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Engineering flat electronic bands in quasiperiodic and fractal loop geometries

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ABSTRACT

Exact construction of one electron eigenstates with flat, non-dispersive bands, and localized over clusters of various sizes is reported for a class of quasi-one-dimensional looped networks. Quasiperiodic Fibonacci and Berker fractal geometries are embedded in the arms of the loop threaded by a uniform magnetic flux. We work out an analytical scheme to unravel the localized single particle states pinned at various atomic sites or over clusters of them. The magnetic field is varied to control, in a subtle way, the extent of localization and the location of the flat band states in energy space. In addition to this we show that an appropriate tuning of the field can lead to a re-entrant behavior of the effective mass of the electron in a band, with a periodic flip in its sign.

Geometrically frustrated lattices (GFLs) supporting flat, dispersionless bands in their energy spectrum with macroscopically degenerate eigenstates have drawn great interest in recent times [1–8]. Initial interest in antiferromagnetic Heisenberg model on frustrated lattices [9–14] has evolved into extensive studies of the gapped flat band states to gapless chiral modes in graphenes [15], in optical lattices of ultracold atoms [16], waveguide arrays [17], or in microcavities having exciton-polaritons [18]. The quenched kinetic energy of an electron in a flat band state (FBS) leads to the possibility of achieving strongly correlated electronic states, topologically ordered phases, such as the lattice versions of fractional quantum Hall states [19]. Recently, the controlled growth of artificial lattices with complications such as in the kagome class has added excitement to such studies [20,21].

Spinless fermions are easily trapped in flat bands [6]. The non-dispersive character of the energy (E)–wave vector (k) curve implies an infinite *effective mass* of the electron, leading to practically its *immobility* in the lattice. Such states are therefore strictly localized either on special sets of vertices, or in a finite cluster of atomic sites spanning finite areas of the underlying lattice. Recently it has been shown that an infinity of such cluster-localized single particle states can be exactly constructed even in a class of deterministic fractals [22]. Apart from its interest in direct relation to the study of GFLs, this work provides an example where eigenvalues corresponding to localized eigenstates in an infinite fractal geometry can be exactly evaluated, a task that is a non-trivial one if one remembers that these fractal systems are free from translational invariance of any kind.

In this communication we unravel and analyze groups of flat, dispersionless energy bands in some tailor made GFLs. The lattices display an interesting competition between long range translational order along the horizontal ($x-$) axis and an aperiodic growth in the transverse directions. In each case, the skeleton is an infinite array of diamond shaped networks (Fig. 1(a)) where hierarchical structures, grown deterministically, are embedded in each arm of the diamond. A uniform magnetic flux threads each elementary plaquette, as will be illustrated in appropriate cases. The motivation behind the present study is two-fold.

First, exploiting the self-similar growth of the hierarchical structures we can implement a real space renormalization group (RSRG) scheme to evaluate the *pinned*, flat band states (FBS) exactly. In all the cases we discuss in this paper the flat band states merge with the localized eigenstates of the infinite hierarchical geometry as higher and higher generations of them are embedded in the arms of the underlying diamonds. Thus, once again, the problem of an exact evaluation of localized states in a fractal geometry is, at least partially, solved.

Second, and a more important aspect of the problem is to look for a possible coexistence of a multitude of dispersive and non-dispersive energy bands in a periodic array of the elementary building blocks. As an arm of the elementary diamond hosts a quasi-periodic or a deterministic fractal of sequentially increasing generation, the flat, dispersive bands are likely get densely packed

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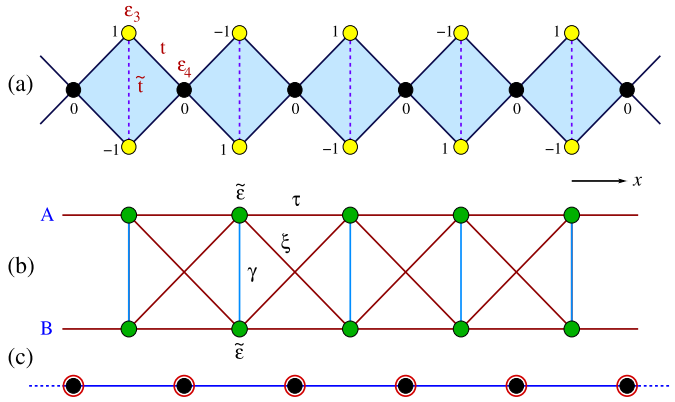

Fig. 1. (Color online.) (a) A typical realization of an elementary array of diamond shaped quadruplets exhibiting a single flat, dispersionless band at $E = 0$, (b) its renormalization into an effective two-arm ladder network with energy dependent potential and nearest and next nearest neighbor interactions and (c) the effective one-dimensional chain obtained after decimating out the top (yellow colored) vertices.

in an environment of dispersive ones. The density of packing may even lead, for a large enough generation of the hierarchical structure, to a re-entrant *dispersive to non-dispersive crossover* in the behavior of the electrons. A recent inspiring work by Danieli et al. [8] has shown that a quasiperiodically modulated flat band geometry may even allow for a precise engineering of the mobility edges.

In addition to this, we anticipate that, a variation in the strength of the magnetic field can lead to a tuning of the curvature of the energy dispersion curves. We can thus achieve a comprehensive control over the group velocity and effective mass of the electron with the help of an external field. Knowing that, a deterministic quasiperiodic or fractal geometry normally offers a completely fragmented, Cantor set-like energy spectrum, this latter study may allow us to control the effective mass of the electron using an external agent such as the magnetic field over arbitrarily small scales of the energy or, equivalently, the wave vector.

We present here a simple analytical method to detect the sharply localized eigenstates that are *pinned* on certain atoms or atomic clusters in a periodic array of diamonds. The non-dispersive character of such states is explicitly worked out. The method is then extended to unravel the entire set of such FBS when each arm of an elementary diamond hosts a quasiperiodic lattice grown according to a deterministic Fibonacci sequence [23], and Berker [24] geometry. Such aperiodic structures with sequentially increasing hierarchy are embedded in the diamond's arm. We indeed find that, as one gradually increases the degree of aperiodicity in the arms, the *pinned* FBS in such periodic approximants turn out to be the localized eigenstates of the systems in their respective thermodynamic limits.

In addition, we observe that, with a deterministic aperiodic geometry of sufficiently large generation embedded in the arms of a diamond array, the interplay of periodicity along the x-axis and the aperiodic order in the transverse directions, produces a highly complex dispersion pattern. The flat, dispersionless bands densely fill the gaps between the dispersive ones, giving rise to the possibility of a quasi-continuous crossover between them as the aperiodic components grow in hierarchy.

The magnetic field piercing the elementary plaquettes in each case is shown to control the group velocity of the electrons, making them more and more immobile as the flux $\Phi \to \Phi_0/2$, where $\Phi_0 = hc/e$ is the fundamental flux quantum. This is an exemplary case of *extreme localization* induced by the magnetic flux as discussed by Vidal and co-workers [11–13]. The magnetic field is shown to flip the sign of the effective mass multiple times within a single Brillouin zone – a remarkable contrast to the ordinary periodic linear lattice. The electron–lattice interaction thus can be fine-tuned from outside by selective choice of the flux threading a plaquette.

In what follows, we present our results. In Section 1 we work out the basic method of analyzing the FBS in an elementary diamond array, and compare the result with the existing ones. Section 2 deals with the Fibonacci-diamond chain, and in Section 3 we elaborately discuss the fractal-diamond networks. In Section 4 we explicitly discuss the generic diamond loop-array where a magnetic field controls the effective mass of the electron making its sign periodically flipped. In Section 5 we draw our conclusions.

1. The Hamiltonian and the pinned eigenstates

We refer to Fig. 1. Spinless, non-interacting electrons are described using a tight-binding Hamiltonian in the Wannier basis, viz.,

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle ij \rangle} t_{ij} \left[c_i^\dagger c_j + h.c. \right] \tag{1}$$

where, ϵ_i is the on-site potential and can assume values equal to ϵ_3 or ϵ_4 depending on the site at the vertex having a coordination number $z = 3$ (yellow circles), or in the bulk, having a coordination number $z = 4$ (black circles). Throughout this paper we shall choose $\epsilon_3 = \epsilon_4$ just to see the effect of the topology of the lattice alone. However, the symbols will be in use to facilitate any discussion. The nearest neighbor hopping integral $t_{ij} = t$ along the arm of the diamond, and $t_{ij} = \tilde{t}$ along the diagonal connecting the vertices with coordination number two. The Schrödinger equation, written equivalently in the form of the difference equation,

$$(E - \epsilon_i)\psi_i = \sum_j t_{ij}\psi_j \tag{2}$$

allows us to decimate out the "black" vertices of the diamond network to map the original array on to an effective two-arm ladder (Fig. 1(b)) (with arms marked A and B) comprising identical (green colored) atomic sites with renormalized on-site potential $\tilde{\epsilon} = \epsilon_3 + 2t^2/(E - \epsilon_4)$. The renormalized hopping integral along the arm of the ladder now becomes $\tau = t^2/(E - \epsilon_4)$, and the inter-arm hopping becomes $\gamma = \tilde{t} + 2t^2/(E - \epsilon_4)$. The decimation generates a second neighbor hopping (brown line) inside a unit plaquette of the ladder and along the diagonal, viz., $\xi = t^2/(E - \epsilon_4)$.

The difference equation for the ladder network may now be cast using 2×2 matrices, in the form [25]:

$$\left[\begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} - \begin{pmatrix} \tilde{\epsilon} & \gamma \\ \gamma & \tilde{\epsilon} \end{pmatrix} \right] \begin{pmatrix} \psi_{n,A} \\ \psi_{n,B} \end{pmatrix} = \begin{pmatrix} \tau & \xi \\ \xi & \tau \end{pmatrix} \begin{pmatrix} \psi_{n+1,A} \\ \psi_{n+1,B} \end{pmatrix} + \begin{pmatrix} \tau & \xi \\ \xi & \tau \end{pmatrix} \begin{pmatrix} \psi_{n-1,A} \\ \psi_{n-1,B} \end{pmatrix} \tag{3}$$

It is easy to check that both the 'potential matrix' (comprising $\tilde{\epsilon}$ and γ) and the 'hopping matrix' (with τ and ξ) commute, and hence can be simultaneously diagonalized by a similarity transform. Eq. (3) can then be easily decoupled, in a new basis defined by $\phi_n = \mathbf{M}^{-1}\psi_n$. The matrix $\mathbf{M}$ diagonalizes both the 'potential' and the 'hopping' matrices. The decoupled set of equations are free from any 'cross terms' and reads, in terms of the original on-site potentials and hopping integrals, as:

$$\left[E - \left(\epsilon_3 + \tilde{t} + \frac{4t^2}{E - \epsilon_4} \right) \right] \phi_{n,A} = \frac{2t^2}{E - \epsilon_4} (\phi_{n+1,A} + \phi_{n-1,A})$$
$$(E - \epsilon_3 + \tilde{t})\phi_{n,B} = 0 \tag{4}$$

The first equation represents a periodic array of identical atomic sites with renormalized on-site potential $\epsilon_3 + \tilde{t} + 4t^2/(E - \epsilon_4)$, and nearest neighbor hopping integral $2t^2/(E - \epsilon_4)$. The second