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Engineering bands of extended electronic states in a class of topologically disordered and quasiperiodic lattices

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ABSTRACT

We show that a discrete tight-binding model representing either a random or a quasiperiodic array of bonds can have the entire energy spectrum or a substantial part of it absolutely continuous, populated by extended eigenfunctions only, when atomic sites are coupled to the lattice locally, or non-locally from one side. The event can be fine-tuned by controlling only the host–adatom coupling in one case, while in two other cases cited here an additional external magnetic field is necessary. The delocalization of electronic states for the group of systems presented here is sensitive to a subtle correlation between the numerical values of the Hamiltonian parameters – a fact that is not common in the conventional cases of Anderson localization. Our results are analytically exact, and supported by numerical evaluation of the density of states and electronic transmission coefficient.

1. Introduction

Electronic wave functions in a disordered lattice exhibit an exponentially localized envelope in space – a phenomenon, commonly known as the Anderson localization [1–4]. The problem has kept itself alive over all these years in condensed matter physics, and has given quantum transport properties of disordered systems intriguing twists and turns. The recent development of fabrication and lithographic techniques has taken the phenomenon of Anderson localization beyond the electronic systems, substantiated by remarkable experiments incorporating localization of light [5,6], ultrasound in three-dimensional elastic networks [7], or even plasmonic [8,9] and polaritonic [10,11] lattices. Direct observation of the localization of matter waves [12–16] in recent times has made the decades old phenomenon even more exciting.

The key point in Anderson localization is the dimensionality. Within the tight binding approximation, the electronic wave functions are localized for dimensions $d \leq 2$ (the band center in the off diagonal disorder case is an exception). For $d > 2$ with strong disorder, the wave function decays exponentially [2,3]. Extensive analyses of the localization length [17,18], density of states [19], and multi-fractality of the single particles states [20,21] have consolidated the fundamental ideas of disorder induced localization. Intricacies of the single parameter scaling hypothesis – its validity [22], variance [23], or even violation [24,25] in low dimensional systems – provided the finer details of the localization phenomenon that have subsequently been supported by experimental measurements of conductance distribution in quasi-one-dimensional gold wires [26].

However, in low dimensions, or more specifically, in one-dimensional disordered lattices even a complete delocalization of electronic states can be seen. This path breaking result was initially put forward by Dunlap et al. [27] in connection with a sudden enhancement of conductance of a class of polyanilenes on protonation. Known as the *random dimer model* (RDM) the phenomenon is attributed to certain special kinds of positional correlation in the potential profiles. The investigation of delocalization of eigenstates in correlated disordered models was taken up further over the years and interesting results such as the relation of localization length with the density of states [28] were put forward. The work extended to quasi-one-dimensional systems as well for which the Landauer resistance and its relation to the localization length was examined in detail [29] for a two-leg ladder model, an extensive extension of which was later done by Sedrakyan et al. [30]. Controlled disorder induced localization and delocalization of eigenfunctions took a considerable volume in contemporary literature, exploring solid non-trivial results involving electron or phonon eigenstates [31–33]. Extended eigenfunctions in all such works mostly appear at special discrete set of energy eigenvalues.

Eventually, the possibility of a controlled engineering of spectral continuum populated by extended single particle states and even a metal–insulator transition in one, or quasi-one-dimensional discrete systems have also been discussed in the literature [34–36].

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But, on the whole, the general exponentially localized character of the eigenfunctions prevails, and the possibility of having a mixed spectrum of localized and extended states in a disordered system (under some special positional correlations) is now well established.

Can one generate, going beyond the RDM, a full band of only extended eigenfunctions in a disordered system with $d \leq 2$? If yes, what would be the minimal models capable of showing such unusual spectra? This is the question that we address to ourselves in the present communication. We put forward examples of a class of essentially one-dimensional disordered and quasiperiodic lattices where a *complete delocalization* of electronic states can be engineered, and *absolutely continuous* bands can be formed in the energy spectrum. This is shown to be possible when an infinite disordered or quasiperiodic array of two kinds of 'bonds' is side coupled to a single or a cluster of quantum dots (QD) from one side at a special set of vertices. Minimal requirements are discussed in detail. In some of the examples cited here, the attachment of the dots form local loops which can be pierced by a constant magnetic field, breaking the time reversal symmetry of electron-hopping only locally, along the edges of such closed loops. The engineering of bands of extended states is shown to be the result of a definite numerical correlation in the values of the electron hopping amplitude along the chain (backbone) and the coupling of the linear backbone with the side coupled dots, the strength of the magnetic field or both.

It should be mentioned that an early report of an RDM-kind of correlation leading to extended eigenfunctions in a Fibonacci superlattice was put forward by Kumar and Ananthakrishna [37]. The insight into the phenomenon was immediately provided by Xie and Das Sarma [38]. However, the fact that certain specific *numerical relationship* among a subset of parameters of the Hamiltonian is capable of producing, absolutely continuous *bands* of extended eigenfunctions is uncommon and, to the best of our knowledge, has not been addressed until very recently [39].

We consider two bonds A and B arranged along a line forming an infinite linear chain. The sequence of the bonds may be random or quasiperiodic [40], offering either a pure point spectrum or a singular continuous one. The bonds connect identical atomic sites, an infinite subset of which is coupled to similar atoms (mimicing single level quantum dots (QD)) from one side giving the system a quasi one-dimensional flavor. The disorder (or, quasiperiodic order) thus has a topological character. In addition to the basic interest of going beyond the RDM, two other facts motivate us in undertaking such a work.

First, the Fano–Anderson effect [41,42] caused by the insertion of a bound state into a continuum is an exciting field, and has been investigated recently in nanoscale systems [43]. In this context, our study provides examples where one can observe at least one effect of inserting multiple bound states, in fact, an infinity of them in a *singular continuum*, or a pure point spectrum.

Second, the present advanced stage of growth techniques has motivated in depth studies of quasiperiodic nanoparticle arrays in the context of ferromagnetic dipolar modes [44] or plasmon modes [45]. Also, the use of a scanning tunnel microscope (STM) tip to fabricate structures atom by atom, viz., Xe on Ni substrates [46], or nanometer size gold particles on metals [47], or, putting individual atoms of Si substrate [48] has stimulated a lot of work in this field [49,50]. Our results can motivate future experiments in this direction.

In Section 2 we describe the lattice models. In Section 3, within Subsections 3.1 and 3.2 the local, non-local and the mixed cases introduced in Section 2 are discussed, with explicit remarks on the density of states profiles in each case. Subsection 3.3 specially deals with the special case of a Fibonacci quasiperiodic chain, using a real space renormalization group (RSRG) scheme. Section 4 describes the two terminal transmission coefficient, while Section 5 provides a critical discussion on the evolution of the parameter space under the RSRG scheme and its relation with the extendedness of the wave function. In Section 6 we briefly point out a triplet of other geometries which are less restrictive compared to the ones discussed here, and in Section 7 we draw our conclusion.

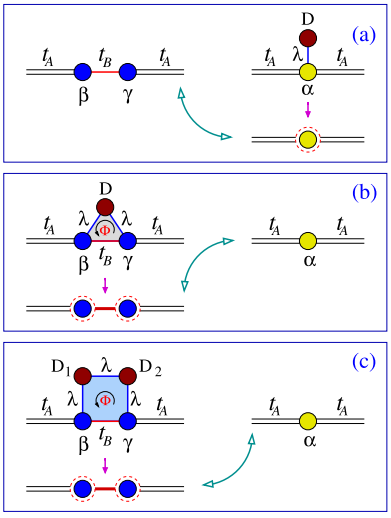

Fig. 1. (Color online.) Building blocks of the quasi-one-dimensional lattices described in the text. In each case the backbone is a linear array of two kinds of bonds A (double line) and B (red single line), such that a B-bond is always flanked by two A-bonds on either side. The atomic sites on the backbone are marked as α, β and γ as described in the picture. The hooping integrals are appropriately described by t_A and t_B. (a) A QD (D) is locally connected to the α-site. This D–α cluster is "renormalized" into an effective site (yellow circle surrounded by red dotted lines). (b) A QD (D) is non-locally coupled to the β–γ pair. The D–β–γ cluster is then renormalized into the immediate lower geometry, pointed by the arrow. (c) The QDs D_1 and D_2 exhibit a mixed connection to β–γ pair. The block β–D_1–D_2–γ is renormalized to the diatomic molecule shown by the arrowhead. In every case, the linear chain (disordered or quasiperiodic) is formed by arranging the cluster linked by the bent cyan double arrowheads in the desired order.

2. The model

We refer the reader to Fig. 1 where the basic structural units are displayed. The backbone in each case is an infinite array of a single (red) bond B and a double bond A. We shall restrict ourselves to a geometry where the single 'B' bonds do not come pairwise. Thus we have a kind of 'anti-RDM' here. This is not always needed though, as will be discussed in the concluding section.

Three cases are separately discussed. The simplest one is that of a local connection (LC), where a single QD (marked as D in Fig. 1(a) is tunnel-coupled to a site α flanked by two A-bonds. The second case discusses a non-local connection (NLC), where a QD (D) is tunnel-coupled to both the sites residing at the extremities (β and γ in Fig. 1(b)) of a B-bond. The final geometry describes a mixed connection (MC), where two inter-coupled QDs D_1 and D_2 are connected to the extremities of a B-bond (i.e. to β and γ sites) as shown in Fig. 1(c). In the two latter cases a uniform magnetic field is applied in a direction perpendicular to the plane of every closed loop. The system in each case is described by a tight-binding Hamiltonian.

We show that, for a particular algebraic relationship between the nearest-neighbor hopping integrals t_{ij} along the backbone and the backbone-QD coupling λ, the infinite topologically disordered or quasiperiodic chain of scatterers yields absolutely continuous energy bands in the spectrum. In the case of LC (Fig. 1(a)) there will be two continuous subbands. In the NLC and MC cases (Figs. 1(b) and 1(c)) a single absolutely continuous band spans the entire energy spectrum when, in addition to the algebraic rela-