

Density of states and localization of electrons in a tight-binding model on the Penrose tiling

E. S. Zijlstra and T. Janssen

Institute for Theoretical Physics, University of Nijmegen, Toernooiveld, NL-6525 ED Nijmegen, The Netherlands

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The density of states is studied for periodic and open boundary conditions in the vertex model of the Penrose tiling. For one gap in the spectrum the gap labeling is done explicitly. Localization of wave functions is studied by $2p$ norms in a series of approximants for one value of the energy by means of a contour integration in the first Brillouin zone. The results show that a surface can smoothen out a spiky density of states. We find evidence for extended wave functions.

I. INTRODUCTION

Since the discovery of aperiodic crystals, such as quasicrystals, it has been an important issue how quasiperiodicity affects physical properties. Theoretically, efforts have gone into calculating properties of relatively simple model systems with a quasicrystalline structure and into *ab initio* calculations of approximants, crystals with large unit cells that have the same local atomic structure as a quasicrystal. In this paper we present calculations for one of the most frequently used models with quasicrystalline structure, the two-dimensional Penrose tiling with fat and skinny rhombuses. We have restricted ourselves to the so-called vertex model, which is a tight-binding model, where one electronic basis state is positioned on each vertex, and where the edges of the rhombuses represent bonds of equal strength. A few things are exactly known for this model. In the center of the spectrum, at $E=0$, a sharp peak in the density of states is present, which after some confusion^{1,2} was shown to correspond to highly degenerate, strictly localized states^{3,4} with an exact lower bound on their abundance of $81-50\tau \approx 9.83\%$ of all states,^{5,6} where τ is the golden mean, $\tau=(\sqrt{5}+1)/2$. Because of the bipartite property of the Penrose tiling the spectrum is symmetric with respect to $E=0$. Properties for $E \neq 0$ are only approximately known through (i) studies of finite clusters of the Penrose tiling with open or fixed boundary conditions,^{1,3,7-11} (ii) approximate studies of the infinite tiling,¹¹⁻¹³ and (iii) studies of periodic Penrose lattices (PPL's), a special class of approximants of the Penrose tiling. Where the first method requires huge clusters in order to reduce the influence of the surface, which can be looked at as a line of defects, and where the studies of the infinite tiling need simplifying assumptions, of which the validity is not clear, in order to keep the calculations tractable, the third method does not have these disadvantages, for there is no approximation other than a slightly modified structure and no surface is present, since periodic boundary conditions can be used. Contrary to the infinite Penrose tiling, which satisfies matching rules for the skinny and fat rhombuses everywhere, a PPL has two violations of the matching rules per unit cell,¹⁴ from which it follows that the density of mismatches is inversely proportional to the number of sites per unit cell. By considering PPL's with ever larger unit cells the structure of the Penrose tiling can arbitrarily well be approximated. In this paper we study what effects quasiperiodicity may have on the fine structure of the electronic density of states and we

look at localization of wave functions by calculating participation ratios.

In order to obtain the density of states of the Penrose tiling, Rieth and Schreiber¹⁵ diagonalized the vertex model tight-binding Hamiltonian of a PPL with 3571 sites per unit cell with periodic boundary conditions, and evaluated the results as a set of histograms with a resolution $\Delta E = 5 \times 10^{-2}$ in units of the strength of a bond. They concluded that the density of states is irregular and strongly fluctuating, and that this result is not substantially changed when using open boundary conditions. *Ab initio* calculations have shown that realistic models for approximant phases of three-dimensional quasicrystals also have a spiky density of states,¹⁶ with spikes of width 10–20 meV,¹⁷ which are due to densely distributed almost dispersionless bands.¹⁶ The flatness of these bands has been used in combination with Boltzmann transport theory to explain exotic experimentally observed transport properties of quasicrystals,^{17,18} e.g., high zero-temperature electrical resistivity. Based on the observation that the spikes become more dense in higher approximants, Fujiwara and co-workers^{17,19} have argued that in the quasiperiodic limit the density of states is extremely singular with spikes at all energies and of all widths. On the other hand, Hafner and co-workers^{20,21} have pointed out that the amplitude of the fine structure may decrease in the quasiperiodic limit, so that only the most pronounced peaks and (pseudo)gaps remain, a view that is supported by the fact that, with the exception of one tunneling spectroscopy experiment²² of the decagonal quasicrystal $\text{Al}_{73}\text{Ni}_{17}\text{Co}_{10}$, no spikes have been observed.²³⁻²⁵ The following alternative explanations have been brought up for the experimental absence of spikes: (1) Much used techniques, such as photoemission spectroscopy at room temperature or x-ray spectroscopy, have a resolution that is too low to observe spikes.^{24,25} (2) Tunneling experiments, which have a high resolution, probe the surface of a material, which may be in a different, nonquasicrystalline, phase than the bulk.²³ (3) The local density of states of the first few atomic layers of the surface might be smeared out by surface states and surface resonances, since even if the quasicrystalline phase is persistent up to the surface, it is known that details of the density of states in the energy range of 50 meV depend on the atomic order on several inter atomic distances.²³ (4) *Ab initio* calculations and simple model calculations do not take into account the effect of electron scattering, which can

change the density of states on an energy scale of 10–200 meV.²³ (5) Possibly deterministic models like the Penrose tiling do not realistically describe quasicrystals. Instead, in reality, randomness might be present. This idea is supported by Yamamoto and Fujiwara,²⁶ who have calculated the density of states of a PPL with 3571 sites per unit cell with random phason strain, by calculating four \mathbf{k} points in the first Brillouin zone, and then using a very simple estimation for the density of states, assuming that the bands are so flat, that it only matters how they overlap with each other. They found an enormously spiky density of states with many gaps, which disappear when randomness is introduced. In Sec. III it will be shown that this extreme spikiness is probably a result of their calculational method. Nevertheless, the conclusion that randomness can smear out the density of states is probably correct. Still, it is unclear which explanation should be used to understand the absence of spikes in experiments. This paper tries to give a partial answer to this problem by calculating the density of states of the Penrose tiling to an accuracy that is as high as possible, which gives the possibility to check the reasoning of Hafner and co-workers^{20,21} for a concrete case, and by doing a calculation with open boundary conditions, which shows that the presence of an unreconstructed surface can smoothen out the density of states of an approximant.

Nothing is rigorously known about the localization of wave functions in the Penrose tiling, except that there are strictly localized states at $E=0$. Localization properties have, among other methods, been studied by means of $2p$ norms,^{7,15,27} which are a generalization of participation numbers. For a tight-binding eigenstate ψ that is properly normalized, such that $\sum_n |\psi_n|^2 = 1$, where the sum is over all sites in one unit cell of an approximant, the $2p$ norm is defined by

$$\|\psi\|_{2p} \equiv \sum_n |\psi_n|^{2p}, \quad (1)$$

and the generalized participation ratio is defined by

$$p_{2p} \equiv \frac{\|\psi\|_{2p}^{-1/(p-1)}}{N}, \quad (2)$$

where N is the number of sites per unit cell. The generalized participation ratio, which always lies in the interval $[0,1]$, gives an indication of the percentage of sites participating with a substantial amplitude in a wave function. Note that $p=2$ gives the ordinary participation ratio. Considering participation ratios of a series of approximants, and assuming that the same critical wave function $\psi(\mathbf{r}) \propto |\mathbf{r}|^{-\alpha}$, $1/p \leq \alpha < 1$, is approximated ever better for higher approximants, it can be shown that the generalized participation ratio of ψ scales in two dimensions with unit-cell size N as²⁷

$$p_{2p} \propto N^{(1-p\alpha)/(p-1)}. \quad (3)$$

Except for the wave function of the lowest energy in the spectrum, which has been studied separately for PPL's with up to 167 761 sites per unit cell,¹⁵ only the average scaling behavior of groups of wave functions in finite energy intervals has been studied. Agreement was found with Eq. (3), where by using the 8-norm and PPL's of maximally 1364

sites per unit cell an exponent $\frac{3}{8} < \alpha < \frac{5}{8}$ was found,²⁷ and where by using the ordinary participation ratio (the 4-norm) and finite clusters with up to 4000 sites $\alpha \approx 0.55$ was found,¹⁵ which was also found in the above-mentioned study of the wave function of lowest energy.¹⁵ Note that Ref. 27 uses the center model of the Penrose tiling, which is not the vertex model, so that in principle, there is no reason why these results should be the same. In this paper we study the participation ratio and a generalized participation ratio with $p=4$ of PPL's with maximally 64 079 sites per unit cell at fixed energy, without averaging over an energy range, by means of a method that, to our knowledge, is new. We have found that the wave functions at $E=3.0$ eV are probably extended.

This paper is organized as follows. In Sec. II a few comments are made about properties of PPL's and how they can be generated through the cut-and-project formalism. In Sec. III the method and results are given for the density-of-states calculations. Also some comments are made about the numerical convergence of the density of states. The gap labeling of a gap at $E=2.7$ eV is done explicitly. In Sec. IV the method and results are given for the calculation of the participation ratio at fixed energy. We conclude in Sec. V.

II. MODEL

The Penrose tiling can be obtained with the cut-and-project method.²⁸ Approximants are usually generated with the multigrid method,^{14,27} but in this section we give a recipe for obtaining PPL's with the cut-and-project formalism, where the notation of Janssen²⁸ is followed. If in the internal space the vectors $e_n = (\cos \frac{2}{5}\pi n, \sin \frac{2}{5}\pi n)$, $n=0, \dots, 4$ are approximated by

$$\begin{aligned} e_0 &= (1, 0), \\ e_1 &= \left(\frac{\tau_1 - 1}{2}, \sin \frac{2}{5}\pi n \right), \\ e_2 &= \left(-\frac{\tau_1}{2}, (\tau_2 - 1) \sin \frac{2}{5}\pi n \right), \\ e_3 &= \left(-\frac{\tau_1}{2}, (1 - \tau_3) \sin \frac{2}{5}\pi n \right), \\ e_4 &= \left(\frac{\tau_1 - 1}{2}, (\tau_3 - \tau_2 - 1) \sin \frac{2}{5}\pi n \right), \end{aligned} \quad (4)$$

where $\tau_1 = (F_{n+2} + F_n)/(F_{n+1} + F_{n-1})$, $\tau_2 = (F_{n-1} + F_{n-3})/(F_n + F_{n-2})$, and $\tau_3 = 1 + (F_{n-1}/F_{n+1})(F_{2n}/F_{2n-1})$, with F_i Fibonacci numbers, $F_0=0$, $F_1=1$, $F_{i+1}=F_i+F_{i-1}$, and if $\gamma_i=0$, $i=0, \dots, 4$, then an approximant of the Penrose pattern is obtained with a unit cell that has the shape of a fat rhombus and $F_{2n+3} + F_{2n+1}$ vertices per unit cell, and that has mirror symmetry in the short diagonal of its unit cell. If $\tau_2 = 1 + (F_{n+1}/F_{n-1})(F_n + F_{n-2})/(F_{n+3} + F_{n+1})$, and $\tau_3 = (F_{n+4} + F_{n+2})/(F_{n+3} + F_{n+1})$, and τ_1 is the same as above, an approximant is obtained with a unit cell that has the shape of a skinny rhombus, and $F_{2n+4} + F_{2n+2}$ vertices per unit cell, and that has mirror symmetry in the long diagonal of its unit cell. These

TABLE I. Number of subdiagonals N_{sub} of H_{even}^2 for various approximants after permutation.

N	N_{even}	N_{sub}
1 364	646	72
2 207	1 082	115
3 571	1 726	116
5 778	2 853	121
9 349	4 577	190
15 127	7 504	192
24 476	12 079	315
39 603	19 704	301
64 079	31 781	498

approximants are called periodic Penrose lattices, and they are special because they violate the matching rules of the Penrose tiling minimally.¹⁴

In the vertex model, vertices correspond to atoms with one electronic basis state and edges of the tiles correspond to bonds of equal strength. To indicate orders of magnitude, we choose an edge to have a length of 2 \AA , and the corresponding bonds to have a strength of 1 eV .

III. DENSITY OF STATES

Because of the bipartite property of the Penrose tiling the Hamiltonian squared can be written as a direct sum,

$$H^2 = H_{\text{even}}^2 \oplus H_{\text{odd}}^2, \quad (5)$$

where H_{even}^2 (H_{odd}^2) acts only on the N_{even} (N_{odd}) coefficients of all even (odd) sites, ψ_{even} (ψ_{odd}). We diagonalized H_{even}^2 , after having permuted it to band diagonal form, with a LAPACK routine²⁹ for a series of approximants and for various \mathbf{k} points in the asymmetric unit of the first Brillouin zone. Table I gives the number of even lattice points of some approximants and the number of subdiagonals of H_{even}^2 after permutation. We obtained the density of states of an approximant using linear interpolation of its band structure. We then convoluted the result with a Gaussian of finite width. In Fig. 1 we show the density of states of a PPL with 64 079 sites per unit cell that was convoluted with a Gaussian of width 20 meV . The normalization is such that the integral of the density of states equals unity. Only $E > -0.4 \text{ eV}$ is shown since the density of states is symmetric with respect to $E=0$. The difference between the density of states of Fig. 1 and that of one approximant lower (with 39 603 sites per unit cell) gives an indication of how well Fig. 1 approximates the density of states of the Penrose tiling at the given resolution. The maximum of the absolute value of this difference is indicated in Fig. 1 as the error. Figure 1 was calculated with seven \mathbf{k} points in the asymmetric unit of the first Brillouin zone. It was checked that using only three \mathbf{k} points gives the same result up to a difference that is much smaller than the indicated error.

Figure 2 gives the density of states for approximants of the Penrose tiling at a ten times higher resolution than Fig. 1. These results have not converged to those of the infinite Penrose tiling. The indicated error is the maximum of the absolute value of the difference between each plot and the

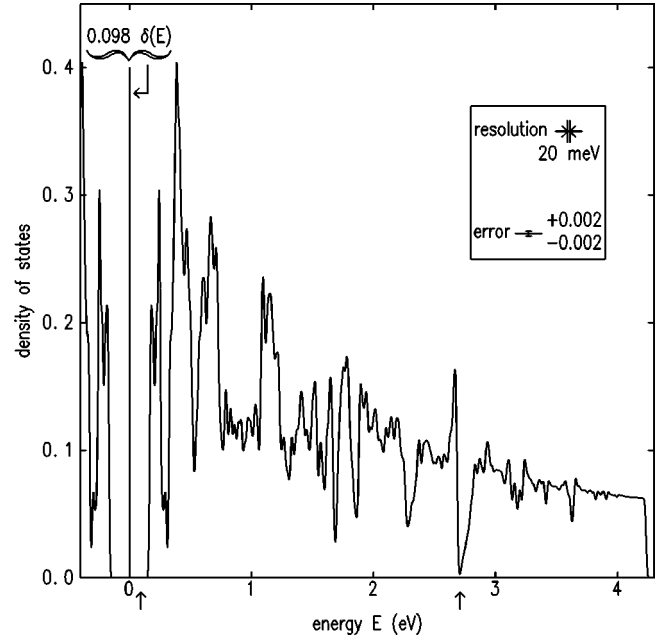


FIG. 1. The density of states of the Penrose tiling, convoluted with a Gaussian of width 20 meV . The δ peak due to strictly localized states at $E=0$ is not smoothed. The error bar indicates how much the result, which was obtained by numerical methods, might deviate from the exact result. Because the density of states is symmetric with respect to $E=0$, only a small part of the negative-energy axis is shown. Arrows indicate the two gaps for which the gap labeling is considered in the text. The density of states does not vanish completely near $E=2.7 \text{ eV}$ due to the smoothing.

same calculation with approximately four times fewer \mathbf{k} points. Comparing Figs. 2(a) and 2(c), which show the density of states of two different PPL's, we see that the higher approximant has spikes with lower amplitude, as was also observed by Hafner and co-workers^{20,21} Comparing Fig. 2(d), which has open boundary conditions in one direction, to Fig. 2(c), we see that an unreconstructed surface can smoothen out the density of states.

When calculating the density of states it is important to monitor the numerical error. Some methods converge faster than other methods, and it is even known that some methods do not converge at all.³⁰ Figure 2(b), e.g., shows the density of states of a PPL with 1364 sites per unit cell, calculated with the method of Yamamoto and Fujiwara.²⁶ The error, which was estimated by comparing to a calculation involving more \mathbf{k} points, is not shown, since it is greater than 1.0, from which it is clear that in the calculations of Yamamoto and Fujiwara²⁶ no convergence was obtained with respect to the number of \mathbf{k} points. In Table II we compare the numerical errors in the density of states of a PPL with 24 476 sites per unit cell, as calculated by three commonly used methods as a function of the number of \mathbf{k} points in the asymmetric unit. In all cases the error shown is the maximum of the absolute value of the difference of the density of states and a reference density of states, which was calculated with the same method, using 273 \mathbf{k} points in the asymmetric unit. The three methods are: (1) counting the number of states in a set of histograms of width 20 meV ; (2) representing each eigenstate of the Hamiltonian as a Gaussian with full width half maximum 20 meV , centered at its eigenvalue, and (3)

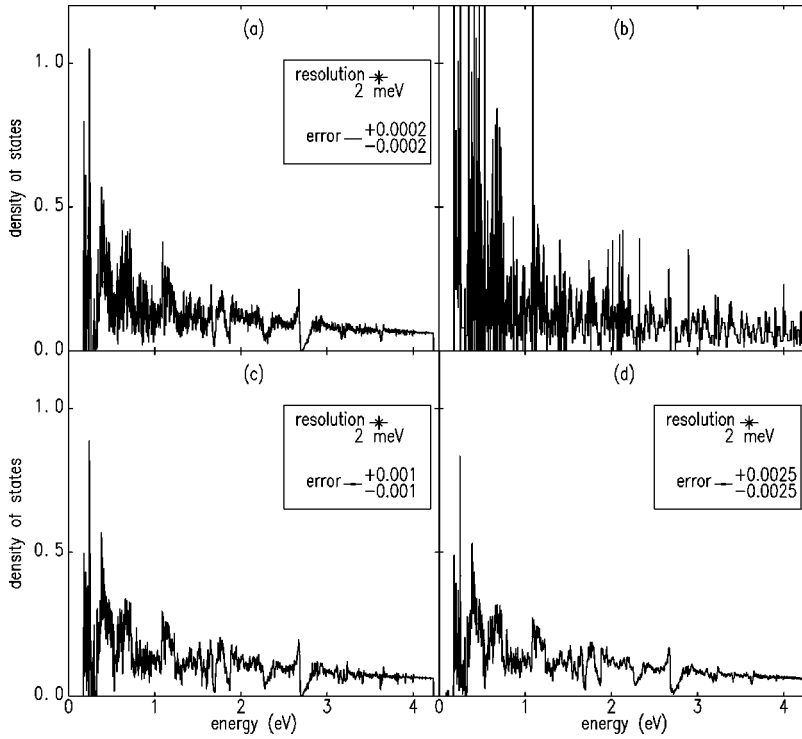


FIG. 2. The density of states of approximants of the Penrose tiling. (a), (c), and (d) were convoluted with a Gaussian of width 2 meV. (a) and (b) give the density of states for a PPL with 1364 sites per unit cell, where (a) was calculated as indicated in the text, and (b) was calculated by the method of Yamamoto and Fujiwara (Ref. 26). No error is indicated for (b), since it is greater than 1.0. (c) and (d) give the density of states of a PPL with 24 476 sites per unit cell, where (c) has periodic boundary conditions, and (d) has periodic boundary conditions in one direction and open boundary conditions in the other direction, with two unit cells in between the two surfaces. The higher approximant studied in (c) has spikes with a lower amplitude than (a), and these spikes can partially disappear by introducing a surface, as is seen in (d).

linear Brillouin-zone integration followed by convolution with a Gaussian of width 20 meV. The last method, which we have used in this paper, is seen to give the best results. It is important to realize that linear interpolation alone, without any smoothening, does not treat Van Hove singularities correctly,³⁰ even when arbitrarily many \mathbf{k} points are used.

At $E = 0.1$ eV and $E = 2.7$ eV we found gaps in the spectra of the high approximants. Table III gives both the widths Δ of these gaps, which were found by calculating 273 \mathbf{k} points in the asymmetric unit of the first Brillouin zone, and the numerical values of the integrated density of states (IDOS), which is defined by

$$\text{IDOS}_E \equiv \int_{-\infty}^E (\text{density of states}) dE. \quad (6)$$

From the data of Table III it seems likely that both gaps will be open in the quasiperiodic limit $N \rightarrow \infty$. The IDOS at $E = 2.7$ eV can be seen to converge rapidly with increasing approximant size N . In fact, since an integer number of bands is on either side of a gap, the IDOS in the gap of an approximant can be written as a fraction. In case of the gap at $E = 2.7$ eV the results of Table III are

TABLE II. Comparison of numerical errors of often used methods for calculating the density of states.

Number of \mathbf{k} points	Error in density of states, using		
	(1) Box counting	(2) Gaussian broadening	(3) Linear interpolation
1	0.024	0.025	
3	0.015	0.008 5	0.004 6
7	0.004 4	0.000 82	0.000 25
21	0.001 2	0.000 20	0.000 071
73	0.000 3	0.000 05	0.000 017

$$\text{IDOS}_{2.7} = 1 - \frac{F_{m-2}}{F_m + F_{m+2}}, \quad m = 17, \dots, 21, \quad (7)$$

where m is defined to be $m \equiv 2n + 2$ for approximants with skinny unit cells and $m \equiv 2n + 1$ for fat approximants. Probably, the IDOS in the infinite tiling is given by the limit

$$\lim_{m \rightarrow \infty} \text{IDOS}_{2.7} = -\frac{2}{5} + \frac{4}{5} \tau, \quad (8)$$

which is in agreement with the gap labeling theorem for the Penrose tiling, which predicts³¹ that all gaps in the infinite tiling must be at an IDOS of the form $(n + m\tau)/20$, with n and m integers. It is unlikely that the limit (8) is not correct, for Eq. (7) would have to deviate from the given fraction from a certain approximant on. Imagine that it would happen in the first approximant that we have not calculated, a PPL with $N = 103\,682$, then the deviation would be of order $1/N$. From Table III it can be seen that approximately four deci-

TABLE III. Width Δ and IDOS of the gaps at 0.1 eV and 2.7 eV for a few approximants.

N	$E = 0.1$ eV		$E = 2.7$ eV	
	Δ (meV)	IDOS	Δ (meV)	IDOS
9 349	170.8	0.549 58	14.4	0.894 427 211 5
15 127	169.0	0.549 15	19.6	0.894 427 183 2
24 476	170.8	0.549 31	17.4	0.894 427 194 0
39 603	170.7	0.549 13	19.9	0.894 427 189 9
64 079	^a	0.549 21	^a	0.894 427 191 4
∞		$\geq 0.549 15$ ^b		0.894 427 191 0 ^c

^aNot calculated.

^bThis value is the exact lower bound $41 - 25\tau$, derived from data of Arai *et al.* (Ref. 5).

^cThis is $-2/5 + (4/5)\tau$, which is derived in the text.

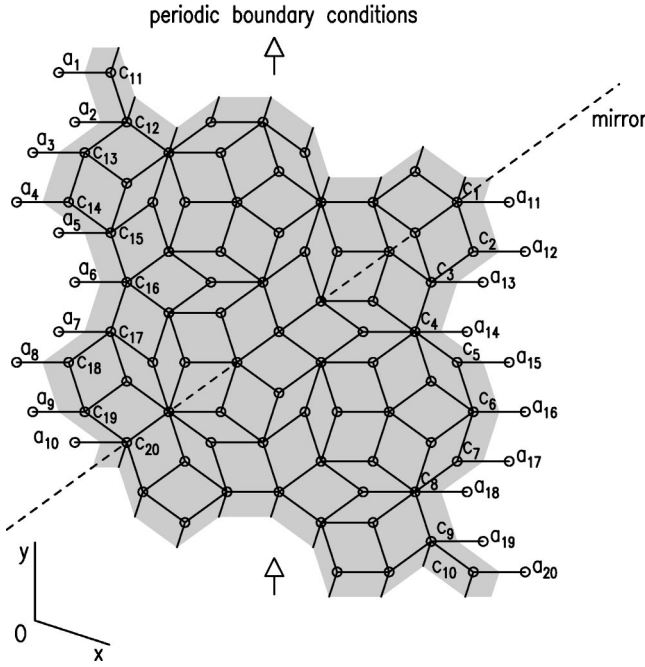


FIG. 3. The unit cell of a PPL with $N = 76$ is shaded. The dotted line indicates mirror symmetry. Note that the x and y direction are not perpendicular. In the y direction periodic boundary conditions are applied and in the x direction the unit cell is periodically repeated, but only those sites are shown that have at least one bond connecting it to a site within the shaded region. These sites are labeled by $a_1 \dots a_{20}$. Fixed boundary conditions can be applied by choosing constant values for $a_1 \dots a_{20}$. In the text it is explained how one can find such $a_1 \dots a_{20}$ that the obtained wave function is, apart from a phase factor $\exp(i\pi k_x)$, periodic in the x direction.

mal places that seemed to have converged numerically in the previous approximant, would have to be changed. For higher approximants this becomes even more unlikely. The IDOS at $E=0.1$ eV does not converge as rapidly, and therefore we cannot do the gap labeling for this gap, but the numerical values in Table III are at least consistent with the predicted value of Arai *et al.*⁵, which is also indicated in Table III.

IV. LOCALIZATION

In this section we calculate the participation ratio resolved density of states at $E=3.0$ eV for a series of approximants, and look how it scales as a function of unit-cell size. The reason that we restrict ourselves to one value of the energy is that our method, which works for fixed energy, requires less time and memory on a computer than direct diagonalization of Hamiltonian matrices, so that we can calculate participation ratios for relatively high approximants. We plan to discuss energy dependence in a later work. The choice to study $E=3.0$ eV is to a certain extent arbitrary: We wanted to study an energy $E>2.0$ eV because we had seen that the density of states converges more rapidly for those energies. We chose $E=3.0$ eV because it lies in the center of the selected energy range.

First we explain our method by showing how it works for the tight-binding Hamiltonian H of a PPL with 76 sites per unit cell, which is indicated schematically in Fig. 3, but in principle, it works for any tight-binding Hamiltonian, and in

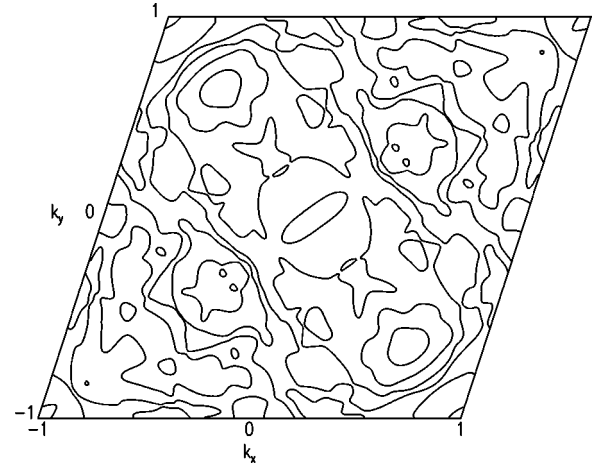


FIG. 4. $E=3.0$ eV contour lines in the unit cell of the reciprocal lattice of a PPL with 24 476 sites per unit cell. k_x and k_y are normalized such that they are between -1 and 1 .

practice, we used H_{even}^2 of a series of PPL's, which is more time efficient on a computer, and which immediately gives ψ_{even} , and we obtained the odd part of the wave function by $\psi_{\text{odd}} = (H/E)\psi_{\text{even}}$. The goal of our method is to obtain contour lines $E(k_x, k_y) = 3.0$ eV, so that we can perform contour integrations in the first Brillouin zone. First, we show how we can obtain all possible $k_x(E, k_y)$, where in the y direction periodic boundary conditions are applied, and we search all compatible periodic boundary conditions in the x direction. We exploited the fact that a solution with periodic boundary conditions can always be written as a linear combination of solutions with fixed boundary conditions. This is illustrated in Fig. 3, where we have numbered the sites outside the shaded unit cell by a_1, \dots, a_{20} , and the corresponding sites in the unit cell by c_1, \dots, c_{20} , and where the fixed boundary conditions $\{a_1=1, a_i=0, i=2, \dots, 20\}$, $\{a_1=0, a_2=1, a_i=0, i=3, \dots, 20\}$, etc., form a complete set. By solving for all these fixed boundary conditions,

$$(H - E)\psi = \text{fixed boundary conditions}, \quad (9)$$

where ψ is a column vector containing the coefficients of all sites in the shaded area including the c_i 's, and where E is the constant energy, $E = 3.0$ eV, we obtain the linear dependence

$$\begin{pmatrix} c_1 \\ \vdots \\ c_{20} \end{pmatrix} = M \begin{pmatrix} a_1 \\ \vdots \\ a_{20} \end{pmatrix}, \quad (10)$$

where the j th column of the matrix M contains the solutions c_i for the j th set of fixed boundary conditions. Equation (9) is a system of linear equations, which we have solved with the sparse Harwell Subroutine Library³² (HSL) package ME48. By using iterative refinement, keeping the results in extended precision, M can be obtained in machine precision.³³ By requiring

$$\begin{pmatrix} c_1 \\ \vdots \\ c_{10} \end{pmatrix} = e^{i\pi k_x} \begin{pmatrix} a_1 \\ \vdots \\ a_{10} \end{pmatrix}, \quad (11)$$

and

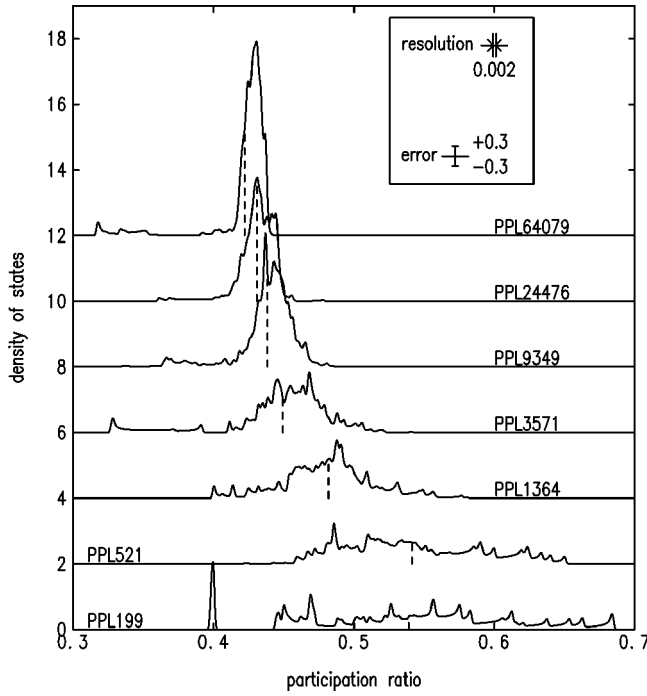


FIG. 5. Participation ratio resolved density of states at $E=3.0$ eV as obtained by contour integration in the unit cell of the reciprocal lattice for a series of approximants with up to 64 079 sites per unit cell. The results have been smoothened by convoluting them with a Gaussian with width equal to the indicated resolution. For clarity, the zeros of the density-of-states axis of the various plots have been shifted with respect to each other. The dotted lines indicate the centers of mass of each distribution. The normalization is consistent with that of Sec. III, such that $\int_0^1 (\text{density of states}) dp$ gives the density of states at $E=3.0$ eV. The indicated error is an estimation of the maximum error of the highest approximant; all other PPL's have errors of, at most, 0.06. For high approximants, the distribution of the participation ratio is a relatively narrow function. The center of mass seems to approach a constant value of $p \approx 0.4$. This indicates that the wave functions are either extended or critical with $\alpha < 0.5$.

$$\begin{pmatrix} c_{11} \\ \vdots \\ c_{20} \end{pmatrix} = e^{-i\pi k_x} \begin{pmatrix} a_{11} \\ \vdots \\ a_{20} \end{pmatrix}, \quad (12)$$

and substituting Eq. (10) for the c_i 's, we obtain a generalized eigenvalue problem, which can be solved by LAPACK (Ref. 29) in a standard way. The generalized eigenvalues of Eq. (11) give the compatible periodic boundary conditions in the x direction, and the eigenvectors give the corresponding fixed boundary conditions. By solving Eq. (9) again for these fixed boundary conditions we obtain the wave function $\psi(E, k_x, k_y)$. Contours can easily be recognized if k_x is obtained for sufficiently many k_y values, and if the two mirror planes of a properly chosen unit cell of the reciprocal lattice are used. Figure 4 gives the contour lines of a PPL with 24 476 atomic sites per unit cell, as an illustration. The contour integration

$$\rho(p) = \int_C \frac{\delta(p_C - p)}{|\nabla_k E|} dl, \quad (13)$$

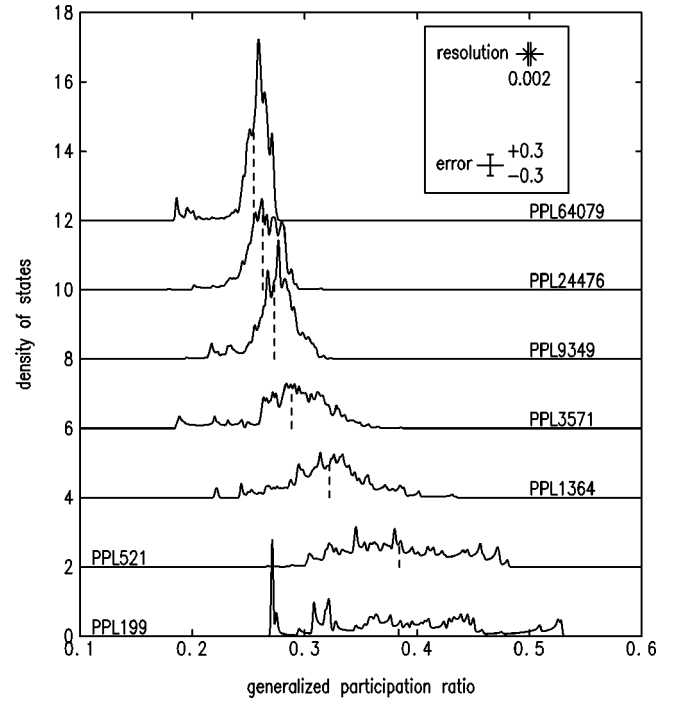


FIG. 6. The 8-norm related generalized participation ratio resolved density of states at $E=3.0$ eV for a series of approximants. The same remarks hold as for Fig. 5. The center of mass (dotted lines) seems to approach a constant value, which indicates that the wave functions are either extended or critical with $\alpha < 0.25$.

where p_C is the (generalized) participation ratio along the contour as obtained by linear interpolation between calculated points, and where $\partial E / \partial k_x$ and $\partial E / \partial k_y$ are linearly interpolated expectation values of the wave functions, gives the density of states resolved for the (generalized) participation ratio $\rho(p)$.

Results for the participation ratio p and for the 8-norm related generalized participation ratio p_8 are given in Fig. 5 and Fig. 6. For low approximants ($199 < N < 9349$) the distributions of p and p_8 are quite broad, and they seem to follow a power-law behavior according to Eq. (3), but for higher approximants ($N > 24\,476$) the distributions become more narrow, and seem to tend to finite values, so that in the quasiperiodic limit p and p_8 might be well-defined quantities, and the wave functions are either extended or critical with $\alpha < 0.25$. It is interesting to speculate about the generality of these results. Clearly, they conflict conclusions of previous studies,^{15,27} namely that states in the Penrose tiling are critical, but the reason is obviously that we have been able to study higher approximants. They also contradict the results of Rieth and Schreiber¹⁵ for the state of minimum energy, but, as was already remarked there,¹⁵ this state seems to be quite specific, and it might not reflect a general behavior. More detailed studies will be necessary to test the general validity of the present results.

V. OUTLOOK

We found that the density of states of the Penrose tiling is less spiky than expected,^{15,27} but due to computational limitations we could not obtain a better resolution than 20 meV. We saw that the density of states of approximants, which can

easily be calculated with a high resolution, is really spiky, and that higher approximants have a lower amplitude of the spikes, as has been noticed in other quasiperiodic systems before.^{20,21} Also we saw that an unreconstructed surface can smoothen the density of states through surface states and surface resonances, in agreement with an earlier prediction.²³ Because of computational limitations we cannot decisively conclude whether these effects explain the absence of spikes in experiments.^{23–25} As already indicated in Sec. I, other effects, e.g., chemical and structural disorder, may also play a role. In the future we plan to study the local density of states at a surface, which might show the effect of surface states even stronger.

For $E=3.0$ eV we could, by means of contour integrations in the reciprocal space, obtain the density of states, resolved for the participation ratio p and for p_8 , of a series of approximants. For high approximants we found that p and p_8

maybe approach finite limiting values, which would indicate that the Penrose tiling has extended states at $E=3.0$ eV. This is surprising,^{15,27} and it would be interesting to repeat the same calculation for other energies and higher approximants, to see if our results are general for all energies and persistent in larger systems.

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