An efficient method to compute the scattering properties of long periodic waveguides

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Abstract. By properly combining finite element techniques and the transfer matrix approach we propose a method to calculate numerically the scattering properties of non-integrable very long periodic waveguides at a low computational cost. We verify the performance of our proposal by comparing with standard finite element method computations of conductance for three different waveguide geometries.

1. Introduction
The complex scattering of waves (electronic, electromagnetic, acoustic, etc) through guiding devices has been a subject of interest for a long time. In particular, it is well known that transport properties depend strongly on the time- and length-scales involved, being the waveguide length $L$ one of the most relevant scales. Even though there are well established theoretical approaches to study transport (for example, in mesoscopic systems we can mention theories of random matrices or ballistic sigma-models) it is desirable to verify them by the use of numerical experiments. However, due to computational standard limitations, a serious problem one has to face when performing numerical transport experiments is to approach the often invoked theoretical limit $L \to \infty$.

In this paper we consider the electronic/electromagnetic wave transport through non-integrable two-dimensional (2D) waveguides. We focus our attention on periodic waveguides and show that by properly combining finite element methods and the transfer matrix approach we are able to obtain the scattering properties of very long periodic waveguides at a low computational cost.

The outline of this paper is as follows. In Section 2 we review the concepts of scattering and transfer matrices and describe the method we propose to compute the scattering properties of periodic waveguides. In Section 3 we introduce the generalized ripple billiard which is the non-integrable 2D waveguide model we use to verify the performance of our proposal. Then, in Section 4 we validate our method by comparing with standard finite element method computations of conductance for three different waveguide geometries. Finally, we conclude in Section 5.

2. Definitions and Method
2.1. The scattering matrix $S$

The $S$-matrix is the most fundamental quantity for analyzing wave scattering phenomena in various fields of physics, for it provides us with the most complete scattering data [1].
The longitudinal wave vector functions in the leads are

where \( \psi_{\text{left}} \) and \( \psi_{\text{right}} \) correspond to the lead into the mode probability amplitude for a left (right)-incoming mode. The transmission and reflection amplitudes given, respectively, by \( t \) and \( r \) matrices, where \( M \times M \) matrices, where \( M \) is the highest mode given by the largest \( m \) beyond which the longitudinal wave vector \( k_m = \sqrt{2mE/h^2 - m^2\pi^2/d^2} \) becomes complex.

The elements of the transmission \( (t \text{ and } t') \) and reflection \( (r \text{ and } r') \) matrices are the transmission and reflection amplitudes given, respectively, by \( t_{nn}(E) = (a_n^R/a_n^L)\sqrt{k_n/k_m}, \) \( t'_{nn}(E) = (b_n^L/b_n^R)\sqrt{k_n/k_m}, \) \( r_{mn}(E) = (b_n^L/a_n^L)\sqrt{k_n/k_m}, \) and \( r'_{mn}(E) = (a_n^R/b_n^R)\sqrt{k_n/k_m}. \) Here, \( a_n^R \) \( (a_n^L) \) is the amplitude of the forward traveling plane wave \( \text{exp}[ik_n^{LR}(x)]\sqrt{2/d}\sin(m\pi y/d) \) on the left (right) lead corresponding to the \( m \)-th transversal mode. Similarly, \( b_n^R \) \( (b_n^L) \) is the amplitude of the backwards traveling plane wave \( \text{exp}[-ik_n^{LR}(x)]\sqrt{2/d}\sin(m\pi y/d) \) on the left (right) lead. See [2, 3] for details. The \textit{square}d modulo element \( |t_{n,m}|^2 \) \( \text{(|t'_{n,m}|^2)} \) gives the probability amplitude for a left (right)-incoming mode \( m \) to be transmitted to the right (left) lead into the mode \( n. \) Similarly, \( |r_{n,m}|^2 \) \( \text{(|r'_{n,m}|^2)} \) is the probability for a left (right)-incoming mode \( m \) to be reflected to the left (right) lead into mode \( n. \)
Figure 2. Scheme of a two-dimensional waveguide composed by two cavities $C_1$ and $C_2$ (with transfer matrices $T_1$ and $T_2$, respectively) connected in series.

2.2. The transfer matrix $T$

The transfer-matrix method can be used when the total system can be broken into a sequence of subsystems that interact only with adjacent subsystems. Then, having as a reference the scattering setup of Figure 1, the $T$-matrix relates waves in the left lead to waves in the right lead as

$$\psi_R = T\psi_L.$$  \hspace{1cm} (6)

With the notation above the $T$-matrix and the waves in the left and right leads are written as

$$T = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad \psi_L = \begin{pmatrix} a_L \\ b_L \end{pmatrix}, \quad \psi_R = \begin{pmatrix} a_R \\ b_R \end{pmatrix}. \hspace{1cm} (7)$$

A useful property of the $T$-matrix in the study of scattering systems is the serial multiplication: Consider two waveguide cavities $C_1$ and $C_2$, see Figure 2, whose transfer matrices are $T_1$ and $T_2$, respectively. If the amplitudes of the waves related through $T_1$ are $(a^{(1)}, b^{(1)})$ and $(a^{(2)}, b^{(2)})$ (the left and right wave coefficients corresponding to $C_1$) and the amplitudes of the waves related through $T_2$ are $(a^{(2)}, b^{(2)})$ and $(a^{(3)}, b^{(3)})$ (left and right wave coefficients corresponding to $C_2$), then the $T$-matrix of the combined scattering system composed by the cavities $C_1$ and $C_2$ connected in series is given by the matrix product $T = T_2 T_1$, where $T$ relates the left $(a^{(1)}, b^{(1)})$ and right $(a^{(3)}, b^{(3)})$ wave coefficients of the combined scattering system. Moreover, the serial multiplication property can be generalized to any finite number of cavities: Let's consider a waveguide scattering system composed by $N$ cavities $C_i$ connected in series, each one having a transfer matrix $T_i$, then the transfer matrix of the complete waveguide system is given by

$$T = \prod_{i=1}^{N} T_i. \hspace{1cm} (8)$$

2.3. Proposal

Since both, the $S$-matrix and the $T$-matrix, describe an scattering process they could be expressed in terms of the other’s matrix elements. For the scattering setup we consider here, see Figure 1, they are given as [4]

$$T(S) = \begin{pmatrix} t - r'[t']^{-1} r' & r'[t']^{-1} \\ -[r']^{-1} r & [t']^{-1} \end{pmatrix}, \hspace{1cm} (9)$$

$$S(T) = \begin{pmatrix} \alpha - \delta [\delta]^{-1} \gamma & [\delta]^{-1} \\ \alpha - \beta [\delta]^{-1} \gamma & \beta [\delta]^{-1} \end{pmatrix}. \hspace{1cm} (10)$$

Then, the procedure we propose to obtain the scattering properties of periodic waveguides is as follows: (i) compute the scattering matrix $S_0$ of the unitary cell $C_0$, one period of
the waveguide, by standard finite element method (FEM) computations; (ii) construct the corresponding transfer matrix $T_0$ by the use of Equation (9); (iii) calculate the transfer matrix $T$ of the waveguide composed by $N$ unitary cells connected in series by the use of Equation (8), which in this case reduces to $T = (T_0)^N$ since the scattering system is periodic; (iv) compute the scattering matrix $S$ of the waveguide by the use of Equation (10). The advantage of our approach is that the FEM is used only for one cell, allowing for higher geometrical resolution, and hence more accurate calculations of transport quantities than in the standard method where the FEM is used for the whole length of the waveguide. The iteration of the transfer matrices implies lower computational cost than FEM computations.

Once the $S$-matrix is known it is possible to compute transmission, reflexion, shot noise, conductance, etc. See for example [4]. In particular, we will be interested below in the dimensionless conductance, which is well described by the Landauer-Buttiker formula [5]

$$G = \text{Tr}(tt^\dagger).$$

### 3. The waveguide model

To test the method described above we use a 2D periodic waveguide which is composed by $N$ periods (unitary cells) of the generalized ripple billiard, defined by two walls given by the functions

$$g(x) = d + A_1\xi_1(x),$$
$$f(x) = A_2\xi_2(x),$$

where $d$ is the average width of the billiard, $A_{1,2}$ stand for the amplitudes of modulation, and $\xi_{1,2}(x)$ are periodic functions with period $L_x$: $\xi_{1,2}(x + L_x) = \xi_{1,2}(x)$. See Figure 3.

When $\xi_1(x) = \cos(2\pi x/L_x)$, $L_x = 2\pi$, and $A_2 = 0$ in Equation (12) the standard ripple billiard is recovered. See for example [6], Chapter 6. An attractive feature of the generalized ripple billiard is that its classical phase space undergoes the generic transition to global chaos as the amplitudes $A_{1,2}$ increase. Then, results from the analysis of this system are applicable to a large class of systems, namely non-degenerate, non-integrable Hamiltonians [6, 7]. Various transport and dynamical properties of the ripple billiard have been investigated in both, classical [2, 3, 8] and quantum regimes [2, 3, 9, 10, 11, 12, 13, 14, 15] in its two versions: finite (one or few periods of modulation) [2, 3, 8, 10, 11, 15] and infinite [12, 13, 14]. Hence, the ripple billiard has become a paradigm in studies of quantum chaos.

Below we use three waveguide geometries characterized by the choice of $g(x)$ and $f(x)$ as follows.

#### 3.1. Waveguide with one rippled wall

Here we consider the standard ripple billiard as in [2, 3]; so we choose $\xi_1(x) = \cos(2\pi x/L_x)$, $L_x = 2\pi$, and $A_2 = 0$ in Equation (12). See Figure 3(a).

#### 3.2. Waveguide with rippled walls and constant width

Here we choose $\xi_1(x) = \xi_2(x) = \cos(2\pi x/L_x)$, $L_x = 2\pi$, and $A_1 = A_2$ in Equation (12); so that $g(x) - f(x) = d$. See Figure 3(b).

#### 3.3. Waveguide with rippled walls and constant cross section

For this case we write $g(x)$ and $f(x)$ in the parametric form [16] $\vec{f}(t) = (x(t), f(t))$ and $\vec{g}(t) = \vec{f}(t) + d\vec{N}$, respectively, with $\vec{N} = \vec{N}(t)/||\vec{N}(t)||$ and $\vec{N}(t) = (x''(t)f'^2(t) - x'(t)f'(t)f''(t),$
Figure 3. (a) Waveguide with one rippled wall, (b) waveguide with rippled walls and constant width, and (c) waveguide with rippled walls and constant cross section. Here, the size of all waveguides is equal to four unitary cells; i.e. $N = 4$.

By choosing $\xi_2(x) = \cos(2\pi x/L_x)$ and $L_x = 2\pi$ in Equation (12); i.e. $f(x) = A_2 \cos(x)$, we get for the parametrization of $g(x)$

$$
\gamma(t) = \left( t + d - \frac{A_2 \sin(t)}{\sqrt{A_2^2 \sin^2(t) + 1}} , \ A_2 \cos(t) + \frac{d}{\sqrt{A_2^2 \sin^2(t) + 1}} \right).
$$

Here, the constant cross section of the waveguide is $d$. See Figure 3(c). Waveguides with constant cross section are also known as unidirectional waveguides since, in their classical limit, they show perfect particle transmission. See for example [16].

4. Results

In Figures 4, 5, and 6 we show plots of the dimensionless conductance $G$ as a function of the normalized energy $E/E_0$ for waveguides with one rippled wall, waveguides with rippled walls and constant width, and waveguides with rippled walls and constant cross section, respectively. See also Figure 3. $E_0$ is given by Equation (4) with $k_m = 0$ and $m = 1$. The values of the geometrical parameters are given in the corresponding figure captions. In all three cases we present results for waveguides composed by $N = 2, 5, 10, 25,$ and $50$ unitary cells.

In Figures 4-6 black curves correspond to the calculation of $G$ using the standard finite element methods (see details in [17]). While the corresponding computation of $G$, based on the transfer matrix approach, is shown as red dots. We observe a good global correspondence of both sets of data. However, closer inspection reveals important differences that indicate that our approach is more efficient and accurate. Specifically, the standard finite element method shows gaps not produced by our method, see, e.g., Figure 4, $N = 25$ for $E/E_0 < 4$. We believe these gaps are incorrect given that the standard method shows also various places where $G$ reaches values higher than allowed by flux conservation, that is, higher than the corresponding number of open modes, see, e.g., Figure 4, $N = 25$ in $6 \leq E/E_0 \leq 8$. These errors appear because the number of finite elements per unit cell $N_e$ used in the standard method is smaller than the corresponding number $N_c$ used for a single cell in our combined method. $N_e$ is necessarily smaller than $N_c$ since the standard method requires larger computational resources. Further evidence that our method is more accurate is that it reproduces the expected $N - 1$ small oscillations in the transmission bands for periodic systems, see Figures 4-6 for $N > 10$. 


5. Conclusions

We have proposed a method, based on a combination of finite element methods and the transfer matrix approach, to calculate the scattering properties of non-integrable periodic waveguides. Even though we have used the generalized ripple billiard to validate our proposal, the applicability of our method should not be restricted to this waveguide geometry.

We stress that our proposal offers a very efficient and low computational cost technique, as compared with standard finite element methods. As a rough example, we mention that the calculation of the conductance $G$ reported in Figures. 4-6, using the standard finite element methods (black curves), for the waveguides of size $N = 50$ took about $30$hrs. While the
corresponding computation of $G$, based on the transfer matrix approach (red dots), took only 20mins (moreover, consider that most of this time was used to obtain the scattering matrix of the unit cell $S_0$).

We expect to successfully apply this method to calculate statistically the scattering properties of surface disordered waveguides, where large waveguide ensembles are needed.

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6. References

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