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Electronic properties of the octagonal tiling: a new renormalization-group calculation

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Abstract. — We present a new renormalization-group calculation of the octagonal tiling excitation spectrum. Two new self-similar octagonal tilings are introduced, a triangle-kite and a triangle-dart tiling, which are entangled with the standard rhombus-square tiling. The decimation procedure involved in the renormalization group calculation transforms each tiling onto a different one and goes back to the (rescaled) original tiling after three steps. The local and average density of states are calculated. In the case of a Laplacian-like tight-binding Hamiltonian, on the standard rhombus-square octagonal tiling, our results compare reasonably well to numerically derived spectra and improve some previous renormalization group calculations. In the pure hopping case, the renormalization is shown to be inaccurate by comparing to numerical density of states obtained by a continued fraction method.

1. Introduction.

There has been much interest in quasiperiodic systems since the discovery of quasicrystals [1]. Considerable effort has been devoted to the understanding of electronic behavior in such structures, intermediate between periodic and random. The kind of long range order (quasiperiodicity) that is nevertheless present has not yet allowed for a simplified framework like, for instance, the one that Bloch theorem and k-space calculations provide in the presence of translational symmetry. However, some quasiperiodic tilings present inflation-deflation symmetries that permit real-space renormalization-group (RSRG) methods to be applied.

For 1D quasiperiodic lattices, several skillful and powerful RSRG approaches have been developed in order to investigate the electronic properties. The most influential method is the dynamical-map method introduced by Kohmoto, Kadanoff and Tang [2], and independently by Ostlund et al. [3], which associates the energy spectrum of an infinite 1D quasiperiodic structure to a trace map and a map invariant of periodic systems (approximants) which are successively constructed according to well known inflation rules. Another widely used RSRG method is the real-space decimation methods developed by several groups [4-7]. All these methods, which are exact in one dimension, have provided a very detailed knowledge of the spectral properties, in terms of the nature of the spectrum and of the eigenfunctions (for a recent review, see [24]).
In comparison with the 1-dimensional systems, much fewer work has been devoted to the electronic properties of 2D quasiperiodic tilings [8-14], and, owing to their complexity, most of it has been purely numerical. Detailed investigations [9, 10] showed that the rhombus tilings (ten-fold symmetric Penrose and octagonal tilings) pure hopping spectrum have a central peak which is a delta function associated with a special kind of localized state, i.e., the confined state. In the Penrose case, two finite gaps separate this peak from the rest of the spectrum, while there is no numerical evidence for gaps surrounding this central peak in octagonal tilings.

In addition to these numerical calculations, RSRG approaches [13, 14] have been proposed for these 2D-structures. The problem in using RSRG decimation methods in 2D comes from the difficulty in getting a compact renormalization group. The latter is obtained by neglecting some interactions upon renormalization, which leads therefore to approximated spectra. The first RSRG scheme for 2D quasiperiodic lattice was proposed by Sire and Bellissard [13] for the quasiperiodic octagonal tiling (paved by rhombus and square as basic tiles) on the basis of the Schur formula for calculating the renormalized Hamiltonian on the decimated structure. These authors calculate the support of the spectrum for a tight binding Hamiltonian which includes a hopping term between neighbors and a diagonal term proportional to the site coordination number. It is possible to weight the diagonal and off-diagonal contributions and for instance interpolate between a « molecular » level situation and a Laplacian-like model. Another RSRG decimation approach was then developed, which uses a more elaborate decimation and calculate the local density of states (LDOS) of Penrose tiling [14].

In this paper we follow the latter method and calculate the octagonal tiling density of states. While in the previous calculation on this tiling [13], the decimation proceeded in one step from the tiling to its deflated scaled version, here it takes three successive steps with only one kind of sites being eliminated at each step. The two intermediate steps correspond to eight-fold symmetric quasiperiodic point sets. By consistently defining edges in these point sets, they give rise to two new tilings, the Triangle-Dart (TD) and Triangle-Kite (TK) octagonal tilings. The standard octagonal tiling is hereafter called the Rhombus-Square (RS) tiling. Our result improve upon the previous ones in that the full expected spectrum is recovered in the « molecular » level limit (while one branch was missing near $E = 7$ in Ref. [13]), and also because the total band width is also better approached in the Laplacian-like case. In addition the DOS and LDOS are calculated and the pure hopping case is considered. This paper is organized as follows. In section 2, the three octagonal tilings are presented and their mutual transformations analyzed. The RSRG approach is described in section 3. In section 4, the calculated spectra are given, along with a discussion.

2. Self-similar entangled octagonal sets.

The well-known RS octagonal tiling [15, 16] and its acceptance zone are presented in figures 1a and 1b. According to the acceptance zone description, the RS sites can be classified into seven types corresponding to different local environments. The seven types of sites, i.e., c, s, p, q, m, r and e, which are displayed in figure 1c have the frequency $n_c = \omega$, $n_s = 2 \omega^2$, $n_p = \omega^3$, $n_q = \omega^4$, $n_m = 2 \omega^5$, $n_r = \omega^6$ and $n_e = \omega^7$ with $\omega = \sqrt{2} - 1$.

The RS octagonal tiling presents a well-known self-similar property. Removing c, s, and q types of sites and joining the remaining sites with new edges, one obtains a new RS octagonal lattice with a rescaled factor $\lambda = 1 + \sqrt{2}$. This is exactly the decimation that was done in one step in reference [13]. Here, we first remove type c sites and add new edges on the long diagonal of the original RS rhombi. This immediately gives a new lattice made of two different tiles, a triangle and a kite (Fig. 2a). This new tiling is still eight-fold symmetric (its acceptance zone has an eight-fold symmetric star shape) and is called the TK tiling. Its seven types of sites are illustrated in figure 2b.
We now eliminate sites of types 6 and 7 in the TK tiling. Note that those sites correspond to the original « s » sites of the RS tiling. After proper edge addition, a new tiling is defined which is composed of basic triangles and darts. It is called the TD octagonal tiling (Fig. 3a) and its eight types of sites are displayed in figure 3b. It is easy to see that after removing the type 8 sites in the TD tiling, one finally obtains the RS tiling with a rescaled factor \( \lambda \). The type 8 sites in the TD tiling correspond to the type q sites of the original RS tiling. So one can see that for an RS octagonal tiling, if we remove c type, s type, and q type sites successively, we obtain a TK, TD and finally a rescaled RS tiling. In the following we shall
Fig. 2. — The Triangle-Kite tiling: a) a piece of the tiling, b) the seven types of sites with their local environment.

Also denote TK, TD, and RS the decimations which transform the RS, TK, and TD point sets into the TK, TD, and RS point sets, respectively. These three transformations will be used to derive a (approximate) compact renormalization group to study the electronic properties of these octagonal tilings. Note the important following point: for these intermediate tilings, the hopping terms of the Hamiltonians are not restricted to be along the edges that define the tiles. More complex interactions are generated upon renormalization, and will be given below.
Fig. 3. — The Triangle-Dart tiling. a) A piece of the tiling; b) the eight types of sites with their local environment.
3. Renormalization group for octagonal tilings.

We consider the following general tight-binding Hamiltonian:

\[ H = \sum_i \epsilon_i |i\rangle \langle i| + \sum_{ij} \nu_{ij} |i\rangle \langle j| \]  

(1)

where \( \epsilon_i \) is the site energy and \( \nu_{ij} \) is the hopping integral between sites \( i \) and \( j \). The Green function \( G(H) \) is defined as

\[ (Z - H) G(H) = I \quad \text{with} \quad Z = E + i\eta \]  

(2)

The sites of the original lattice are called of type 1 or 2 corresponding respectively to those sites being kept and those being decimated. After decimation, one has

\[ (Z - H_{11}') G_{11}(H_{11}') = I \]  

(3)

where \( H_{11}' \) is the renormalized Hamiltonian for the new set composed of only type 1 sites, which is given by

\[ H_{11}' = H_{11} + H_{12}(Z - H_{22})^{-1} H_{21} \]  

(4)

In order to calculate the DOS, we use the generating function formalism introduced by Tremblay and Southern [17], and proved to be useful for self-similar and quasiperiodic structures [18-20]. Let us define the generating function by

\[ F(H) = 2 \ln \left( \int_{-\infty}^{\infty} \prod_i \left[ \exp \left( \sum_j \nu_j \right) \right] \right) \]  

(5)

where \( U^T = (u_1, u_2, \ldots, u_\nu) \) and \( u_j \) are continuous variables defined on the sites. Successive decimation gives

\[ F(H) = -\sum_{k=1}^{\kappa_{\text{max}}} \ln \left\{ \det (Z - H_{22}^{(k)}) \right\} + \text{constant} \]  

(6)

in which \( \kappa \) denotes that the corresponding variables belong to \( k \)-th decimation. Now, the DOS \( \rho(E) \) can be deduced from the derivative of the generating function \( F(H) \)

\[ \rho(E) = -\frac{1}{\pi} \text{Im} \left( \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{\nu} G_{ii} \right) = \lim_{N \to \infty} \frac{1}{N\pi} \frac{\partial \text{Im} (F(H))}{\partial E} \]  

(7)

For 1D quasiperiodic structures, suitable choice of \( H_{22}^{(k)} \) often make \( (Z - H_{22}^{(k)})^{-1} \) and \( \det (Z - H_{22}^{(k)}) \) exactly solvable and hence give the LDOS and DOS. However, in the 2D case, even though one chooses an \( H_{22}^{(k)} \) corresponding to solvable small clusters, the successive decimations make the treatment of \( H_{22}^{(k)} \) as difficult as that of the original Hamiltonian because of the increasing number of the parameters in the Hamiltonian of the renormalized structures. Some approximations have to be made in order to get a compact renormalization group, such that the number of parameters remains constant under decimation. Usually \( H_{22}^{(k)} \) is approximated by a local Hamiltonian constructed on small clusters whose mutual interactions are ignored [13].

In the octagonal case, we use the three above transformations TK, TD and RS in order to generate the renormalization. To obtain the RSRG transformations equations, let us first
construct the Hamiltonian for the different structures. We assume that different types of sites have different site energies. For the RS octagonal lattice, the seven kinds of site energies are \( \{ t_1, t_2, t_3, t_4, t_5, t_6, t_7 \} \) corresponding to seven types of sites, c, s, p, q, m, r, and e. The site energies of the TK and TD tilings take the values \( \{ t_1, t_2, t_3, t_4, t_5, t_6, t_7 \} \) and \( \{ e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8 \} \), respectively. The three types of hopping integrals \( t_j, \nu, k_j \) in the three tilings, are illustrated in figure 4. In our RSRG, we only consider the contribution of the nearest-neighbor decimated sites to the renormalized site energies. According to equation (4), we obtain the following equations for the TD transformation:

If we define

\[
C = 1/(Z - t_2) \quad p_1 = t_1(1 + 2 t_4 C), \quad p_2 = t_5^2 C \\
p_3 = p_1/(1 - 2 p_2 C), \quad p_4 = 2 p_2^2 C/(1 - 2 p_2 C)
\]

![Fig. 4.](image)

**Fig. 4.** — Definition of the Hamiltonian hopping parameters: a) rhombus-square tiling; b) triangle-kite tiling; c) triangle-dart tiling.
then one gets,
\[ t_1 = t_v + 4t_1^2C + 2p_1p_3C + \frac{2p_3^2C}{1-2(p_2 + p_3)C} \]
\[ t_2 = t_v + 3t_1^2C + \frac{2p_3^2C}{1-3p_2C} \]
\[ t_3 = t_v + 2t_3^2C \]
\[ t_4 = t_p \]
\[ \nu_6 = \nu_1 + 2t_5^2C \]
\[ \nu_5 = \nu_1 + 2t_5^2C \]
\[ \nu_3 = \nu_1 + t_4^2C \]
\[ \nu_4 = \nu_1 + t_4^2C \]
\[ \nu_1 = t_6 + 2t_1t_2C \]
\[ \nu_2 = t_6 + t_1t_2C \]
\[ \nu_3 = t_6 + t_1t_2C \]
\[ \nu_4 = t_6 + t_1t_2C \]
\[ \nu_5 = t_6 + t_1t_2C \]
\[ \nu_6 = t_6 + t_1t_2C \]
\[ \nu_7 = t_6 + t_1t_2C \]
\[ \nu_8 = t_6 + t_1t_2C \]
and
\[ D_m = C^2 - t_5^2 \]
\[ D_1 = C^2 - 2p_2^2 + p_3^2 \]
\[ D_2 = C^2 - 2p_2^2 + p_3^2 \]
\[ F(H_{RS}) = F(H_{TD}) - \mu_n N \ln D_m - \mu_r N \ln D_r - \mu_c N \ln D_c + \text{constant} \]

\( N \) is the number of sites in RS octagonal lattice. In equations (9), \( D_m, D_1, \) and \( D_2 \) are exact determinants associated with the local clusters of c-type sites around sites of type m, r, and e, respectively. In the equation for \( \nu_i \), we have neglected some higher order contributions of \( t_8 \).

Now we perform the TK transformation from TK to TD, i.e., decimate sites of types 6 and 7 in TK tiling (those sites correspond to the s sites in the original RS tiling). Defining \( R = Z - \nu_6 \), \( S = Z - \nu_7 \), the RSRG equations of the TK transformation are given by:
\[ e_1 = e_1 + 8 \nu_1^2R \]
\[ e_2 = e_2 + 6 \nu_1^2R + 2 \nu_2^2S \]
\[ e_3 = e_3 + 4 \nu_1^2(R + S) \]
\[ e_4 = e_4 + 2 \nu_1^2R + 6 \nu_5^2S \]
\[ e_5 = e_5 + 2 \nu_1^2R + 2(\nu_1^2 + \nu_2^2)S \]
\[ e_6 = e_6 + \nu_1^2R + 2 \nu_3^2S + 2 \nu_3^2R \]
\[ e_7 = e_4 + 4 \nu_1^2 \frac{R}{1 - \nu_8 R} \]
\[ e_8 = e_8 + 2 \nu_5^2S \]
\[ k_1 = 2 \nu_1 \nu_4 R \]
\[ k_2 = \nu_1 \nu_4 R \]
\[ k_3 = 2 \nu_1 \nu_6 S \]
\[ k_4 = 2 \nu_1 \nu_6 S \]
\[ k_5 = \nu_1 \nu_4 R + \nu_1 \nu_5 S \]
\[ k_6 = \nu_1 + 2 \nu_3^2 \frac{R}{1 - \nu_8 R} \]
\[ k_7 = \nu_1 + \nu_6 \nu_6 S \]
\[ k_8 = \nu_7 S \]
\[ k_9 = \nu_1^2 R^2 \frac{R}{1 - \nu_8^2 R^2} \]

and
\[ F(H_{TD}) = F(H_{TK}) - \nu_x N \ln D_1^{TD} - 2 \frac{n_c}{A^2} N \ln D_2^{TD} + \text{constant} \]

with
\[ D_1^{TD} = R^2 - \nu_8^2 \]
\[ D_2^{TD} = S^2 \]
where \( \nu = 2 - \sqrt{2} \) is the frequency of rhombi in the RS tiling, and \( D_{1}^{1D} D_{2}^{1D} \) come from the contributions of two-site molecular cluster (6-type of site) and single site (7-type site) (see Fig. 3), respectively.

Finally when the RS transformation is applied to the Tk tiling, a new RS octagonal tiling is obtained with the following renormalized Hamiltonian parameters:

\[
\begin{align*}
\tau' \ &= \ e_7 + k_8 W, \quad \tau' \ &= \ e_6 + 2 k_7 W, \quad \tau_4' \ &= \ e_4 + 3 k_3 W, \quad \tau_4 \ &= \ e_4 + (k_1^2 + 2 k_7^2) W \\
\tau_1' \ &= \ e_1 + 2 k_1 W, \quad \tau_1' \ &= \ e_2 + k_1 W, \quad \tau_0' \ &= \ e_1, \\
t_1' \ &= \ k_1, \quad t_2' \ &= \ k_2 + k_7 k_8 W, \quad t_3' \ &= \ k_5 + k_3 k_7 W \\
t_4' \ &= \ k_4 + 2 k_1 k_7 W, \quad t_5' \ &= \ k_6, \quad t_6' \ &= \ k_6 \\
\end{align*}
\]

where \( W = Z - e_8 \). The generating function for the TK lattice is given by

\[
F (H_{TK}) = F (H_{RS}) - \frac{n_c}{k} \ln W. \tag{13}
\]

Now we have derived a RG from an RS octagonal lattice to a new RS octagonal lattice. If one starts from TK or TD octagonal lattice, the above RSRG transformations can also give the corresponding renormalized parameters for these TK or TD octagonal tilings. Since all these tilings have one special site, with perfect eight-fold point symmetry which survives the whole sequence of decimations, the local density of states at this site can be calculated from the RG equations (8), (10) and (12). Using the recursion relations (9), (11), (13) for the generating function, one can calculate the (average) density of states of the octagonal tiling.

4. Results and discussion.

4.1 LAPLACIAN-LIKE HAMILTONIANS. — We focus the discussion on the excitation spectrum of the RS tiling. Figure 5 shows the support of the spectrum for the Laplacian-like Hamiltonian generated by taking \( \tau = \tau' \), \( t_1 = t_2 = t_3 = t_4 = t \), \( t_5 = t_6 = 0 \), \( 0 < t < 1 \) in which \( z_r = 3, 4, 5, 6, 7, 8 \) is the coordination number of the seven types of sites c, s, p, q, m, e, respectively. The case \( t = 1 \) corresponds to the spectrum of the discrete Laplacian on that tiling. We can see that the present calculation improves the previous one\[13\] in both limits, \( t = 0 \) and

![Fig. 5. — Spectrum of the Laplacian-like Hamiltonian with 0 ≤ t ≤ 1](image-url)
Fig. 6. — Spectrum of the Hamiltonian related to that in figure 5 and discussed in the text.

Fig. 7. — Density of states for the pure hopping model as obtained from the renormalization group: a) average DOS; b) local DOS on the site with 8-fold symmetry.
Indeed, the case \( t = 0 \) corresponds to disconnected sites and one should therefore find a spectrum made of discrete levels equal to the different coordination numbers, with relative degeneracies following the relative occurrence of these different types of sites. While there are few 7-fold coordinated sites, the energy \( E = 7 \) was nevertheless absent of the spectrum in reference [13] when \( t = 0 \), but appears here, with the correct degeneracy. Furthermore, for \( t = 1 \) the exact lower edge of the spectrum is known to be precisely zero; here it falls around 0.4, closer to this exact value. We have also calculated the spectrum of a related Hamiltonian corresponding to \( \{ e_i = (1-t) z_i, \ t_1 = t_2 = t_3 = t_4 = t, \ t_5 = t_6 = 0, \ 0 < t < 1 \} \), shown in figure 6, for the sake of comparison with numerical results [12]. The two spectra agree quite well in the weak hopping range.

4.2 Pure Hopping Models. — Figures 7a and b displays the density of states, total and local, for the pure hopping model \( \{ e_i = 0, \ t_1 = t_2 = t_3 = t_4 = 1, \ t_5 = t_6 = 0 \} \). In this case, numerical calculations on large approximants show a one-band spectrum, without internal gaps. The approximate renormalization, quite reliable in the weak coupling regime, is expected to give only poor results in the present case and, indeed, our calculation gives a quite different spectrum especially in its central part. Note, however, that it is sensitive to the confined states at energy zero, since a peak appears at that energy in the DOS. The fact that this peak does not appear in the 8-fold symmetric site LDOS is also encouraging since it is not expected here because the corresponding wave function vanishes at those sites.

In order to further test our LDOS renormalization calculation, we have numerically calculated the LDOS at an 8-fold site, inside a very large approximant, using a continued fraction [21] (or recursion [22]) method. Figure 8 shows the result for 3 different numbers of continued fraction coefficients. The first curve, figure 8a, corresponds to 20 coefficients, i.e. the LDOS is correct up to the 40-th moment. Note that it agrees with the recent calculation of Jagannathan [23], which used the same number of coefficients. We then push the calculation up to 60 coefficients (Fig. 8b) and finally 120 coefficients (Fig. 8c) (240 exact moments !) to further analyze the effect of the long range quasiperiodic-like order. Note that we took care of having a large enough approximant unit cell in order not to be sensitive to the periodic boundary conditions. A first comment is that it clearly confirms the non-accuracy of the renormalization in the pure hopping case (compare Figs. 7b and 8c !). A second point is that the LDOS is highly non-smooth and intricate, and that there is a marked tendency for the local minima (in the case of a small number of continued fraction coefficients) to give rise to gaps, especially just near \( E = \pm 2 \). This does not mean that the total DOS will have these gaps. Note however that preliminary calculations done on a quite different site (3-fold coordinated) also showed the same tendency. Finally, as far as the confined state at \( E = 0 \) is concerned, we found that it is almost the only spectral region which is sensitive to changing the asymptotic value of the continued fraction coefficient, and in particular we do not get a vanishing LDOS as expected. This suggests that if ever the DOS has a gap separating the delta peak from the rest of the spectrum, as in the Penrose tiling case for example, this gap is certainly very small.

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Fig. 8. — Local density of states for a 8-fold coordinated site as obtained from a continued fraction calculation with varying the number of continued fraction levels: a) 20 levels; b) 60 levels; c) 120 levels.

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