Bound States In and Out of the Continuum in Nanoribbons with Wider Sections: A Novel Algorithm based on the Recursive S-Matrix Method

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A novel method to find bound states in general tight-binding Hamiltonians with semi-infinite leads is reported. The method is based on the recursive S-matrix method, which allows to compute iteratively the S-matrix of a general system in terms of the S-matrices of its subsystems. The condition that the S-matrices of the subsystems must accomplish to have a bound state at energy $E$ is established. Energies that accomplish this relation, can be determined with high accuracy and efficiency by using the Taylor series of the S-matrices. The method allows to find bound states energies and wavefunctions in (BIC) and out (BOC) of the continuum, including degenerate ones. Bound states in nanoribbons with wider sections are computed for square and honeycomb lattices. Using this method, the bound states in a graphene nanoribbon with two quantum-dot-like structures which are reported to have BICs by using another technique are verified. However, this new analysis reveals that such BICs are double, one with even and the other with odd wavefunction, with slightly separated energies. In this way, the new method can be used to efficiently find new BICs and to improve precision in previously reported ones.

1. Introduction

Bound states in a quantum system have normalizable wavefunctions that are nonzero only in a finite region of the space or decay to zero when the position goes to infinity. For finite closed systems, all wavefunctions are bound states, with discrete energies that can be calculated by diagonalizing the Hamiltonian. Let us consider a general tight binding Hamiltonian with $N$ sites

$$\hat{H} = \sum_{n=1}^{N} \varepsilon_n |n\rangle \langle n| + \sum_{n,m=1}^{N} t_{nm} |n\rangle \langle m|$$

where $|n\rangle$ is the Wannier function at site $n$ with site-energy $\varepsilon_n$, and $t_{nm}$ is the hopping integral between sites $n$ and $m$. The energy $E_m$ of Hamiltonian with eigenfunction $|\psi_m\rangle = \sum_{n=1}^{N} a_{m,n} |n\rangle$ solves the matrix equation

$$\begin{pmatrix} \varepsilon_1 & t_{12} & \cdots & t_{1N} \\ t_{21} & \varepsilon_2 & \cdots & t_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ t_{N1} & t_{N2} & \cdots & \varepsilon_N \end{pmatrix} \begin{pmatrix} a_{m,1} \\ a_{m,2} \\ \vdots \\ a_{m,N} \end{pmatrix} = E_m \begin{pmatrix} a_{m,1} \\ a_{m,2} \\ \vdots \\ a_{m,N} \end{pmatrix}$$

The matrix in Equation (2) is the matrix representation of the Hamiltonian in the base of the Wannier functions $|\psi_m\rangle$. In other words, by calculating the eigenvalues and eigenvectors of the Hamiltonian matrix, we find the $N$ energies and eigenfunctions of the system. Numerically, this calculation can be done by using standard procedures for diagonalization, such as those in the Math Kernel Library. However, numerical diagonalization is computationally expensive in large systems, as occurs in systems with leads.

A lead is a semi-infinite structure formed by the periodical repetition of a unitary cell in one direction, while the other side of the lead is connected to the scattering region. Leads act as waveguides for incoming and outgoing Bloch waves (open channels), but they may also contain evanescent functions that decay exponentially to zero away from the scattering region (closed channels). The scattering matrix (S-matrix) of the system relates the coefficients of incoming Bloch waves to those of outgoing Bloch waves. Consequently, the dimension of the S-matrix is equal to the number of open channels in the leads. Due to the periodic nature of the leads, energies associated with Bloch waves form continuum energy bands. Bound states do not overlap with any of the Bloch waves, because wavefunctions associated with Bloch waves are non-normalizable, but they couple to evanescent modes. Bound states in the continuum (BIC) have energies at values where there are open channels, so they coexist with the energy-bands in leads. On the other hand, bound states out of the continuum (BOC) have energies at values with non-open channels.

The S-matrix of a system contains all the effects caused by the scattering region on its surroundings. It can be found by direct inversion, which could be done efficiently in sparse systems. Also, the S-matrix can be calculated from the S-matrices of their subsystems by using the recursive scattering matrix method.
The S-matrix is related to the energy by

\[ E = \cos(\mathbf{k} \cdot \mathbf{a}) = \left| \mathbf{a}_A^{(n)} \mathbf{S}_A^{(n)} \mathbf{a}_B^{(n)} \right| \]

where \( \mathbf{a}_A^{(n)} \) and \( \mathbf{a}_B^{(n)} \) are the coefficients of the incoming and outgoing waves, respectively.

2. Algorithm to Find Bound-States

Let us consider a general tight-binding system with attached semi-infinite atomic chains (auxiliary chains). These auxiliary chains have sites with null site-energy and are connected between first neighbors by hopping integrals \( t_c \). Due to the periodicity of auxiliary chains, the amplitude coefficient of the \( n \)-th site in the \( n \)-th auxiliary chain (\( a_{n,m} \)) is given as a linear combination of an incoming and an outgoing wave:

\[ a_{n,m} = A_n^{(i)} e^{-ikm} + A_n^{(o)} e^{ikm} \]

where \( A_n^{(i)} \) and \( A_n^{(o)} \) are, respectively, the coefficients of the incoming and the outgoing waves in the \( n \)-th auxiliary chain, and \( k \) is related to the energy by \( E = 2t_c \cos(k) \). The case \( m = 0 \) corresponds to the site where the auxiliary chain is attached.

Let us consider another system \( B \) with auxiliary chains and denote the coefficients of the incoming and outgoing waves in these chains as \( B_n^{(i)} \) and \( B_n^{(o)} \), respectively. According to the RSM, doing \( B_n^{(i)} = A_n^{(i)} \) for \( n = 1, \ldots, N \) allows to model the system that results from the joining of systems \( A \) and \( B \), as exemplified in Figure 1. Notice that these equalities remove the corresponding auxiliary chains. This fact can be used to compute recursively the S-matrix of any system from the S-matrix of its subsystems. By starting from the site and bond structures, which have analytical S-matrices, any tight-binding structure can be modeled by following the RSM, including multiterminal cases with general leads. Moreover, the RSM has been extended to find the Taylor series of the S-matrix to arbitrary order. The S-matrix of a system is a function of energy, then its Taylor series allows us to compute the exact derivatives of the S-matrix with respect to the energy.

2.1. Determination of Energies

Let us assume that we want to find the bound states of a general system \( C \) with leads, as the one shown in Figure 1a. Due to the leads, the number of sites in system \( C \) is infinite, and then the bound states cannot be exactly solved by numerical direct diagonalization. Following the RSM, we can divide system \( C \) into two subsystems \( A \) and \( B \), as shown in Figure 1b. Sites in the frontier of this division are connected to auxiliary chains. In this way, scattering matrices of systems \( A \) and \( B \) can be calculated independently as functions of the energy. S-matrix of system \( A \) satisfies

\[ \begin{pmatrix} A_i \cr L_i \end{pmatrix} = \begin{pmatrix} S_A & S_{AL} \\ S_{LA} & S_L \end{pmatrix} \begin{pmatrix} A^{(i)} \\ L^{(i)} \end{pmatrix} \]

(4)

where

\[ A^{(i)} = \begin{pmatrix} A_1^{(i)} \\ A_2^{(i)} \\ \vdots \\ A_N^{(i)} \end{pmatrix}, \quad L^{(i)} = \begin{pmatrix} L_1^{(i)} \\ L_2^{(i)} \\ \vdots \\ L_N^{(i)} \end{pmatrix} \]

(5)

with coefficients \( L_i^{(i)} \) associated with incoming (+) and outgoing (−) Bloch functions (open channels) in the leads. Since bound states should not couple to open channels, we are only interested in cases where \( L^{(i)} = 0 \). Let us assume that for \( A^{(i)} = A_i^{(i)} \) this occurs, then Equation (4) implies

\[ S_{LA} A_i^{(i)} = 0 \]

(6)

and

\[ A_i^{(-)} = S_A A_i^{(+)} \]

(7)

Equation (6) is accomplished if the incoming wave from the auxiliary chains is fully reflected into the auxiliary chains, which occurs when

\[ \| A_i^{(+)} \| = \| A_i^{(-)} \| \]

(8)
Figure 1. a) System C: An infinite nanoribbon with a wider section. An instance with $N_L = 3$, $N = 5$, and $M = 6$ sites is shown. b) Joining systems A and B through the RSMM, we can model system C. Auxiliary chains are represented by blue lines. c) Joining systems A’ and B’ through the RSMM, we obtain system A. d) Eigenvalues of $S_A S_B$ for energies between $E = 2|t|$ and $E = 3|t|$. Dashed lines identify energies where the condition for bound states is satisfied by one of the eigenvalues. e) Wavefunctions associated with the bound-state energies in color and radius scales.

An analogous procedure may be followed for system B to obtain

$$E_{B,i}^{(+) -} = S_B B_{i}^{(+) -}$$

(9)

Since system C is recovered by doing $A^{(+) -} = B^{(+) -}$, we conclude that $A_{i}^{(+) -}$ corresponds to a bound state of system C if it accomplishes Equations (7) and (8), and

$$A_{i}^{(+) -} = S_B A_{i}^{(+) -}$$

(10)

where Equation (9) was used. Since S-matrix is unitary, then Equation (8) is satisfied whenever Equations (7) and (10) are satisfied. On the other hand, combining Equations (7) and (10) leads us to

$$A_{i}^{(+) -} = S_B S_A A_{i}^{(+) -}$$

(11)

Consequently, there is a bound state at energy $E$ whenever $S_B S_A$ has an eigenvalue one. Observe that in 1D systems this condition is in agreement with the one reported in ref. [13].

The algorithm to determine numerically the bound state energies consists of calculating the eigenvalues $\lambda_i$ of the matrix product $S_A S_B$ for different energies within an interval of interest, obtaining a set of curves for the imaginary and real parts of the eigenvalues. For example, Figure 1d shows the real and imaginary parts of the eigenvalues of $S_A S_B$ for the system in Figure 1a. In this case, we find bound states at energies $E_1 = 2.36481|t|$ and $E_2 = 2.82856|t|$.

To optimize the searching of bound states, we can use the procedures explained in ref. [4] to find the order-N Taylor series of each eigenvalue of $S_A S_B$

$$\lambda_i (E_0 + \Delta E) = \sum_{n=0}^{N} c_{i,n} (\Delta E)^n$$

(12)

Exact derivatives of $\lambda_i(E)$ are then given by $\lambda_i^{(n)}(E_0) = n! c_{i,n}$. In this way, we may use the Newton–Raphson method to find bound states with high accuracy and efficiency by looking for the zeroes of the imaginary-part of any of the eigenvalues $\lambda_i(E)$. Once a zero of the imaginary-part is located at energy $E$, we must confirm that the corresponding real-part is one to conclude that we have found a bound state.

2.2. Determination of Wavefunctions

Once a bound state energy is found, the corresponding eigenfunction can also be calculated by using the RSMM.

First, according to Equation (3) we have $a_i = A_i^{(+)} + A_i^{(-)}$, where $a_i$ is a vector that contains the amplitude coefficients of sites connected to auxiliary chains (in Equation (3), those with $m = 0$) and
A^{(+)}$ is the eigenvector of $S_0 S_0$ with eigenvalue one, as stated in Equation (11). By using Equation (7), we have

$$a_i = (I + S_A) A^{(+)}$$

(13)

This allows us to find amplitude coefficients for the sites shared by subsystems A and B. Now, let us divide system A into two subsystems A' and B' as exemplified in Figure 1c. Then, by analogy, coefficients at the frontier of this division can be calculated from

$$a'_i = (I + S_{A'}) A'^{(+)i}$$

(14)

Scattering matrices of systems A' and B' satisfy, respectively

$$
\begin{pmatrix}
A'^{(-)} \\
L'^{(-)}
\end{pmatrix}
= 
\begin{pmatrix}
S_{A'} \\
S_{L'A'}
\end{pmatrix}
\begin{pmatrix}
A^{(+)} \\
L^{(+)}
\end{pmatrix}
$$

(15)

and

$$
\begin{pmatrix}
A'^{(-)} \\
B'^{(-)}
\end{pmatrix}
= 
\begin{pmatrix}
S_{A'B'} \\
S_{B'A'}
\end{pmatrix}
\begin{pmatrix}
A^{(+)i} \\
B^{(+)i}
\end{pmatrix}
$$

(16)

Using the RSMM, system A is recovered by taking

$$A'^{(+)i} = B'^{(+)i}$$

(17)

In this way, amplitude coefficients for sites in the frontier between A' and B' are given by $a'_i = A'^{(+)}_i = A'^{(-)}_i$. Since we are solving the wavefunction for the case of $A^{(+)} = A^{(-)}$, then we do not observe overlaps with Bloch modes in the leads, i.e., $L^{(+)} = 0$. Consequently, Equation (15) leads to

$$A'^{(-)} = S_A A'^{(+)}$$

(18)

On the other hand, Equations (16) and (17) give us

$$A'^{(-)} = S_{B'A'} A'^{(+)} + S_{B'B'} A'^{(-)}$$

(19)

Combining Equations (14), (18), and (19), we obtain

$$a'_i = (I + S_A) \left(I - S_{B'B'} S_{A'} \right)^{-1} S_{B'A'} A'^{(+)}$$

(20)

Notice that this expression can always be evaluated, even if the number of frontier sites in the left-side of B' is different to that in the right-side.

Subsystems A' and B' can be redefined to have different sites at the frontier. In this way, we can obtain all the amplitude coefficients for sites in A. An analogous procedure can be followed to evaluate the amplitude coefficients for sites in B. For nondegenerate states, it is worth to mention that wavefunctions can be chosen to be real by multiplying them by a suitable phase constant.[32]

### 2.3. Other Forms of Division

There are many ways of defining systems A and B. For example, in Figure 2a by starting with blocks X, Y, and Z, we show two options to define systems A and B. In the first case, A = XY and B = Z, the condition to obtain a bound state requires that

$$Y^{(z)}_{R,i} = Z^{(z)}_{i}$$

(21)

and

$$\|Y^{(z)}_{R,i}\| = \|Y^{(z)}_{R,i}\| \neq 0$$

(22)

where the last inequality is required to avoid trivial solutions of (11). The S-matrix of block Y, $S_Y$, allows us to write

$$\begin{pmatrix}
Y^{(z)}_{L,i} \\
Y^{(z)}_{R,i}
\end{pmatrix} = S_Y \begin{pmatrix}
Y^{(+)}_{L,i} \\
Y^{(+)}_{R,i}
\end{pmatrix}$$

(23)

Due to conservation of probability current density (which makes the $S_Y$ a unitary matrix), we also have

$$||Y^{(+)}_{L,i}|| + ||Y^{(+)}_{R,i}|| = ||Y^{(-)}_{L,i}|| + ||Y^{(-)}_{R,i}||$$

(24)

where the left-side is proportional to the probability current density that enters the block Y, while the right-side is that leaves this block. If we consider $S_Y^{-1} Y^{(z)}_{R,i} \neq 0$, Equations (22)–(24) lead us to

$$\|Y^{(z)}_{L,i}\| = \|Y^{(z)}_{R,i}\| \neq 0$$

(25)

To obtain $A = XY$, blocks X and Y are joined by using $X^{(z)} = Y^{(z)}_{L,i} + Y^{(z)}_{R,i}$, so, in particular,

$$X^{(z)}_{i} = Y^{(z)}_{L,i}$$

(26)

Notice that Equations (25) and (26) are the conditions to obtain a bound state in the second case, where $A = X$ and $B = Y$. In other words, Equations (21) to (26) demonstrate that condition to find a bound state is independent of the particular form of division as long as $S_Y^{-1} Y^{(z)}_{R,i} \neq 0$.

This freedom in the form of division allows us to propose convenient definitions of A and B. For example, in Figure 2, we propose two alternative definitions of systems A and B. In both cases, system A contains all the sites of the system C but has coupled (b) ten and (c) one auxiliary chains. By joining systems A and B through the RSMM, these coupled chains are removed, so we obtain the same system of Figure 1a in both cases. Real and imaginary parts of eigenvalues are shown below each instance. The number of eigenvalues is equal to the number of auxiliary chains coupled to system A. Consequently, we can define a case with only one eigenvalue, as occurs in Figure 2c, which may be more convenient to analyze. However, it is worth mentioning that for systems with many sites in the dispersion region, eigenvalue curves are smoother in cases with more auxiliary chains, which is desirable when using the Newton–Raphson method. Moreover, cases with a single eigenvalue cannot resolve if the energy has degeneracy, but this can be achieved by changing the form of division to a case with more eigenvalues every time the bound state condition is satisfied.
On the other hand, once a bound state energy is found, the determination of the wavefunction can be optimized by adding auxiliary chains to system $A'$, because in this way such sites become frontier sites and Equation (20) can be used to obtain their amplitude coefficients at once.

According to the demonstration above, the method could fail for certain forms of division where $S_{Y_{LR}} = 0$, because in these cases $Y_{L_i}^{(2)} = 0$, which corresponds to a trivial solution of Equation (11). $Y_{L_i}^{(2)} = 0$ means that there is not exchange of probability density current across the division between systems $A = X$ and $B = YZ$. This occurs for bound states whose wavefunction is null for all sites in one of the subsystems, $A$ or $B$. Consequently, the example in Figure 2c would have failed if the coupled chain in system $A$ would have been in a site where the wavefunction has a node. However, this issue may be avoided by exploring the condition for bound states with different positions of the coupled chain or by exploring other forms of division.

### 3. Bound States in Square-Lattice Nanoribbons

In the following, we present bound states in square-lattice nanoribbons with a wider section calculated by using the method in Section 2. In all cases, we consider null site-energies and hopping integral between nearest neighbors $t < 0$.

For the system of Figure 1a with $N = 50$, $N_L = 40$, and $M = 100$, the energies of the first five bound states, shown in Figure 3 are a) $-3.9956984703$, b) $-3.9944369231$, c) $-3.9841130904$, d) $-3.9819853501$, and e) $-3.9787213144$ in units of $|t|$. Leads in this system have at least one open channel for energies between $-2[1 + \cos(\frac{\pi}{N_L+1})]|t|$ and $2[1 + \cos(\frac{\pi}{N_L+1})]|t|$, i.e., between energies $-3.9941316$ and $3.9941316$ for this instance. Consequently, energies (a) and (b) are BOCs while (c)–(e) are BICs. All these eigenvalues are nondegenerate, and since Hamiltonian is symmetrical under horizontal and vertical reflections, these wavefunctions are necessarily symmetric or antisymmetric under these reflections. Energy (a) is the ground state and, as expected, its wavefunction does not have nodes. All

![Figure 2](https://example.com/fig2.png)

Figure 2. a) Two alternative forms of defining systems $A$ and $B$ by starting from three blocks $X$, $Y$, and $Z$. b,c) Examples of systems $A$ and $B$ whose joining through the RSMM lead us to the same system of Figure 1a (top) and the corresponding real and imaginary parts of the eigenvalues of $S_{Y_{LR}}^2$ in each case (bottom). The eigenvalue with the greatest real part is highlighted with a thick red line, while other eigenvalues are shown in gray.
other wavefunctions have line nodes, whose number increases for bound states with greater energies. Also observe that amplitude in the leads is not zero for all eigenfunctions, but they decay in the leads.

For the case of $N = 13$, $N_L = 7$, and $M = 27$, Figure 4a shows six BICs at the same energy $E = 0$. Figure 4b illustrates the wavefunctions of two of these BICs. Since these bound states are degenerate, eigenvectors $A_j^{(i)}$ in Equation (11) were orthogonalized by using the Gramm–Schmidt algorithm, leading us to orthogonalized wavefunctions. Due to degeneracy, symmetries under horizontal and vertical reflections in the wavefunctions are not guaranteed. There are different values of $N$, $N_L$, and $M$ for which the system of Figure 1a has BICs at $E = 0$. Figure 4c illustrates them by varying the values of $M$ and $N_L$ for fixed $N = 38$ and $N = 39$, where the color scale represents the number of BICs at $E = 0$. For cases with $M = j(N + 1) - 1$, where $j = 1, 2, 3, \ldots$, there are $N - N_L$ BICs at $E = 0$. Wavefunctions in these cases have vertical nodal lines every $N + 1$ sites. This can be observed in the examples of Figure 4b, where all wavefunctions have a vertical nodal line at the center of the system. In general, if $m = (N - i + 1)/i$ is an integer for some integer $i$, there are BICs at $E = 0$ whenever $M = j(m + 1) - 1$ and $M > N_L$. It is important to mention that all wavefunctions associated with BICs at $E = 0$ are null in the leads, which is expected, because at this energy there are no evanescent modes, and so any bound state cannot extend into the leads. However, disorder would couple the wavefunctions to open channels in the leads, making these BICs metastable.

4. Bound States in Graphene Nanoribbons

In the following, we determine bound states in armchair graphene nanoribbons (AGNRs). The first case considered is a two-quantum-dot-like junction in an AGNR shown in Figure 5a. Hydrogen passivation was considered by taking the hopping parameters of the dimers at the border of the AGNR as $t_{d} = 1.12t$ (green bonds in Figure 5a), with $t$ being the parameter in all other cases. This system was previously ex-
Figure 5. a) AGNR with two wider sections. The hopping parameter for the border dimers (green) was taken as 1.12 \(t\) with \(t\) being the parameter for the rest of cases (black), \(L\) measures the distance between wider sections by counting the number of border dimers; this instance corresponds to \(L = 5\).

b–g) Bound state wave functions \(\psi\) of structure (a) with positive energies. h) Bound state energies of structure (a) as function of \(L\). i–k) Bound state wave functions for the case of a single wider section. (bottom) Number of open channels in the leads (\(N_C\)) as a function of energy for BIC and BOC identification.

explored by Gonzalez et al. in search of BICs with a method that consisted in determining energies for which there is a peak in the DOS but not in conductance. Three different BICs were reported with that method for energies 0.05, 0.46, and 0.62 in units of \(|t|\). For the same system, the method hereby proposed allowed us to find six different bound states for positive energies at \(E_{1,1} = 0.050492\), \(E_{1,2} = 0.050633\), \(E_{1,3} = 0.455494\), \(E_{2,2} = 0.456079\), \(E_{3,1} = 0.619317\), and \(E_{3,2} = 0.619912\). By rounding these energies to two decimal places, they can be grouped into pairs \(E_{1,1}, E_{1,2}\), and \(E_{3,1}, E_{3,2}\), each pair matching those previously reported. The six wavefunctions were calculated and are presented in Figure 5b–g. Observe that the wavefunctions within a pair only differ in their symmetry under vertical reflections, one with even and the other with odd wavefunction, and both contribute to the same charge distribution reported in ref. [24]. To understand the origin of these pairs of bound states, we analyze the case of a single quantum-dot junction, finding bound states at energies \(E_1 = 0.050563\), \(E_2 = 0.455786\), and \(E_3 = 0.619607\), whose wavefunctions are shown in Figure 5i–k. Notice that each of these energies lie between a pair of energies of the double defect bound states. Figure 5h presents \(E_{i,k} - E_i\) as a function of the distance \((L)\) between quantum dots. Observe that as \(L\) grows, the energy pairs \(E_{i,k}\) rapidly approach each other, until they ultimately converge at \(E_i\). This behavior is analogous to bonding and antibonding states in molecular orbitals. In these terms, the even and odd symmetry under vertical reflections in the wavefunction of each pair is explained as a constructive and destructive interference phenomenon, respectively, caused by the overlapping of the wavefunctions that are centered in each quantum dot.

The second AGNR explored has a central region formed by a series of continuous expansions and contractions in the width of the ribbon. There are 13 different bound state energies. Their wavefunctions are presented in Figure 6. Except for the two with the lowest energies and the two closest to zero, all the cases have one open channel and therefore are BICs. The eigenfunctions have no common behavior regarding whether they are totally confined to the wider sections or if they decay in the leads, showing robustness of the method under different circumstances. Also, observe that the function corresponding to the lowest energy has no nodes, as expected for a ground state, and the number of nodes increases as the energy grows. AGNRs with continuous width variation as the ones shown in Figure 6 have been explored by Gröning et al., who experimentally obtained conductance maps that are in great agreement with the tight-binding simulated charge density. Thus, experimental observation of the bound states theoretically predicted here may be possible using techniques as the one abovementioned.

5. Discussion and Conclusions

In this paper, we have presented a new method based on the RSMM to calculate energies and wavefunctions of bound states
in general tight-binding systems with infinite leads. The method consists in dividing the system into two subsystems. Then we calculate eigenvalues of a matrix $S_B S_A$ (11) that is given in terms of the S-matrices of such subsystems. Whenssoever an eigenvalue becomes one, there is a bound state. We have used this method to determine BICs and BOCs in square- and honeycomb-lattice nanoribbons with wider sections. In real nanoribbons, these wider sections may be present by design or as fabrication defects. We observe in Figure 3 that even slight width variations may induce BICs. The analysis of Figure 4 explores the impact of defect size in the appearance of BICs. The AGNR shown in Figure 5 allowed to observe the bound state interference between BICs centered in each quantum dot. On the other hand, the multiple wider sections in AGNR of Figure 6 induce the formation of many BICs and constitute an accessible structure for experimental BIC observation.

The number of eigenvalues to be analyzed in search for bound states can be controlled as there are multiple ways to define the subsystems. They only must satisfy that by joining them through the RSMM the system is recovered. The number of eigenvalues depends on the number of auxiliary chains in each subsystem. In this way, we have proposed alternatives with different number of eigenvalues. By analyzing the eigenvalues in each alternative, we show that any of them is useful to find the bound states. In particular, we have proposed in Figure 2c an alternative where one of the subsystems has only one site, leading us to a single
eigenvalue of $S_A S_A$, which is convenient. However, we pointed out that in cases with more auxiliary chains, curves of eigenvalues are smoother, which is also desirable. Moreover, when the wavefunctions are being calculated, it is better to maximize the number of sites with attached auxiliary chains. In practice, we can change the way the subsystems are defined to explore the advantages of each definition.

The method allows us to compute bound-state energies with high precision and can be used standalone or together with other methods to determine energy of BICs. Machine precision is achieved in a few iterations following the Newton–Raphson method, where exact first derivatives of the eigenvalues of $S_A S_A$ are computed by using Taylor series of the S-matrices. On the other hand, we can explore the occurrence of bound states in a selected domain of interest, where other methods have reported BICs. For example, BICs in Figure 5 were previously reported by Gonzalez et al., where they identified peaks in the density of states that are not present in the transmission spectrum as signals of BICs. Energy of these BICs was reported with two decimal places. By exploring the vicinity around such energies with the method hereby proposed, we confirm these BICs. But actually, there are two BICs for each reported energy. The energy of each pair differs by the 4th decimal digit. Their corresponding wavefunctions have the same absolute value, which make them indistinguishable when the charge distribution is analyzed through the Green’s function. The origin of this pair of energies is analogous to the bonding and antibonding states in molecular orbitals and are the result of the linear combination of BICs orbitals centered in each quantum-dot structure. Even when the method reported here can work independently to find BICs, we believe that the technique that occupies the density of states and the transmission spectrum is useful to find regions of interest by inspection. Then, the method proposed here may focus on these regions to find energies and wavefunctions of the bound states with high precision. In terms of computational effort, this method is on par with the one that compares density of states with transmission spectrum, because all relevant quantities of both methods can be obtained recursively from the $S$-matrix of the system $C$. In fact, $S$-matrices of system $A$ and $B$ are just the ones used in the last iteration of the RSMM to obtain system $C$, so they become available during the recursive process. Furthermore, as explained in Section 2.3, by using convenient forms of division, time to diagonalize $S_A S_A$ can be neglectable.

We expect that the predicted BICs in this paper could be verified in experimental setups. In particular, those in Figure 6 correspond to a system that has been realized recently to study topological border states. Other cases may be explored in acoustic or optical systems. Simulations of tight-binding Hamiltonians using ultracold atoms in an optical lattice constitute another possible way to observe BICs, as these techniques are in current development and have already allowed to explore diverse quantum phenomena.

It is worth to mention that this method does not add any additional approximations beyond the tight-binding approach. Moreover, the method can also be considered for continuous systems where a discretization process results in an effective tight-binding model, as occurs in quantum billiards. To analyze specific systems, it is only necessary to set adequate parameters in the tight-binding Hamiltonian. Realistic parameters can be obtained from a Wannierization of density functional theory band structure calculations and from the density functional-based tight-binding method. Recent developments as the use of neural networks may also provide a path to obtain more realistic parameters for arbitrary systems.

Even when we have applied the method to nanoribbons with wider sections, it can also be used on systems with other kind of defects, such as impurities, vacancies, dislocations, etc., including point, line, and planar defects. This method could also be useful to study the formation of charge islands in graphene nanoribbons with edge disorder. Analysis of these scenarios is currently under development.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

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