Evolution with size in a locally periodic system: scattering and deterministic maps

V Domínguez-Rocha and M Martínez-Mares

Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa, Apartado Postal 55-534, 09340 México Distrito Federal, Mexico

E-mail: vdr@xanum.uam.mx and moi@xanum.uam.mx

Received 14 February 2013, in final form 25 April 2013
Published 21 May 2013
Online at stacks.iop.org/JPhysA/46/235101

Abstract

In this paper, we study the evolution of the wavefunction with the system size in a locally periodic structure. In particular, we analyse the dependence of the wavefunction with the number of unit cells, which also reflects information about its spatial behaviour in the system. We reduce the problem to a nonlinear map and find an equivalence of its energy regions of single periodicity and weak chaos, with the forbidden and allowed bands of the fully periodic system, respectively. At finite size the wavefunction decays exponentially with the system size, as well as in space, when the energy lies inside a region of single periodicity, while for energies in the weak chaotic region it never decays. At the transition between those regions the wavefunction still decays but in a $q$-exponential form; we find that the decay length is a half of the mean free path, which is larger than the lattice constant.

PACS numbers: 05.60.Gg, 05.45.Ac, 72.10.-d, 72.20.Dp

1. Introduction

Crystalline materials occupy a special place in the solid state physics. Despite the fact that in real life the majority of the solids are noncrystalline, crystals help to understand a lot of the properties of the solid matter. At the macroscopic scale crystalline solids are considered as infinite periodic systems, which are well described by the band theory [1]. However, the propagation of electrons through a locally periodic system, which consists of a finite number $N$ of repeating elements [2], has been of great interest due to the practical applications in designing artificial materials with specific features. That is the case of layered periodic structures or finite superlattices [3–5], and man-made devices fabricated with optical lattices to model condensed matter systems [6–10]. Furthermore, the applicability of locally periodic structures cover a wide range that includes structurally chiral materials [11], microwave [12], photonic [13–15] and phononic [16, 17] crystals, as well as elastic or acoustic systems [18–20].
The study of locally periodic structures is mainly concerned with the band formation for several cases of fixed $N$, where each one is analysed separately to look for the emergence of the allowed and forbidden bands [21–24]. In all cases, the precursors of the band structure of the corresponding fully periodic system, which is almost formed when $N$ is large enough, can be observed [2]. An interesting question that immediately arises is how or when the properties of fully periodic systems are reached. Therefore, to answer this question it is necessary to study the evolution of the system as $N$ increases. This procedure allows us to get additional information about the band formation; that is, the evolution to the infinite system should not be the same for energies in the gap than those in an allowed band of the fully periodic system.

Since the standard method of band theory for crystals is not applicable for finite systems, the scattering approach becomes very important in the determination of their transport properties. In particular, the transfer matrix method [25] is a powerful tool that has been successfully applied in the study of the transmittance, conductance or resistance, for example, through a finite sequence of scattering elements along one dimension [15, 23, 26]. However, for nonlinear (as well as linear) arrays of scatterers, the electronic transport is described by the scattering matrix instead of the transfer matrix. That is the case of a double Cayley tree whose conductance was analysed at fixed generation (the generation plays the same role as $N$) [27]. On the other hand, the behaviour of the conductance on a double Cayley tree as a function of the generation was studied in [28]. There, a remarkable equivalence between the electronic transport and the dynamics of an intermittent low-dimensional nonlinear map has been exhibited; the map presents regions of weak chaos and of single periodicity, whose Lyapunov exponents are zero and negative, which indicates the conducting and insulating phases, respectively [29]. The conductance oscillates with the generation in the weakly chaotic attractors of the map, indicating conducting states. In the attractors of single periodicity, the conductance decays exponentially as is typical for insulating states, but at the transition the intermittency of the map makes the conductance to reach the insulating phase in a $q$-exponential form. Therefore, there exist typical length scales on the different energy regions that remain to be understood.

A scaling analysis of the conductance is one way to obtain information about the metallic or insulating behaviour of a system [30]. But, the conductance is a global quantity and not much can be said about the local character in the system. Therefore, it is important to study the wavefunction directly, whose spatial behaviour should reflect whether a system behaves as a conductor or not.

The purpose of this paper is to analyse the evolution of the wavefunction with $N$ and once this is done, look at its spatial behaviour in a locally periodic structure in one dimension. This study allows us to determine the nature of the several states in the system, answer the question posed above and find a physical interpretation of the typical length scales in the problem. In order to do this, we consider a locally periodic potential that is formed by a sequence of individual scattering potentials. For our purpose, it is not necessary to consider an open system on both edges. Therefore, without any loss of generality, we avoid unnecessary complications and restrict the system to have only one entrance. We solve the problem analytically for arbitrary individual potentials using the scattering matrix formalism. Following the same ideas in [28], we reduce the problem to the analysis of the dynamics of an intermittent low-dimensional nonlinear map.

We organize the paper as follows. In the following section, we present the scattering approach to our linear chain of scatterers. In the same section, the recursive relation satisfied by the scattering matrix, when an individual scatterer is added, is reduced to a nonlinear map. The scaling analysis and the spatial dependence of the wavefunction are presented in section 3. We present our conclusions in section 4.
2. A serial structure of quantum scatterers

2.1. Scattering approach

The quantum system that we consider is a one-dimensional locally periodic whose separation between adjacent scatterers is \( a \) that we will refer to as the lattice constant. This chain consists of \( N \) identical scatterers, each one described by the potential \( V_b(x) \) of arbitrary shape and range \( b \), as shown in figure 1. The unit cell consists of a free region of size \( a - b \) plus the potential of range \( b \), except in the first one where the size of the free region is \( a - b/2 \). Our chain lies in the semispace at the right of the origin, bounded on the left (\( x = 0 \)) by a potential step of high \( V_0 \gg E \), where \( E \) is the energy of the quantum particle; the right side of the chain remains open. We assume that each scatterer is described by a unitary scattering matrix \( S_b \) that has the following structure:

\[
S_b = \begin{pmatrix} r_b & t'_b \\ t_b & r'_b \end{pmatrix},
\]

where \( r_b \) (\( r'_b \)) and \( t_b \) (\( t'_b \)) are the reflection and transmission amplitudes for incidence on the left (right) of the potential, respectively.

As we will see below, the evolution of several properties of the system with the number of scatterers can be obtained from the scattering matrix of the system. Therefore, we write the scattering matrix \( S_N \) that describes the system with \( N \) scatterers, in terms of the one with \( N - 1 \) of them, \( S_{N-1} \), by adding an individual scatterer using the combination rule of scattering matrices. The combination of \( S_{N-1} \) and \( S_b \) gives the following recursive relation, namely

\[
S_N = r'_b + t_b \frac{1}{e^{-2ik(a-b)} - S_{N-1}r'_b} S_{N-1}t'_b,
\]

where \( k = \sqrt{2ME/\hbar^2} \), with \( M \) being the mass of the particle. The initial condition for this recursive relation is the scattering matrix \( S_0 \) associated with the scattering due to the potential step but measured at \( x = b/2 \).

2.2. Reduction to a nonlinear map

Since \( S_N \) relates the amplitude of the outgoing plane wave to the amplitude of the incoming one to the system, it is a \( 1 \times 1 \) unitary matrix that can be parameterized just by a phase, \( \theta_N \), as

\[
S_N = e^{i\theta_N}.
\]
Figure 2. (a) Bifurcation diagram for a chain of delta potentials with $ua = 10$. We plot only the last 30 iterations of $N = 1000$ for the phase as a function of $ka$ starting with an initial condition $\theta_0 = \pi$. We also plot the analytical results given by equations (12) and (17), but they are indistinguishable from the numerics. (b) Finite $N$ Lyapunov exponent $\Lambda_1(N)$ as a function of $ka$ for $N = 1000$. Theoretical result $\lambda_1$ given by (22) is also plotted; it is indistinguishable from $\Lambda_1(N)$ for very large $N$. Inset: $\Lambda_1$ for $N = 20$.

The recursive relation (2) can be seen as a one-dimensional nonlinear map. That is,

$$ f(\theta_{N-1}) = -\theta_{N-1} + 2 \arctan \frac{\text{Im}(r'_b a'_b + \alpha_b e^{i\theta_{N-1}})}{\text{Re}(r'_b a'_b + \alpha_b e^{i\theta_{N-1}})}, $$

modulo $\pi$. Here, $\alpha_b = t_b e^{i\phi/2} e^{i(k(a-b))}$, $e^{i\phi} = t'_b / t_b$, and $\text{Re}(a')$ and $\text{Im}(a')$ denote the real and imaginary parts of $a'$, respectively. Because the reflected wave at the potential step acquires an additional phase $\theta_{\text{step}}$, then $S_0 = e^{i\theta_0}$, where $\theta_0 = \theta_{\text{step}} + kb$, which is the initial condition for the map.

Although the nonlinear map (4) is valid for arbitrary individual potentials, it is necessary to consider a particular case to look for the characteristics of the map. Let us assume for a moment that an individual potential is just a delta potential of intensity $v$ and null range, $b = 0$. In this case, $r_b = r'_b = -u/(u - 2ik)$ and $t_b = t'_b = -2ik/(u - 2ik)$, where $u = 2Mv/\hbar^2$ [31]. The corresponding bifurcation diagram for $ua = 10$ and $\theta_0 = \pi$ is shown in figure 2(a), from which we observe ergodic windows between the windows of periodicity 1. The width of an ergodic window depends on the potential intensity, as well as on the energy; it is wider for higher values of $ka$ (when referring to the delta potential we will speak of $ka$ instead of $k$), as is expected, since for higher energies the effect of the potential is smaller. In the ergodic window, $\theta_N$ fluctuates, while in the window of periodicity 1 it reaches a fixed value when $N$ is very large.

Figure 2(a) suggests that in a window of periodicity 1, (2) reaches a fixed point solution for $S_N$, while it does not in an ergodic window. If we look for the fixed point solutions of equation (2), then we find that in fact, in windows of periodicity 1, $S_N$ has the fixed point solutions of the form (3), $e^{i\theta_e}$. We will see below that one solution is stable, the other is an unstable one (the solution shown in figure 2 for $ua = 10$ with $\theta_0 = \pi$ is a stable one; see figure 3(a)). In an ergodic window, (2) still has fixed point solutions but not of the form (3), which represents a $1 \times 1$ unitary matrix; they are of the form $w_\pm = |w_\pm| e^{i\theta}$, with $\theta$ being the value around which $\theta_N$ fluctuates with an invariant density. These solutions are...
marginally stable (see below) [32]. The stable and marginally stable fixed point solutions can be summarized as

\[
S_\infty = \begin{cases} 
  e^{\alpha_k} & \text{for } k_{c,\alpha} < k < k_{c,\alpha}' \\
  w_\pm & \text{for } k_{c,\alpha}' < k < k_{c,\alpha} \\
  e^{\alpha_k} & \text{for } k_{c,\alpha} < k < k_{c,\alpha}' 
\end{cases}
\]

(5)

where \( k_{c,\alpha} \) and \( k_{c,\alpha}' \) denote the critical values of \( k \) on the left and right edges of the corresponding ergodic window (see (10) below);

\[
e^{\alpha_k} = \frac{1}{r_\alpha b} \left[ \mp \sqrt{(\text{Re } \alpha_b)^2 - |t_b|^2} + i \text{Im } \alpha_b \right]
\]

(6)

for \(|\text{Re } \alpha_b(k)| > |t_b(k)|^2\) and

\[
w_\pm = \frac{i}{r_\alpha b} \left[ \pm \sqrt{|t_b|^2 - (\text{Re } \alpha_b)^2} + \text{Im } \alpha_b \right]
\]

(7)

for

\[
|\text{Re } \alpha_b(k)| \leq |t_b(k)|^2.
\]

(8)

such that

\[
\tan \theta = \frac{\text{Im}(i r_\alpha b^* \alpha_b^*)}{\text{Re}(i r_\alpha b^* \alpha_b^*)}.
\]

(9)

The equality in (8) determines the critical values \( k_{c,\alpha} \) and \( k_{c,\alpha}' \); that is

\[
|\text{Re } \alpha_b(k_c)| = |t_b(k_c)|^2,
\]

(10)

where \( k_c \) denotes \( k_{c,\alpha} \) or \( k_{c,\alpha}' \). At a critical attractor, \( \theta \) takes the value \( \theta(k_c) = \theta_c \), where

\[
\tan \theta_c = \frac{\text{Im}[i r_\alpha b^* \alpha_b^*(k_c)]}{\text{Re}[i r_\alpha b^* \alpha_b^*(k_c)]}.
\]

(11)

The condition (8) is equivalent to that for allowed bands in the infinite linear chain of scatterers [33]. Therefore, we have found a correspondence between the windows of single periodicity (or chaotic) and forbidden (or allowed) bands in the limit \( N \to \infty \), in a similar
way as happens for the double Cayley tree studied in [28]. Equation (10) defines the left and right edges of the chaotic windows.

The dynamics of the map is expected to be different on each type of windows of the bifurcation diagram. To observe the trajectories on each region of $k$ we need to go back to the particular case of delta potentials. For this case, (6) gives

$$e^{i\theta_k} = -\frac{2ka}{ua} e^{-i\Delta [\pm x(ka) + iy(ka)]},$$

(12)

where

$$x(ka) = \sqrt{\left(\cos ka + \frac{ua}{2ka} \sin ka\right)^2 - 1}$$

$$y(ka) = \sin ka - \frac{ua}{2ka} \cos ka$$

(13)

for $|\cos ka + (ua/2ka) \sin ka| > 1$, while (7) gives

$$w_\pm = \frac{2ka}{ua} e^{-i\Delta [\pm x'(ka) + y(ka)]},$$

(14)

where

$$x'(ka) = \sqrt{1 - \left(\cos ka + \frac{ua}{2ka} \sin ka\right)^2}$$

(15)

for

$$\left|\cos ka + \frac{ua}{2ka} \sin ka\right| \leq 1,$$

(16)

which is the condition for allowed bands in the Kronig–Penney model [34]. From (14), it is easy to see that the phase of $w_\pm$ is given by (see (9))

$$\theta = -ka + (m + 1)\pi, \quad m = 0, 1, \ldots$$

(17)

The band edges are obtained from the equality in (16), namely

$$\tan \frac{k_{cm} a}{2} = \left\{ \begin{array}{ll}
\frac{ua}{k_{cm} a}, & \text{for } m \text{ odd} \\
-\frac{2k_{cm} a}{ua}, & \text{for } m \text{ even},
\end{array} \right.$$  

(18)

and $k_{cm} a = m\pi$, for $m$ odd and even. At the band edges, $\theta(k_{cm} a) = \theta_{cm}$, with $\theta_{cm} = -k_{cm} a + (m + 1)\pi$. For the first chaotic window ($m = 1$), $k_{c1} a = 2.28445 \ldots$ and $k_{c1} a = \pi$, $\theta_{c1} = 3.99873 \ldots$ and $\theta'_{c1} = \pi$, for $ua = 10$ as shown in figure 2 and further numerical calculations. Equations (12) and (17) coincide with the numerical results on both sides and inside of the first chaotic window, as is shown in figure 2(a).

The trajectories of the map for this example are shown in figure 3 for some values of $ka$. In panel (a), $ka = 2$, where $ka$ is inside the window of period 1; we observe that all trajectories (we show only two) diverge from a fixed point (repulsor) and converge to another stable fixed point (attractor) as $N \to \infty$; the attractor corresponds to $\theta_c \approx 3.61$. Panels (b) and (d) show intermittent trajectories at the tangent bifurcations when $ka = 2.2846$ and 3.141 45, very close to the transitions from the chaotic side. In panel (c), deep inside the chaotic window, the trajectories never converge. Therefore, we observe that the behaviour of the trajectories for two initial conditions strongly depends on the specific region to which $ka$ belongs. The dynamics of the map can be analysed by means of the sensitivity to initial conditions, something that we do next.
2.3. Sensitivity to initial conditions

The dynamics of the nonlinear map (4) is characterized by the sensitivity to initial conditions. For finite $N$, it is defined by [28]

$$
\Xi_N = \left| \frac{d\theta_0}{d\theta_0} \right| \equiv e^{N\lambda_1(N)},
$$

(19)

where $\theta_0$ is the initial condition and $\lambda_1(N)$ is the finite $N$ Lyapunov exponent, whose dependence on $N$ is shown as an argument (the subscript 1 will be clear below). For the map (4), $\Xi_N$ satisfies the following recursive relation:

$$
e^{N\lambda_1(N)} = \frac{|b_0|^4}{|r_jg_0^* + \alpha_0 s_0|} e^{(N-1)\lambda_1(N-1)}.
$$

(20)

In figure 2(b), we plot $\Lambda_1(N)$ obtained from (20) for the delta potentials as a function of $k\alpha$, for $N = 1000$. We observe that $\Lambda_1(N)$ is negative in the windows of period 1, indicating that $\Xi_N$ decays exponentially with $N$ when $N$ is very large. This means that any trajectory in the map converges rapidly to a fixed point, as happens in figure 3(a). In the chaotic windows, $\Lambda_1(N)$ goes to zero in the limit $N \to \infty$. The $\Xi_N$ does not depend on $N$ and nothing can be said about the convergence of any trajectory; this situation corresponds to figure 3(c). For a finite number of iterations, $\Lambda_1(N)$ is still negative in the windows of period 1, but it oscillates around zero in the chaotic windows. This can be seen in the inset of figure 2; the amplitude of those oscillations tends to zero as $N$ increases; this is a signal of weak chaos [29, 35]. Here, we are interested in the behaviour of $\Xi_N$ with $N$.

With this evidence, we can assume that, in the limit $N \to \infty$, $\Lambda_1(N) \to \lambda_1$ and $\Xi_N \to \xi_N$, where $\xi_N$ is the sensitivity to initial conditions defined by

$$
\xi_N = e^{N\lambda_1},
$$

(21)

where $\lambda_1$ is the Lyapunov exponent of the map, which is given by

$$
\lambda_1 = \ln \frac{|b_0|^4}{|r_jg_0^* + \alpha_0 s_0|}.
$$

(22)

For one of the two roots expressed in (6), which is valid for $k$ in a window of period 1, $\lambda_1$ is positive. This means that the fixed point solution is unstable. The second solution is a stable one since $\lambda_1$ is negative. It is the last one, the only that appears in figure 2(a) due to the initial condition that has been chosen. In the chaotic windows, there are two values of $\lambda_1$ that correspond to the two solutions $w_{\pm}$, one positive and another negative, both at the same distance from zero, for any initial condition. In this case, both values of $\lambda_1$ have to be taken into account. We find that the actual Lyapunov exponent that agrees with $\Lambda_1(N)$, which has been obtained iteratively for very large $N$, is the average of those values, which is zero. In figure 2(b), we compare $\lambda_1$ of (22) with $\Lambda_1(N)$ calculated iteratively by means of (20), for the delta potentials. For $N = 1000$, we observe that both results are indistinguishable. Therefore, (21) says that $\xi_N$ decays exponentially with $N$ for $k$ in the windows of period 1 and remains constant in the chaotic windows. These results are verified in panels (a) and (c) of figure 4, where we compare (21) with the numerical calculations for the delta potential.

The behaviour of the sensitivity to initial conditions is very different at the critical attractors, since there an anomalous dynamics occurs due to the tangent bifurcation [36, 37]. A critical attractor is located at the point $(k_c, \theta_c)$, where $k_c$ denotes $k_{x_n}$ or $k_{x_n}$ and $\theta_c, \theta_{x_n}$ or $\theta_{x_n}$. If we make an expansion of $\theta_N$ close to $\theta_c$, then the result is given by

$$
\theta_N - \theta_c = (\theta_{N-1} - \theta_c) + \alpha(\theta_{N-1} - \theta_c)^2 + \cdots,
$$

(23)
where \( z = 2 \) and \( u = \pm |r_{{k_c}}(k_c)|^2 \). Due to the known properties of this nonlinearity of the tangent bifurcation [37], we expect that the sensitivity obeys a \( q \)-exponential law for large \( N \). That is, \( \xi_{N \to \infty} = \xi_N \), where

\[
\xi_N \propto e^{N\lambda(q)} = (1 - (q - 1)N\lambda_q)^{-1/(q-1)},
\]

with \( q = 2 - 1/z = 3/2 \) and \( \lambda_{3/2} = zu = \mp 2|r_{{k_c}}(k_c)|^2 \). The minus and plus signs correspond to trajectories at the left and right (right and left) of the point of tangency \( \theta_c = \theta_{\ell_{\ell_{\ell}}}(\theta_c = \theta_{r_{r_{r}}}) \), respectively; that is, \( \xi_N \) decays with \( N \) with a power law when \( \theta_{N-1} - \theta_{\ell_{\ell_{\ell}}} < 0 \) (\( \theta_{N-1} - \theta_{r_{r_{r}}} > 0 \)) and grows faster than exponential when \( \theta_{N-1} - \theta_{\ell_{\ell_{\ell}}} > 0 \) (\( \theta_{N-1} - \theta_{r_{r_{r}}} < 0 \)).

In panels (b) and (d) of figure 4, we show the behaviour of \( \Xi_N \) with \( N \) at the edges \( k_{c_{c}}a \) and \( k_{c_{c}}a \), obtained from the numerical calculation for the delta potential, and compare them with (24). In (b), it is clear that \( \Xi_N \) behaves as \( \xi_N \) of (24) at \( ka = k_{c_{c}}a \) for very large \( N \). That is not the case at the right edge \( ka = k_{c_{c}}a \) where \( \Xi_N \) remains constant with \( N \). This pathological behaviour is because \( k_{c_{c}}a \) corresponds to a resonance and there the delta potentials become invisible.

3. Behaviour of the wavefunction

3.1. Evolution of the wavefunction with the system size

The wavefunction in the region between the individual potentials can be written as a superposition of plane waves travelling to the left and right. If we normalize it in such a way that the amplitude after the last scatterer is 1, then the square modulus of the wavefunction in the region between the scatterers \( n \) and \( n + 1 \), labelled by \( n (n = 0, 1, \ldots, N) \), can be written as

\[
|\psi^{(N)}_{n_{a}}(x)|^2 = \frac{e^{N\lambda_q(N)}}{e^{N\lambda_q(n)}} \cos^2[k(x - na - b/2) + \theta_{n/2}],
\]

\( 1 \) The \( q \)-exponential is defined as \( \exp_q(x) = [1 + (1 - q)x]^{1/(1-q)} \) for \( x, q \in \mathbb{R} \). The ordinary exponential is recovered when \( q = 1 \), while for \( q = 3/2 \) the \( q \)-exponential becomes \( \exp_{3/2}(x) = (1 - x/2)^{-2} \).
where \( q = 1 \) for \( k \) in the windows of single period and of weak chaos; \( q = 3/2 \) at the transition from the chaotic side. We see from (25) that at the position \( x \), the amplitude of the wavefunction depends on \( N \) only through the numerator. This means that we can replace \( N \) by \( N - 1 \) to find the wavefunction at the same position for a chain made of \( N - 1 \) scatterers. Hence, the following recursive relation is satisfied by the square modulus of the wavefunction:

\[
|\psi_n^{(N)}(x)|^2 = \frac{e_q^{N\Lambda_q(N)}}{e_q^{N-1}\lambda_q(N-1)} |\psi_n^{(N-1)}(x)|^2.
\] (26)

An iteration process leads us to

\[
|\psi_n^{(N)}(x)|^2 \approx e_q^{N\Lambda_q(N)} |\psi_n^{(0)}(x)|^2,
\] (27)

where \( \psi_n^{(0)}(x) \) is the wavefunction at \( x \) in the absence of any scatterer.

The factor in front of the right-hand side of (27) is just the sensitivity to initial conditions for finite \( N \) (see (19)). Therefore, the evolution of \( |\psi_n^{(N)}(x)|^2 \) with \( N \) is given by \( \Xi_N \), as shown in figure 4. This behaviour resembles the evolution of the conductance with the system size in a double Cayley tree [28]. For energies in a window of period 1, \( |\psi_n^{(N)}(x)|^2 \) decays exponentially with \( N \), for \( N \gg 1 \), with a typical decay length which we identify with a localization length due to the similar scaling behaviour of the conductance with \( N \) [28]; this localization length is given by

\[
\zeta_1 = \frac{a}{|\lambda_1|}.
\] (28)

When \( |\lambda_1| > 1 \), on the one hand, the localization length is smaller than the lattice constant; this occurs far from the transition to the chaotic side, close to the transition \( \zeta_1 > a \). On the other hand, for energies in the chaotic window, \( |\psi_n^{(N)}(x)|^2 \) never decays but oscillates as \( N \) increases; there, \( \lambda_1 = 0 \) such that a localization length cannot be defined. However, at the transition from the chaotic side the wavefunction shows a power law decay with \( N \) (see figure 4(b)). The typical decay length, that we identify with a localization length too, is given by

\[
\zeta_{1/2} = \frac{a}{|\lambda_{1/2}|} = \frac{a}{2|r_b'(k_c)|^2}.
\] (29)

What is very interesting here is that the term on the right-hand side of the second equality is \( \ell/2 \), where

\[
\ell = \frac{a}{|r_b'(k_c)|^2},
\] (30)

which is a definition of the mean free path [38, 39]. This equation means that the mean free path is larger than the lattice constant. This result is in agreement with the one obtained from Esaki and Tsu, where \( \ell \sim 3a \), in a supperlattice [40]. For our particular case of a delta potential with \( ua = 10 \), \( \ell \approx 1.21a \) for \( k_c a = 2.28445 \ldots \) and \( \ell \approx 1.4a \) for \( k_c a = \pi \). The behaviour of the wavefunction in the space can let us understand the nature of the states on the different energy regions.

### 3.2. Spatial behaviour of the wavefunction

In the limit of very large \( N \), \( \Lambda_q(N) \to \lambda_q \) and the squared modulus of the wavefunction given by (25) can be written as

\[
|\psi_n^{(N)}(x)|^2 = \frac{e_q^{N\lambda_q}}{e_q^{\lambda_q}} \cos^2[k(x - na - b/2) + \theta_n/2].
\] (31)
For $k$ far from the critical attractors, $q = 1$ and the ordinary exponential function is recovered. In this case, the spatial behaviour of the wavefunction is given by

$$
|\psi_n^{(N)}(x)|^2 = e^{-(N-n)a/\xi_1} \cos^2[k(x - na - b/2) + \theta_n/2].
$$

(32)

This equation means that when the energy is in a window of period 1, the wavefunction decreases exponentially in space from the boundary ($n = N$) to inside of the system ($n < N$). In this case, the quantum particle is spread over few $\xi_1$s. It is in this sense that we interpret $\xi_1$ as a localization length. This localization length is smaller than the period of our locally periodic structure, $a$, except very close to the transition region. This situation is illustrated in figure 5(a) for the chain of delta potentials.

For energies in the weakly chaotic windows, $\xi_1 \to \infty$ and the wavefunction becomes extended through the system, as can be seen in figure 5(c).

Near the transition, at the weakly chaotic attractors, (31) can be written as

$$
|\psi_n^{(N)}(x)|^2 = \left( \frac{1 \pm na/2\xi_3/2}{1 \pm Nna/2\xi_3/2} \right)^2 \cos^2[k(x - na - b/2) + \theta_n/2].
$$

(33)

where we used that $\lambda_{3/2} = \mp a/\xi_{3/2}$. The plus (minus) sign in (33) corresponds to the left (right) chaotic attractor. This equation clearly shows a power law decay from the boundary. That is, the wavefunction is still localized but the localization is not exponential, but $q$-exponential. It is interesting to note that the localization length is $\xi_{3/2} = \ell/2$. The factor $1/2$ is due to the fact that the localization length is measured from the maximum of the wavefunction, which in this case is at the boundary of the system, while the mean free path implicitly assumes the width of a wave packet; according to Esaki and Tsu [40], the mean free path in a superlattice is the uncertainty in the position. In figure 5(b), we can observe the power law decay of the squared modulus of the wavefunction for the chain of delta potentials. Figure 5(d) shows the behaviour of the squared modulus of the wavefunction at the attractor on the right.
side of the chaotic window. In this case, the system is invisible since \( k_c a = \pi \) corresponds to a resonance and the wavefunction has nodes just at the delta potentials.

4. Conclusions

We considered a locally periodic structure in one dimension, which consists of a chain of potentials of arbitrary shape. We studied the evolution of the wavefunction of the chain when the system size increases. This procedure helped us to observe the behaviour of the wavefunction in space when the size of the system remains fixed.

Since the system is not fully periodic, we cannot use the traditional band theory. Instead of that we take advantage of a recursion relation of the scattering matrix, in terms of the number of scatterers, to reduce the problem to a nonlinear map. Through this method all information about the behaviour of the system was obtained from the dynamics of this map. In this way, we could understand how and when the band theory of the fully periodic chain is reached by the knowledge of the type of evolution of the wavefunction with the system size. We found an equivalence between the periodic and weakly chaotic regions of the map and the forbidden and allowed bands, respectively. This equivalence is similar to that remarked in the literature for the conductance of a double Cayley tree, where it is null in the windows of period 1, and oscillates in regions of weak chaos. Also, we found that the wavefunction at a given position scales with the system size in a similar way as the conductance does. In a window of period 1, far from the transition to the chaotic window, the wavefunction decays exponentially with a typical length scale, which is smaller than the lattice constant. Very close to the transition from the window of period 1, this typical length becomes larger than the lattice constant. This behaviour drove us to interpret the typical scale as a localization length. We corroborated this interpretation by the exponential localization of the wavefunction close to the boundary of the finite system. In the chaotic region, the wavefunction does not decay and a localization length cannot be defined.

At the transition between periodic and weakly chaotic regions, but from the chaotic side, the wavefunction scales as a power law. This implies that it is still localized but with a \( q \)-exponential form. The localization length was found to be one half of the mean free path. We demonstrate analytically that the mean free path is larger than the lattice constant, in complete agreement with a result found in the literature for a superlattice.

Finally, it is worth mentioning that our development considers independent quantum particles such that classical waves can also be used. In particular, one-dimensional elastic systems are strong candidates to simulate our quantum system by means of elastic rods with narrow notches [19].

Acknowledgments

The authors thank RA Méndez-Sánchez and G Báez useful discussions. MMM is grateful with the Sistema Nacional de Investigadores, Mexico, and with MA Torres-Segura for her encouragement. VDR thanks financial support from CONACyT, Mexico, and partial support from C Jung through the CONACyT project no. 79988.

References

[1] Ashcroft N W and Mermin N D 1976 Solid State Physics (Glendale, CA: Thomson Learning) chapter 8
[2] Griffiths D J and Steinke C A 2001 Am. J. Phys. 69 137
[3] Pacher C, Rauch C, Strasser G, Gornik E, Elsholz F, Wacker A, Kießlich G and Schöll E 2001 Appl. Phys. Lett. 79 1486
[4] Morozov G V, Sprung D W L and Martorell J 2002 J. Phys. D: Appl. Phys. 35 2091
[5] Morozov G V, Sprung D W L and Martorell J 2002 J. Phys. D: Appl. Phys. 35 3052
[6] Courtaude E, Houde O, Clément J F, Verkerk P and Henneguin D 2006 Phys. Rev. A 74 031403
[7] Ponomarev A V, Madroñero J, Kolovsky A R and Buchleitner A 2006 Phys. Rev. Lett. 96 050404
[8] Wang T, Javanainen J and Yelin S F 2007 Phys. Rev. A 76 011601
[9] Olson S E, Terraciano M L, Bashkansky M and Fatemi F K 2007 Phys. Rev. A 76 061404
[10] Houston N, Rius E and Arnold A S 2008 J. Phys. B: At. Mol. Opt. Phys. 41 211001
[11] Reyes J A and Laktutai A 2006 Opt. Commun. 259 164
[12] Luna-Acosta G A, Schanze H, Kuhl U and Stöckmann H J 2008 New J. Phys. 10 043005
[13] Lipson R H and Lu C 2009 Eur. J. Phys. 30 S33
[14] Estevez J O, Arriaga J, Méndez Blas A and Agarwal V 2009 Appl. Phys. Lett. 94 061914
[15] Archuleta-Garcia R, Moctezuma-Enriquez D and Manzanares-Martinez J 2010 J. Electromagn. Waves Appl. 24 351
[16] Vasseur J O, Hladky-Hennion A-C, Djafari-Rouhani B, Duval F, Dubus B, Pennec Y and Deymier P A 2007 J. Appl. Phys. 10 114904
[17] Vasseur J O, Deymier P A, Djafari-Rouhani B, Pennec Y and Hladky-Hennion A-C 2008 Phys. Rev. B 77 085415
[18] Sigalas M M and Economou E N 1994 J. Appl. Phys. 75 2845
[19] Morales A, Flores J, Gutiérrez L and Méndez-Sánchez R A 2002 J. Acoust. Soc. Am. 112 1961
[20] Sánchez-Pérez J V, Caballero D, Martínez-Sala R, Rubio C, Sánchez-Dehesa J, Meseguer F, Linares J and Gálvez F 1998 Phys. Rev. Lett. 80 5325
[21] Kouwenhoven L P, Hekking F W J, van Wees B J, Harmans C J P M, Timmering C E and Foxon C T 1990 Phys. Rev. Lett. 65 361
[22] Sprung D W L, Wu H and Martorell J 1993 Am. J. Phys. 61 1118
[23] Pereyra P 1998 Phys. Rev. Lett. 80 2667
[24] Exner P, Tater M and Vaněk D 2001 J. Math. Phys. 42 4050
[25] Gilmore R 2004 Elementary Quantum Mechanics in One Dimension (Baltimore, MD: Johns Hopkins University Press) p 15
[26] Azbel M Y 1982 Phys. Rev. B 25 849
[27] Avishtah Y and Luck J M 1992 Phys. Rev. B 45 1074
[28] Martínez-Mares M and Robledo A 2009 Phys. Rev. E 80 045201
[29] Jiang Y, Martínez-Mares M, Castaño E and Robledo A 2012 Phys. Rev. E 85 057202
[30] Lee P A and Ramakrishnan T V 1985 Rev. Mod. Phys. 57 287
[31] Mello P A and Kumar N 2005 Quantum Transport in Mesoscopic Systems: Complexity and Statistical Fluctuations (New York: Oxford University Press) p 53
[32] Wolf A, Swift J B, Swinney H L and Vastano J A 1985 Physica D 16 285
[33] Merzbacher E 1998 Quantum Mechanics 3rd edn (New York: Wiley) p 101
[34] Kronig R de L and Penney W G 1931 Proc. R. Soc. Lond. A 130 499
[35] Heiligenthal S, Dahms T, Yanchuk S, Jüngling T, Flunkert V, Kantner I, Schöll E and Kinzel W 2011 Phys. Rev. Lett. 107 254102
[36] Geisel T and Thomaes S 1984 Phys. Rev. Lett. 52 1936
[37] Baldovin F and Robledo A 2002 Europhys. Lett. 60 518
[38] Mello P A 1988 Phys. Rev. Lett. 60 1089
[39] Mello P A and Stone A D 1991 Phys. Rev. B 44 3559
[40] Esaki L and Tsu R 1970 IBM J. Res. Dev. 14 61