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Electrons and Phonons on the Square Fibonacci Tiling

RONI ILAN, EDO LIBERTY, SHAHAR EVEN-DAR MANDEL, and RON LIFSHITZ

School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel

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We study the Schrödinger equation for an off-diagonal tight-binding hamiltonian, as well as the equations of motion for out-of-plane vibrations on the separable square Fibonacci quasicrystal. We discuss the nature of the spectra and wave functions of the solutions.

Keywords Separable quasicrystals; electronic spectrum; phonon spectrum; square Fibonacci tiling

1. Separable Quasicrystal Models

Much research has been conducted on the properties of excitations in quasicrystals, ever since the early interest in this question [1] and up to this day [2]. Many exact results have been found for 1-dimensional ($1d$) quasicrystals, yet the properties of excitations in $2d$ and $3d$ quasicrystals are known to a much lesser degree. Furthermore, the different models that have been mostly studied—such as $1d$ chains, the standard decagonal, octagonal, and icosahedral tilings, or actual structural models of real quasicrystals—do not allow one to easily focus on the dimensional dependence of the physical properties of quasicrystals, though some interesting heuristic arguments have been given by Sire [3].

One of us [4] has recently studied the geometric properties and calculated the diffraction pattern of the square and cubic Fibonacci tilings, suggesting that they be used as models for $2d$ and $3d$ quasicrystals (with obvious generalization to any higher dimension). The advantage of these prototypical models of d-dimensional quasicrystals is that they are separable—certain problems, such as the eigenvalue problems studied here, can be decomposed into d separate one-dimensional problems, yielding straightforward solutions, while allowing directly to focus on the effect of dimensionality on the problem being studied. The most apparent disadvantage of these models is that they do not occur in "real" quasicrystals, yet they should not be dismissed as irrelevant because they can be artificially constructed using, for example, conducting nanowires, coupled nanomechanical resonators, or photonic quasicrystals.

The square Fibonacci tiling is constructed by taking two identical grids—each consisting of an infinite set of lines whose inter-line spacings follow the well-known Fibonacci sequence of short (S) and long (L) distances—and superimposing them at a 90° angle, as shown in Fig. 1. This construction can be generalized, of course, to any quasiperiodic

Address correspondence to Roni Ilan, School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978 Israel. E-mail: ronlif@post.tau.ac.il

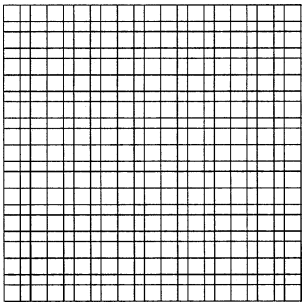

FIGURE 1 A section of the square Fibonacci tiling.

sequence as well as to higher dimensions. If the original $1d$ sequence has inversion symmetry the generated $2d$ and $3d$ quasicrystals will have square and cubic point group symmetry, respectively.

2. Electrons and (Scalar) Phonons

Here we take advantage of the separability of the square (and cubic) Fibonacci tilings to study two problems: (1) The tight binding hamiltonian with zero onsite energy and hopping amplitudes t for vertices connected by long (L) edges, 1 for vertices connected by short (S) edges, and zero for vertices that are not connected by edges; and (2) The normal modes of out-of-plane vibrations of a network of unit masses connected by springs according to the square Fibonacci tiling, with spring constants k for long edges, and 1 for short edges.

The 2-dimensional Schrödinger equation for the connected-neighbor tightbinding hamiltonian is given by

$$\begin{aligned} &t_{n+1}\Psi(n+1,m) + t_n\Psi(n-1,m) \\ &\quad + t_{m+1}\Psi(n,m+1) + t_m\Psi(n,m-1) = E\Psi(n,m), \end{aligned} \tag{1}$$

where $\Psi(n,m)$ is the value of a $2d$ eigenfunction on a vertex labeled by the two integers n and m, and E is the corresponding eigenvalue. The hopping amplitudes t_j are equal to 1 or t according to the Fibonacci tiling as described above. The equations of motion for the network of springs is obtained from the Schrödinger equation (1) by replacing t_j by the spring constant k_j , replacing E by $(k_{n+1} + k_n + k_{m+1} + k_m) - \omega^2$, where ω is the normal frequency, and viewing $\Psi(n,m)$ as the out-of-plane displacement of the (n,m) vertex. The generalization of Eq. (1) to three or any higher dimension is obvious.

With no additional assumptions other than the absence of diagonal hopping or diagonal springs this 2-dimensional eigenvalue problem, as well as its higher dimensional versions, are all separable. Two-dimensional eigenfunctions can be expressed as products

$$\Psi_{ij}(n,m) = \Psi_i(n)\Psi_j(m), \tag{2}$$

with eigenvalues

$$E_{ij} = E_i + E_j, \quad \text{or} \quad \omega_{ij}^2 = \omega_i^2 + \omega_j^2, \tag{3}$$

where $\Psi_i(n)$ and $\Psi_j(n)$ are two of the eigenfunctions of the corresponding $1d$ eigenvalue equation on the Fibonacci chain, with eigenvalues E_i and E_j or ω_i^2 and ω_j^2 , respectively.

Separable quasiperiodic hamiltonians have been studied on such models in the past [5], mainly focusing on square or cubic periodic lattices with constant hopping amplitudes (or springs) and on-site energies (or masses) that follow the same quasiperiodic sequence in all directions. These so-called "diagonal" models are separable if one requires the on-site energies (or masses) to be of the form $V(n, m, \ldots) = V_x(n) + V_y(m) + \ldots$, in which case they have solutions as above.

3. Adding Energies

When solving the $1d$ tight-binding problem using the standard methods of transfer matrices and trace maps [1] one finds for any t that the nth approximant, with F_n atoms per unit cell, has a spectrum containing F_n continuous bands, where F_n is the nth Fibonacci number. As n increases and the quasicrystal is approached, the bands become narrower, and in the limit $n \to \infty$ the spectrum becomes singular-continuous, containing a Cantor-like set of points whose total bandwidth (Lebesgue measure) is zero. Figures 2(a–c) show these bands for

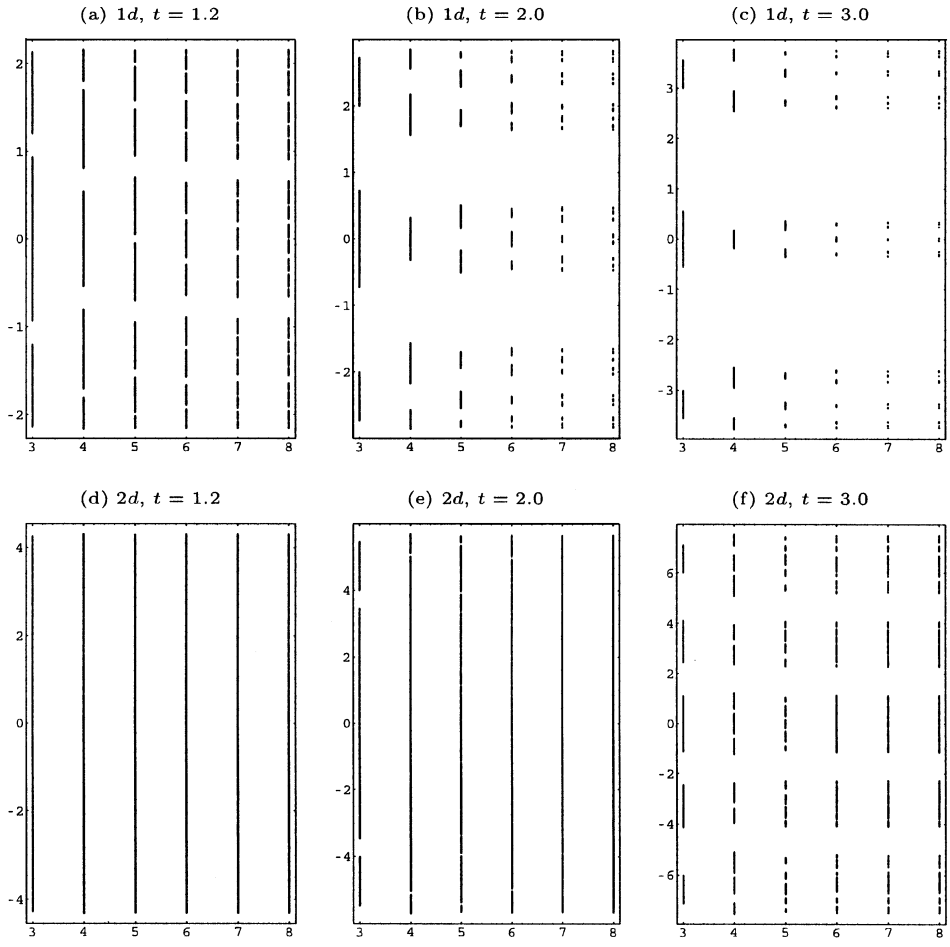

FIGURE 2 Energy spectra of the first few $1d$ and $2d$ approximants with $t = 1.2$, 2.0, and 3.0. In (a–c) the number of bands for the 3rd to the 8th approximants are 3, 5, 8, 13, 21, and 34. In (d) there is a single band for all approximants; in (e) the number of bands are 3, 3, 9, 13, 19, and 31; and in (f) there are 5, 13, 23, 47, 87, and 213 bands.

the first few approximants for three values of the parameter t. One sees that as t increases away from the periodic ($t = 1$) structure the gaps that are formed become increasingly wider.

When adding two such spectra as in Eq. (3) we first note that due to the degeneracy of $E_{ij} = E_{ji}$ the maximum number of bands for the nth approximant, if there is no overlap at all, is $F_n(F_n + 1)/2$. The degree of overlap depends on t. We find three distinct behaviors which can be described qualitatively as follows:

(1) For large enough t the gaps in the $1d$ spectrum are sufficiently wide such that the $2d$ spectrum contains well separated bands (Fig. 2(f)). As n increases the total number of bands increases and in the limit $n \to \infty$ the $2d$ spectrum becomes singular-continuous with zero total bandwidth.
(2) For t close to 1, gaps in the $1d$ spectrum are suficiently small such that the $2d$ bands greatly overlap, forming a single or a few bands even in the $n \to \infty$ limit [Fig. 2(d)]. The spectrum of the $2d$ quasicrystal is therefore absolutely continuous.
(3) For intermediate t a peculiar situation exists (observed also in the diagonal models [5]) where even though the total number of bands increases with n the total integrated bandwidth tends to a finite value (Fig. 2(e)). It is not clear to us at this point whether the spectrum of the $2d$ quasicrystal in this case contains an absolutely continuous part or whether it remains singular-continuous as in $1d$.

Clearly, the transitions betw een the different behaviors are pushed to higher values of t as the dimension increases and additional $1d$ spectra are added. We shall provide elsewhere a detailed analysis of the phase diagram of this system as a function of t and dimension. We shall also describe the differences between electrons and phonons.

4. Multiplying Wave Functions

An intriguing paradox arises in light of the discussion above. Since for any t the $1d$ spectrum is singular-continuous, all $1d$ eigenfunctions $\psi_i(n)$ are critical, decaying as a power laws from different points n_0. Any product of two such functions, as in Eq. (2), must be critical on the $2d$ quasicrystal as well, yet we have observed that for t close to 1 the spectrum is continuous, implying that the wave functions must be extended.

We would like to conjecture that the resolution of this paradox stems from the high degeneracy of each eigenvalue when bands overlap and merge into one as in Fig. 2(d). In general, many different pairs of $1d$ eigenvalues E_i and E_j may add up to the same $2d$ eigenvalue E. Each eigenfunction $\Psi_{ij}(n, m)$ with eigenvalue E is critical, all peaked at different points (n_0, m_0) on the $2d$ quasicrystal, with substantial overlap due to their slow spatial decay. It is plausible that one could construct linear combinations of these critical eigenfunctions that are extended over the whole infinite quasicrystal. We intend to investigate this conjecture in the near future.

To support our conjecture, we conclude by showing that for any value of t the eigenfunctions with energy $E = 0$ are extended over the $2d$ quasicrystal. First recall that for any $1d$ eigenfunction $\Psi_i(n)$ with energy E_i, the function $(-1)^m \psi_i(m)$ is a $1d$ eigenfunction with energy $-E_i$. Therefore, $\Psi_i(n, m) = (-1)^m \psi_i(n)\psi_i(m)$ is a $2d$ eigenfunction with energy $E = 0$. Thus, for the nth approximant, the energy $E = 0$ is F_n-fold degenerate (a similar situation arises for the labyrinth tiling [6]). Since the $1d$ eigenfunctions form a complete set that spans all functions on the Fibonacci chain, one can perform a change of basis to an alternative complete set $\phi_j(n) = \sum_i c_{ji}\psi_i(n)$ whose members are all extended. The $2d$ eigenfunctions $\Phi_j(n, m) = (-1)^m \phi_j(n)\phi_j(m)$, all with energy $E = 0$ are extended over the whole $2d$ quasicrystal.

We should conclude with a cautionary remark that all our conclusions rely on the fact that the behavior for finite $2d$ approximants survives in the infinite limit. This is not obvious until proven rigorously as in $1d$.

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