

## Metal-Insulator Transition in an Aperiodic Ladder Network: An Exact Result

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We prove that a tight-binding ladder network composed of atomic sites with on-site potentials distributed according to the quasiperiodic Aubry model can exhibit a metal-insulator transition at multiple values of the Fermi energy. For specific values of the first and second neighbor electron hopping, the result is obtained exactly. With a more general model, we numerically calculate the two-terminal conductance. The numerical results corroborate the analytical findings.

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The classic problem of electron localization in low dimensional quantum systems has remained alive over the last 50 years, since its proposition in 1958 by Anderson [1]. It is now well known that in one dimension (1D) even for arbitrarily weak disorder (almost) all the one-electron states are exponentially localized [1,2] and one never encounters mobility edges, that is, energy eigenvalues separating localized (insulating) states from the extended (conducting) ones, though positional correlations among the constituent “atoms” have been shown to lead to some unscattered (extended) states in an otherwise disordered one-dimensional lattice [3–6].

Quasiperiodic lattices, such as a 1D single band Aubry-Andre (AA) chain [7] have also played their part in the quest of mobility edges in 1D. In an AA chain of lattice constant  $a$ , the on-site potential described by,  $\epsilon_n = \lambda \cos(Qna)$  with  $Q$  being an irrational multiple of  $\pi$ . An AA model represents an almost periodic lattice which is different from a randomly disordered system, and displays a special kind of “order”, called the quasiperiodic order. The system, however, lacks translational periodicity. In one dimension with nearest neighbor hopping integral  $t$ , and with a site potential given by  $\epsilon_n$  as above, the amplitude  $f_n$  of the wave function at the  $n$ th site of the lattice can be obtained from the eigenvalue equation

$$[E - \lambda \cos(Qna)]f_n = t(f_{n+1} + f_{n-1}). \quad (1)$$

When  $\lambda > 2t$  all the single particle states are exponentially localized with Lyapunov exponent  $\ln(\lambda/2t)$ , while  $\lambda < 2t$  makes the states (all of them) extended [7,8]. One gets a metal-insulator (MI) transition in parameter space, but no mobility edges in energy exist for this model. A second important feature of this model is its self duality, which means that if one makes the transformation [8] from  $f_n$  to  $g_m = \sum_{n=-\infty}^{\infty} f_n e^{-imnQa}$ , then the coefficients  $g_m$  satisfy  $[E - 2t \cos(Qma)]g_m = (\lambda/2)(g_{m+1} + g_{m-1})$ . The  $g_m$  equation is exactly of the same form as Eq. (1) with the roles of  $t$  and  $\lambda$  interchanged. It can be shown [8] that if the eigenstates given by  $g_m$  are localized in reciprocal space,

then the eigenstates of Eq. (1) will be extended in real space, and vice versa. Incidentally, several variants of the Aubry model have also been examined to detect the signature of mobility edges even in one dimension [9–11].

In this Letter we investigate the electronic spectrum of an AA-ladder network built by fixing two identical AA chains laterally (see Fig. 1). The motivation behind the present work is twofold. First, we wish to investigate if the interplay of the quasi-one-dimensional structure of the network and the AA duality, which is still preserved, leads to a possibility of an MI transition. If it is true, then a ladder network such as this, could be used as a switching device, the design of which is of great concern in the current era of nanofabrication. Interestingly, research in AA models in one dimension and its variations has been rekindled recently in the context of potential design of aperiodic optical lattices [12,13]. Therefore, the question of the existence of MI transition in a system with “pure” AA potential can be addressed with a renewed interest. Second, the ladder networks have recently become extremely important in the context of understanding the charge transport in double-stranded DNA [14,15]. Experimental results on DNA transport report wide ranges of behavior, from almost insulating [16], semiconducting [17], to even metallic [18], which can be attributed to many experimental complications, such as the preparation of the sample, sample-electrode contact, etc. In addition to this, Mrevlishvili [19] experimentally observed oscillations in the specific heat of

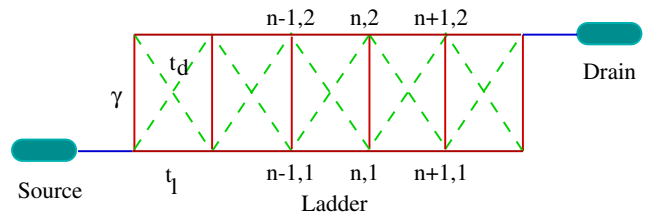


FIG. 1 (color online). Schematic view of a ladder attached to two electrodes.

DNA structures at low temperatures, results that have been subsequently explained by Moreira *et al.* [20] considering a quasiperiodic sequence of the nucleotides. The results of Ref. [20], compare remarkably well with numerical results obtained for *Ch22* human chromosomes. The helical structure of the double-stranded DNA is expected to affect the periodicity of the effective site potentials on the ladder, and introduce incommensurate periods in the system. In view of this, the examination of the electronic spectrum of a ladder network comprising of aperiodically varying site potentials might throw new light into the behavior of electrons, both in the context of basic physics and possible technological applications including DNA devices.

We adopt a tight-binding formalism, incorporate nearest and next-nearest-neighbor hopping inside a plaquette of the ladder and show that such a system exhibits a reentrant MI transition. Most interestingly, for a selected set of the Hamiltonian parameters we exactly prove the existence of mobility edges. Let us refer to Fig. 1. The Hamiltonian of the ladder network is given by,

$$\mathbf{H} = \sum_n \epsilon_n \mathbf{c}_n^\dagger \mathbf{c}_n + \mathbf{t} \sum_n \mathbf{c}_n^\dagger \mathbf{c}_{n+1} + \text{H.c.}, \quad (2)$$

where

$$\mathbf{c}_n = \begin{pmatrix} c_{n,1} \\ c_{n,2} \end{pmatrix}, \quad \epsilon_n = \begin{pmatrix} \epsilon_{n,1} & \gamma \\ \gamma & \epsilon_{n,2} \end{pmatrix}, \quad \mathbf{t} = \begin{pmatrix} t_l & t_d \\ t_d & t_l \end{pmatrix}. \quad (3)$$

In the above,  $c_{n,j}$  ( $c_{n,j}^\dagger$ ) are the annihilation (creation) operator at the  $n$ th site of the  $j$ th ladder,  $\epsilon_{n,1} = \epsilon_{n,2} = \lambda \cos(Qna)$  is the on-site potential at the  $n$ th site of the  $j$ th ladder,  $\gamma$  is the vertical hopping between the  $n$ th sites of the two ladders,  $t_l$  is the nearest neighbor hopping integral between the  $n$ th and the  $(n+1)$ th sites of every arm and  $t_d$  is the next nearest neighbor hopping within a plaquette of the ladder (see Fig. 1).

We describe the system in a basis defined by the vector

$$\mathbf{f}_n = \begin{pmatrix} f_{n,1} \\ f_{n,2} \end{pmatrix}, \quad (4)$$

where,  $f_{n,j}$  is the amplitude of the wave function at the  $n$ th site of the  $j$ th arm of the ladder ( $j = 1, 2$ ). In this basis, our task is to solve the difference equations  $(E\mathbf{I} - \epsilon_n)\mathbf{f}_n = \mathbf{t}(\mathbf{f}_{n+1} + \mathbf{f}_{n-1})$ . To show the existence of multiple mobility edges in such a system in an analytical way, we choose  $t_d = t_l$ , make the duality transformation to the reciprocal space for each arm of the ladder and arrive at a difference equation,

$$[E - 2t_l \cos(Qma)]\mathbf{I} - \{2t_l \cos(Qma) + \gamma\}\sigma_x \mathbf{g}_{m,j} = (\lambda/2)\mathbf{I}(\mathbf{g}_{m+1,j} + \mathbf{g}_{m-1,j}), \quad (5)$$

where,  $\sigma_x$  is the usual Pauli matrix. We now diagonalize the  $\sigma_x$  matrix by a similarity transformation using a matrix  $\mathbf{S}$ , and define  $|\phi_m\rangle = \mathbf{S}|g_m\rangle$ . The difference equation (5) now decouples into

$$(E + \gamma)\phi_{m,2} = (\lambda/2)(\phi_{m+1,2} + \phi_{m-1,2}), \quad (6)$$

$$[E - \gamma - \Delta \cos(Qma)]\phi_{m,1} = (\lambda/2)(\phi_{m+1,1} + \phi_{m-1,1}). \quad (7)$$

Here,  $\phi_{m,1}$  and  $\phi_{m,2}$  are the elements of the column vector  $\phi_m$  and  $\Delta = 4t_l$ . It is interesting to observe that, the Eq. (6) above corresponds to a perfectly ordered chain with nearest neighbor hopping integral equal to  $\lambda/2$  in the reciprocal space. This implies that, for  $-\lambda - \gamma < E < \lambda - \gamma$  we have a gap less continuous spectrum in the reciprocal space. Equation (7) on the other hand, represents the familiar single band Aubry model for which all states are localized or extended if  $\Delta > \lambda$ , or,  $\Delta < \lambda$  respectively. We can now extract information about the nature of eigenfunctions by considering the two Eqs. (6) and (7) simultaneously.

*Case I.*— $|E + \gamma| < \lambda$  and  $\Delta > \lambda$ . We focus on the pair of Eqs. (6) and (7). When  $E$  lies within this range, we are within the ‘‘continuous band’’ of extended states (in the reciprocal space). This means that the density of states corresponding to Eq. (6) is nonzero at all energies lying within this range and therefore  $\phi_{m,2} \neq 0$  irrespective of the

choice of  $\Delta$ . Therefore,

$$S_{21}g_{m,1} + S_{22}g_{m,2} \neq 0 \quad (8)$$

for all  $m$  in dual space. This implies that,

$$\lim_{n \rightarrow \infty} [S_{21}f_{n,1} + S_{22}f_{n,2}] = 0 \quad (9)$$

in real space.  $S_{ij}$  are the elements of the matrix  $\mathbf{S}$ . If the average density of states corresponding to Eq. (7) is non-zero, then Eq. (7) tells us that  $\lim_{m \rightarrow \infty} \phi_{m,1} = 0$ , as we have chosen  $\Delta > \lambda$  [8]. This implies that,

$$\lim_{m \rightarrow \infty} [S_{11}g_{m,1} + S_{12}g_{m,2}] = 0 \quad (10)$$

in dual space, and,

$$S_{11}f_{n,1} + S_{12}f_{n,2} \neq 0 \quad (11)$$

for all values of  $n$  in real space. Now, the density of states for an Aubry model is nonzero in the immediate neighborhood of  $E = \gamma$  (the band center) [8]. We can therefore definitely say from Eqs. (9) and (11) that, both  $f_{n,1}$  and  $f_{n,2}$  will be nonzero for any arbitrary value of  $n$ . This ensures that all the states for the Aubry ladder will be extended at the center of the band. However, interesting changes are observed as one looks away from the band center. It is known [7,8] that the density of states of an infinite one band Aubry model is highly fragmented. This means we shall have zero values of the density of states (i.e., no state

at all) scattered throughout the spectrum. Whenever the density of states is zero, we shall have

$$S_{11}f_{n,1} + S_{12}f_{n,2} = 0 \quad (12)$$

for all  $n$ . Considering Eqs. (9) and (12) together, it becomes quite clear that both  $f_{n,1}$  and  $f_{n,2}$  have to be equal to zero as  $n \rightarrow \infty$  in order that the Eqs. (8) and (11) are simultaneously satisfied. This means that the eigenstates are localized away from the center of the band. We thus have extended wave functions at the band center flanked by the exponentially localized states on either side for  $-\lambda - \gamma < E < \lambda - \gamma$  and  $\Delta > \lambda$ .

It is to be noted that in the true quasiperiodic limit the spectrum of an Aubry model exhibits more than one subband separated by global gaps. Within each subband one has a highly fragmented band structure with infinitesimal energy gaps (for an infinite system). So, in principle, following the argument given above, one should encounter an infinite number of mobility edges. However, for realistic systems electron-electron interactions or the lead-sample connection will broaden the energy levels and the infinitesimal gaps will not persist. Only mobility edges which reside in the vicinity of the finite gaps separating the subbands will survive.

*Case II.*— $|E + \gamma| > \lambda$  and  $\Delta > \lambda$ . In this energy regime  $E$  lies outside the band corresponding to the ordered system [Eq. (6)], the corresponding density of states is zero (as there are no states at all). One then has,

$$S_{21}f_{n,1} + S_{22}f_{n,2} = 0 \quad (13)$$

for all  $n$ . If, on the other hand, the density of states corresponding to Eq. (7) is nonzero, then

$$S_{11}f_{n,1} + S_{12}f_{n,2} \neq 0 \quad (14)$$

for all  $n$ . Therefore, from Eqs. (13) and (14) we observe that,  $f_{n,1}$  and  $f_{n,2}$  both remain nonzero for all values of  $n$ . This means, the eigenstates are extended for these values of energy. Thus, for  $\Delta > \lambda$ , the eigenvalue spectrum for the Aubry ladder, in real space, exhibits the existence of localized and extended states separated by mobility edges and a reentrant metal-insulator transition is clearly visible. One can follow a similar chain of arguments to show that all states will be localized in real space for  $\Delta < \lambda$ . There are no mobility edges here.

For a more general choice of the Hamiltonian parameters (with  $t_l \neq t_d$  and  $\epsilon_{n,1} \neq \epsilon_{n,2}$ ), an analytical approach becomes difficult. We have numerically calculated the conductance of an Aubry ladder with various sets of parameters using a Green's function formalism. Though one has true quasiperiodicity only in an infinite system, for which we already have given an analytical proof for the existence of MI transition (for a special set of parameters), it is known that even finite systems grown following a quasiperiodic order are capable of exhibiting the localization effects [8–10]. For example, in finite laboratory-grown

Fibonacci multilayers experimental evidence of localization of light has already been reported [21]. Therefore, though for an ideal infinite system several exotic spectral features may not be unlikely, in our cases of interest, as we have worked in the parameter regime where the single band AA model has exponentially localized states only, expecting the localization fingerprints in a finite AA ladder is quite legitimate. In the present calculation MI transition and mobility edges are found even when the simplification in the values of the hopping integrals are not made.

To calculate the conductance, a finite Aubry ladder is attached to two semi-infinite one-dimensional metallic electrodes (Fig. 1), described by the standard tight-binding Hamiltonian and parametrized by constant on-site potential  $\epsilon_0$  and nearest-neighbor hopping integral  $t_0$ . For low bias voltage and temperature, the conductance  $g$  of the ladder is determined by the Landauer conductance formula [22]  $g = (2e^2/h)T$ , where the transmission probability  $T$  is given by [22]  $T = \text{Tr}[\Gamma_S G_L^r \Gamma_D G_L^a]$ .  $\Gamma_S$  and  $\Gamma_D$  correspond to the imaginary parts of the self-energies due to coupling of the ladder with the two electrodes and  $G_L$  represents the Green's function of the ladder [23–25]. In Fig. 2 we present the behavior of the conductance for the cases when  $\gamma = 0$ , and  $t_l = t_d$ , and the general case for a nonzero  $\gamma$ , and  $t_l \neq t_d$  is shown in Fig. 3. In every case the pictures of the density of states are superposed to show that we have eigenstates existing in energy regimes for which the conductance is zero. This speaks of localized eigenstates and

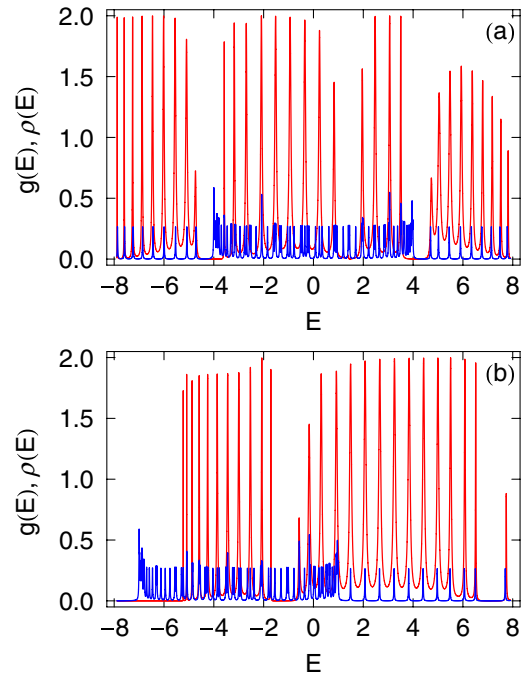


FIG. 2 (color online).  $g$ - $E$  (red color) and  $\rho$ - $E$  (blue color) curves for a 60-rung ladder. (a)  $\gamma = 0$  and (b)  $\gamma = 3$ . Other parameters are,  $Q = (1 + \sqrt{5})/2$ ,  $t_d = t_l = 3$ ,  $\epsilon_0 = 0$ ,  $t_0 = 4$ , and  $\lambda = 4$ . We have chosen  $c = e = h = 1$ .

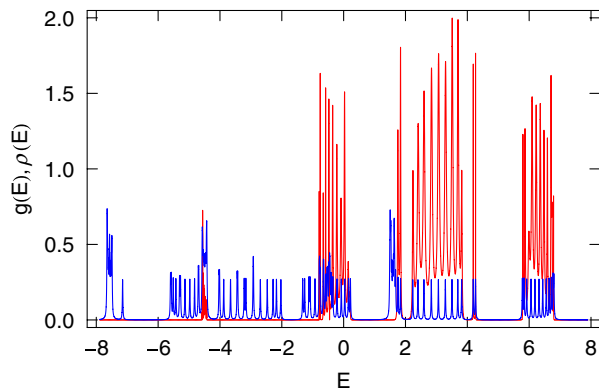


FIG. 3 (color online).  $g$ - $E$  (red color) and  $\rho$ - $E$  (blue color) curves for a general AA-ladder with 60 rungs. Here,  $\gamma = 3$ ,  $Q = (1 + \sqrt{5})/2$ ,  $t_d = 1$ ,  $t_l = 2$ ,  $\epsilon_0 = 0$ ,  $t_0 = 4$ , and  $\lambda = 4$ . We have chosen  $c = e = h = 1$ .

the transition from the conducting (high  $g$ ) to nonconducting phase is clear.

Before we end, it should be pointed out that though the results presented in this communication are for zero temperature, they should be valid even for finite temperatures ( $\sim 300$  K) as the broadening of the energy levels of the ladder due to its coupling with the electrodes will be much larger than that of the thermal broadening [22]. The inter-ladder hopping  $\gamma$  will shift the spectra corresponding to Eqs. (6) and (7) relative to each other, thus making it possible, in principle, to tune the positions of the mobility edges. This aspect may be utilized in designing a tailor made switching device.

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