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Engineering electronic states of periodic and quasiperiodic chains by buckling

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ABSTRACT

The spectrum of spinless, non-interacting electrons on a linear chain that is buckled in a non-uniform, quasiperiodic manner is investigated within a tight binding formalism. We have addressed two specific cases, viz., a perfectly periodic chain wrinkled in a quasiperiodic Fibonacci pattern, and a quasiperiodic Fibonacci chain, where the buckling also takes place in a Fibonacci pattern. The buckling brings distant neighbors in the parent chain to close proximity, which is simulated by a tunnel hopping amplitude. It is seen that, in the perfectly ordered case, increasing the strength of the tunnel hopping (that is, bending the segments more) absolutely continuous density of states is retained towards the edges of the band, while the central portion becomes fragmented and host subbands of narrowing widths containing extended, current carrying states, and multiple isolated bound states formed as a result of the bending. A switching "on" and "off" of the electronic transmission can thus be engineered by buckling. On the other hand, in the second example of a quasiperiodic Fibonacci chain, imparting a quasiperiodic buckling is found to generate *continuous subband(s)* destroying the usual multifractality of the energy spectrum. We present exact results based on a real space renormalization group analysis, that is corroborated by explicit calculation of the two terminal electronic transport.

1. Introduction

Localization of single particle quantum states has been an ubiquitous phenomenon, observed primarily as a consequence of disorder in a system, and is traditionally called the Anderson localization [1]. The pivotal result in the field of disorder-induced localization is that, the single particle eigenstates of a Hamiltonian describing a disordered lattice should be exponentially localized for dimension $d \leq 2$, and even for $d > 2$ for strong disorder. The effect is strongest in one dimension where all the states are localized for any strength of disorder. The envelope of the wave function decays exponentially with respect to a given location in the lattice [2,3]. These results have been aptly justified by various calculations related to the localization length [4,5] and the density of states [6]. The single parameter scaling hypothesis – its validity [7], variance [8], or even violation [9,10] in low dimensional systems within a tight-binding approximation has also enriched the field.

This picture is to be contrasted with the effect of quasiperiodic order [11,12] in one dimensional lattices where the single particle excitations are *critical* and exhibit a power law localization with a multifractal character in general [13]. Resistance for such systems exhibits power law growth as well as the size of the lattice increases [14–16]. The exotic spectral properties of quasiperiodic lattices occupied an immense volume of literature over the past three decades, and even today, the unusual behavior of quantum conductance in such systems are of immense interest [17].

In this communication, we revisit the effect of 'deterministic disorder', introduced in an infinitely long one dimensional chain of atomic sites by buckling the chain in *local segments*, and throughout its length, following a quasiperiodically ordered sequence. Bent quantum wires have been studied previously in the context of ballistic transport characteristics [19]. Single and multiply bent two dimensional quantum wires were examined in respect of localized, doubly split one electron states [20]. Apart from these, winding chains have been considered as models of conducting polymers [21,22]. The winding brings sites that were distant neighbors in the unperturbed system to close proximity, and a tunnel hopping provides additional paths for the electron. The lattice becomes a topologically disordered (deterministic though) system in the spirit of Guinea and Vergés [23], who discussed the effect of

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fluctuating coordination numbers in a linear chain, caused by dangling branches coupled from a side, or bridging two distant sites in a one dimensional lattice. Such tunneling has been shown [21,22] to have profound influence on quantum transport, leading to large localization lengths in disordered polymers, which is indicative of a metal-insulator (MI) transition in such systems. Real polymers of course, include interaction between different constituent chains, the coupling between the adjacent chains being mediated by the overlapping hydrogen orbitals. In several cases the main spectral features can be explained by an effective tight binding model with next nearest neighbor hopping integrals. The effect of second neighbor hopping is also studied for quasi one dimensional organic polymer ferromagnetic systems and have unraveled a plethora of information [24]. Buckling a chain makes such longer range interactions possible in a natural way, and thus deserves close scrutiny.

In addition, a quasiperiodic order in chains and their bending are two important ingredients that have been shown to arise in the recent field of two dimensional materials, a graphene nanoribbon for example [18]. This provides an extra motivation for studying the present model.

We examine two different cases. At first, we consider a perfectly periodic chain of atoms within a tight binding approximation. Buckling is introduced in a Fibonacci quasiperiodic sequence [11] such that the chain bends after every n and m atoms, the numbers n and m being distributed in a Fibonacci pattern. Tunnel hopping is introduced across such clusters and it is seen that for large strength of the tunnel hopping amplitude, which may be thought to be caused by large bending of the local segments, the energy spectrum turns out to be extremely interesting. The outer edges of the spectrum retain the character of a pure, one dimensional chain of atoms, while the central part, spanning between $E = \epsilon \pm 2t$, feels the 'disorder' and breaks up into multiple subbands populated by extended eigenstates as well as sharply localized bound states. Thus wrinkling the chain appropriately one can look into the possibility of a switching action as one sweeps the Fermi energy from the domain of absolutely continuous spectrum to the fragmented one, mixed with transparent and localized states.

In the second example, we consider a quasiperiodic Fibonacci chain to begin with. The tunnel hopping, spanning the second neighbors, but in a restricted sense, also follows a Fibonacci sequence. This introduces a competing quasiperiodic order. The introduction of the tunnel hopping in this case results in something totally different. We have encountered several cases where an appropriate choice of the tunnel hopping is seen to generate *absolutely continuous* subbands in the otherwise fragmented Cantor set energy spectrum, typical of a Fibonacci lattice [11] making the system conduct over specified energy intervals.

In what follows, we discuss our findings in details. In section 2 we lay down the models and the methods followed. Section 3 contains the results for both the cases addressed here, and in section 4 we draw our conclusions.

2. The model and the method

2.1. The perfectly periodic chain with quasiperiodic buckling

Let us refer to Fig. 1 which shows a linear chain of atomic scatterers (violet spheres). The chain is assumed to be buckled after every n and m atoms, where we have taken the sequence of n and m following a Fibonacci distribution. That is, the chain is inhomogeneously distorted and the distorted segments are distributed as, *na*, *ma*, *na*, *na*, *ma*, ..., where, a is the uniform lattice spacing. This is the typical arrangement of constituents in a binary Fibonacci chain comprising of say, two letters L ans S, and grown following the algorithm $L \to LS$ and $S \to L$ [11]. The Hamiltonian

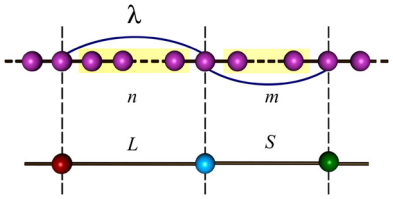

Fig. 1. (Color online) A one-dimensional chain of atoms with identical quantum dots each of having on-site potentials ϵ and hopping integral t with long range hopping λ (blue line) across n-atoms and across m-atoms which follow a Fibonacci sequence, as discussed in text. The figure below indicates the *renormalized* version of the buckled ordered chain with restricted long range hopping.

describing the system and written in a tight binding approximation reads

$$H = \epsilon \sum_i |i\rangle\langle i| + \sum_{ij} t_{ij}|i\rangle\langle j| \tag{1}$$

In this case, ϵ is the uniform on-site potential describing the parent ordered chain. The hopping integral $t_{ij} = t$ for the nearest neighboring sites on the linear backbone, and $t_{ij} = \lambda_n$ or λ_m depending on whether the buckling (shown by the blue line), connecting the vertices along the chain and across a segment of n sites or a segment of m sites. However, in the subsequent discussion, we shall stick to the case where, $\lambda_n = \lambda_m = \lambda$, which shows interesting spectral behavior.

Using a set of difference equations

$$(E - \epsilon)\psi_i = \sum_{ij} t_{ij}\psi_j \tag{2}$$

It is simple to reduce the original chain depicted in Fig. 1 to a linear Fibonacci chain with two kinds of (effective) bonds L and S (see Fig. 1) which follow a Fibonacci pattern $LSLLSLSLLSLLS$..... This results in three kinds of (effective) on-site potentials namely, ϵ_α, ϵ_β and ϵ_γ, representing vertices flanked by LL, LS or SL bonds. The hopping integrals along the effective L or S bonds are designated by t_L and t_S respectively. These on-site potentials and the hopping integrals are given by

$$\begin{aligned}
\epsilon_\alpha &= \epsilon + 2t\frac{U_{n-1}(x)}{U_n(x)} \\
\epsilon_\beta &= \epsilon + t\left[\frac{U_{n-1}(x)}{U_n(x)} + \frac{U_{m-1}(x)}{U_m(x)}\right] \\
\epsilon_\gamma &= \epsilon_\beta \\
t_L &= \lambda + \frac{t}{U_n(x)} \\
t_S &= \lambda + \frac{t}{U_m(x)}
\end{aligned} \tag{3}$$

Here, $x = (E - \epsilon)/2t$, and $U_n(x)$ is the n-th order Chebyshev polynomial of the second kind. The resulting *effective* Fibonacci chain (Fig. 1(b)) is then further renormalized using the standard decimation procedure, viz., by 'folding' it backward using the deflation rule $LS \to L'$ and $L \to S'$. The recursion relations relating to the potentials and the hopping matrix elements at one length scale to the next, given by

$$\begin{aligned}
\epsilon'_\alpha &= \epsilon_\gamma + \frac{t_L^2 + t_S^2}{E - \epsilon_\beta} \\
\epsilon'_\beta &= \epsilon_\gamma + \frac{t_S^2}{E - \epsilon_\beta} \\
\epsilon'_\gamma &= \epsilon_\alpha + \frac{t_L^2}{E - \epsilon_\beta}
\end{aligned}$$

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