#### Localization properties of Krönig-Penney incommensurate potentials

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By means of the renormalization approach we study the localization properties of a one-dimensional system of  $\delta$ -like potential barriers, whose heights are modulated incommensurately with respect to their separation. We show how to distinguish different types of localized states present in the spectrum. Our study shows that in the case of slowly varying potential heights, the Lyapunov coefficient of exponentially localized states approaches zero linearly in correspondence to energies where a transition to power-law localized states is present. A second transition to extended states is then observed. The consequences on the transmittivity of the system are described.

### I. INTRODUCTION

Great attention has been devoted recently to the study of quasiperiodic potentials. Their main feature is the lack of translational invariance; this is realized, for instance, by assigning randomly fluctuating values to the site energies of the lattice, adopting one of the two following schemes. The first is to choose a quasiperiodic sequence of values for the site energies according to a given inflation rule<sup>1</sup> (for instance, Fibonacci, Thue-Morse, or Rudin-Shapiro inflation rules), and the second is to superimpose another periodic potential to the periodic energies of the lattice whose periodicity is incommensurate with the lattice constant.<sup>2</sup> The main purposes of these studies are a clear analysis of the electronic spectrum, with a definition of its absolutely continuous part, singularly continuous part, and pure point part, as well as a description of the localization properties of eigenstates.

A possible way to treat these types of potentials is in the frame of tight-binding models, where we assign to the discrete lattice site a single energy (or more, according to the number of orbitals on the site) and hopping interactions between adjacent sites. Here we consider the problem of equally spaced potential barriers of  $\delta$  functions with variable heights. If these heights are chosen randomly,<sup>3</sup> the model can be taken as a starting point for the study of the properties of a one-dimensional disordered system, and it has been exploited mainly in the case of the presence of a static electric field.<sup>4</sup> This variation of the classical Krönig-Penney model can be a useful tool to investigate quasiperiodic sequences,<sup>5-8</sup> incommensurate potentials<sup>9-12</sup> and, in particular, the properties of quasiperiodic superlattices.<sup>13</sup>

In this work we focus on the problem of equally spaced potential barriers of  $\delta$  functions whose heights are assigned according to the incommensurate potential:

$$V_n = V_0 \cos(Qn^{\nu}) \tag{1}$$

with  $Q = 2\pi \alpha$ ,  $\alpha$  irrational number and  $\nu > 0$ . In the

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case v=1 this potential has been widely studied in the tight-binding approximation (Aubry model<sup>14</sup>); in the case v < 1 the heights of the  $\delta$  functions are asymptotically slowly varying, while for v > 1 this potential simulates the properties of a disordered system. We use this potential in the case v < 1, and v=1 with an appropriate choice of the number  $\alpha$ , to give a simple description of the energy spectrum of a one-dimensional crystal which can present extended as well as different kinds of localized states. In particular we put in evidence the presence of exponentially localized and power-law localized states in separate energy regions; this determines two transitions: from exponentially localized to power-law localized states. This occurs at the edges of every energy band of the system.

The paper is organized as follows. In Sec. II we show how the renormalization approach can be exploited to distinguish different kinds of localization of eigenstates. In Sec. III we give a detailed description of the spectrum of the incommensurate Krönig-Penney model through the Lyapunov exponent  $\gamma(E)$  and the transmission coefficient, devoting particular attention to transitions between different regimes of localization. In Sec. IV we show some examples of exponentially localized states and power-law localized states. Section V contains the conclusions.

### **II. POINCARÉ MAP FOR THE KRÖNIG-PENNEY MODEL AND RENORMALIZATION APPROACH**

#### A. Discrete Schrödinger equation for the Krönig-Penney potential

Let us consider the Schrödinger equation for an electron traveling in a one-dimensional crystal with potential barriers of  $\delta$  functions:

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \sum_n V_n \delta(x - na)\right] \Psi(x) = E \Psi(x) , \qquad (2)$$

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where  $V_n$  is the heights of the  $\delta$  barriers and a is the space between them; in the following, the energy will be given in atomic units and the lengths in units of a = 1. A simple and efficient method to study the progressive scattering by the  $\delta$ -function potential barriers has been provided by Bellisard *et al.*<sup>15</sup> Their procedure can be summarized as follows: the eigenfunction of the Schrödinger equation (2) between the (n-1)th and nth  $\delta$  in a plane wave with coefficients  $A_n$  and  $B_n$ :

$$\Psi(x) = A_n e^{i\sqrt{E}x} + B_n e^{-i\sqrt{E}x} \quad (n-1 < x < n)$$

The conditions of continuity of the function and of the discontinuity of its derivative across each  $\delta$  provide recursive relations for the wave functions calculated on three consecutive  $\delta$ -function positions, which can be put in the matrix form

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = \begin{pmatrix} \cos\sqrt{E} + V_n \frac{\sin\sqrt{E}}{\sqrt{E}} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix},$$

where  $\Psi_n = \Psi(x = n)$ . We are thus left with the solution of an equivalent discrete Schrödinger equation:

$$t(E)(u_{n+1}+u_{n-1})+a_n(E)u_n=Eu_n , \qquad (3)$$

where

$$a_n(E) = -V_n \frac{\sqrt{E} \sin(\sqrt{E})}{2\cos(\sqrt{E})} , \quad t(E) = \frac{E}{2\cos(\sqrt{E})} . \quad (4)$$

It can be shown<sup>16</sup> that for each solution of Eq. (3), with conditions (4), there is a unique solution of Eq. (2) with  $\Psi_n = u_n$ . Thus the band structure derived from Eq. (3) is identical to the original solution of the Krönig-Penney model: allowed energy bands corresponding to itinerant solutions of the form  $\Psi_n \sim e^{ikn}$  are determined by the condition  $|\xi(E)| \leq 1$ , where

$$\xi(E) \equiv \cos(\sqrt{E}) + \frac{V_n \sin(\sqrt{E})}{2\sqrt{E}} ,$$
  
$$\xi(E) \equiv \cos(k) .$$
 (5a)

Forbidden energy regions corresponding to nonsquare integrable solutions of the form  $\Psi_n = e^{qn}$  (q real) are found for  $|\xi(E)| > 1$ ; in this case it holds that

$$|\xi(E)| = \cosh(q) . \tag{5b}$$

For the tight-binding problem (3) the renormalization approach<sup>17</sup> can be usefully exploited. Moreover, also the transfer-matrix technique<sup>18</sup> is easily used to investigate the transmission properties of a sample of the system.

#### B. Localization properties and renormalization approach

Through the calculation of the Green function, the renormalization approach allows us to investigate the most important physical properties of the system, such as the energy spectrum, the density of states, and so on. Here we are interested in the localization properties of the slowly varying incommensurate Krönig-Penney model described by the tight-binding equation (3). The application of the renormalization approach to the system described by Eq. (3) leads to the following recursive transformations:<sup>17</sup>

$$\varepsilon_{0}^{(N-1)}(E) = \varepsilon_{0}^{(N-2)}(E) + t_{0,N-1}^{(\text{eff})}(E) \frac{1}{E - \varepsilon_{N-1}^{(N-2)}(E)} \times t_{N-1,0}^{(\text{eff})}(E) , \qquad (6a)$$

$$\varepsilon_N^{(N-1)}(E) = a_N(E) + t(E) \frac{1}{E - \varepsilon_{N-1}^{(N-2)}(E)} t(E) , \qquad (6b)$$

$$t_{0,N}^{(\text{eff})}(E) = t_{0,N-1}^{(\text{eff})}(E) \frac{1}{E - \varepsilon_{N-1}^{(N-2)}(E)} t(E)$$
  
=  $t_{N,0}^{(\text{eff})}(E)$ . (6c)

By progressive elimination of the sites  $1, \ldots, N-1$  of the lattice defined by Eq. (4), Eqs. (6) allow us to obtain two fundamental quantities: the normalized energy of site 0,  $\varepsilon_0^{(N-1)}(E)$ , and the effective interaction  $t_{0N}^{(\text{eff})}(E)$  between sites 0 and N. For the knowledge of the electronic properties of the system it is useful to calculate  $\varepsilon_0^{(N-1)}(E)$ because it directly gives the matrix element  $G_{00}(E)$  of the Green function of the system through the relation

$$G_{00}(E) = 1 / [E - \varepsilon_0^{(N-1)}(E)]$$
.

On the other hand, the most significant quantity for the study of the localization properties of the eigenstates is the energy-dependent hopping effective interaction  $t_{0N}^{(\text{eff})}(E)$ . Its physical meaning is in fact the effective interaction between sites 0 and N; this can remain different from zero or rapidly decreases to zero during the renormalization in the case of traveling or localized states and gaps, respectively. Therefore  $t_{0N}^{(\text{eff})}$  gives a nonambiguous criterion for distinguishing the two situations. Given the total equivalence between the tight-binding Eq. (3) and the Schrödinger Eq. (2) for the Krönig-Penney problem, this criterion can automatically be applied to the wave functions of our system.

From the quantitative point of view,  $t_{0N}^{(eff)}(E)$  allows us to calculate the Lyapunov coefficient  $\gamma(E)$  through the asymptotic relation<sup>19</sup>

$$\gamma(E) = -\lim_{N \to \infty} \frac{1}{N} \ln |t_{0N}^{(\text{eff})}(E)| .$$
(7)

The general expression (7) can be evaluated for any arbitrary energy E. In correspondence with extended states we obtain  $\gamma(E)=0$ ; in correspondence with exponentially localized states decreasing as  $e^{-\gamma N}$ , the Lyapunov coefficient  $\gamma(E)$  provides the inverse localization length of the wave function. In particular,  $\gamma(E)$  can also be evaluated within forbidden energy gaps where no state is present.

Here we show that the effective hopping interaction  $t_{0N}^{(eff)}(E)$  can also be usefully exploited for the determination of *power-law* localized states, i.e., when the amplitude  $c_N$  of the wave function decreases as  $N^{-\sigma}$ ; in this case the power  $\sigma$  is available from the asymptotic relation

$$\sigma = -\lim_{N \to \infty} \frac{\ln |c_N|}{\ln(N)} . \tag{8}$$

Starting from the infinite one-dimensional lattice, we can decimate the sites between  $n = -\infty$  and n = 0, between n = 0 and n = N, and between n = N + 1 and  $n = +\infty$ . We arrive to a renormalized equivalent lattice of only two sites, 0 and N, and the corresponding effective Hamiltonian can be written in the form

$$H_{\text{eff}}(E) = \begin{bmatrix} \varepsilon_0(E) + \varepsilon_L(E) & t_{0N}^{(\text{eff})}(E) \\ t_{0N}^{(\text{eff})}(E) & \varepsilon_N(E) + \varepsilon_R(E) \end{bmatrix},$$

where with  $\varepsilon_L(E)$  and  $\varepsilon_R(E)$  we have indicated the contributions to the effective self-energies of sites 0 and N given by the renormalization transformations in the regions  $-\infty < n < 0$  and  $N < n < +\infty$ , respectively. From  $H_{\text{eff}}(E)$ , by a direct inversion of  $[E - H_{\text{eff}}(E)]$ , we can obtain the Green-function matrix elements  $G_{00}(E)$ ,  $G_{NN}(E)$ , and  $G_{0N}(E)$  of the original system. Moreover, if  $E_a$  is an eigenvalue of  $H_{\text{eff}}(E)$ , and we choose the energy E much nearer to it than to any other eigenvalue, it is easy to show that the amplitude  $c_N$  of the wave function  $\Psi_a$  of  $H_{\text{eff}}$ , at the site N, is simply related to the off-diagonal matrix element of the Green function by

$$c_N(E) \approx \frac{E - E_a}{c_0^*} G_{0N}(E)$$

for  $E \sim E_a$ , where  $c_N = \langle \Psi_a | N \rangle$  and  $c_0 = \langle \Psi_a | 0 \rangle$ . The relation between  $G_{0N}(E)$  and  $t_{0n}^{(\text{eff})}(E)$  is given by

$$G_{0N}(E) = \frac{-t_{0N}^{(\text{eff})}(E)}{[E - \varepsilon_0(E) - \varepsilon_L(E)][E - \varepsilon_N(E) - \varepsilon_R(E)] - [t_{0N}^{(\text{eff})}(E)]^2} = \frac{-t_{0N}^{(\text{eff})}(E)}{[E - \varepsilon_N(E) - \varepsilon_R(E)]}G_{00}(E)$$

and, for  $E \sim E_a$ ,

$$G_{0N}(E) \sim \frac{-t_{0N}^{(\text{eff})}(E)}{[E - \varepsilon_N(E) - \varepsilon_R(E)]} \frac{|c_0|^2}{E - E_a} ;$$

thus it follows that, if  $E \sim E_a$ ,

$$|c_N(E)| \approx \left| \frac{c_0(E)}{E - \varepsilon_R(E) - \varepsilon_N(E)} t_{0N}^{(\text{eff})}(E) \right| \,.$$

Since  $\varepsilon_N$  is a bounded quantity, it is clear that  $\ln|c_N|/N$ and  $\ln|t_{0n}^{(\text{eff})}(E)|/N$  have the same asymptotic limit, coherently with the result contained in the form (7) for the Lyapunov coefficient. From the above relation we obtain

$$\frac{\ln|c_N(E)|}{\ln(N)} = \frac{\ln|t_{0N}^{(\text{eff})}(E)|}{\ln(N)} + \frac{\ln|c_0(E)| - \ln|E_a - \varepsilon_R(E) - \varepsilon_N(E)|}{\ln(N)} .$$
(9)

This means that there is a tight connection between the asymptotic behaviors of  $\ln|c_N(E)|/\ln(N)$  and of  $\ln|t_{0N}^{(\text{eff})}(E)|/\ln(N)$ . Therefore this latter quantity can be used to individuate with great precision the transition between different kinds of localization. The advantage of this procedure derives from the fact that the behavior of  $t_{0N}^{(\text{eff})}(E)$  can be studied, for each energy, by means of a systematic iteration of the Eqs. (6) starting from the site N=0 independently from the spatial position of the localized eigenstate. However, because the quantity  $\ln(N)$  approaches infinity very slowly, the precise value of the power  $\sigma$  for the localization of the state can be determined just taking into consideration the coefficients  $c_N$  of the wave function, through Eq. (9).

# **III. BEHAVIOR OF THE LYAPUNOV COEFFICIENT**

The solution of the Schrödinger equation (2) when the heights or  $\delta$  functions are all equal to  $V_0$  is well known.<sup>20</sup> It can be described as a sequence of energy bands (separated by gaps) with the lower forbidden gap edges

fixed at energies  $E = n^2 \pi^2$ , and higher edges at energies depending from the strength of the (positive) potential  $V_0$ . The situation for the forbidden zone edges is reversed for negative  $V_0$ .

The problem we are interested in is to find how the properties of the electronic spectrum are modified when a dependence of the heights  $V_n$  from the site number n is imposed. This can be realized, for instance, by assigning random values to  $V_n$ , as in the Anderson tight-binding model of disordered systems. In this case it can easily be shown that the functional dependence of localization lengths of the eigenstates can be interpreted with the law given by Thouless,<sup>21</sup> with the correction near E = 0 given by Kappus and Wegner.<sup>22</sup> Another way to realize an aperiodic version of the Krönig-Penney model is to assign the form of potential (1) to the heights  $V_n$ . We can remember that if the site energies of a one-dimensional lattice in the tight-binding model are assigned according to potential (1), its electronic spectrum presents very interesting characteristics.<sup>14,2</sup> In the case v > 1 the potential is asymptotically rapidly varying, and in the case  $v \ge 2$  it is, from the point of view of the localization properties of eigenstates, a pseudorandom potential. If v=1, the main characteristic of the band structure is the deep fragmentation (the gaps form a Cantor set) depending on the value of  $\alpha$ . From the point of view of the spatial localization of eigenstates, for v=1 no mobility edge is present; in fact for  $V_0 < 2$  the states are all extended, and for  $V_0 > 2$  they are all exponentially localized. In the case when  $\nu < 1$  the spectrum presents (when  $V_0 \leq 2$ ) extended states for  $|E| < |2 - V_0|$ , and exponentially localized states for  $|2-V_0| < |E| < |2+V_0|$  with a behavior of the inverse localization length that is a linear function of the energy near the mobility edges located at  $E = \pm (2 - V_0)$ .<sup>19,23,24</sup> For this reason we have decided first to investigate the Krönig-Penney model with the heights of the  $\delta$  functions modulated according to potential (1) and 0 < v < 1. To simplify the analysis we now consider the case of repulsive barriers  $V_n > 0$  for any n. For this reason we have slightly modified potential (1) in the following form:



FIG. 1. Schematic representation of the potential barriers of  $\delta$ -function form. In the background is plotted the periodic sequence of barriers with constant height  $V_0 = 5$ ; in the foreground are shown the barriers with heights modulated according to potential (10), Q = 1.2,  $\nu = 0.7$ , and  $V_0 = 2.5$ . Energies are in atomic units.

$$V_{n} = V_{0} [1 + \cos(Qn^{\nu})] . \tag{10}$$

The potential we are considering is shown schematically in Fig. 1, where  $V_0=2.5$ ; the modulated  $\delta$  functions are superimposed on the periodic Krönig-Penney model, where all the heights are equal to 5. A first characterization of the localization properties of the energy spectrum can be obtained from the behavior of the Lyapunov coefficient. In Fig. 2 we compare the plot of  $\gamma(E)$  for the incommensurate Krönig-Penney model [potential given by Eq. (10)], with  $V_0=2.5$  (full line), and for the usual periodic model (dashed line). The numerical results for  $\gamma(E)$  within the forbidden energy gaps of the periodic Krönig-Penney model perfectly agree with the values obtained from Eq. (5b), i.e., with



FIG. 2. Behavior of the Lyapunov coefficient as a function of energy in the periodic Krönig-Penney model (heights equal to 5; dashed line) and in the aperiodic model [Eq. (10) of the text; full line] with  $V_0=2.5$ , Q=1.2, and  $\nu=0.7$ . Energies are in atomic units.

$$\gamma(E) = \operatorname{arccosh} \left| \cos(\sqrt{E}) + \frac{V_0 \sin(\sqrt{E})}{2\sqrt{E}} \right|$$

In the picture we reproduce the first two allowed bands [where  $\gamma(E)=0$ ] and the beginning of the third one. It can be seen that the Lyapunov coefficients in the two situations are almost coincident in correspondence with the left borders of the forbidden energy gaps of the periodic case, which are independent of  $V_n$ , and are located at  $E_n = n^2 \pi^2$ . Instead, in correspondence with the right borders of the gaps [whose positions depend from the values of  $V_n$ ] a significant difference exists, and a linear behavior of  $\gamma(E)$  is observed.

We have seen from Fig. 2 that the intervals of energy where  $\gamma(E)$  is different from zero in the periodic (corresponding to gaps) and aperiodic systems (corresponding to exponentially localized states) are practically coincident. The case where  $\gamma(E)=0$  is more ambiguous in the incommensurate model because it does not necessarily correspond to extended states, but also to a localization weaker than the exponential one. In the incommensurate Krönig-Penney model, we encounter a transition from extended to power-law localized states when we approach the region of exponentially localized states from the side of extended states. This occurs, of course, around the edges of each gap of the system. With respect to the single connected band of the tight-binding model with the same site energies and all interactions equal to a given constant, here we have a system with an infinite number of bands, where the density of states is not symmetrical with respect to the center of each band; therefore we also expect that the distribution of the different kinds of localized states will be asymmetrical at the borders of the gaps. We can control the transition between the different kinds of localization, for different values of the energy E without explicit calculation of wave functions, using the method presented in Sec. II by renormalizing the equivalent lattice, starting from the origin. When we approach the borders of a gap of the periodic case from the extended states regions, in the incommensurate case we observe that the quantity  $-\ln |t_{0N}^{(eff)}(E)| / \ln(N)$  as a function of N begins to oscillate around constant values different from zero: this is the sign of the presence of power-law localized states. These values increase when we approach the zones of exponentially localized states: the sign of the transition toward this stronger form of localization is the linear behavior of  $-\ln|t_{0N}^{(eff}(E)|/\ln(N)$  with N. This transition is shown in Fig. 3(a), where we have taken into consideration the region of localized states at  $E \sim 18$ . We have found that the intervals containing power-law localized states are in general rather wide: for energies corresponding to the first gap (right border) of the periodic Krönig-Penny model, in the incommensurate case we observe the transition from exponentially localized states to power-law localized states at  $E \sim 3.47$  and the transition to extended states at  $E \sim 3.55$ ; in correspondence with the second gap of the periodic case (left border) we have, in the incommensurate case, a transition from extended to power-law localized states at  $E \sim 8.60$ , from power-law to exponentially



FIG. 3. (a) Change of the behavior of the ratio  $-\ln|t_{0}^{(eff)}(E)|/\ln(N)$  in correspondence with the transition from exponentially localized states (linear behavior) to power-law localized states (plateau) when the values  $V_0=2.5$ , Q=1.2, and v=0.7 are chosen. We observe that this transition occurs in correspondence with the beginning of the band of the periodic case (E=17.74). (b) Change of the behavior of  $-\ln(\text{transm.})/\ln(N)$  when the extended state energy range is approached.

localized states at  $E \sim 9.87$ , and (right border) a transition to power-law localized states at  $E \sim 17.75$  and a transition to extended states at  $E \sim 18.20$ . We can also control these transitions by means of the transmission properties of our system. For instance, from Fig. 3(b) we can see that at  $E \sim 18$  the quantity  $-\ln(\text{transm.})/\ln(N)$ , as a function of N, oscillates around a constant value, different from zero, and the transmittivity decreases, according to a power law, approaching zero. When we arrive at  $E \sim 18.20$  the extended nature of eigenstates determines an oscillating behavior of  $-\ln(\text{transm.})/\ln(N)$ around the value zero.

We conclude this section by observing that if we assign  $V_0$  a negative value (attractive barriers), the role of the borders of the forbidden energy gaps is inverted, so that in the incommensurate case the values of  $\gamma(E)$  are modified at energies near the left borders of the forbidden gaps of the periodic case. If we consider the modulation potential in form (1), we can observe the two effects combined. In fact, for  $\nu = 1$ , if we assign Q a value very near  $\pi$  we realize a slowly varying aperiodic modification of the situation of alternating positive and negative heights. The results when Q = 3.1415 are shown in Fig. 4.



FIG. 4. Behavior of the Lyapunov coefficient as a function of energy (in atomic units) for a periodic Krönig-Penney model [Eq. (1) of the text with  $Q = \pi$ ,  $V_0 = 5$ , and v = 1; dashed line] and for an incommensurate model [Eq. (1) of the text with Q = 3.1415,  $V_0 = 5$ , and v = 1; full line].

## IV. DIFFERENT KINDS OF LOCALIZATION OF EIGENSTATES AT THE METAL-INSULATOR TRANSITION

In this section we want to underline some characteristics of the wave functions of localized states, looking for a connection between their spatial behavior and the spatial distribution of the potential barriers. The central point is that the incommensurate potential breaks the translational invariance of the system by a well-defined analytic law; thus the spatial distribution of the barriers can be easily visualized [Fig. 5(a)].



FIG. 5. Comparison between the distribution of potential barriers for the incommensurate model [Eq. (10) of the text with Q = 1.2,  $V_0 = 2.5$ , and v = 0.7] from  $N \sim 1700$  to  $N \sim 2400$  and the plot of  $\ln |c_n|^2$  for a series of exponentially localized states at energies corresponding to the second forbidden gap of the periodic Krönig-Penney model. The energies (in atomic units) of the series are  $E \sim 12$ , 14, 15, 16, 17 for plots (a), (b), (c), (d), and (e), respectively.



FIG. 6. Profile of a power-law localized state corresponding to the values  $V_0=2.5$ , Q=1.2, and v=0.7 in the potential of Eq. (10) and E=17.88 (atomic units).

In the case of exponentially localized states we expect to obtain a linear behavior of the envelope of the plot of  $\ln |c_N|^2$  as a function of *n* in the asymptotic region  $(N \rightarrow \infty)$ . The plots shown in Fig. 5(b) confirm this conjecture. If we look at the deep structure of the wave functions we can observe an alternation of oscillating and linearly decreasing parts for  $\ln |c_N|^2$ . A qualitative interpretation of this kind of structure can be given from the correspondence between the decaying parts of  $\ln |c_N|^2$ (which are a sign of the scattering process suffered by the electron) and the presence of  $\delta$  functions in space, and also from the correspondence between the oscillating parts of  $\ln |c_N|^2$  (absence of scattering effects) and the lack of effects of the  $\delta$  functions. To illustrate this point, in Fig. 5(a) we show the structure of the potential barriers in a zone of the system from  $N \sim 170$  to  $N \sim 2400$ ; in correspondence, in Fig. 5(b) we present a series of eigenstates at various energies, chosen from  $E \sim 9.9$  to  $E \sim 17.8$ . In practice we obtain that  $|c_N|^2$  has exponentially decreasing behavior in the regions where the electrons feel scattering from the potential barriers, otherwise they are oscillating. The global envelope of the wave function is thus exponential. By comparison with Fig. 5(a) we observe that, as we approach the band edge, regions without scattering centers increase in size with respect to regions with scatterers, and correspondingly the width of the plateaus with oscillating  $|c_N|^2$  values also increases.

The envelope of a power-law localized state is of course very different. We show an example in Fig. 6, which corresponds to the value E = 17.88, where a power-law localized state is present [see Fig. 3(b)].

Let us finally consider the Krönig-Penney model with randomly distributed heights of  $\delta$  functions, a model used also to analyze transitions from exponentially to powerlaw localized states in the presence of electric fields.<sup>4</sup> We can analyze this case through the localization and transmission properties of pseudorandom Krönig-Penney



FIG. 7. Behavior of the logarithm of transmittivity as a function of the length N of the sample for three energies near  $E = \pi^2$ (E = 9.896, 9.8696, and 9.870, in atomic units) and  $V_0 = 5$ , Q = 1.2, and v = 2.5 in the potential of Eq. (1).

model realized with potential (1) and v > 2. We find that, like in the random case, the value of  $\gamma(E)$  is different from zero for any value of E, except for  $E = n^2 \pi^2$ ; moreover the transmittivity, at these energies, is equal to 1, as a confirmation of the extended nature of these states.<sup>3</sup> It can be interesting now to investigate the behavior of the transmittivity of finite samples of the system in the energy regions  $E \sim n^2 \pi^2$ .

Our numerical results for the transmittivity show that if we go very near the values  $E = n^2 \pi^2$ , the transmittance, as a function of *n*, ceases to be exponentially decreasing and also approaches zero with a slower law for very long samples ( $N = 10^5$ ). In Fig. 7 we compare the behavior of the logarithm of transmittivity for energies approaching  $E = \pi^2$ . We can see that for energies differing of the order of  $\sim 5 \times 10^{-4}$  from  $\pi^2$  the transmittivity decreases almost exponentially; for E = 9.8696 the decreasing rate is slower.

### **V. CONCLUSIONS**

In this paper we have studied the localization properties of an incommensurate Krönig-Penney model in the tight-binding framework, exploiting the renormalization procedure. We have observed that exponentially localized states appear at energy intervals corresponding to forbidden gaps in the periodic case; a correspondence between the spatial structure of the wave function and the spatial distribution of the  $\delta$ -function barriers has been suggested. For each band of the spectrum, power-law localized states are present between exponentially localized and extended states; this confirms similar results for incommensurate tight-binding models.<sup>25</sup> Correspondingly, a power-law behavior of the transmittivity as a function of the length of the sample can be observed. Finally, we have studied the pseudorandom form of the incommensurate potential showing that around the energy values  $E = n^2 \pi^2$  the decreasing rate of the transmittivity is slower than exponential.

<sup>1</sup>See, for instance, T. Schneider, D. Würtz, A. Politi, and M. Zannetti, Phys. Rev. B 36, 1789 (1987); Q. Niu and F. Nori, Phys. Rev. Lett. 57, 2057 (1986); Z. Cheng, R. Savit, and R. Merlin, Phys. Rev. B 37, 4375 (1988); M. Dulea, M. Johansson, and R. Riklund, *ibid.* 47, 8547 (1993).

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