolution of the system, and iii) ensures that left and right eigenvectors are identically equivalent.

Quantum mechanics, and specifically the Schrödinger equation, was initially formulated to describe electronic excitations in the presence of spatially varying potentials. In such a paradigm, the electrons do not have a ‘lifetime’ in that they do not spontaneously decay. Then, provided there is invariance in time, the wavefunction may be decomposed using Fourier time-components: $\Psi(r,t) = \psi(r)e^{iEt/\hbar}$. As such, their energies ought to be real in all cases such that there is no imaginary component that would cause a temporal decay of the particle.

However, as the ideas of quantum mechanics permeate into more complex systems, this fixation upon the Hermiticity of eigenvalue problems has been relaxed as the constituent excitations are capable of temporal decay, in the cases of, e.g., excitons\textsuperscript{15}, plasmons\textsuperscript{16,17}, and phonons\textsuperscript{18,19}, or of variations in their phase through gain and loss in the case of, e.g., photons\textsuperscript{20,21} or plasmons\textsuperscript{22}. As a result, the field of non-Hermitian topological protection has been delved into in earnest with a more general 36-fold way of non-Hermitian topological invariants being developed\textsuperscript{5,23}.

In such systems, radical departures from the basic Hermitian model are observed. For example: i) the emergence of exceptional points whereat the bulk bands develop imaginary components\textsuperscript{24–27}, ii) a richer variety of topological protections due to the increased number of possible symmetries\textsuperscript{23,28}, iii) the non-Hermitian skin effect in the absence of chiral symmetry\textsuperscript{29–31}, and iv) the non-Hermitian anomalous skin effect wherein edges states are attenuated and amplified in the presence of chiral symmetry\textsuperscript{29,32,33}. This final effect shall be the most relevant for the present work.

The system we consider herein is a bipartite Kronig-Penney\textsuperscript{34,35} model with negative-strength Dirac-delta potentials, as shown in figure 1, that is constructed in order to effectively mimic the SSH model\textsuperscript{36,37}. The bipartition may be achieved by either varying the distances or the baseline potentials between the two Dirac-deltas within and without the unit-cell. It is crucial that the strengths of the Dirac-delta potentials themselves are made to be identical. In this way, no on-site potential is introduced that would trivially distinguish the sublattices within the tight-binding model. As such, chiral symmetry is not destroyed trivially from the get-go.

The paper is divided into five parts. Firstly, the simple tight-binding Schrödinger equation is introduced for the present system whose tight-binding parameters are derived in Appendix C. Secondly, the bulk solution is investigated wherein the low-energy effective Hamiltonian is seen to be non-Hermitian as a result of the overlap matrix. The topology is shown, however, to be exactly the same as in the standard Hermitian SSH model thereby symmetry-protecting the edge states. Thirdly, the finite solution is presented through a simple second quantisation procedure upon the tight-binding model. Fourthly, results for the two cases in which the distances and baseline potentials are varied are presented separately. In both cases, the non-Hermitian anomalous skin effect is observed. Finally, conclusions are drawn upon the nature of this theory in relation to general tight-binding models.
II. THE TIGHT-BINDING SCHRÖDINGER EQUATION

The bulk tight-binding time-independent Schrödinger equation (TISE) that applies to the unit-cell as shown in Fig. 1 reads \( H(k)\psi_k = E(k)S(k)\psi_k \). Explicitly, it takes the following form:

\[
\begin{pmatrix}
\epsilon & h(k) \\
(h^*(k) & \epsilon)
\end{pmatrix}
\begin{pmatrix}
C_{A,k} \\
C_{B,k}
\end{pmatrix} = E(k)
\begin{pmatrix}
1 & g(k) \\
g^*(k) & 1
\end{pmatrix}
\begin{pmatrix}
C_{A,k} \\
C_{B,k}
\end{pmatrix},
\]

(1)

The detail of the on-diagonal matrix element \( \epsilon \) is unimportant, however it may not be trivially ignored at this point due to the presence of non-zero off-diagonal elements within \( S(k) \), and the nearest-neighbour off-diagonal matrix elements are \( h(k) = te^{ikv} + t' e^{-ikw} \) and \( g(k) = \eta e^{ikv} + \eta' e^{-ikw} \). The analytic calculation of all the tight-binding parameters \( \epsilon, t, t', \eta, \eta' \) may be found in the Appendix C, and it is guaranteed by the validity of the tight-binding approximation that \( \epsilon, t, t' < 0 \) and \( 0 \leq \eta, \eta' \leq 1 \).

The convention in most tight-binding approximations is to simply ignore the overlap matrix because it either does not contribute meaningfully due to its negligibility when compared with the Hamiltonian matrix, as is the case in the SSH model\(^{36,38,39} \), or it has no effect on the interesting low-energy physics that occurs within the vicinity of the Fermi energy, as is the case in graphene\(^{40,41} \). However, in the present case, neither of these situations is in principle realised.

As such, the low-energy effective Hamiltonian that defines a well posed energy-eigenvalue matrix equation \( \mathcal{H}(k)\psi_k = E(k)\psi_k \), whose eigenvectors \( \psi_k \) are crucially unchanged, is \( \mathcal{H}(k) = S^{-1}(k)H(k) \) where:

\[
\mathcal{H}(k) = \begin{pmatrix}
\epsilon(k) + i\gamma(k) & f(k) \\
f^*(k) & \epsilon(k) - i\gamma(k)
\end{pmatrix},
\]

(2)

and the matrix elements are:

\[
\begin{align*}
\epsilon(k) &= [\epsilon - \eta t - t' \eta' - (t' \eta + \eta t)\cos(kd)](1 - |g(k)|^2)^{-1}, \\
f(k) &= [h(k) - \epsilon g(k)](1 - |g(k)|^2)^{-1}, \\
\gamma(k) &= [t\eta' - t'\eta] \sin(kd)(1 - |g(k)|^2)^{-1}.
\end{align*}
\]

(3)

This effective Hamiltonian is then in an identical form to the one previously studied in Ref. 10.

As such, the Schrödinger equation is now: \( \mathcal{H}(k)\psi_k = E(k)\psi_k \), and the low-energy effective Hamiltonian, since it is a 2x2 matrix, may be decomposed in terms of the Pauli matrices \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) as:

\[
\mathcal{H}(k) = d_0(k)I_2 + d(k) \cdot \sigma,
\]

(4)

where \( d_0(k) = \epsilon(k) \) and \( d(k) = (d_x(k), d_y(k), d_z(k)) \) with \( d_x(k) = \text{Re}[f(k)], \quad d_y(k) = \text{Im}[f(k)] \) and \( d_z(k) = i\gamma(k) \).

In the simple SSH Hermitian system, \( d_z = 0 \) and so the topological invariant that protects via the presence of chiral symmetry resides within the winding of \( d = (d_x, d_y, 0) \). This also applies within non-Hermitian systems wherein \( d_x \neq 0 \) as long as it is possible to adiabatically deform the two systems to one another. As such, the \( d_0(k)I_2 \) is not important with respect to the topological information and symmetry protection. Indeed, its contribution to the eigenvalues may be trivially removed without affecting the underlying topology of the Hamiltonian\(^{42} \).

However, an important point must be made that may be overlooked about the matrix elements \( h(k) \) and \( g(k) \). Since they exist upon the off-diagonals of \( H(k) \) and \( S(k) \), they are in fact defined up to a phase. This ‘gauge’ ambiguity is present in all tight-binding models be they the SSH model\(^{36} \) or that for graphene.\(^{43} \) If the problem were to be solved without addressing this issue now, then the (non-Hermitian) Zak phase\(^{29,44} \), \( \theta_Z \), as given by:

\[
\theta_Z = i\int_{-\pi/d}^{+\pi/d} dk \left[ \langle \psi_L | \partial_k | \psi_L \rangle + \langle \psi_R | \partial_k | \psi_R \rangle \right],
\]

(5)

where \( L, R \) signify the normalised left and right eigenvectors of \( \mathcal{H}(k) \), would be quantised into units of \( \pi \) plus the intra-unit-cell width \( v \).\(^{37} \) Furthermore, the winding of \( f(k) \) would not be well-defined as zero or one in the trivial and non-trivial regions, respectively.

This is in fact exactly the same ambiguity encountered when dealing with the exact system\(^{37} \), which was solved by Zak\(^{45} \) originally. In both cases, the objective is to make the unit-cell wavefunction centro-symmetric about the unit-cell mid-point.

In the real-space solution, the wavefunction has to be symmetric about the middle of the unit-cell such that no extra contribution to \( \theta_Z \) is acquired as a result of the imbalance in ‘polarisation’ across the unit-cell. Here, as is clear in the expressions for \( h(k) \) and \( g(k) \), a similar effect is manifest in that there is a phase difference of \( e^{ikv} \) between the two sites that constitute the unit-cell basis. As a result, a calculation of \( \langle \psi_L | \partial_k | \psi_L \rangle \) will yield this phase in addition to the standard curvature contribution. Then we would have that \( \theta_Z = v, \pi + v \) within the trivial and non-trivial regions respectively; an ill-defined and unquantised number.

Thus, instead of \( h(k) = te^{ikv} + t'e^{-ikw} \) and \( g(k) = \eta e^{ikv} + \eta' e^{-ikw} \), we should have \( h(k) = t + t'e^{-ikd} \) and \( g(k) = \eta + \eta' e^{-ikd} \). This may be accomplished simply by defining \( \tilde{H}(k) = U(k)H(k)U^{-1}(k) \), \( \tilde{S}(k) = U(k)H(k)U^{-1}(k) \), and \( \tilde{\psi} = U(k)\psi \) where:

\[
U(k) = \begin{pmatrix}
e^{ikv/2} & 0 \\
0 & e^{-ikv/2}
\end{pmatrix}.
\]

(6)

Then, dropping the tildes for brevity and clarity, the new effective Hamiltonian \( \mathcal{H}(k) = S^{-1}(k)\mathcal{H}(k) \) is identical to the old one except that the off-diagonal elements are now in terms of the newly-defined \( h(k) \) and \( g(k) \). As a result, these elements now look identical to the standard SSH model, which is known to host topological chiral-symmetry protected edge states\(^{36} \).
III. THE BULK SOLUTION

Solving the above eigenvalue problem presented through Eq. (2), we find that:

\[ E_{\pm}(k) = \varepsilon(k) \pm \sqrt{f(k)^2 - \gamma^2(k)}, \]

and so, if \( \gamma(k) > |f(k)| \) then we have complex energy solutions. Indeed, this may be seen in a clearer fashion by using Eq. (3) to observe that:

\[ E_{\pm}(k) = \varepsilon(k) \pm \frac{\sqrt{\nu^2 + \omega^2 + 2\nu\omega \cos(kd) - \beta^2 \sin^2(kd)}}{1 - |g(k)|^2}, \]

where \( \nu = t - \eta \epsilon, \omega = t' - \eta' \epsilon \) and \( \beta = t \eta' - t' \eta \).

Since the band gaps are defined at the edge of the Brillouin zone at \( k = \pm \pi/d \), we see that the topological phase transition is governed solely by the behaviours of \( \nu \) and \( \omega \) with respect to each other. The value of \( \beta \) then determines whether any region within the Brillouin zone possesses complex energies and as a result introduces the concept of exceptional points.

The argument of the square-root in Eq. (8) may be manipulated to become:

\[ F(\phi) = (\nu + \omega)^2 + 4 \cos^2(\phi) [\nu \omega - \beta^2 \sin^2(\phi)], \]

where \( \phi = kd/2 \). This expression is clearly always positive if \( \nu \omega > \beta^2 \) however, when \( \nu \omega < \beta^2 \), it may become negative depending on the value of \( \phi \). The minimum of this may be shown to occur when \( \cos(2\phi_{\min}) = -\nu \omega / \beta^2 \). Thus, at this minimum point, the argument evaluates as:

\[ F(\phi_{\min}) = -(\omega^2 - \beta^2)(\nu^2 - \beta^2)\beta^{-2}. \]

In order that \( F(\phi_{\min}) < 0 \) it must be that either \( |\omega| > |\beta| \) and \( |\nu| > |\beta| \) or \( |\omega| < |\beta| \) and \( |\nu| < |\beta| \). However, since it is also required that \( \nu \omega < \beta^2 \), the only way in which \( F(\phi_{\min}) \) may be negative is if \( |\omega| < |\beta| \) and \( |\nu| < |\beta| \), as was first presented by Yuce and Oztas.

This is never achieved within physical tight-binding models, however, as it ought not to. This may be understood either numerically for the present system, as is shown in Appendix A, or qualitatively by considering the dimmerised and non-bipartite limits of the system. When totally dimerised it will be that \( t \rightarrow t_{\text{max}} = \tau, t' \rightarrow 0 \), \( \eta \rightarrow 1, \eta' \rightarrow 0 \) such that \( t \eta' \) and \( t' \eta \) both remain non-zero so that \( \beta \neq 0 \). Then \( \nu \rightarrow \tau - \epsilon, \omega \rightarrow 0, \beta \sim 0 \) (or in the opposite dimerised limit \( \nu \rightarrow 0, \omega \rightarrow \tau - \epsilon, \beta \sim 0 \)). So in this limit, \( |\omega| < |\beta| \) yet \( |\nu| > |\beta| \) and so \( F(\phi_{\min}) \) cannot be negative at these limits.

This is true unless it becomes that \( |\tau| > |\epsilon| \) in which case \( |\nu| < |\beta| \) and so \( F(\phi_{\min}) \) becomes negative. This scenario may not occur physically, however, since it would indicate that it is energetically more favourable to execute a hop between lattice sites than it is to remain on the current site. In other words, the basis upon which the tight-binding model is built was poorly chosen. This may be seen most clearly in Fig. 2(a) wherein \( F(\phi_{\min}) \) is plotted in the \( t - \eta \) plane. The black regions indicate the areas in which \( F(\phi_{\min}) < 0 \), which begin at the points \( t = \pm |\epsilon| \) for \( \eta = \eta' = 1 \):

\[ t = \eta(t'\eta' - \epsilon) \pm (t' - \eta' \epsilon) \sqrt{\eta^2 + \eta'^2 - 1}, \quad \forall \eta, \eta' \neq 1, \]

The other limit is when the bipartition vanishes at the band gap closing point whereat \( t = t' = \eta' = 0 \) such that \( \nu = \omega = 0 \). Clearly, here, \( |\nu| > |\beta| \) and \( |\omega| > |\beta| \) and so \( F(\phi_{\min}) \) cannot be negative here either.

As a result, in all physical tight-binding models, the bands are always real. This has the added caveat that the exceptional points defined by \( |f(k)| = |\gamma| \) in fact annihilate one another as they coincide with the topological transition point whereat \( \nu = \omega \) and \( k = \pm \pi/d \).

This result follows naturally since the original Hamiltonian of our problem is demonstrably Hermitian in nature. It is the only effective low-energy tight-binding Hamiltonian that has a non-Hermitian character. Moreover, this non-Hermitian character enters in since we may not neglect the overlap of the neighbouring basis wavefunctions. As such, we say that this Hamiltonian is \( \mathcal{PT} \)-symmetric since it possesses real eigenvalues in the absence of Hermiticity. Yet, as will be seen, this non-Hermiticity is highly non-trivial with respect to the behaviours of the edge states. Indeed, it must be stressed that this-to-be-seen behaviour is a physical effect of the system and not an artefact of the tight-binding approximation; the exact solution to the problem exhibits this same phenomenon.

The \( \mathcal{PT} \)-symmetry operator is given by \( \mathcal{PT} = \sigma_z K \) where \( K \) is the complex conjugation operator. Then it is clear that \( [\mathcal{PT}, \mathcal{H}] = 0 \). Since \( |f(k)|^2 - \gamma^2(k) > 0 \) always, as above, the present class of Hamiltonian may be adiabatically deformed into its Hermitian counterpart. This is because, as long as the band gap does not close in such a deformation, then the exceptional points are never encountered. Then, through a simple transformation, the \( \gamma(k) \) term may be eliminated from the tight-binding Hamiltonian. Hence the topological character is that of the basic SSH model, i.e. non-trivial, and is given by the \( \mathcal{Z} \)-invariant that resides in the winding number of the off-diagonal element \( f(k) \) (or the Zak phase).

In fact, since the advent of non-Hermitian topological classifications, we may go further and identify that this Hamiltonian belongs to the BDI class that is characterised by the following symmetries: particle-hole (PHS), time-reversal (TRS), and chiral (CS). Mathematically, these are expressed as:

\[ \begin{align*}
\text{PHS} & : \hat{C}^{-1} \mathcal{H}^\mathcal{T}(k) \hat{C} = -\mathcal{H}(-k), \\
\text{TRS} & : \hat{T}^- \mathcal{H}^* (k) \hat{T}^- = \mathcal{H}(-k), \\
\text{CS} & : \hat{\Gamma}^{-1} \mathcal{H}^\mathcal{T}(k) \hat{\Gamma} = -\mathcal{H}(k),
\end{align*} \]

where \( \hat{C} = \sigma_z, \hat{T}^- = \mathbb{1}_2 \) and \( \hat{\Gamma} = \hat{C} \hat{T}^- = \sigma_z \). As such, it possesses chiral symmetry guaranteed by \( \hat{\Gamma} = \sigma_z \).
However, and this is the crucial difference with Hermitian problems, the chiral and sublattice symmetries are not identical. The definition of sublattice symmetry is\textsuperscript{23}:

\begin{equation}
\text{SLS} : \hat{S}^{-1} \mathcal{H}(k) \hat{S} = -\mathcal{H}(k),
\end{equation}

which may be shown to be present for the current effective Hamiltonian with \( \hat{S} = \sigma_z - i\gamma(k)(\sigma_x - i\sigma_y)/f(k) \). It is clear then that these two symmetries (chiral and sublattice) coincide in the Hermitian limit wherein \( \gamma(k) \to 0 \). It is interesting to note that this sublattice symmetry operator is \( k \)-dependent and acts upon the wavefunctions to mix their weights \( c_A \) and \( c_B \) together (due to the presence of the off-diagonal Pauli matrices \( \sigma_{x,y} \)).

Now, since the effective Hamiltonian \( \mathcal{H}(k) \) belongs to the BDI class, according to the periodic table of invariants\textsuperscript{8} we seek a \( \mathbb{Z} \oplus \mathbb{Z} \) invariant, \textit{i.e.} the sum of two separate and distinct invariants.

These invariants are the parametric winding number in the complex plane of the off-diagonal matrix element\textsuperscript{36}, here \( f(k) \), which may be calculated through:

\begin{equation}
\mathcal{W} = \frac{1}{2\pi i} \int_{-\pi/d}^{+\pi/d} dk \frac{d}{dk} \ln[f(k)],
\end{equation}

and shown to be equivalent to the Zak (one-dimensional Berry) phase, and the winding number of the imaginary part of the energy.\textsuperscript{30,46} Since the energy is always real, this second winding number is identically zero and so we seek the simple \( \mathbb{Z} \)-invariant given by the winding number of \( f(k) \), \( \mathcal{W} \), as one would expect since this non-Hermitian system inherits its topological character from its Hermitian counterpart.

A crucial point to make here, this being the novel aspect of this paper, is that the analysis of the topological character of the above Hamiltonian is in fact completely general. It does not only apply to the present Kronig-Penney system. Given a tight-binding Schrödinger equation as in Eq. (1), the effective Hamiltonian will always be non-Hermitian and \( \mathcal{PT} \)-symmetric as in Eq. (2). Therefore, the overlap matrix within all tight-binding models will act to attenuate or amplify any edge states observed in the system; an effect that will be seen subsequently.

Moreover, the addition of the further overlap variables, \( \eta \) and \( \eta' \) within the bulk tight-binding model leads to a modified phase space for the winding number \( \mathbb{Z} \)-invariant.

The band gaps defined through Eq. (8) close at \( \nu = \omega \), \textit{i.e.} \( t - \eta e = t' - \eta' \epsilon \), and so:

\begin{equation}
\eta = (t - t')\epsilon^{-1} + \eta',
\end{equation}

defines the topological transition point in the phase-space of \( t - \eta \). When there is no overlap, in which case \( \eta = \eta' = 0 \), the transition point is \( t' = t \), as expected. However, when not so, \( \eta \) varies linearly with \( t \) with a gradient of \( \epsilon^{-1} \) and \( \eta \)-intercept of \( \eta' = t' - t^{-1} \) as may be seen in Fig. 2(b). This then shines light on one of the important points of this work; namely that the influence of \( \epsilon \) is only relevant if there is a finite overlap between neighbouring sites, \( \eta, \eta' \). Indeed, within \( E(k) \), \( \epsilon \) may be ignored as a trivial energy shift if (and only if) \( \eta = \eta' = 0 \). So too here is the topological transition unaffected by \( \epsilon \) if \( \eta = \eta' = 0 \).

Within the tight-binding Kronig-Penney model the phase space ought to be restricted to the positive quadrant, \( \eta, \eta' > 0 \) and \( t, t' > 0 \), since there is no effect, akin to a gauge potential or gain and loss, that would alternately change the signs of the nearest-neighbour tight-binding parameters.

### IV. THE FINITE SOLUTION

To solve the finite system we now go beyond first quantisation, wherein the tight-binding parameters were determined, and extend to a second quantisation in terms of ladder operators. To do so, we consider the Schrödinger equation within the bulk as initially defined in Eq. (1) and postulate the second quantised full-chain Hamiltonian and overlap operators that would generate this bulk equation upon the imposition of periodic boundary conditions, \textit{i.e.} Bloch’s theorem. Such a postulation is a simple task since only nearest-neighbour interactions are considered. So \( \hat{H} |0\rangle = E\hat{S} |0\rangle \) is found where \( |0\rangle \) is the vacuum state and the Hamiltonian and overlap operators are expressed in terms of lattice-site creation and annihilation operators, \( \hat{c}_{\alpha i}^{\dagger} \) and \( \hat{c}_{\alpha i} \) respectively, as:

\begin{equation}
\hat{H} = \sum_i \left[ \epsilon \left( \hat{c}_{A i}^{\dagger} \hat{c}_{A i} + \hat{c}_{B i}^{\dagger} \hat{c}_{B i} \right) + t \left( \hat{c}_{A i}^{\dagger} \hat{c}_{B i} + \hat{c}_{B i}^{\dagger} \hat{c}_{A i} \right) + t' \left( \hat{c}_{A(i+1)}^{\dagger} \hat{c}_{B i} + \hat{c}_{B i}^{\dagger} \hat{c}_{A(i+1)} \right) \right],
\end{equation}
\[
\hat{S} = \sum_i \left[ \left( \hat{c}_{A_i} \hat{c}_{A_i} + \hat{c}_{B_i} \hat{c}_{B_i} \right) + \eta \left( \hat{c}_{A_i} \hat{c}_{B_i} + \hat{c}_{B_i} \hat{c}_{A_i} \right) + \eta' \left( \hat{c}_{A_{(i+1)}} \hat{c}_{B_i} + \hat{c}_{B_i} \hat{c}_{A_{(i+1)}} \right) \right],
\]  

(17)

This also makes demonstrably clear the gauge ambiguity in defining the positions of the lattice sites within the unit cell. When Fourier-transforming the ladder operators they may always be chosen up to an arbitrary phase, which manifests itself non-trivially in the calculation of any geometric phases within the bulk.

Then, the matrix eigenvalue equation \( \hat{H} |0\rangle = E \hat{S} |0\rangle \) must be solved numerically for an arbitrary number of unit cells. Edge and defect states should then be observed at the junction of two separate chains that have differing bulk topological invariants. At the edges the chain terminates with the vacuum and, since the vacuum always has a bulk invariant of zero, if the unit cell is topologically non-trivial then edge states will exist.

In this context, the total wavefunction is simply \( \Psi(x) = \sum_i |c_{A_i}\Psi_A(x, x_{A_i}) + c_{B_i}\Psi_B(x, x_{B_i})\rangle \), where \( c_{\alpha i} \) are the weightings of the wavefunction upon the lattice site \( i \) of the sublattice \( \alpha \) and the wavefunctions \( \Psi_\alpha(x, x_{\alpha i}) \) are those as shown in Eq. (C2) and derived in Appendix B.

Then, typical Hamiltonian and overlap matrices (with \( N = 3 \) as an example) would be:

\[
\begin{align*}
\hat{H} & = \begin{pmatrix}
\varepsilon & t & 0 & 0 & 0 & 0 \\
t & \varepsilon' & 0 & 0 & 0 & 0 \\
0 & t' & \varepsilon & 0 & 0 & 0 \\
0 & 0 & t & \varepsilon' & 0 & 0 \\
0 & 0 & 0 & t & \varepsilon & 0 \\
0 & 0 & 0 & 0 & 0 & \varepsilon
\end{pmatrix}, \\
\hat{S} & = \begin{pmatrix}
1 & \eta & 0 & 0 & 0 & 0 \\
\eta & 1 & \eta' & 0 & 0 & 0 \\
0 & \eta' & 1 & \eta & 0 & 0 \\
0 & 0 & \eta & 1 & \eta' & 0 \\
0 & 0 & 0 & \eta' & 1 & \eta \\
0 & 0 & 0 & 0 & \eta & 1
\end{pmatrix},
\end{align*}
\]

(18)

where \( \varepsilon \) is a different on-site potential that occurs at the edges. It must be stressed that solving the problem with these modified edge on-site potentials does not affect the symmetry protection of the states since this is guaranteed by the presence of chiral symmetry within the bulk Hamiltonian, which is maintained here. It is only the boundary conditions that change. This is again a demonstration of the effect of the overlap matrix since all on-site potentials may be ignored when \( \eta = \eta' = 0 \) but, when this is not the case, the on-site potentials are the edges are crucially important.

V. RESULTS

Having obtained the full tight-binding Schrödinger equation \( \hat{H} |0\rangle = E \hat{S} |0\rangle \) in second quantised form and in terms of the relevant system parameters, as in Eqs. (16,17), the solution from this point is a numerical one. We consider here two separate scenarios.

The first is to consider the case in which only the distances between the Dirac-delta potentials are modulated with the baseline potentials kept constant and equal to zero. This therefore mimics the system as initially studied in Ref. 37. The second is to consider the opposite case in which the distances are held constant whilst varying the baseline potentials between the delta potentials.

In the first case, the tight-binding parameters, as shown in Eq. (C4), in fact simplify under the prescription that \( V_e = V_w = 0 \) (see Fig. 1 for details of \( V_{e,w} \)) to:

\[
\begin{align*}
\varepsilon & = E_0 \left[ 1 + 2 \left( e^{-2\kappa v} + e^{-2\kappa w} + 2e^{-2\kappa d} \right) \right], \\
t & = E_0 (3 + \kappa v) e^{-\kappa v}, \quad t' = E_0 (3 + \kappa w) e^{-\kappa w}, \\
\eta & = (1 + \kappa v) e^{-\kappa v}, \quad \eta' = (1 + \kappa w) e^{-\kappa w},
\end{align*}
\]

(19, 20, 21)

where \( E_0 = -\hbar^2 \kappa^2 / (2m) \) is the energy of a lone symmetric Dirac-delta of potential \( V \) and \( \kappa = -mV/\hbar^2 \). Then, in order to mimic Ref. 37, we take natural units

FIG. 3. (Colour on-line) A selection of figures applying to the system wherein only the distances between the Dirac-deltas are varied. Panel (a): the bulk bands with \( v = .49, w = .51 \). Panel (b): the bulk bands with \( v = .3, w = .7 \). Panels (c,d): the finite bands for \( N = 19 \) (b) and \( N = 20 \) (c) lattice sites with \( v = a, w = 1 - a \) and boundary conditions as in Eq. (22). Panels (e,f): the 10th (e) and 11th (f) edge state wavefunctions for \( a = .55 \) corresponding to the mid-gap modes of panel (d). Panels (g,h): the same edge state wavefunctions for \( a = .8 \).
of $h = m = 1$, a Dirac-delta strength of $V = -10$ and vary the distances between the Dirac-deltas as $v = a$ and $w = d - a$ such that the unit-cell length, which will be taken to be $d = 1$, remains constant.

Then, using Eq. (8), the bulk bands of the system may be plotted for a range of values for the $a$-parameter, a pair of which are shown in Figs. 3(a,b). As observed, for $a \sim d/2$, the bands appear similar to the conventional Hermitian SSH model with a mid-gap point given by $E_0 = -mV^2/(2h^2)$. However, as $a$ departs from this value the bands flatten, which is not unusual, but the mid-gap point departs from $E_0$ as a result of the exponential terms in Eq. (19).

As mentioned, the precise construction of the boundary conditions for the finite chain is integral. Within the bulk, the on-site potential is uniform and is given by $\epsilon$ in Eq. (19). However, the derivation of this expression is within the nearest-neighbour approximation in the bulk. At the edge, there is only one nearest-neighbour. As such, the on-site potentials of the edges are in fact:

$$\epsilon_v = E_0 \left[ 1 + 2e^{-2\kappa v} \right], \quad \epsilon_w = E_0 \left[ 1 + 2e^{-2\kappa w} \right],$$

where $\epsilon_v$ and $\epsilon_w$ apply if the final hopping is of the $v$-type, $t$, or $w$-type, $t'$, respectively. This boundary condition generates the band spectra as shown in Fig. 3(c,d) and corresponds to ‘open’ boundary conditions whereby the states are allowed to decay to infinity at the edges. As may be seen, there exist mid-gap edge states in both cases of $N = 19$ and $N = 20$ that are seemingly identical to the standard SSH solution$^{36}$.

As may be seen in Figs. 3(e,f), the edge state wavefunctions of the even $N = 20$ case are confined to a single sublattice only, i.e. all $c_B$ components are identically zero, thereby showing it to be an eigenstate of the chiral operator $\hat{\Gamma} = \sigma_z$ and thus protected by the presence of this symmetry$^{46}$. Furthermore, as shown in Figs. 3(g,h), it displays the non-Hermitian phenomenon of attenuation and amplification at either edge as a result of the $i\gamma(k)$ term within the bulk effective Hamiltonian.

Now, for the second case, we take the distances to be constant as $v = w = d/2$ with $d = 1$ and vary the baseline potentials symmetrically as $V_v = +T$ and $V_w = -T$ whilst maintaining the Dirac-delta potentials strengths as $V = -10$. As a result, the wavevectors read:

$$\kappa_v = \kappa + \frac{T}{V}, \quad \kappa_w = \kappa - \frac{T}{V}.$$  

Now, provided that $|T|$ never exceeds $V^2$, these wavevectors will always be positive as required for bound solutions. There thus comes a point in $|T|$ whereat the present theory breaks down. Furthermore, for sufficiently large $|T|$, next-nearest-neighbour interactions will begin to become influential.

In this case, the tight-binding parameters read:

$$\epsilon = -\frac{h^2}{2m} \left( \kappa^2 - \frac{T^2}{V^2} \right) \left[ 1 + 4 \left( \cosh \left( TdV^{-1} \right) e^{-\kappa d} + \cosh \left( 2TdV^{-1} \right) e^{-2\kappa d} \right) \right],$$

$$t = -\frac{h^2}{2m} \left( \kappa^2 - \frac{T^2}{V^2} \right) \left[ \frac{1}{2\kappa} \left( \kappa^2 + \frac{T^2}{V^2} \right) + \left( \kappa^2 + 2\kappa \frac{T}{V} + \frac{T^2}{V^2} \right) d \right] e^{-Td(2V)^{-1} + 2\cosh \left( Td(2V)^{-1} \right)} e^{-\kappa d/2},$$

$$t' = -\frac{h^2}{2m} \left( \kappa^2 - \frac{T^2}{V^2} \right) \left[ \frac{1}{2\kappa^2} \left( \kappa^2 + \frac{T^2}{V^2} \right) + \left( \kappa^2 - 2\kappa \frac{T}{V} + \frac{T^2}{V^2} \right) d \right] e^{+Td(2V)^{-1} + 2\cosh \left( Td(2V)^{-1} \right)} e^{-\kappa d/2},$$

$$\eta = \frac{1}{2} \left( 1 - \frac{T^2}{\kappa^2 V^2} \right) \left[ \kappa Td^{-1} e^{-Td(2V)^{-1}} + 2\cosh \left( Td(2V)^{-1} \right) \right] e^{-\kappa d/2},$$

$$\eta' = \frac{1}{2} \left( 1 - \frac{T^2}{\kappa^2 V^2} \right) \left[ \kappa Td^{-1} e^{+Td(2V)^{-1}} + 2\cosh \left( Td(2V)^{-1} \right) \right] e^{-\kappa d/2}.$$  

Fig. 4 shows all the relevant plots of the bulk bands, finite bands and edge states of this second system under consideration. In panels (a,b), the bulk bands appear SSH-like however in panel (c), whereat $T = 25$, both bands have clearly ‘inverted’. This phenomenon is mirrored in the finite system where the lower(upper) bulk bands touch at around $T \sim \pm 20(\pm 25)$.

These are unphysical effects that emerge as a result of the negligence of next-nearest-neighbour hoppings. Indeed, when $T = 25$ then $\kappa_w = 7.5$ and $\kappa_v = 12.5$ at which point the motivation for the ignorance of next-nearest-neighbour hoppings, which are proportional to $e^{\pm TdV^{-1}}$, becomes unfounded. Such terms are non-illuminating and so will not be presented. Suffice it to say that the protection of the edge states, in this case with $V = -10$ and $d = 1$, only extends up to $|T| \sim 25$. After this point nothing concrete may be said about the natures of the edge states since the nearest-neighbour assumption becomes invalid.

However, within the nearest-neighbour limit of $|T| < 25$, the edge states, as shown in panels (c,f,g,h), exhibit the same behaviours of being initially Hermitian, wherein the edge states are shared equally between the ends, but later non-Hermitian, wherein the edge states are atten-
V. SUMMARY AND CONCLUSION

A tight-binding approximation of the Kronig-Penney model in the presence of negative strength Dirac-delta potentials has been developed. In doing so, it became apparent that the overlap matrix, which is often ignored for simplicity, had a non-trivial influence on not only the physics within the bulk but also on the behaviour and nature of the topological edge states in the finite system.

Such a matrix caused the effective Hamiltonian to be non-Hermitian and to in fact belong to the BDI class of topological invariants. As such, the sought invariant was \( \mathbb{Z} \oplus \mathbb{Z} \) where these invariants were the winding numbers of the off-diagonal matrix element and the imaginary part of the energy. Since the original system was Hermitian, it had to be that the energy eigenvalues were real even in the low-energy description. As such, the Hamiltonian was observed to be \( \mathcal{PT} \)-symmetric thereby allowing it to be adiabatically deformed to its Hermitian counterpart. As a result, it inherited the topology of its Hermitian counterpart, which is a \( \mathbb{Z} \)-invariant given by the winding of the off-diagonal matrix element or the Zak phase.

One might ask to the relevance of the revelation that the overlap matrix may not be ignored in certain cases but not in others. Indeed, when considering the elementary system of polyacetylene, which the basic SSH model was developed to describe, the \( sp \)-\( 1 \) hybridisation of the carbon atoms presupposes the negligibility of the overlap matrix. The in-plane carbon atoms form alternately single and double covalent bonds with their neighbours through their \( 2s \), \( 2p_z \) and \( 2p_y \) orbitals leaving a single electron free in the \( 2p_z \) orbital. This electronic state then forms the tight-binding model for the lattice, which is the SSH model. Such a \( 2p_z \) orbital is extremely well-localised and so the overlap between neighbouring sites is minimal.

However, as we have seen here, the overlap matrix plays an important role if the basis wavefunctions do not possess this supremely strong localisation or if they are brought together thereby causing the functions to have an enhanced overlap. Indeed, this has been investigated before\(^{41} \) but not in relation to any topological edge states.

Yet, the topological protection of edge states is not unique to electronic systems. Indeed, since it is a feature of wave-like excitations (recall that the topological character may be found within the wavefunction through the Zak or Berry phase), symmetry protected states may be observed in photonic\(^ {47-50} \), phononic\(^ {51-53} \), magnonic\(^ {54-56} \), and plasmonic\(^ {57-63} \) systems. In such systems, especially photonic and plasmonic systems, the interactions are often long-ranged and any localised states, with which a tight-binding model may be constructed, have evanescent tails far from their lattice sites. Then the overlap matrix would be important to account for especially if the tight-binding model is not found through first-principles but instead through some \textit{ad hoc} fitting procedure. In such a case, an accidental ignorance of the overlap matrix could limit the predictive power of the constructed model.

VI. ACKNOWLEDGEMENTS

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FIG. 5. (Colour online) Panel (a): simultaneous plots of $|\nu| - |\beta|$ and $|\omega| - |\beta|$ for the two cases as considered in the main text of: (a) varying the distances between the Dirac-delta potentials as $v = a$, $w = d - a$ with a constant baseline potential $V_0 = 0$, and (b) varying the baseline potentials are $V_v = -T$ and $V_w = +T$ with $v = w = d/2$.

63 L. Wang, R.-Y. Zhang, M. Xiao, D. Han, C. T. Chan, and W. Wen, New Journal of Physics 18, 103029 (2016).

Appendix A: Numerical Proof that $F(\phi_{\text{min}})$ is Never Negative

As discussed in Section III, the argument of the square root in the expression for the bulk energy eigenvalues cannot be negative otherwise the energies becomes complex and exceptional points are introduced to the Brillouin zone. For the two cases as studied within Section V, the behaviours of $|\nu| - |\beta|$ and $|\omega| - |\beta|$ will now be presented to show that it is never that both $|\nu| < |\beta|$ and $|\omega| < |\beta|$ simultaneously.

Recalling that $\nu = t - \eta$, $\omega = t' - \eta'$ and $\beta = t\eta - t'\eta'$ the relations between $\nu$, $\omega$ and $\beta$ may be plotted as in Fig. 5 using the tight-binding parameters as laid out in Eqs. (19-21) for panel (a) and Eqs. (24-28) for panel (b). As may be clearly seen, $|\nu| - |\beta|$ and $|\omega| - |\beta|$ are never both negative at the same point and so $F(\phi_{\text{min}}) \geq 0$ for all range of physical parameters (meaning that $\epsilon, t, t' < 0$ and $0 \leq \eta, \eta' \leq 1$). It is important to note, however, that the fact that $|\nu| - |\beta|$ and $|\omega| - |\beta|$ do become negative in the second case of panel (b) may very well be an indication of the breakdown of the tight-binding approximation there since the bulk bands invert and the finite bands touch when $T \sim \pm(20 - 25)$. Regardless, however, $|\nu| - |\beta|$ and $|\omega| - |\beta|$ are never simultaneously negative and so $F(\phi_{\text{min}})$ is always positive as required.

Appendix B: The Solution to the Solitary Asymmetric Dirac-delta

For a bipartite Kronig-Penney model with Dirac-delta potentials that have negative strengths we seek negative energy solutions. A lone Dirac-delta potential possesses a single bound state that exponentially localises to the potential site.

The solution of the lone asymmetric bound state proceeds in the standard scattering way. Assuming the Dirac-delta potential to be situated at $x = x_0$, we solve:

$$H(x)\Psi(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right] \Psi(x) = E\Psi(x), \quad (B1)$$

where $V(x) = V_0\delta(x - x_0) + V_1\theta(x_0 - x) + V_2\theta(x - x_0)$, with the standard solution for the wavefunction of:

$$\Psi(x, x_0) = \theta(x_0 - x)(Ae^{i\kappa x} + Be^{-i\kappa x}) + \theta(x - x_0)(Ce^{i\kappa x} + De^{-i\kappa x}), \quad (B2)$$

and seek negative energy solutions such that $q_j = i\kappa_j$, where these wavevectors are found by solving the TISE in each
from which it may be seen that: 

\[ q_j = \hbar^{-1} \sqrt{2m(E - V_j)} \implies \kappa_j = \hbar^{-1} \sqrt{2m(V_j - E)}. \]  

(B3)

As a result, the wavefunction must be well-defined at \( \pm \infty \) and thus \( A = D = 0 \) thereby yielding:

\[ \Psi(x, x_0) = \theta(x_0 - x)Be^{\kappa_1x} + \theta(x - x_0)Ce^{-\kappa_2x}. \]  

(B4)

Now we enforce the continuity of the wavefunction at \( x = x_0 \) and so observe that \( B = Ce^{-(\kappa_1 + \kappa_2)x_0} \). Furthermore, the wavefunction must be normalised as:

\[ 1 = \int_{-\infty}^{+\infty} dx |\Psi(x, x_0)|^2 = C^2e^{-2(\kappa_1 + \kappa_2)x_0} \int_{-\infty}^{x_0} dx e^{2\kappa_1x} + C^2 \int_{x_0}^{+\infty} dx e^{-2\kappa_2x}, \]  

(B5)

from which it may be seen that:

\[ C = \sqrt{\frac{2\kappa_1\kappa_2}{\kappa_1 + \kappa_2}} e^{\kappa_2x_0}. \]  

(B6)

Thus:

\[ \Psi(x, x_0) = \sqrt{\frac{2\kappa_1\kappa_2}{\kappa_1 + \kappa_2}} \left[ \theta(x_0 - x)e^{\kappa_1(x - x_0)} + \theta(x - x_0)e^{-\kappa_2(x - x_0)} \right]. \]  

(B7)

To find the energy of this bound state we integrate the TISE once in the vicinity of the potential since we cannot impose that the derivative of the wavefunction be continuous at the potential due to the presence of the Dirac-delta. Thus:

\[ E \int_{x_0}^{x_0+\epsilon} dx \Psi(x, x_0) = -\frac{\hbar^2}{2m} \int_{x_0}^{x_0+\epsilon} dx \Psi''(x, x_0) + \int_{x_0}^{x_0+\epsilon} dx [V\delta(x) + V_1\theta(x_0 - x) + V_2\theta(x - x_0)]\Psi(x, x_0), \]  

(B8)

which becomes, in the limit of \( \epsilon \to 0 \):

\[ -\frac{\hbar^2}{2m} [\Psi'(x_0^+, x_0) - \Psi'(x_0^-, x_0)] + V\Psi(x_0, x_0) = 0, \]  

(B9)

where the superscripts \( \pm \) signify to take \( \Psi'(x, x_0) \) to the limit of \( x_0 \) within the regions \( x > x_0 \) (plus) and \( x < x_0 \) (minus). Thus we see that:

\[ \frac{\hbar^2}{2m}(\kappa_1 + \kappa_2) + V = 0, \]  

(B10)

and so, taking Eq. (B10) together with Eq. (B3), the energy of the bound state, after some unilluminating algebra, is:

\[ E = \frac{1}{2}(V_1 + V_2) - \frac{mV^2}{2\hbar^2} - \frac{\hbar^2(V_1 - V_2)^2}{8mV^2}. \]  

(B11)

Clearly, when \( V_1 = V_2 = 0 \) we recover the standard result of a symmetric Dirac-delta \( E_0 = -mV^2/(2\hbar^2) \). Moreover, when \( V_1 = V_2 = U \neq 0 \) we see that \( E = U + E_0 \), i.e. the potentials act as trivial energy shifts; they only have a non-trivial effect when \( V_1 \neq V_2 \).

Taking Eq. (B11) and substituting it into the \( \kappa_j \) of Eq. (B3), yields the wavevectors as:

\[ \kappa_{1,2} = \sqrt{\frac{m}{\hbar^2}(V_{1,2} - V_{2,1}) + \frac{m^2V^2}{\hbar^4} + \left(\frac{V_1 - V_2}{2V}\right)^2}. \]  

(B12)

As such, we may see that:

\[ \kappa_{1,2} = \sqrt{\frac{(V_{1,2} - V_{2,1}) + mV^2}{2\hbar^2}} = \pm \left[ -\kappa + \frac{1}{2V}(V_{1,2} - V_{2,1}) \right], \]  

(B13)

where \( \kappa = -mV/\hbar^2 \), such that \( E_0 = \kappa V/2 \), is the wavevector of a lone symmetric Dirac delta potential. Since it cannot physically be that \( \kappa_1,2 < 0 \) (such that the correct behaviour at infinity is maintained), the minus sign must be chosen here. As such:

\[ \kappa_1 = \kappa - \frac{1}{2V}(V_1 - V_2), \quad \kappa_2 = \kappa - \frac{1}{2V}(V_2 - V_1). \]  

(B14)

So, in summary, the lone asymmetric Dirac-delta potential hosts a single bound state with negative energy given by Eq. (B11) and wavefunction as in Eq. (B7) where the wavevectors too may be found in Eq. (B14). This wavefunction will constitute the atomic orbitals (basis wavefunctions) of our tight-binding model.
Appendix C: The Matrix Elements of the Expansion

The full problem, within the bulk as shown in Fig. 1, is to solve the time-independent Schrödinger equation as in Eq. (B1): $H(x)\Psi(x) = E\Psi(x)$, in the presence of a spatially varying potential given by:

$$V(x) = \sum_i \left\{ V[\delta(x - x_Ai) + \delta(x - x_Bi)] + V_v\theta(x_{Bi} - x)\theta(x - x_Ai) + V_v\theta(x_{A(i+1)} - x)\theta(x - x_{Bi}) \right\},$$

(C1)

where the sum over $i$ is over a number of unit-cells that is determined by the accuracy required of the model. For small values of $|V|$ and/or $V_v$, this sum must be over several unit-cells however in the nearest-neighbour approximation it need only be between three neighbouring unit-cells, i.e. the central unit-cell and its two neighbours.

Considering the unit-cell as shown in Fig. 1, the atomic wavefunctions for the $A$ and $B$ sublattices are:

$$\Psi_A(x, x_{Aj}) = \sqrt{\frac{2\kappa_v\kappa_w}{\kappa_v + \kappa_w}} \left[ \theta(x_{Aj} - x)e^{\kappa_v(x-x_{Aj})} + \theta(x - x_{Aj})e^{-\kappa_v(x-x_{Aj})} \right],$$

$$\Psi_B(x, x_{Bj}) = \sqrt{\frac{2\kappa_v\kappa_w}{\kappa_v + \kappa_w}} \left[ \theta(x_{Bj} - x)e^{\kappa_v(x-x_{Bj})} + \theta(x - x_{Bj})e^{-\kappa_v(x-x_{Bj})} \right],$$

(C2)

where $\kappa_v = \kappa - (V_v - V_w)/(2V)^{-1}$. As such, the normalisation constant simplifies to $N_c = \sqrt{\kappa_v\kappa_w\kappa_v^{-1}}$. Using these basis wavefunctions, the tight-binding Schrödinger equation may be constructed as:

$$\begin{pmatrix}
H_{AA} & H_{AB} \\
H_{BA} & H_{BB}
\end{pmatrix}
\begin{pmatrix}
c_A \\
c_B
\end{pmatrix}
= E
\begin{pmatrix}
S_{AA} & S_{AB} \\
S_{BA} & S_{BB}
\end{pmatrix}
\begin{pmatrix}
c_A \\
c_B
\end{pmatrix},$$

(C3)

where $H_{mn} = \langle \Psi_m | H | \Psi_n \rangle$, $S_{mn} = \langle \Psi_m |\Phi_n \rangle$ and $c_n$ are the coefficients that yield the unit-cell wavefunction as $\Psi(x) = \theta(x_0 - x)\theta(x - x_3)|c_A\Psi_A(x, x_{A1}) + c_B\Psi_B(x, x_{B1})\rangle$. As will be subsequently shown in this section, the relevant tight-binding parameters may be found as:

$$\epsilon = \frac{\hbar^2}{2m} \kappa_v\kappa_w \left[ 1 + 2 \left( e^{-2\kappa_v\nu} + e^{-2\kappa_v\nu} + e^{-2\kappa_v\nu} + e^{-2\kappa_v\nu} \right) \right],$$

$$t = -\frac{\hbar^2}{2m} \kappa_v\kappa_w \frac{1}{\kappa_v} \left[ \frac{1}{2\kappa_v} \left( \kappa_v^2 + \kappa_w^2 \right) e^{-\kappa_v\nu} + e^{-\kappa_v\nu} + e^{-\kappa_v\nu} \right],$$

$$t' = -\frac{\hbar^2}{2m} \kappa_v\kappa_w \frac{1}{\kappa_v} \left[ \frac{1}{2\kappa_v} \left( \kappa_v^2 + \kappa_w^2 \right) e^{-\kappa_v\nu} + e^{-\kappa_v\nu} + e^{-\kappa_v\nu} \right],$$

$$\eta = \frac{1}{\kappa_v^2 \kappa_w \kappa_v} \left[ \frac{1}{2} \left( e^{-\kappa_v\nu} + e^{-\kappa_v\nu} + \kappa ve^{-\kappa_v\nu} \right) \right],$$

(C4)

such that $H_{AA} = H_{BB} = \epsilon$, $H_{AB} = H^*_{BA} = te^{i\kappa v} + t'e^{-i\kappa v}$, $S_{AA} = S_{BB} = 1$, and $S_{AB} = S^*_{BA} = \eta e^{i\kappa v} + \eta' e^{-i\kappa v}$.

Following the standard, general theory of the tight-binding model, the matrix elements may be evaluated, within the present context as:

$$\langle \Phi_m | H | \Phi_m \rangle = \int_{-\infty}^{+\infty} \frac{dx}{N} \sum_{i,j=1}^N e^{ik(x_m-x_n)} \left[ \theta(x_{ni} - x)e^{\kappa(x-x_{ni})} + \theta(x - x_{ni})e^{-\kappa(x-x_{ni})} \right] \times$$

$$\left[ \frac{\hbar^2}{2mdx^2} + V \sum_{l=-N}^N (\delta(x - x_{nl}) + \delta(x - x_{ml})) \right] \left[ \theta(x_{mj} - x)e^{\kappa(x-x_{mj})} + \theta(x - x_{mj})e^{-\kappa(x-x_{mj})} \right],$$

(C5)

$$\langle \Phi_m | \Phi_m \rangle = \int_{-\infty}^{+\infty} \frac{dx}{N} \sum_{i,j=1}^N e^{ik(x_m-x_n)} \left[ \theta(x_{ni} - x)e^{\kappa(x-x_{ni})} + \theta(x - x_{ni})e^{-\kappa(x-x_{ni})} \right] \times$$

$$\left[ \theta(x_{mj} - x)e^{\kappa(x-x_{mj})} + \theta(x - x_{mj})e^{-\kappa(x-x_{mj})} \right],$$

(C6)

where the sum over $\{i,j\}$ is over pairs of lattice sites, which we restrict to on-site and nearest-neighbours, i.e. $i,j = 0,1,2$, and the sum over $l$ is over a suitable number of Dirac-delta potentials (lattice sites). The prefactor $N$ drops out in the subsequent analysis as it accounts for double counting in the $\{i,j\}$ summation.
Considering first the case wherein $n = m = A$ and $i = j = 1$, i.e. interactions within the unit-cell only, and name this contribution $\epsilon_{AA}$, we see that:

\[
\epsilon_{AA} = \frac{2\kappa_w \kappa_v}{\kappa_w + \kappa_v} \int_{-\infty}^{+\infty} dx \left[ \theta(x_A - x) e^{\kappa_u (x - x_A)} + \theta(x - x_A) e^{-\kappa_v (x - x_A)} \right] \\
\times \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \sum_{i = -N}^{N} [\delta(x - x_{A1}) + \delta(x - x_{B1})] \right] \left[ \theta(x_A - x) e^{\kappa_u (x - x_A)} + \theta(x - x_A) e^{-\kappa_v (x - x_A)} \right] \\
\times \left[ \frac{1}{2} \int_{-\infty}^{+\infty} dx \left[ \theta(x_A - x) e^{\kappa_u (x - x_A)} + \theta(x - x_A) e^{-\kappa_v (x - x_A)} \right] \right] \\
\times \left[ \delta'(x_A - x) e^{\kappa_u (x - x_A)} + \delta'(x - x_A) e^{-\kappa_v (x - x_A)} - 2 \delta(x - x_A) \left( \kappa_w e^{\kappa_u (x - x_A)} + \kappa_v e^{-\kappa_v (x - x_A)} \right) \right] \\
\times \left[ \frac{1}{2} \int_{-\infty}^{+\infty} dx \left[ \theta(x_A - x) e^{\kappa_u (x - x_A)} + \theta(x - x_A) e^{-\kappa_v (x - x_A)} \right] \right] \\
\times \left[ \frac{1}{2} \int_{-\infty}^{+\infty} dx \left[ \theta(x_A - x) e^{\kappa_u (x - x_A)} + \theta(x - x_A) e^{-\kappa_v (x - x_A)} \right] \right] \\
\times \left[ \frac{1}{2} \int_{-\infty}^{+\infty} dx \left[ \theta(x_A - x) e^{\kappa_u (x - x_A)} + \theta(x - x_A) e^{-\kappa_v (x - x_A)} \right] \right] \\
\times \left[ \frac{1}{2} \int_{-\infty}^{+\infty} dx \left[ \theta(x_A - x) e^{\kappa_u (x - x_A)} + \theta(x - x_A) e^{-\kappa_v (x - x_A)} \right] \right]. \tag{C7}
\]

It is a standard result that:

\[
\int_a^b dx f(x) \delta^{(n)}(x - c) = \pm (-1)^n f^{(n)}(c) \theta(c - a) \theta(b - c), \tag{C8}
\]

and so:

\[
\epsilon_{AA} = \frac{2\kappa_w \kappa_v}{\kappa_w + \kappa_v} \left[ E_w \left( e^{2\kappa_u (x_{A1} - x_A)} + e^{2\kappa_v (x_{B1} - x_A)} + 1 \right) + E_v \left( \frac{1}{2} + e^{-2\kappa_v (x_{B1} - x_A)} + e^{-2\kappa_v (x_{A1} - x_A)} \right) \right] \\
- \frac{\hbar^2}{2m} \left[ (\kappa_w - \kappa_v) - (\kappa_w - \kappa_v) + (\kappa_w - \kappa_v) + (\kappa_w - \kappa_v) \right] \\
= \frac{2\kappa_w \kappa_v}{\kappa_w + \kappa_v} \left[ E_w + E_v \left( 1 + e^{-2\kappa_v w} + e^{-2\kappa_v v} + e^{-2\kappa_v d} + e^{-2\kappa_v d} + \frac{\hbar^2}{2m} (\kappa_w + \kappa_v) \right) \right] \\
= \frac{\kappa_w \kappa_v}{\kappa} V \left( 1 + e^{-2\kappa_w w} + e^{-2\kappa_v v} + e^{-2\kappa_v d} + e^{-2\kappa_v d} + \frac{\hbar^2}{2m} \kappa_w \kappa_v \right) \tag{C9}
\]

Thus, the on-site potential is:

\[
\epsilon_{AA} = \frac{1}{\kappa} \kappa_w \kappa_v V \left( 1 + e^{-2\kappa_w w} + e^{-2\kappa_v v} + e^{-2\kappa_v d} + e^{-2\kappa_v d} \right) - \frac{1}{2\kappa} (\kappa_v E_w + \kappa_w E_v). \tag{C10}
\]
Now we find the on-site potential for the B sublattice as:

\[
\epsilon_{BB} = \frac{2\kappa_w\kappa_v}{\kappa_w + \kappa_v} \int_{-\infty}^{+\infty} dx \left[ \theta(x_{B1} - x)e^{\kappa_v(x-x_{B1})} + \theta(x - x_{B1})e^{-\kappa_w(x-x_{B1})} \right] \times \\
\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right] \sum_{i=-N}^{N} \left[ \delta(x - x_{A1}) + \delta(x - x_{B1}) \right] \left[ \theta(x_{B1} - x)e^{\kappa_v(x-x_{B1})} + \theta(x - x_{B1})e^{-\kappa_w(x-x_{B1})} \right] = \frac{2\kappa_w\kappa_v}{\kappa_w + \kappa_v} \int_{-\infty}^{+\infty} dx \left[ E_v + V[\delta(x - x_{B1}) + \delta(x - x_{B1}) + \delta(x_{B1} - x) + \delta(x - x_{B1})] \right] e^{2\kappa_v(x-x_{B1})} \\
- \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} dx \left[ \delta'(x_{B1} - x) e^{2\kappa_v(x-x_{B1})} + \delta'(x - x_{B1}) e^{(\kappa_v - \kappa_w)(x-x_{B1})} \right] - 2\delta(x - x_{B1}) \left( \kappa_v e^{2\kappa_v(x-x_{B1})} + \kappa_w e^{(\kappa_v - \kappa_w)(x-x_{B1})} \right) \\
- \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} dx \left[ \delta'(x_{B1} - x) e^{(\kappa_v - \kappa_w)(x-x_{B1})} + \delta'(x - x_{B1}) e^{-2\kappa_w(x-x_{B1})} \right] - 2\delta(x - x_{B1}) \left( \kappa_v e^{(\kappa_v - \kappa_w)(x-x_{B1})} + \kappa_w e^{-2\kappa_w(x-x_{B1})} \right), \quad (C11)
\]

which evaluates as:

\[
\epsilon_{BB} = \frac{2\kappa_w\kappa_v}{\kappa_w + \kappa_v} \left( E_v + V \left( e^{2\kappa_v(x_{B0} - x_{B1})} + e^{2\kappa_v(x_{A1} - x_{B1})} + \frac{1}{2} \right) \right) + \frac{E_v}{2\kappa_w} + V \left( \frac{1}{2} + e^{-2\kappa_w(x_{A2} - x_{B1})} + e^{-2\kappa_w(x_{B2} - x_{B1})} \right) \\
- \frac{\hbar^2}{2m} \left[ \kappa_v - (\kappa_v - \kappa_w) - \kappa_v - \kappa_w + (\kappa_v - \kappa_w) + \kappa_v - \kappa_v - \kappa_v \right] \\
= \frac{2\kappa_w\kappa_v}{\kappa_w + \kappa_v} \left( E_v + V \left( 1 + e^{-2\kappa_v v} + e^{-2\kappa_w w} + e^{-2\kappa_w d} + e^{-2\kappa_v d} \right) \right) + \frac{E_v}{2\kappa_w} + V \left( \frac{1}{2} + e^{-2\kappa_v v} + e^{-2\kappa_w w} + e^{-2\kappa_w d} + e^{-2\kappa_v d} \right) - \frac{1}{2\kappa} (\kappa_v E_v + \kappa_w E_v), \quad (C12)
\]

and thus we see that \( \epsilon_{AA} = \epsilon_{BB} \) as it ought to be. In fact, this expression may be simplified further since \( V/\kappa = -\hbar^2/m \) to become:

\[
\epsilon_{AA} = \epsilon_{BB} = \epsilon = -\frac{\hbar^2}{m} \kappa_w \kappa_v \left( 1 + e^{-2\kappa_v v} + e^{-2\kappa_w w} + e^{-2\kappa_w d} + e^{-2\kappa_v d} \right) + \frac{\hbar^2}{2m} \kappa_w \kappa_v \\
= -\frac{\hbar^2}{2m} \kappa_w \kappa_v \left[ 1 + 2 \left( e^{-2\kappa_v v} + e^{-2\kappa_w w} + e^{-2\kappa_v d} + e^{-2\kappa_w d} \right) \right], \quad (C13)
\]
Now, moving onto the intra-cell hopping term $t_{AB}$ with $i = 1$, $j = 1$:

$$
t_{AB} = e^{ik(x_{B1} - x_{A1})} \frac{2\kappa_u \kappa_v}{\kappa_w + \kappa_v} \left\{ \int_{-\infty}^{+\infty} dx \left[ \theta(x_{A1} - x) e^{\kappa_u (x-x_{A1})} + \theta(x-x_{A1}) e^{-\kappa_u (x-x_{A1})} \right] \times \\
\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V + \sum_{d=-N}^{N} \delta(x - x_{Ai}) \right] \left[ \theta(x_{B1} - x) e^{\kappa_v (x-x_{B1})} + \theta(x-x_{B1}) e^{-\kappa_v (x-x_{B1})} \right] \\
- \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} dx \left[ \theta(x_{B1} - x) e^{\kappa_u (x-x_{A1})} + \theta(x-x_{B1}) e^{-\kappa_u (x-x_{A1})} \right] \\
\times \left[ \delta'(x_{B1} - x) e^{\kappa_v (x-x_{B1})} + \delta'(x-x_{B1}) e^{-\kappa_u (x-x_{B1})} \right] - 2\delta(x-x_{B1}) \left( \kappa_v e^{\kappa_v (x-x_{B1})} + \kappa_u e^{-\kappa_u (x-x_{B1})} \right) \right\} \\
= e^{ik(x_{B1} - x_{A1})} \frac{2\kappa_u \kappa_v}{\kappa_w + \kappa_v} \left\{ \int_{-\infty}^{x_{A1}} dx \left[ E_v + V \left[ \delta(x - x_{A0}) + \delta(x-x_{B0}) + \delta(x-x_{A1}) \right] \right] e^{\kappa_u (x-x_{A1})} \\
+ \int_{x_{A1}}^{x_{B1}} dx \left[ E_v + V \left[ \delta(x - x_{A1}) + \delta(x-x_{B1}) \right] \right] e^{\kappa_u (x-x_{A1})} \\
- \frac{\hbar^2}{2m} \int_{x_{A1}}^{x_{B1}} dx \left[ \delta'(x_{B1} - x) e^{\kappa_v (x-x_{B1})} + \delta'(x-x_{B1}) e^{-\kappa_u (x-x_{B1})} \right] - 2\delta(x-x_{B1}) \left( \kappa_v e^{\kappa_v (x-x_{B1})} + \kappa_u e^{-\kappa_u (x-x_{B1})} \right) \right\}. \quad \text{(C14)}
$$

This becomes:

$$
t_{AB} = e^{ik(x_{B1} - x_{A1})} \frac{2\kappa_u \kappa_v}{\kappa_w + \kappa_v} \left\{ \left[ E_v + \frac{E_w}{2(\kappa_w + \kappa_v)} + \frac{E_v(x_{B1} - x_{A1}) + V}{2} \right] e^{\kappa_u (x-x_{A1})} \\
+ V \left( e^{(\kappa_u + \kappa_v)x_{A0} - \kappa_u x_{A1} - \kappa_u x_{B1} - \kappa_u w x_{B1} - \kappa_u x_{A1} + \frac{1}{2} e^{(\kappa_w + \kappa_v) x_{A1} - \kappa_u x_{B1} - \kappa_u w x_{A1}}} \right) \\
+ V \left( \frac{1}{2} e^{-\kappa_u (x_{B1} + \kappa_u w x_{B1} + \kappa_u x_{A1})} + e^{(\kappa_u + \kappa_v)x_{A2} - \kappa_u x_{B1} + \kappa_u x_{A1} + \kappa_u w x_{B1} + \kappa_u w x_{A1}} + e^{(\kappa_w + \kappa_v) x_{B2} + \kappa_u w x_{B1} + \kappa_u x_{A1}} \right) \\
- \frac{\hbar^2}{2m} \left[ (\kappa_u + \kappa_v) e^{-\kappa_u (x_{A1} - x_{B1})} - 2\kappa_u e^{\kappa_v (x_{A1} - x_{B1})} - 2\kappa_u e^{-\kappa_u (x_{A1} + \kappa_u w x_{B1} + \kappa_u x_{A1} + \kappa_u w x_{B1})} \right] \right\} \\
= \frac{2\kappa_u \kappa_v}{\kappa_w + \kappa_v} \left\{ \left[ E_v + \frac{E_w}{2\kappa} + E_v V \right] e^{-\kappa_u v} + \frac{\hbar^2}{2m} (\kappa_u + \kappa_v) e^{-\kappa_v v} \\
+ V \left( e^{-\kappa_u (x_{B1} + \kappa_u w x_{B1} + \kappa_u x_{A1})} + \frac{1}{2} e^{\kappa_w + \kappa_v} \right) + \frac{1}{2} e^{-\kappa_u v} + \frac{1}{2} e^{-\kappa_u v} + e^{\kappa_u (x_{B1} + \kappa_u w x_{B1} + \kappa_u x_{A1})} \right\}. \quad \text{(C15)}
$$

Now, again $\kappa_v + \kappa_w = 2\kappa$, and so:

$$
t_{AB} = e^{ikr} \frac{\kappa_u \kappa_v}{\kappa} \left\{ \left[ \frac{E_v + E_w}{2\kappa} + E_v V + \frac{\hbar^2 \kappa}{m} \right] e^{-\kappa_u v} + \frac{V}{2} (e^{-\kappa_u v} + e^{-\kappa_v v}) \\
+ V \left( e^{-\kappa_u (x_{B1} + \kappa_u w x_{B1} + \kappa_u x_{A1})} + \frac{1}{2} e^{\kappa_w + \kappa_v} \right) + \frac{1}{2} e^{-\kappa_u v} + e^{-\kappa_u v} e^{-2\kappa d} \right\}. \quad \text{(C16)}
$$

Thus, to first order (ignoring any $e^{-\kappa d}$ terms) and recalling that $\kappa = -mV/\hbar^2$:

$$
t_{AB} = \frac{\kappa_u \kappa_v}{\kappa} \left\{ \left[ \frac{E_v + E_w}{2\kappa} + E_v V \right] e^{-\kappa_u v} + \frac{V}{2} (e^{-\kappa_u v} + e^{-\kappa_v v}) \right\} e^{ikr}. \quad \text{(C17)}
$$
Now, we again move onto the inter unit cell hopping $\tilde{t}_{BA}$ between $i=1$ and $j=2$, which is given by:

$$\tilde{t}_{BA} = e^{ik(x_{A2} - x_{B1})} \frac{2\kappa_w\kappa_v}{\kappa_w + \kappa_v} \left\{ \int_{-\infty}^{+\infty} dx \left[ \theta(x_{B1} - x) e^{\kappa_v(x-x_{B1})} + \theta(x - x_{B1}) e^{-\kappa_v(x-x_{B1})} \right] \times \right. $n

$$ \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \sum_{l=-N}^{N} \left[ \delta(x - x_{A1}) + \delta(x - x_{B1}) \right] \left[ \theta(x_{A2} - x) e^{\kappa_v(x-x_{A2})} + \theta(x - x_{A2}) e^{-\kappa_v(x-x_{A2})} \right] $$

$$ - \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} dx \left[ \theta(x_{B1} - x) e^{\kappa_v(x-x_{B1})} + \theta(x - x_{B1}) e^{-\kappa_v(x-x_{B1})} \right] $$

$$ \times \left[ \delta'(x_{A2} - x) e^{\kappa_v(x-x_{A2})} + \delta'(x - x_{A2}) e^{-\kappa_v(x-x_{A2})} - 2\delta(x - x_{A2}) \left( \kappa_w e^{\kappa_v(x-x_{A2})} + \kappa_v e^{-\kappa_v(x-x_{A2})} \right) \right] \right\} (C18)$$

This becomes:

$$\tilde{t}_{BA} = e^{ik(x_{A2} - x_{B1})} \frac{2\kappa_w\kappa_v}{\kappa_w + \kappa_v} \left\{ \frac{E_w + E_{w}}{2(\kappa_w + \kappa_v)} + E_{w}(x_{A2} - x_{B1}) + V \left( e^{(\kappa_w + \kappa_v)x_{B1} - (\kappa_w x_{A2} + \kappa_v x_{B1})} + e^{(\kappa_w + \kappa_v)x_{A1} - (\kappa_w x_{A2} + \kappa_v x_{B1})} + \frac{1}{2} e^{(\kappa_w + \kappa_v)x_{B1} - (\kappa_w x_{A2} + \kappa_v x_{B1})} \right) \right. $$

$$ + V \left( \frac{1}{2} e^{-((\kappa_w + \kappa_v)x_{A1} - (\kappa_w x_{A2} + \kappa_v x_{B1})} + e^{-(\kappa_w + \kappa_v)x_{B2} + (\kappa_w x_{A2} + \kappa_v x_{B1})} + e^{-(\kappa_w + \kappa_v)x_{A3} + (\kappa_w x_{A2} + \kappa_v x_{B1})} \right) $$

$$ - \frac{\hbar^2}{2m} \left[ (\kappa_w + \kappa_v) e^{-(\kappa_v + \kappa_w)x_{A2} + \kappa_v x_{A2} + \kappa_v x_{B1}} - 2\kappa_w e^{\kappa_v(x_{B1} - x_{A2})} - 2\kappa_v e^{(\kappa_v + \kappa_w)x_{A2} + \kappa_v x_{B1} + \kappa_v x_{A2}} \right] \right. $$

$$ = e^{ikw}\kappa w \kappa v}{K} \left\{ \left( \frac{E_{w} + E_{w}}{4\kappa} + E_{w} - x_{A2} + x_{B1} + V \right) e^{\kappa_w w} + \frac{\hbar^2}{2m} (\kappa_w + \kappa_v) e^{-\kappa_w w} \right. $$

$$ + V \left( e^{-\kappa_w w} + \left( \kappa_v + \kappa_w \right) e^{-(\kappa_v + \kappa_w)w} + e^{-\kappa_v w + \kappa_w w} + \left( \kappa_v + \kappa_w \right) e^{\kappa_v w} \right) \right\} $$

$$ = e^{ikw}\kappa w \kappa v}{K} \left\{ \left( \frac{E_{w} + E_{w}}{2\kappa} + E_{w} + V \right) e^{-\kappa_w w} + \frac{\hbar^2}{m} \left( e^{-\kappa_v w} + \left( \kappa_v + \kappa_w \right) e^{\kappa_v w} \right) \right. $$

$$ + V \left( e^{-\kappa_v w} + e^{-\kappa_v w} \right) e^{-2\kappa_d} + V \left( e^{-\kappa_v w} + e^{-\kappa_v w} \right) e^{-\kappa_v w} \right\}. (C19)$$

This may too be seen to reduce to the previous result. So, to first order:

$$\tilde{t}_{BA} = \frac{\kappa_w \kappa_v}{K} \left( \frac{E_{w} + E_{w}}{2\kappa} + E_{w} \right) e^{-\kappa_w w} + \frac{V}{2} \left( e^{-\kappa_v w} + e^{-\kappa_v w} \right) e^{ikw}. (C20)$$

Thus, to first order in the nearest-neighbour interactions, the effective tight-binding 2x2 matrix Hamiltonian is:

$$H = \begin{pmatrix} \epsilon & t_{AB} + \tilde{t}_{AB} \\ t_{BA} + \tilde{t}_{BA} & \epsilon \end{pmatrix}, (C21)$$
where $t_{AB} = t_{BA}^*$, $\bar{t}_{AB} = \bar{t}_{BA}^*$, and:

$$
\epsilon = -\frac{\hbar^2}{2m} \kappa_w \kappa_v \left[ 1 + 2 \left( e^{-2\kappa_v v} + e^{-2\kappa_w w} + e^{-2\kappa_d d} + e^{-2\kappa_d d} \right) \right],
$$
(C22)

$$
t_{AB} = \frac{\kappa_w \kappa_v}{\kappa} \left[ \left( \frac{1}{2\kappa} (E_v + E_w) + E_v v \right) e^{-\kappa_v v} + \frac{V}{2} \left( e^{-\kappa_v v} + e^{-\kappa_w v} \right) \right] e^{i k v}.
$$
(C23)

$$
\bar{t}_{AB} = \frac{\kappa_w \kappa_v}{\kappa} \left[ \left( \frac{1}{2\kappa} (E_v + E_w) + E_w v \right) e^{-\kappa_w w} + \frac{V}{2} \left( e^{-\kappa_w w} + e^{-\kappa_w w} \right) \right] e^{-i k w}.
$$
(C24)

On the other hand, the matrix elements of the overlap matrix may be found simply as follows. The on-diagonals are equal to one because the basis wavefunctions are normalised correctly. Then the off-diagonals follow as:

$$
\eta_{AB} = \frac{2\kappa_w \kappa_v}{\kappa_w + \kappa_v} e^{i k (x_{B1} - x_{A1})} 
\times \int_{-\infty}^{+\infty} dx \left[ \theta(x_{A1} - x) e^{\kappa_w (x - x_{A1})} + \theta(x - x_{A1}) e^{-\kappa_w (x - x_{A1})} \right] \left[ \theta(x_{B1} - x) e^{\kappa_v (x - x_{B1})} + \theta(x - x_{B1}) e^{-\kappa_v (x - x_{B1})} \right] 
= \frac{\kappa_w \kappa_v}{\kappa} \left[ \frac{1}{2\kappa} \left( e^{-\kappa_v v} + e^{-\kappa_w v} \right) + v e^{-\kappa_v v} \right] e^{i k v},
$$
(C25)

and:

$$
\bar{\eta}_{BA} = \frac{2\kappa_w \kappa_v}{\kappa_w + \kappa_v} e^{i k (x_{B1} - x_{A1})} 
\times \int_{-\infty}^{+\infty} dx \left[ \theta(x_{A1} - x) e^{\kappa_v (x - x_{B1})} + \theta(x - x_{B1}) e^{-\kappa_v (x - x_{B1})} \right] \left[ \theta(x_{A2} - x) e^{\kappa_w (x - x_{A2})} + \theta(x - x_{A2}) e^{-\kappa_w (x - x_{A2})} \right] 
= \frac{\kappa_w \kappa_v}{\kappa} \left[ \frac{1}{2\kappa} \left( e^{-\kappa_v w} + e^{-\kappa_w w} \right) + w e^{-\kappa_v v} \right] e^{-i k w},
$$
(C26)

thus:

$$
S = \left( \frac{1}{\eta_{BA} + \bar{\eta}_{BA}} \right),
$$
(C27)

where $\eta_{AB} = \eta_{B1}$ and $\bar{\eta}_{AB} = \bar{\eta}_{BA}$ as:

$$
\eta_{AB} = \frac{\kappa_w \kappa_v}{\kappa} \left[ \frac{1}{2\kappa} \left( e^{-\kappa_v v} + e^{-\kappa_v v} \right) + v e^{-\kappa_v v} \right] e^{i k v},
$$
(C28)

$$
\bar{\eta}_{AB} = \frac{\kappa_w \kappa_v}{\kappa} \left[ \frac{1}{2\kappa} \left( e^{-\kappa_v w} + e^{-\kappa_v w} \right) + w e^{-\kappa_v w} \right] e^{-i k w}.
$$
(C29)