Electric-field effect on the transmittivity of aperiodic Kronig-Penney crystals

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We describe the effect of a static and uniform electric field on the electronic transport properties of one-dimensional periodic and deterministic aperiodic systems described by the Kronig-Penney model. We study the crystal transmittivity as a function of the length of the sample and of the field strength. In the periodic case we interpret the results exploiting the tilted band scheme and point out regions with a more than exponential decreasing rate of transmittivity. In the case of an incommensurate slowly varying potential we interpret the fine structure of the transmittivity by means of a continuous approximation. In the pseudorandom case we confirm the delocalization effect of the field and we compare the results with the purely random case. [S0163-1829(97)05727-5]

I. INTRODUCTION

The electronic and transport properties of one-dimensional systems under an applied electric field have been deeply studied both for their theoretical interest and for applicative aspects. It is now clear that the spectrum of a periodic single band system in the presence of field is composed of discrete eigenvalues (Stark ladder).[1] In the case of a multiband system, several analytical and numerical contribution have assessed the possibility of interband tunneling of the electron with enhancement of the transport, induced by resonances among states belonging to different ladders.[2–4] The presence of disorder in the system has further added interest to this topic: one of the most interesting results is that the electric field may delocalize the states of the disordered Kronig-Penney crystal changing the wave-function decay from exponential to power law, up to the possibility of extended states.[5–14]

On the other hand, less known is the effect of electric field on the spectral properties of systems that can be considered intermediate between the purely periodic and the purely random case. These systems are defined by the peculiar form of their potential; interesting and well-studied examples are given by the incommensurate potentials,[15] by the potentials defined in terms of inflation rules,[16] and by the hierarchical potentials.[17,18] For them, in general, the character of the states and the corresponding transport properties in the absence of the electric fields according to the nature (absolutely continuous or singularly continuous) of the spectrum are now well defined. The effect of an applied electric field has been discussed in the case of one-dimensional hierarchical models[19] and to prove the existence of the Wannier-Stark ladders in one-dimensional quasiperiodic systems.[20] By means of tight-binding Hamiltonians, field-induced localization has also been proved for Fibonacci and Thue-Morse lattices,[21] and for incommensurate potentials.[22]

The purpose of this paper is to analyze the effect of a static and uniform electric field f on the localization and transport properties of one-dimensional incommensurate or pseudorandom systems described by means of the Kronig-Penney model. Several interesting properties have been put in evidence for this aperiodic model in the absence of field, in particular the metal-insulator transition and the power-law localization of a part of the spectrum.[23]

The Hamiltonian for the Kronig-Penney crystal in the presence of an electric field can be written in the form (Rydberg units are adopted)

$$H=-\frac{d^2}{dx^2}+\sum_n V_n\delta(x-na)-fx, \qquad (1)$$

where V_n is the law assigned to the heights of the δ-function potential barriers and a is the constant spacing between them (in the following we choose a as the unit of length); $f=eF$, where e is the modulus of the electric charge and F the intensity of the uniform electric field. We remember that, when $f=0$ and in the simplest case of periodic distribution of potential barriers, i.e., when $V_n=V_0$ for any n, the condition for the presence of allowed energy bands is given by[24]

$$\cos(\sqrt{E})+\frac{V_0\sin(\sqrt{E})}{2\sqrt{E}}\leqslant 1. \qquad (2)$$

This relation is satisfied for an infinite number of energy intervals whose width increases for increasing energy. If the delta functions have positive heights V_0, the right border of the mth allowed energy band is at the potential-independent positions $E_m^{(R)}=m^2\pi^2$, while the left border $E_m^{(L)}$ can be obtained from

$$\cos(\sqrt{E_m^{(L)}})+\frac{V_0\sin(\sqrt{E_m^{(L)}})}{2\sqrt{E_m^{(L)}}}=(-1)^{m+1}. \qquad (3)$$

For instance, in the case of a Kronig-Penney periodic model where $V_n=V_0=5$ the spectrum begins with a gap that ends at $E\sim 3.8$, and the second gap is bound by the energy values $E\sim 9.86$ and $E\sim 17.8$. In the case of negative potential barriers, the condition of the left and right borders is reversed.

These simple considerations, valid for the periodic systems, cannot be used when the law defining the potential strengths V_n has a more complex form, for instance, when the heights assume random values. In this case it can be convenient to exploit a Poincaré map[25] that provides the transfer matrix for the wave functions of the Hamiltonian (1) calculated on three consecutive δ-function barriers. In the presence of an electric field, the ladder approximation is generally adopted, which consists in substituting the potential term fx in the Hamiltonian (1) by a step potential that varies by the constant value $-f$ at each site n and is constant at adjacent sites; this allows one to take the wave function of the electron traveling in the system between the $(n-1)$th and the nth delta function as a plane wave of the form $\psi(x)=Ae^{ik(n)x}+Be^{-ik(n)x}$. The effect of the electric field is to insert in the wave vector k a dependence from the number of barrier n of the form $k_n=\sqrt{E+fn}$. The corresponding transfer matrix involving $\psi(x=n-1)$, $\psi(x=n)$, and $\psi(x=n+1)$ is given by[6]

$$T_{n,n+1}=\begin{pmatrix} \cos(k_{n+1})+\dfrac{k_n}{k_{n+1}}\dfrac{\sin(k_{n+1})}{\sin(k_n)}\cos(k_n)+V_n\dfrac{\sin(k_{n+1})}{k_{n+1}} & +\dfrac{k_n}{k_{n+1}}\dfrac{\sin(k_{n+1})}{\sin(k_n)} \\ 1 & 0 \end{pmatrix}. \tag{4}$$

The total transmittivity of an incoming free electron through a crystal of length N can then be calculated by means of the expression[6]

$$T_N=\frac{k_0}{k_N}\frac{|\exp(2ik_N)-1|^2}{|c_{N+2}-c_{N+3}\exp(-ik_N)|^2}, \tag{5}$$

where we have indicated $c_N=\psi(x=N)$. The transfer matrix written above can be associated to the discrete tight-binding equation

$$t_{n,n+1}(E)c_{n+1}+t_{n,n-1}(E)c_{n-1}+a_n(E)c_n=Ec_n, \tag{6}$$

where

$$a_n(E)=-\frac{V_nE\sin(k_{n+1})/k_n}{\cos(k_{n+1})+(k_n/k_{n+1})[\sin(k_{n+1})/\sin(k_n)]\cos(k_n)}, \tag{7a}$$

$$t_{n,n+1}(E)=\frac{E}{\cos(k_{n+1})+(k_n/k_{n+1})[\sin(k_{n+1})/\sin(k_n)]\cos(k_n)}, \tag{7b}$$

$$t_{n,n-1}(E)=\frac{E(k_{n-1}/k_n)\sin(k_n)/\sin(k_{n-1})}{\cos(k_n)+(k_{n-1}/k_n)[\sin(k_n)/\sin(k_{n-1})]\cos(k_{n-1})}. \tag{7c}$$

The effective tight-binding equation (6) can describe situations with different values of the "forward" and "backward" hopping interactions (7b) and (7c). The transfer matrix (4) and the expression (5) provide an accurate numerical technique to study the transmission properties of incommensurate and pseudorandom Kronig-Penney potentials under an applied electric field. Moreover, the tight-binding Eq. (6) allows us to obtain an intuitive prediction of the results, exploiting the analytic form and a suitable real-space picture of the potential.

This paper is organized as follows. In Sec. II we consider the periodic Kronig-Penney model and show that from a suitable real-space scheme the regions of oscillating or decreasing transmittivity of the sample can be inferred. In Sec. III we focus on incommensurate Kronig-Penney models and we give a continuous approximation to predict regions of allowed and forbidden zones for the electronic propagation. In Sec. IV we handle the case of the pseudorandom Kronig-Penney model and compare it with the behavior of the purely random potential. Section V contains the conclusions.

II. THE PERIODIC KRONIG-PENNEY MODEL IN AN ELECTRIC FIELD

Let us consider a periodic Kronig-Penney potential with delta functions with positive heights V_0. An energy-site representation of the bands of the system can be realized; in the simple case with $f=0$ this can be done by plotting the allowed regions by horizontal strips with borders $E_m^{(L)}$ and $E_m^{(R)}$ separated by horizontal strips, corresponding to the gaps, where the propagation is forbidden. In this case the energy of the incoming electron is contained in an allowed or in a forbidden region for the entire length of the sample, and correspondingly the transmittivity is respectively oscillating or exponentially decreasing.

When a static uniform electric field is superimposed to the system, the horizontal strips of the case $f=0$ are tilted with negative slope equal to the field intensity f.[26] The borders of the allowed bands as functions of the length N of the sample are given by the relations $E_m^{(L)}-fN$ and $E_m^{(R)}-fN$. We can see (Fig. 1, inset) that that in this case, for any given energy E, for increasing length of the sample, the particle encounters an alternation of allowed and forbidden zones; this is the origin of the complete localization of the spectrum. When we plot the quantity $-\ln T_N$ as a function of the length N, the regions of decrease of the transmittivity correspond to jumps in the plots. From the positions of $E_m^{(L)}$ and $E_m^{(R)}$ and the slope $-f$ of the strips, the starting and ending points of the oscillating parts and of these jumps can be exactly predicted. For a given energy E the regions corresponding to the jumps have as border points:

$$n_L^{(j)}=\frac{m^2\pi^2+E}{f}, \quad n_R^{(j)}=\frac{E_m^{(R)}+E}{f}, \tag{8a}$$

while for the oscillatory regions we have

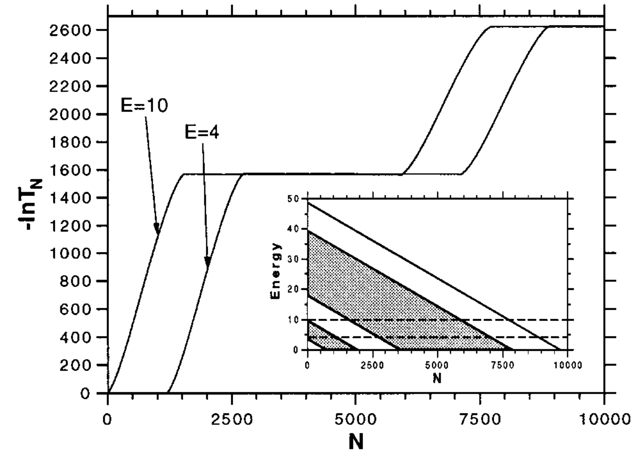

FIG. 1. Behavior of $-\ln T_N$ as a function of N for the periodic Kronig-Penney potential when the height of the barriers is 5; the electric field strength is $f=0.005$ and the two energies are $E=4$, $E=10$. In the inset the tilted band scheme is reproduced, and the two energies considered are indicated with broken lines.

$$n_L^{(o)}=\frac{E_m^{(o)}+E}{f}, \quad n_R^{(0)}=\frac{(m+1)^2\pi^2+E}{f}. \tag{8b}$$

We show in Fig. 1 the behavior of $-\ln T_N$ in a simple periodic system, where the heights of the delta functions are chosen equal to 5 and $f=0.005$, for two different energies E; in the inset the corresponding tilted band scheme is represented. In this picture we can clearly distinguish the regions where $-\ln T_N$ shows oscillatory behavior separated by the regions where $-\ln T_N$ shows a steep increase. These regions correspond (see the inset) to the intervals where the energies (horizontal broken lines) lie in allowed and forbidden zones, respectively. We can observe that $-\ln T_N$ has a nonlinear behavior in the regions just beyond the beginning of the gap; correspondingly, the decrease law for the transmittivity is of the type $T\sim\exp(-\alpha N^{\beta})$ with $\beta>1$. The nonlinearity in the jumps of $-\ln T_N$ has been observed in disordered systems,[27,28] and defined as a form of superlocalization, but Fig. 1 shows that it is present also in periodic systems and that it is a very general effect of the electric field. For instance, in the case $E=10$ the transmittivity decreases faster that exponentially for samples of length $N\lesssim 1000$. This result is more evident for well-separated bands. In fact, in the case of a single band we soon realize that, due to the slope of the allowed band, the distance of the given energy E from the band as a function of the length of the sample increases, determining the more than exponential decrease of transmittivity.[29] This effect does not occur in the absence of electric field because a forbidden energy has in real space a constant distance from the allowed band and therefore the transmittivity has a constant exponential decreasing rate.

III. INCOMMENSURATE SLOWLY VARYING KRONIG-PENNEY MODEL IN AN ELECTRIC FIELD

We investigate now the transmission properties of a Kronig-Penney model where the heights of the barriers are modulated incommensurately with respect to their constant spacing, according to the law

$$V_n=\lambda\ \cos(2\pi\alpha|n|^{\nu}). \tag{9}$$

α is an irrational number and $0<\nu<1$, so as to realize an asymptotic slow variation of V_n. It is well known[30] that a one-dimensional tight-binding Hamiltonian with site energies $a_n=V_n$ and hopping interactions $t_n=1$ presents, for $\lambda\leqslant 2$, two symmetrical mobility edges at $E=\pm(2-\lambda)$ that separate extended states at the center of the spectrum from localized states in its two lateral parts $|2-\lambda|<|E|<|2+\lambda|$. To interpret the presence of mobility edges in the spectrum, for $f=0$, it has been found convenient to introduce a continuous approximation[31] with a pictorial representation of the allowed and forbidden regions of the lattice in the real space. This is realized superimposing the potential V_n to the band of the lattice with $V_n=0$, which extends in the energy interval $-2\leqslant E\leqslant 2$. From the result of this operation it can be observed that the energies of the interval $E\leqslant|2-\lambda|$ are allowed throughout the entire lattice, and this explains the presence of extended states in the corresponding part of the spectrum of the system. For $|2-\lambda|<|E|<|2+\lambda|$ there is an alternation of allowed and forbidden regions of the lattice with corresponding localization of the eigenstates of the spectrum. It can be also observed that the behavior of the transmittivity as a function of the length of the system for $|2-\lambda|<|E|<|2+\lambda|$ is alternatively oscillating and decreasing with a global exponentially decreasing envelope.

The ''continuous approximation'' can be applied also when we map the Kronig-Penney incommensurate potential into a tight binding equation of the form (6), by means of Eqs. (7). We can see that at a given energy E the curves delimiting the allowed energy regions in the real space are given by the functions $a_n(E)\pm 2t(E)$, where $a_n(E)$ and $t(E)$ are obtained by putting $f=0$ in Eqs. (7). It is thus easy to control if the energy E lies in the allowed zone throughout the entire lattice, or if it penetrates the allowed zones only for alternating intervals. In the absence of the electric field the allowed zone is a region delimited by two cosinusoids separated by $2t(E)$.

When the electric field is switched on, the Hamiltonian in Eq. (6) has different ''forward'' and ''backward'' hopping interactions $t_{n,n+1}(E)$ and $t_{n,n-1}(E)$. In this case we have found that the allowed energy zones of the lattice in the real space scheme are delimited by the functions

$$F_n^{(\pm)}(E)=a_n(E)\pm 2\sqrt{t_{n,n+1}(E)t_{n,n-1}(E)}. \tag{10}$$

It is easy to understand from expression (10) that when the electric field is present the allowed band in the real space no longer has the simple form delimited by two shifted cosinusoids. The typical structure of the allowed region as a function of the sample length is shown in the inset of Fig. 2(a), where $\lambda=5$, $2\pi\alpha=0.2$, $\nu=0.7$, $f=0.001$, and calculated at $E=9.5$. We can see that it is made by the alternation of broad and narrow regions with superimposed oscillations at the borders due to the form of $a_n(E)$. The corresponding behavior of $-\ln T_N$ as a function of N [globally shown in Fig. 2(a)] is alternatively oscillating in the intervals of the system where the chosen energy E is inside the allowed region (i.e., when it presents broad parts) and increasing when the energy

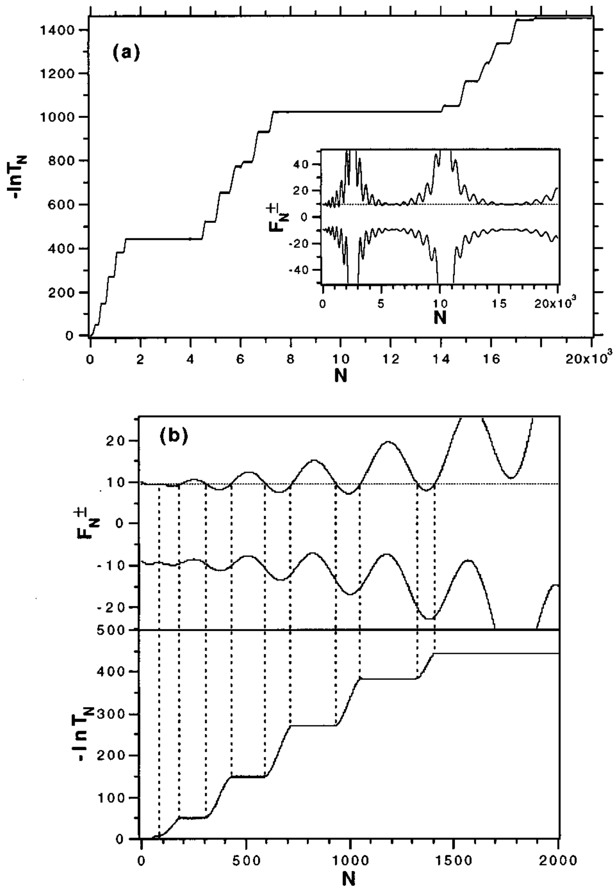

FIG. 2. (a) Behavior of $-\ln T_N$ as a function of N in the slowly varying aperiodic Kronig-Penney model [potential (9)], for $V_0=5$, $2\pi\alpha=0.2$, $\nu=0.7$, $f=0.005$, and $E=9.5$. The upper (F^+) and lower (F^-) borders of the allowed region calculated for the same set of values are reported in the inset. (b) Detail of (a), where the comparison between the behavior of $-\ln T_N$ and the position of the energy with respect to the upper (F^+) and lower (F^-) borders of the allowed region is emphasized.

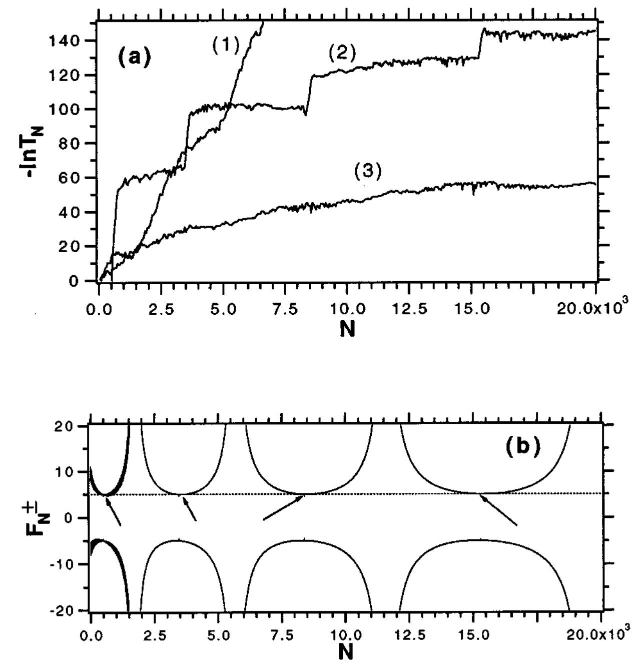

FIG. 3. (a) Behavior of $-\ln T_N$ in the case of barriers of arbitrary sign [potential (9)] for $V_0=1$, $2\pi\alpha=0.2$, $\nu=2.5$, $E=5$, for $f=0$ [plot (1)] and $f=0.01$ [plot (3)] and in the case of positive heights [potential (11)] for $V_0=1$, $2\pi\alpha=0.2$, $\nu=2.5$, $E=5$, and $f=0.01$ [plot (2)]. The jumps in the plot start in the positions indicated by the arrows in the part (b) of the figure. (b) Representation of the upper (F^+) and lower (F^-) borders of the allowed region calculated for the data corresponding to the plot (2) in (a). The points where E touches the borders of the band [corresponding to the jumps of plot (2) in (a)] are indicated by arrows.

is outside the allowed region. The wavy borders of $F_n^{\pm}(E)$ cause the presence of the fine structure of narrow plateaus in each interval of jumps for $-\ln T_N$. From Fig. 2(b) we see that the generalization of the continuous approximation for the Kronig-Penney model in the presence of an electric field gives a very accurate prediction of the behavior of the transmittivity as a function of the length of the system also in the finest structures of the plot. It can be verified that for no energy value the behavior of the transmittivity is oscillating for the entire length of an infinite sample. This is because the chosen energy E in this case is never completely inside the allowed band zone, and it indicates that the electric field in the incommensurate slowly varying model provokes the complete localization of the spectrum, as it does in the case of a periodic system.

IV. THE PSEUDORANDOM KRONIG-PENNEY CRYSTAL IN AN ELECTRIC FIELD

The pseudorandom Kronig-Penney model is defined by potential barriers V_n assigned according to the expression (9), with $\nu>2$. In this case, in fact, for increasing n the potential soon becomes rapidly changing so as to simulate a true random potential,[32] independently of the values of α. As in the random case, for $f=0$ the spectrum of the tight-binding pseudorandom lattice is composed entirely by exponentially localized states but for the points at $E_m=m^2\pi^2$. We have found that the plots of the Lyapunov exponent $\gamma(E)$ (inverse localization length) for infinite systems, as a function of the energy E, in the two cases show similar behavior: that is, a decreasing envelope with minima in correspondence with $E_m=m^2\pi^2$. We have verified also that the curve corresponding to $\gamma(E)$ for the pseudorandom case lies always above the curve for the random case, indicating a stronger localization.

When an electric field is superimposed to a one-dimensional disordered system, one of the most surprising results is the delocalization of its eigenstates, which manifests through a transition from exponential localization to a weaker form of localization (power-law form) and then, for higher values of the field f, to an extended state regime. This fact has been shown analytically[5,8] and numerically by studying the transmittivity of finite samples[6,9,11–13] and going beyond the ladder approximation considering Airy functions instead of plane waves between adjacent barriers.[9,12,13]

Recently a difference in the transmission of a disordered electrified chain has been observed[27,28] in the case of random barriers of fixed sign, with respect to the case of barriers with arbitrary sign. It is therefore convenient to start considering a pseudorandom law for the barrier heights in the form

$$V_n = V_0[1+\cos(2\pi\alpha|n|^{\nu})], \tag{11}$$

where α is an irrational number and $\nu > 2$; in this case the barriers all have positive signs. In Fig. 3(a), plot (1) shows the behavior of $-\ln T_N$ for potential values $V_0 = 1$, $2\pi\alpha = 0.2$, $\nu = 2.5$, and $E = 5$, $f = 0.01$; we can see that it presents jumps similar to the ones observed in the periodic Kronig-Penney model and in the slowly varying aperiodic case. Moreover we observe that the position of the jumps can be predicted again by using a representation in real space for the allowed zones [see Fig. 3(b)], as can be verified by comparing the position of the jumps with the points where the chosen energy E crosses the border of the allowed zones. We can observe also that these borders oscillate too rapidly to allow the detection of steps along the jumps of $-\ln T_N$ as in the slowly varying case.

In the case of the potential (9) with barriers of arbitrary sign, the jumps of $-\ln T_N$ disappear, as can be seen in the plot (3) of Fig. 3(a), in this case the behavior of $-\ln T_N$ is very different from the case $f = 0$ [curve (1)] and it is typical of a regime of power-law localization of eigenstates, similar to what was found in the case of the random potential. We have calculated the height of the plateau reached by the quantity $-\ln T_N/\ln N$ (which is an estimate of the power of decay of the wave function[23]) for various values of E, V_0, and f, and we have verified that it scales as $1/f$ as a function of the field strength f, as predicted in Ref. 8. Moreover we have found that $-\ln T_N/\ln N$ varies as V_0^2 as a function of the amplitude of the potential V_0; these behaviors break down in the proximity of the transition of the wave functions toward the extended regime. Comparing the results of the pseudorandom and the random distribution of the heights V_n (with the same spread of values in the two cases), for the same values of energy E and field f, we have observed that the plateaus of $-\ln T_N/\ln N$ are higher in the pseudorandom case, indicating a stronger localization, coherently with the higher values of the Lyapunov exponent for the same cases found for $f = 0$. As a consequence, the transition from the decreasing to the oscillating behavior of T_N is reached in the pseudorandom case for higher values of f: for instance, if in Eq. (9) $\lambda = V_0 = 1$, $2\pi\alpha = 0.2$, $\nu = 2.5$, and $E = 5$ the transition is observed for $f \sim 2$, while for a random potential with spread of height in the interval $(-1,1)$ this threshold is reached for $f \sim 1.2$.

V. CONCLUSIONS

We have investigated the effect of a static, uniform electric field on the electronic transport of a one-dimensional Kronig-Penney system with potential barriers distributed both periodically and according to a deterministic aperiodic law. We have shown that, to interpret the transmittivity it can be useful to exploit a continuous representation in real space for the energetically allowed zones of the system. This method can be also extended to the pseudorandom case when the barriers are of the same sign and jumps in the plot of $-\ln T_N$ are visible. When the barriers have arbitrary signs, the results found for disordered systems are confirmed: the transmittivity of the system decreases following a power law and, once a threshold value of the field is overcome, a transition toward an oscillating behavior of the transmittivity is observed. This threshold for the field strength is higher in the pseudorandom case than in the corresponding random one, indicating a more localizing character of the pseudorandom potential.

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