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LETTER TO THE EDITOR

Beyond exponential localization in one-dimensional electrified chains

Riccardo Farchioni and Giuseppe Grosso

Dipartimento di Fisica, Università di Pisa and Istituto Nazionale Fisica della Materia, Piazza Torricelli n. 2, 56126 Pisa, Italy

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Abstract. We interpret a new kind of localization in a finite one-dimensional tight-binding model under a weak applied electric field. This phenomenon is quite general and manifests itself in a more than exponential decreasing behaviour of the chain transmittivity. We provide analytic expressions for the transmittivity and confirm the theoretical results by transfer matrix numerical calculations. We show that this phenomenon is present in ordered as well as in aperiodic (incommensurate and pseudorandom systems) irrespective of the number of allowed bands.

The one-dimensional nearest-neighbour tight-binding equation

$$t\left(u_{n+1}+u_{n-1}\right)+V_n u_n=E u_n \tag{1}$$

is the model most used to analyse the localization properties of the electronic states.

In equation (1) the hopping interaction t is chosen as the unit of energies, u_n is the amplitude of the electronic wave function at the nth lattice site, V_n is the site energy and E the electron energy. The exponential localization of all the states by whatever weak random potential V_n is a well known fact [1]. New interest to this subject has been added considering V_n with a period incommensurate with the underlying lattice [2] i.e. when V_n has properties intermediate between the periodic (Bloch) and the random (Anderson) case. For the paradigmatic Harper potential, $V_n = \lambda\cos(2\pi\alpha n)$ with α irrational, Aubry and André [3] have elucidated the role of the strength λ of the potential in comparison with the hopping interaction t, showing that the states are all extended or all localized provided $\lambda < 2t$ or $\lambda > 2t$ respectively. In the case $\lambda = 2t$ all the states are 'critical'. Moreover the study of the Kronig–Penney model, with δ-potential strength incommensurate with the underlying lattice, has made it possible to point out the existence of power law localized states [4] between extended and exponentially localized states.

Further interest in the transport properties of the above topics is added by the presence of an applied static electric field. Once again the random Kronig–Penney model has been widely adopted through the Poincaré map associated with the corresponding Schrödinger equation in order to obtain a finite difference equation of type (1) with appropriate hopping and site energies [5]. An important contribution to the understanding of localization properties of 1D disordered systems under the action of an external field has been provided by Soukoulis *et al* [6]; for small fields they individuate power law localized states, as predicted by Prigodin [7]. This behaviour has been confirmed rigorously by Delyon and coworkers [8]. Numerous successive contributions [9–13] have shown that the states of a 1D random system under the application of an electric field f change their character

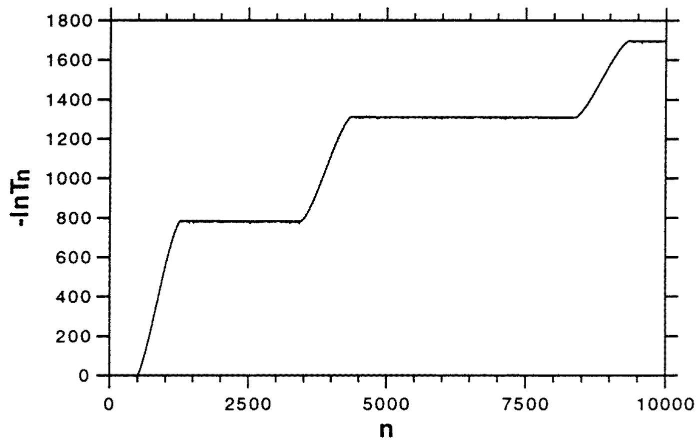

Figure 1. Plot of $-\ln T_n$ as a function of n calculated for a Krönig–Penney model with δ-potential barriers of heights equal to 5, at the energy $E = 5$ and under an applied electric field $f = 0.01$ (Rydberg units are used). The intervals of n corresponding to the jumps and plateaus of $-\ln T_n$ can be predicted on the basis of the tilted band scheme applied to the multiband spectrum of the Krönig–Penney model. A nonlinear behaviour of $-\ln T_n$ can be observed in the extremal parts of the jumps.

from exponential to power law localization and then, beyond a critical field, they become extended. This depends on the type of potential V_n and on the ratio efL/E between the electrostatic energy gained by the electron through the sample of length L, and its energy E [10].

The transmittivity T_n through an ordered 1D multiband system in an electric field as a function of the chain length n shows regions of oscillations (plateaus in the plot of $-\ln T_n$ versus n) and rapid decrease (jumps in the plot of $-\ln T_n$). As an example, we report in figure 1 the numerical results for the transmittivity of a Kronig–Penney δ-potential model, for electron energy $E = 5$ and electric field $f = 0.01$ (Rydberg units are used here); by the tilted band scheme [14] we can soon realize that the growing segments and the plateaus correspond to spatial regions where the travelling electron meets gaps and bands respectively. A similar plot has been obtained by Leo [15] for the transport in ordered and disordered semiconductor superlattices. Recently it has been observed [16] that a similar alternation of jumps and plateaus occurs in disordered Kronig–Penney systems when the potential is composed exclusively by barriers or exclusively by wells. For this class of systems it has also been noticed that the behaviour of $-\ln T_n$, in the regions where the jumps take place, is not strictly linear; in particular, at the beginning of each jump, $-\ln T_n$ grows more than linearly, indicating that the transmittivity decreases more than exponentially there. This phenomenon can be defined as a form of superlocalization and has already appeared in the context of fractal media [17].

The aim of this paper is to give an explanation of the nonlinear behaviour of $-\ln T_n$, starting from the observation that it occurs also in periodic Kronig–Penney systems under an electric field. Here we concentrate mostly on a single band tight binding system, because in this case it is possible to provide also an analytic form of $-\ln T_n$. However, the basic result of our analysis can explain the same effect in periodic and aperiodic tight binding and Kronig–Penney models.

Let us consider first a perfect lattice described by equation (1) with periodic potential

$V_n = a$. It is well known that this problem has itinerant solutions for energies in the interval $[-W + a, W + a]$, where $W = 2t$ is the half bandwidth, with dispersion relation $E(k) = a + 2t\cos(k)$. For energies outside the allowed band ($|E - a|/W > 1$), we can define for the exponentially decaying solutions of (1), the Lyapunov exponent

$$\gamma(E) = \operatorname{arcosh}\left|\frac{E-a}{W}\right| \tag{2}$$

thus $-\ln T_n$ varies linearly with the sample length n, with slope 2γ [1]. We consider then a chain made by segments, and within each of them the energies are all equal (say in the ith segment let the site energies be all equal to a_i). If we think of each segment as a part of a periodic infinite chain and repeat the reasoning leading to equation (2), then we have that for energies external to $[-W + a_i, W + a_i]$ the slope of $-\ln T_n$ versus n is given by $2\gamma_i$. For the chain with different segments the slope of $-\ln T_n$ changes at the beginning of any segment. In the limit of segments constituted by a single site, $-\ln T_n$ can be considered a continuous curve as function of n, with continuously changing slope according to the law

$$-\frac{\mathrm{d}}{\mathrm{d}n}\ln T_n = 2\operatorname{arcosh}\left|\frac{E-a_n}{W_n}\right| \tag{3}$$

where W_n is the half bandwidth at site n, and E is always external to the band at site n.

This is exactly the situation of a single band system where the site energies vary according to the relation

$$a_n = V_0 + efn \tag{4}$$

as required by the presence of an electric field of strength f superimposed to a periodic chain with site energies V_0. Integration of equation (3) thus provides the following analytic expression for $-\ln T_n$

$$\begin{aligned}-\ln T_n = \mp\left(\frac{2}{ef}\right)\bigg\{&|E - \big(V_0 + efn\big)|\operatorname{arcosh}\frac{|E-(V_0+efn)|}{W}\\ &-\sqrt{(E-(V_0+efn))^2 - W^2}\bigg\}\end{aligned} \tag{5}$$

(n outside the tilted band, see figure 2(a)); the minus sign refers to the case $E > a_n + W$, and the plus sign to the case $E < a_n - W$. From figure 2(a) we can see that for $V_0 - W < E < V_0 + W$ the electron is in an allowed band region from $n = 0$ up to the site n^* defined by the condition $V_0 - W + fn^* = E$, thus we expect T_n to oscillate there, and to decrease for $n > n^*$. For $E > V_0 + W$ the electron is in a forbidden region from $n = 0$ up to the point n'^* defined by $V_0 + W + fn'^* = E$, thus T_n decreases; then it oscillates for the sites within the tilted band and beyond n^* it decreases again. For the tight binding periodic case with $V_0 = 0$, $f = 0.01$ and length $N = 1000$ sites, we compare in figure 2(b) the theoretical predictions from equation (5) (continuous line) with transfer matrix [18] numerical calculations of $-\ln T_n$ (circles). We have chosen three energies: $E = -2t$, $E = 0$ and $E = 4t$. In the first case the decreasing behaviour of the transmittivity begins at $n = 0$; in the second case the transmittivity oscillates up to $n^* = 200$, then it decreases; in the third case the decrease of T_n is between $n = 0$ and $n'^* = 200$, it oscillates from $n'^* = 200$ to $n^* = 600$ and then it decreases. In all the cases the numerical results are reproduced with high accuracy by equation (5).

Equation (5) can be given in a form useful for asymptotic regions. Let us define $\alpha = ef/W$ and introduce the index n' to numerate the sites in the regions external to the

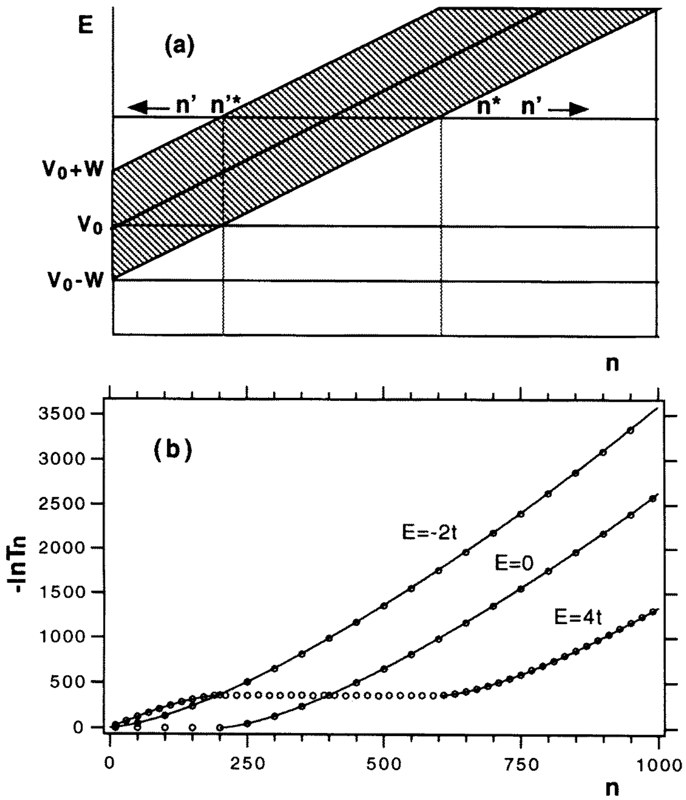

Figure 2. (a) Schematic representation of the tilted band for a single band system with site energies V_0 and half bandwidth W in the presence of a uniform electric field. The slope of the band corresponds to the field strength f. (b) Behaviour of $-\ln T_n$ as a function of n for a single band system with $V_0 = 0$, $W = 2t$. The field intensity is $f = 0.01$. The three energy values correspond to the horizontal lines of figure (a). For $E = -2t$, $-\ln T_n$ grows from $n^* = 0$; for $E = 0$ it oscillates up to $n^* = 200$ and then it grows; for $E = 4t$, $-\ln T_n$ grows up to $n'^* = 200$, it oscillates up to $n^* = 600$, and then it grows again. The circles are numerical results, the lines represent the analytical law (5).

band: in figure 2(a) we see that $n' = n - n^*$ if we leave the band on the right, while $n' = n'^* - n$ if we leave the band on the left. We have then

$$-\ln T_n = \mp\frac{2}{\alpha}\left\{(1+\alpha n')\text{arcosh}\,(1+\alpha n') - \sqrt{(1+\alpha n')^2 - 1}\right\}. \tag{6}$$

Let us consider explicitly the case $V_0 - W \leqslant E \leqslant V_0 + W$; the case $E > V_0 + W$ can be handled along the same lines. In the 'near band' region, $\alpha n' \ll 1$, the leading term of equation (6) is given by the expression

$$-\ln T_n \sim \sqrt{\alpha} n'^{3/2} \qquad (\alpha n' \ll 1) \tag{7}$$

which does not contain the field in the exponent of n'. In the 'far band' region, $\alpha n' \gg 1$ we have

$$-\ln T_n \sim 2n'(\ln 2\alpha n' - 1) \qquad (\alpha n' \ll 1) \tag{8}$$

which is almost linear in n'.

For a multiband system $-\ln T_n$ behaves as in figure 2(b), $E = -2t$, in the regions where the gaps begin, while in the regions at the end of the gaps it behaves as in figure 2(b), $E = 4t$. For example, when a field is applied to a Kronig–Penney model (see figure 1) all the jumps in the function $-\ln T_n$, corresponding to gaps, can be interpreted in this way, and the behaviour of $-\ln T_n \sim n^{3/2}$ predicted by equation (7) is well reproduced in the proximity of the jumps when the influence of the left border of the adjacent band is negligible.

The more than exponential decreasing rate of the transmittivity in the presence of an electric field can be observed not only for periodic one-dimensional tight binding systems, but also for aperiodic and pseudorandom systems where the field modifies the nature of the states localized by the presence of the potential. We consider first an aperiodic system, where the site energies are given by the incommensurate potential [19, 20]

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

with α irrational and $\nu > 0$. It is a well assessed fact [20, 21] that, if $0 < \nu < 1$, the spectrum of the potential (9) has extended states for $E < |2t - \lambda|$ and exponentially localized states for $|2t - \lambda| < E < |2t + \lambda|$; therefore it possesses mobility edges at the energy values $E = \pm(2t - \lambda)$. We can control how the behaviour of the transmittivity changes under the application of an electric field. From figure 3(a), where $\lambda = t$, $2\pi\alpha = 1.2$ and $\nu = 0.7$, we see that for $E = -2t$ the envelope of $-\ln T_n$ has linear dependence from n in the case $f = 0$ (where the energy corresponds to an exponentially localized state), while it is clearly nonlinear for $f = 0.001$.

The origin of the steps which can be observed in the plots of figures 3(a) and 3(b) can be explained in terms of a real space continuous approximation. In the absence of electric fields this is realized by superimposing the potential V_n to the band $[-2t, 2t]$ of the regular lattice; this operation provides a pictorial representation of the allowed and forbidden regions for the travelling electron energy E in the real space [21]. For instance, in the case of potential (9) with $\lambda = t$ and $f = 0$ the interval $-t \leqslant E \leqslant t$ is always allowed for the electron propagation, while for $t < |E| < 3t$ an alternation of allowed and forbidden intervals as function of n appears. Therefore, in the case of figure 3(a), where the energy $E = -2t$ has been chosen, for $f = 0$ we observe the presence of a ladder structure which indicates an alternation of intervals where $-\ln T_n$ oscillates (corresponding to allowed energy zones) and intervals where it grows (corresponding to forbidden energy zones); the overall envelope of $-\ln T_n$ is linear.

When the electric field is applied, all the structure constituted by the band $[-2t, 2t]$ and the potential V_n has to be tilted; we thus obtain finite intervals where the electron lies in an allowed region (corresponding to a plateaus of $-\ln T_n$) and finite intervals where the energy lies alternately in allowed and forbidden regions (corresponding to a ladder structure in the plot). This explains why, for $f = 0.001$ and $E = -2t$ (figure 3(a)), the plot presents a ladder structure, up to $n = 1000$, which is progressively lost beyond this point. As it can be observed, the envelope of the plot shows clearly a more than linear growth rate of $-\ln T_n$. This is better seen in figure 3(b) where $E = 2t$. For $f = 0$ we observe a linear growth behaviour of $-\ln T_n$ with superimposed steps. If $f = 0.001$ the energy lies in a completely allowed interval for $1000 < n < 3000$ where $-\ln T_n$ shows a plateau; for $3000 < n < 5000$ the alternation of allowed and forbidden zones is reflected in the ladder structure superimposed to the clearly nonlinear growth behaviour. Finally, for $n > 5000$ the step structure gradually disappears because in this interval the energy $E = 2t$ lies in a completely forbidden zone.

If in equation (9) a value $\nu > 2$ is assigned, the potential is pseudorandom [19] and, for $f = 0$, all the eigenstates of the spectrum are exponentially localized. It can be observed

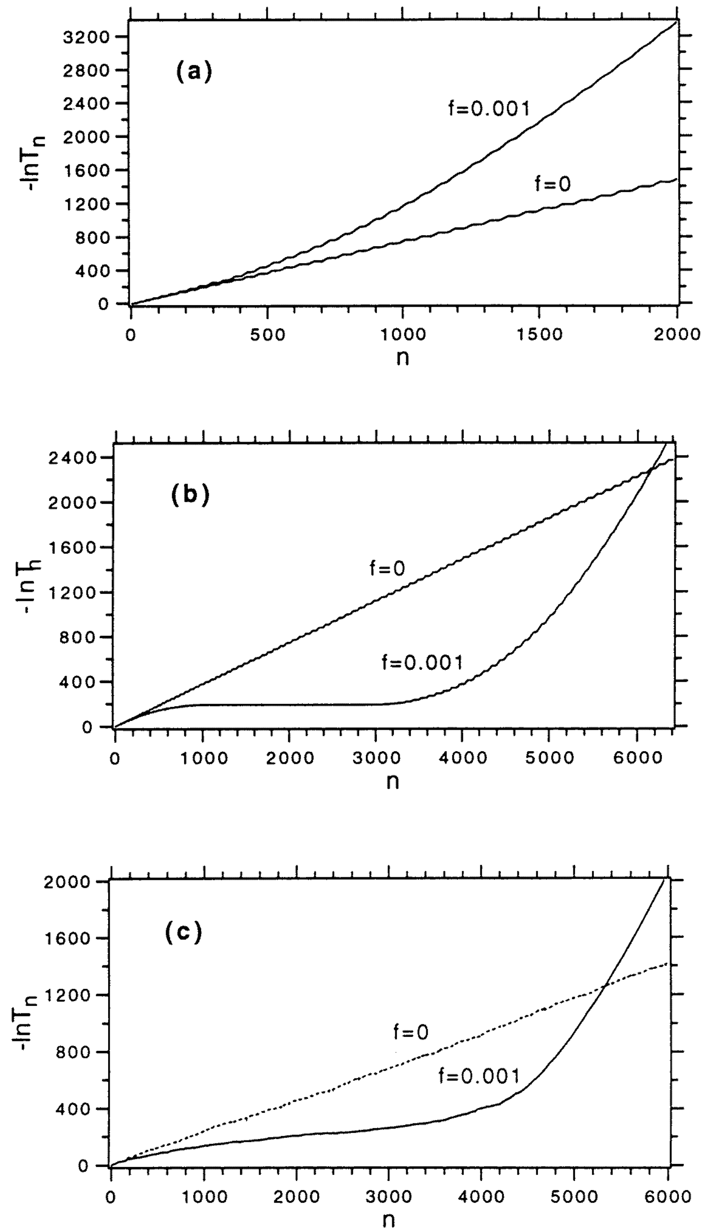

Figure 3. Behaviour of $-\ln T_n$ as a function of n in an aperiodic system (potential (9) with $\lambda = t$ and $2\pi\alpha = 1.2$): (a) $\nu = 0.7$ (slowly varying potential), $E = -2t$; (b) $\nu = 0.7$ (slowly varying potential), $E = 2t$; (c) $\nu = 2.5$ (pseudorandom potential), $E = 2t$. In the three pictures the cases $f = 0$ and $f = 0.001$ are compared.

in figure 3(c), for $\nu = 2.5$, that the growing rate of $-\ln T_n$ is nonlinear and very rapid for $n > 3000$ in comparison with what happens in the region $1000 < n < 3000$, which resembles the plateau of figure 3(b). In the pseudorandom case the step structure is not present because of a very rapid spatial fluctuation of the potential.

Finally, we wish to remark that in a Kronig–Penney model with barriers assigned with the same sign and distributed according to a pseudorandom law, the plot of $-\ln T_n$ presents a structure of jumps and plateaus very similar to that observed in the disordered case [16]; the behaviour of the transmittivity at the beginning of each jump can again be interpreted in the frame proposed in this paper.

In conclusion, we have investigated the phenomenon of the superlocalization in one-dimensional systems in an electric field. It manifests a more than exponential rate of decrease of the transmittivity as function of the length of the sample. For a single band periodic system we have obtained an analytic form which provides for the transmittivity the law $-\ln T_n \sim n^{3/2}$. This behaviour survives also for the regions beyond each band of multiband periodic systems when the bands are not too close, and in the case of aperiodic and pseudorandom potentials.

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