Metal-insulator transition in an aperiodic ladder network: an exact result

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We show, in a completely analytical way, 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 exact. With a more general model, we calculate the two-terminal conductance numerically. The numerical results corroborate the analytical findings and yield a richer variety of spectrum showing multiple mobility edges.

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The classic problem of electron localization in low dimensional quantum systems has remained alive over the last fifty years, since its proposition in 1958 by Anderson [1]. It is now well known that in one dimension 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. Last couple of decades however, have witnessed an interesting twist in the canonical wisdom about localization problem through the advent of the so called correlated disordered models in one dimension. It is now established that even in a one dimensional chain of atomic sites, short range [3, 4] or long range [5, 6] positional correlations between the constituents can induce unscattered (extended) wave functions at specific values of the electron-energy [3, 4] or even a crossover from localized to extended states [5, 6].

The search for a mobility edge in one dimensional lattices has always been an intriguing problem that started earlier with certain aperiodic lattices which bridge the gap between a perfectly periodic lattice and a completely random one. A famous example is the single band Aubry-Andre (AA) model [7] in which the on-site potential in a 1-d chain of lattice constant \( a \) is described deterministically by, \( \epsilon_n = \lambda \cos(Qna) \) with \( Q \) being an irrational multiple of \( \pi \). It is to be appreciated that an AA-model represents a certain class of almost periodic lattices which are much different from conventional randomly disordered systems, and displays a special kind of ‘order’, called the quasiperiodic order. The system however lacks translational periodicity. In a one dimensional chain with nearest neighbor hopping integral \( t \) for example, and with such a potential (also called a Harper potential) the amplitude \( f_n \) of the wave function at the \( n \)th site of the lattice can be obtained from the eigenvalue equation

\[
\lambda = \sum_{m=-\infty}^{\infty} g_m e^{imQn} - \sum_{m=-\infty}^{\infty} f_n e^{-imQn} \quad (2)
\]

then the coefficients \( g_m \) satisfy

\[
[E - 2t \cos(Qna)] g_m = \frac{\lambda}{2}(g_{m+1} + g_{m-1}) \quad (3)
\]

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 1-d [9, 10, 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 the interplay of the quasi-one dimensional structure of the network and the AA duality, which is still preserved, leads to any possibility of a metal-insulator (MI) transition even within the standard form of the Harper potential. 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 1-d and its variations have 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 (Harper) potential can be addressed with a renewed interest. Secondly, 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 range of behavior, from almost insulating [16], semiconducting [17] to even metallic [18], that 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 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 reference 20, compare remarkably well with numerical results obtained for Ch22 human chromosomes. It is to be appreciated that 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 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 re-entrant MI transition. Most interestingly, for a selected set of the Hamiltonian parameters we are able to provide an exact analysis which shows the existence of mobility edges. We begin by referring to Fig. 1 The Hamiltonian of the ladder network is given by,

$$H = \sum_n \epsilon_n c_n^\dagger c_n + t \sum_n c_n^\dagger c_{n+1} + \text{h.c.}$$  \hspace{1cm} (4)

where

$$c_n = \begin{pmatrix} c_{n,1} \\ c_{n,2} \end{pmatrix}, \quad \epsilon_n = \begin{pmatrix} \epsilon_{n,1} & \gamma \\ \gamma & \epsilon_{n,2} \end{pmatrix}, \quad t = \begin{pmatrix} t_1 & t_d \\ t_d & t_l \end{pmatrix}$$  \hspace{1cm} (5)

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, \(\epsilon_{n,1} = \epsilon_{n,2} = \lambda \cos(Qma)\) 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, \(t_1\) 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

$$f_n = \begin{pmatrix} f_{n,1} \\ f_{n,2} \end{pmatrix}$$  \hspace{1cm} (6)

where, \(f_{n,j}\) is the amplitude of the wave function at the \(n\)th site of the \(j\)th arm of the ladder, \(j\) being equal to 1 or 2. Using this basis, our task boils down to obtain solutions of the difference equation

$$(EI - \epsilon_n)f_n = t(f_{n+1} + f_{n-1})$$  \hspace{1cm} (7)

At first, we proceed to show the existence of multiple mobility edges in such a system in an analytically exact way. For this, we choose \(t_d = t_l\), and make the following transformation to the reciprocal space for each arm of the ladder and arrive at a difference equation in the reciprocal space,

$$\left[\{E - 2t_l \cos(Qma)\}I - \{2t_l \cos(Qma) + \gamma\} \sigma_x \right] g_{m,j} = \frac{\lambda}{2} I \left(g_{m+1,j} + g_{m-1,j}\right)$$  \hspace{1cm} (8)

where, \(\sigma_x\) is the usual Pauli matrix. We now diagonalize the \(\sigma_x\) matrix by a similarity transformation using a matrix \(S\), and define \(|\phi_m\rangle = S|g_m\rangle\) The difference equation (8) now decouples into,

$$(E + \gamma)\phi_{m,2} = \frac{\lambda}{2}(\phi_{m+1,2} + \phi_{m-1,2})$$  \hspace{1cm} (9)

$$[E - \gamma - \Delta \cos(Qma)]\phi_{m,1} = \frac{\lambda}{2}(\phi_{m+1,1} + \phi_{m-1,1})$$  \hspace{1cm} (10)

Here, \(\phi_{m,1}\) and \(\phi_{m,2}\) are the elements of the column vector \(|\phi_m\rangle\) and \(\Delta = 4t_l\). It is interesting to observe that, the Eq. (9) 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. Eq. (10) 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. (9) and (10) simultaneously.

**Case I:** \(|E + \gamma| < \lambda\) and \(\Delta > \lambda\)

We focus on the pair of Eqs. (9) and (10). 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. (9) is non-zero at all energies lying within this range and therefore \(\phi_{m,2} \neq 0\) irrespective of the choice of \(\Delta\). Therefore,

$$S_{11}g_{m,1} + S_{22}g_{m,2} \neq 0$$  \hspace{1cm} (11)

for all \(m\) in dual space. This implies that,

$$\lim_{n \rightarrow -\infty} [S_{21}f_{n,1} + S_{22}f_{n,2}] = 0$$  \hspace{1cm} (12)

in real space. \(S_{ij}\) are the elements of the matrix \(S\). If the average density of states corresponding to Eq. (10) is non-zero, then Eq. (10) tells us that \(\lim_{m \rightarrow -\infty} \phi_{m,1} = 0\), as we have chosen \(\Delta > \lambda\) [8]. This, implies that,

$$\lim_{m \rightarrow -\infty} [S_{11}g_{m,1} + S_{12}g_{m,2}] = 0$$  \hspace{1cm} (13)

in dual space, and,

$$S_{11}f_{n,1} + S_{12}f_{n,2} \neq 0$$  \hspace{1cm} (14)
for all values of $n$ in real space. Now, the density of states for an Aubry model is non-zero in the immediate neighborhood of $E = \gamma$ (the band-center) [8]. We can therefore definitely say from Eq. (12) and Eq. (14) that, both $f_{n,1}$ and $f_{n,2}$ will be non-zero 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 is zero (as there are no states at all).

![Figure 2](image2.png)

**FIG. 2:** $g-E$ (red color) and $\rho-E$ (blue color) curves for a ladder of total number of rungs 60. (a) $\gamma = 0$ and (b) $\gamma = 3$. Other parameters are, $Q = (1 + \sqrt{5})/2$, $t_4 = t_1 = 3$, $\epsilon_0 = 0$, $t_0 = 4$ and $\lambda = 4$. We have chosen $c = e = h = 1$.

The spectrum of an Aubry model exhibits more than one mobility edges which reside in the vicinity of the finite gaps separating the sub-bands 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. (9)), the corresponding density of states is zero (as there are no states at all). One then has,

$$S_{21}f_{n,1} + S_{22}f_{n,2} = 0$$

for all $n$. If, on the other hand, the density of states corresponding to Eq. (10) is non-zero, then

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

for all $n$. Therefore, from Eq. (16) and Eq. (17) we observe that $f_{n,1}$ and $f_{n,2}$ both remain non-zero 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 re-entrant 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.

![Figure 3](image3.png)

**FIG. 3:** $g-E$ (red color) and $\rho-E$ (blue color) curves for a general AA-ladder of total number of rungs 60. The parameters are, $\gamma = 3$, $Q = (1 + \sqrt{5})/2$, $t_4 = 1$, $t_1 = 2$, $\epsilon_0 = 0$, $t_0 = 4$ and $\lambda = 4$. We have chosen $c = e = h = 1$.

For a more general choice of the Hamiltonian parameters (with $t_l \neq t_4$ 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, 9, 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 onsite 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 of the ladder $g = (2e^2/h)TR$ where the transmission probability $T$ is given by $T = Tr [\Gamma_S G_L \Gamma_D G_R]$. $\Gamma_S$ 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. All the information about the ladder-to-electrodes coupling are included into these two self-energies as stated above and are described by the Newns-Anderson (NA) chemisorption theory [23, 24]. For the sake of simplicity, here we have assumed that the entire voltage is dropped across the ladder-electrode interfaces and this assumption does not significantly affect the qualitative aspects of the $g$-$E$ characteristics [22, 23]. 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 non-zero $\gamma$, 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 clearly that we have eigenstates existing in energy regimes for which the conductance is zero. This spikes of localized eigenstates and the transition from the conducting (high $g$) to non-conducting phase is clearly visible in each case.

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. (9) and (10) 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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