Strictly localized states on a two-dimensional Penrose lattice

Masao Arai, Tetsuji Tokihiro, and Takeo Fujiwara
Department of Applied Physics, University of Tokyo, Tokyo 113, Japan

Mahito Kohmoto
*Institute for Theoretical Physics, University of California, Santa Barbara, California 93103
and Department of Physics, University of Utah, Salt Lake City, Utah 84112*
(Received 26 October 1987)

Infinitely degenerate states at an energy $E=0$ on a two-dimensional Penrose lattice are investigated in a tight-binding model where atomic orbitals are located at vertices of rhombuses. The states with $E=0$ are all strictly localized and have amplitudes only on some specific vertices, which are three-edge vertices and some non-three-edge vertices. A lower bound on the fraction of them is calculated analytically as $-50\tau+81\approx 9.83\times 10^{-2}$ [$\tau=(\sqrt{5}+1)/2$], which is conjectured to be the exact fraction.

I. INTRODUCTION

There has been much interest in quasicrystals.[1,2] Since the quasicrystalline phase is characterized by quasiperiodicity and long-range-bond orientational order, the physical properties of quasicrystals are expected to be quite different from both periodic and random systems. Several theoretical models had already been investigated before the discovery of the real quasicrystals,[1] i.e., a one-dimensional (1D) Fibonacci lattice[3-7] and 2D (Refs. 8-10) and 3D (Ref. 11) Penrose lattices. In these lattices there is an upper bound of distance to find an exact copy of any original pattern of a finite size, which is called Conway's theorem. From these points of view, they should be distinguished from incommensurate structures such as the Harper model.

Electronic structures of the 1D Fibonacci lattice have been investigated extensively.[3-7] The numerical and analytical studies showed that the energy spectrum is a Cantor set and that wave functions are critical, namely neither localized nor extended. On the other hand, the 2D Penrose lattice has not been much investigated. In a recent work[12] we argued that exponentially localized states do not exist in a system which satisfies Conway's theorem. This general statement is consistent with Sutherland's self-similar wave function[13] and other works on 1D Fibonacci[3-7] and 2D Penrose lattices.[14,15] Using this statement and numerical results we conjectured that the energy spectrum of the 2D Penrose lattice is singular.

Another singular feature of the electronic property on the 2D Penrose lattice is the existence of states whose degeneracy is proportional to the system size. These states were first pointed out by Semba and Ninomiya[16] in the center model[15] and independently by Kohmoto and Sutherland[17] in the vertex model.[15] Recently we investigated these infinitely degenerate states in the center model and found two different kinds of states at the same energy.[18] One is called confined states and they are strictly localized without tails. The other is called string states, which appear on some strings of rhombuses with one three-edge vertex and which are self-similar and fractal.

The existence of confined states is mainly due to the local connectivity of the 2D Penrose lattice. On the other hand, the string states are strongly influenced by its global configuration. The existence and its degeneracy of both states are sensitive to the decoration of the lattice and other details. We found confined states in other 2D lattices, either quasiperiodic or periodic lattices.[19] A simple example of the periodic lattice with confined states is the periodic Penrose lattice.[12] In 3D lattices and the real quasicrystals it is not clear whether confined states exist or not.

In this paper we analyze the infinitely degenerate states at $E=0$ in the vertex model using the basic idea of Ref. 18. We show that all states are strictly localized, i.e., confined states, and that there is no correspondence of string states in the center model. In Sec. II we define the model Hamiltonian and show the general character of confined states. Various explicit wave functions and an exact lower bound of the fraction of confined states are presented in Sec. III. In Sec. IV the fraction is estimated by another method. Section V is a summary.

II. LOCALIZED STATES AND FORBIDDEN SITES

We use a tight-binding Hamiltonian on the 2D Penrose lattice. Atomic orbitals are placed on vertices of rhombuses and we call this model a vertex model. An electron can hop only to nearest-neighbor sites (vertices) which are connected by the edges of rhombuses and we set all transfer integrals to unity. Then the Schrödinger equation for a wave function $|\Psi\rangle=\sum_i \Psi_i\,|i\rangle$ with an energy E is

$$\sum_{\langle i,j\rangle} \Psi_j = E\Psi_i \ , \qquad (2.1)$$

where the summation is over nearest-neighbor sites. Since the basic units of the lattice are rhombuses, the lattice can be divided into two sublattices. In Eq. (2.1) Ψ_j

on the left-hand side and Ψ_i on the right-hand side belong to different sublattices. If we change the sign of the wave function on one sublattice, the resulting wave function becomes an eigenfunction with an energy $-E$. Thus, the energy spectrum is symmetric with respect to $E=0$. Moreover, for the states at $E=0$, since the right-hand side of Eq. (2.1) vanishes, the Schrödinger equation of each sublattice is independent, i.e., bipartite.

For this model it is known that there exist infinitely degenerate states at $E=0$. We will show that these states are also strictly localized and hereafter we call them confined states. Kohmoto and Sutherland[17] found some of these states (Fig. 1). The state in Fig. 1(a) is denoted by type 1 and that in Fig. 1(b) by type 2. We refer to them as KS-ring states because the supporting regions of them form rings. They argued that the fraction of confined states is $f_c \approx 0.0557$ under the conjecture that all confined states have amplitudes only on three-edge vertices (K and Q by de Bruijn's notation[10]). But this conjecture is incorrect and, as we will show in the following, there exist the confined states with amplitudes on the non-three-edge vertices (S, $S5$, and J). In the center model which has atomic orbitals on the centers of rhombuses, both confined states and string states exist at $E=+2$. We showed all eigenstates with $E=+2$ explicitly, and calculated an exact fraction of them.[18] In the following, we apply the same idea and show an exact lower bound on the fraction of the confined states for the vertex model.

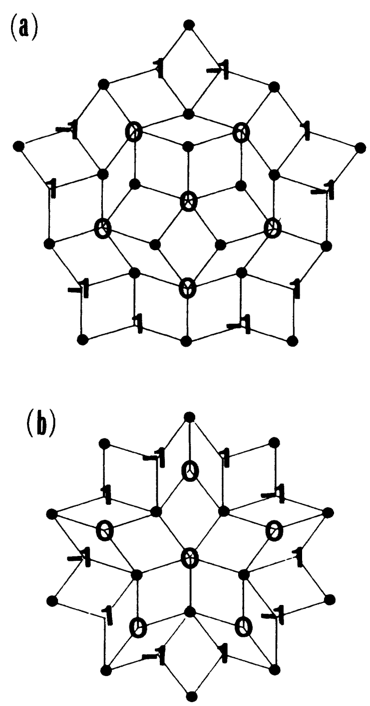

FIG. 1. The confined states found by Kohmoto and Sutherland [(a) type 1 and (b) type 2]. The numbers on the vertices represent the amplitudes of wave functions. Since confined states always sit on one sublattice, the vertices on the other sublattice are shown by solid dots.

We calculated all eigenstates with $E=0$ numerically to specify the character of confined states. We used a lattice with 6545 rhombuses, which has the fivefold rotational symmetry. Because of nonperiodicity of the Penrose lattice, some nontrivial boundary condition is necessary. We used the fixed boundary condition, namely the wave function vanishes outside the lattice. These boundary conditions cause a crucial influence on almost all eigenstates. However, confined states are less affected by the boundary conditions, because their extents are essentially finite regions.

From the result of these calculations, we found that there are specific sites on which any wave function with $E=0$ vanishes (Fig. 2). We call these sites forbidden sites and others allowed sites. Except in the neighborhood of S vertices and $S5$ vertices, three-edge vertices are allowed sites and non-three-edge vertices are forbidden sites. To understand the structure of forbidden and allowed sites, we must consider the structure of three-edge vertices in the 2D Penrose lattice, which we previously discussed in Ref. 18. The results are as in the following.

(1) Any rhombus has one or two three-edge vertices.

(2) All rhombuses with one three-edge vertex are connected by strings and there are no end points in a string.

(3) The smallest strings are five fat rhombuses around S or $S5$ vertices and we call them zeroth S strings and zeroth $S5$ strings, respectively. (Strictly speaking, the zeroth S string is not really a string defined above, but we use this notation in the present paper simply for convenience.)

(4) Strings are generated by $2n$-fold deflation of the zeroth S ($S5$) strings and we call these strings the nth S ($S5$) strings.

From Fig. 2 we observe that non-three-edge vertices on nth S ($S5$) strings for $n \geq 2$ ($n \geq 1$) are forbidden sites. These forbidden sites on strings are connected by bold lines in Fig. 2. These connected forbidden sites divide the whole lattice into finite independent parts. Thus we can treat Eq. (2.1) in each finite region surrounded by strings and all eigenstates with $E=0$ are confined in them. In the finite region, Eq. (2.1) splits into two groups, and each of them corresponds to one sublattice. Figure 2 shows that, in each region surrounded by strings, confined states exist on one sublattice and that all vertices on the other sublattice are forbidden sites. Moreover, the sublattice which has confined states changes from one to the other on strings. From these observations we can summarize the structure of forbidden and allowed sites as in the following.

Rule 1.1. On nth S ($S5$) strings for $n \geq 2$ ($n \geq 1$), non-three-edge vertices are forbidden sites. One-dimensional alignments of these forbidden sites divide the whole lattice into finite independent parts.

Rule 1.2. In an independent part, one sublattice consists of forbidden sites and the other consists of allowed sites. The sublattice of forbidden sites changes from one to the other on strings.

In Fig. 2(a) these rules are broken near the boundary part because of the boundary condition. It seems that the rules are not satisfied at the central parts of the second S strings and of the first $S5$ strings, namely some "allowed" sites have zero amplitudes of a wave function. Though we can use an additional rule to explain them, it is more suitable to consider that these allowed sites have just zero amplitudes of the wave function as a result of solving the Schrödinger equation.

Between strings, since each rhombus has two three-edge vertices which locate diagonally, one sublattice consists only of three-edge vertices. Moreover, it is easily found that the sublattice constructed by three-edge vertices changes from one to the other on strings. Therefore, rules 1.1 and 1.2 can be rewritten as in the following.

Rule 2. Almost all three-edge vertices are allowed sites and almost all non-three-edge vertices are forbidden sites.

Exception 2.1. In the region surrounded by a first S string, five three-edge vertices are forbidden sites and six non-three-edge vertices (S,J) are allowed sites.

Exception 2.2. In the zeroth $S5$ string a non-three-edge vertex $(S5)$ is an allowed site.

If we ignore the above exceptions, this rule is just the conjecture of Kohmoto and Sutherland.[17] We will see later that these exceptions crucially influence the fraction of confined states.

Now we prove these rules. Rules 1 and 2 are equivalent, so we treat rule 2. First, we prove the next two theorems.

Theorem 1. Around $S5$ vertices the solid-dotted sites in Fig. 3(a) are forbidden sites.

Theorem 2. In the region surrounded by strings, two adjacent rhombuses always share one three-edge vertex. If two non-three-edge vertices on one rhombus are for-

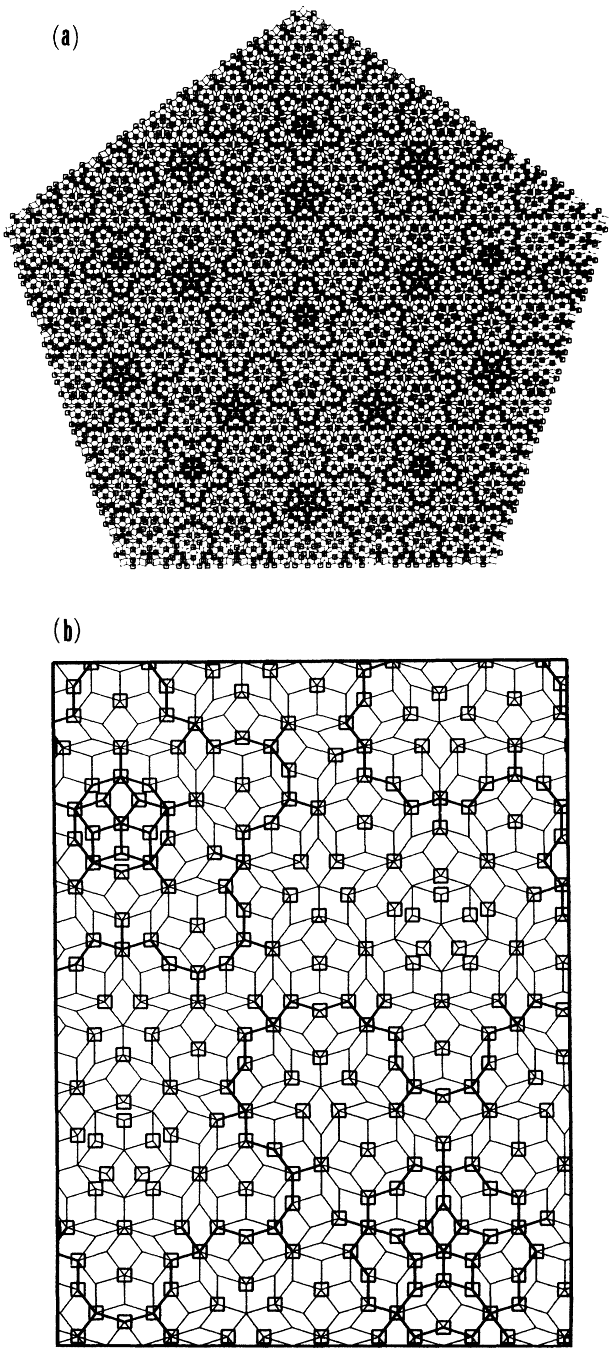

FIG. 2. (a) The results of numerical calculation. The forbidden sites are shown by squares. One-dimensional alignments of forbidden sites are shown by bold lines. (b) Enlarged part of (a). The central S vertex of the fivefold symmetry is located near the upper left-hand corner. The one sublattice consists of allowed sites and the other consists of forbidden sites. The sublattice of forbidden sites changes from one to the other on strings.

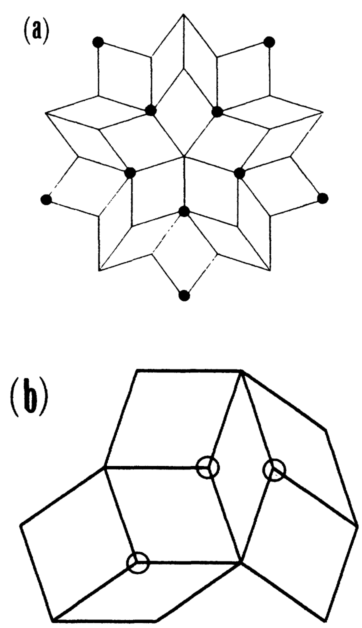

FIG. 3. (a) The local configuration around $S5$ vertices. The solid-dotted vertices are always forbidden sites. (b) An example of the local configuration around three-edge vertices. Three-edge vertices are shown by circles.

bidden sites, non-three-edge vertices on adjacent rhombuses are also forbidden sites.

Theorem 1 is easily shown using the local configuration around $S5$ vertices. Theorem 2 is clear from Fig. 3(b) and from the fact that rhombuses have three-edge vertices locating diagonally. Then rule 2 can be proven in the following way. Between one $(n+1)$th S ($S5$) string and one nth S ($S5$) string for $n \geq 2$ ($n \geq 1$) there always exist zeroth $S5$ strings. Therefore, except in the region surrounded by a first S string or between one first S string and one second S string, all rhombuses can be approached from some zeroth $S5$ string using rhombuses with two three-edge vertices. By using theorems 1 and 2 we find that non-three-edge vertices, except $S5$ vertices, are forbidden sites in these regions. In a first S string and between one first S string and one second S string we can easily verify rule 2 by solving Eq. (2.1). Thus we have proven rule 2.

III. VARIOUS CONFINED STATES AND THEIR FRACTION

We present various confined states under rules 1.1 and 1.2. KS-ring states are easily generalized. Fat rhombuses in the Penrose lattice are also connected by strings.[18] We call them rings in order to distinguish from strings. A thin rhombus in strings shares a K vertex with two fat rhombuses in strings. Another fat rhombus also shares the K vertex. If we use the fat rhombus instead of the thin rhombus, we get a ring. Therefore strings and rings have a one-to-one correspondence. If we put amplitudes $+1$ or -1 on D vertices on these rings, these states are eigenstates with $E=0$ and a generalization of KS-ring states. We refer to them also as KS-ring states. Other eigenstates with $E=0$ which have amplitudes only on three-edge vertices are shown in Fig. 4. The state in Fig. 4(a) is denoted by type 3 and the one in Fig. 4(b) by type 4.

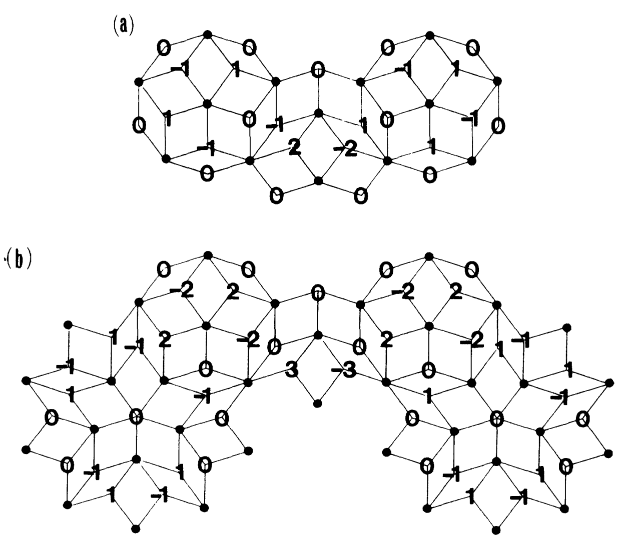

FIG. 4. Another example of the confined states which have amplitude only on three-edge vertices [(a) type 3 and (b) type 4]. The meaning of the symbols on the vertices is identical with those in Fig. 1.

The KS-ring states have the same feature as the string states defined in Ref. 18, namely they have a self-similar and fractal feature. However, the most important difference between KS-ring states and string states is that the KS-ring states can be constructed from the linear combination of smaller states (type 3, type 4, etc.). For example, consider the region between one second S string and one third S string. Along the second S string, KS-ring states exist. However, there are five bridges which connect five equivalent smaller regions (Fig. 5). On these bridges, type-3 and type-4 confined states exist. If we want to get an eigenstate which is linearly independent of type 3 and type 4, we can impose a condition that the wave function vanishes on the bridges. Thus we can treat five regions independently, and the ring structure is not essential along the second S string. The above argument is easily generalized. Along any string (except first strings) the bridges exist. Since we can impose a condition that wave functions vanish on the bridges, we need not consider ring states except types 1 and 2.

The states which have amplitudes on non-three-edge vertices are shown in Figs. 6(a) and 6(b), and we refer to them as type 5 and type 6. On zeroth $S5$ strings enclosed by first $S5$ strings there is no confined state which has an amplitude on an $S5$ vertex. On zeroth $S5$ strings not enclosed by first $S5$ strings, type 5 always exists. Thus type 5 is the unique confined state which has an amplitude on an $S5$ vertex. Around S vertices, local connectivity imposes

$$\Psi_J = -\frac{\Psi_S}{2} , \tag{3.1}$$

where Ψ_S is the amplitude on an S vertex and Ψ_J is that on the J vertices around the S vertex. Thus, similarly to type 5, type 6 is the unique confined state which has amplitudes on an S-vertex and J vertices around it. Therefore, there do not exist other kinds of confined states which have amplitudes on non-three-edge vertices. On

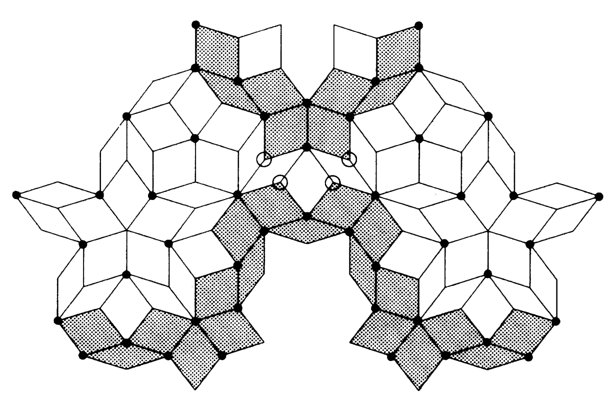

FIG. 5. An example of a bridge. The upper (lower) shaded rhombuses are a part of a third (second) S string. The solid-dotted sites are forbidden sites. The confined states which are independent of types 3 and 4 must vanish on the vertices shown by circles.

the lattice shown in Fig. 2 all confined states are covered by types 1–6. The fraction of the states types 1–6 can be calculated exactly using the inflation-deflation rule.[20] We summarize the results in Table I. The total fraction of types 1–6 is $-50\tau+81 \approx 9.83\times10^{-2}$. This gives a lower bound on the fraction of confined states. If we restrict ourselves to the confined states which have amplitudes only on three-edge vertices, the total fraction of types 1–4 gives their lower bound. The result is 8.01×10^{-2}.

TABLE I. The fraction of various confined states.

Confined states	Their fraction
Type 1	$\frac{1}{\tau^8(\tau^2+1)} \approx 5.883\times10^{-3}$
Type 2	$\frac{1}{\tau^6(\tau^2+1)} \approx 1.540\times10^{-2}$
Type 3	$\frac{1}{\tau^7}+\frac{1}{\tau^{10}} \approx 4.257\times10^{-2}$
Type 4	$\frac{1}{\tau^{11}}+\frac{5}{\tau^{10}(\tau^2+1)} \approx 1.626\times10^{-2}$
Type 5	$\frac{1}{\tau^8}-\frac{1}{\tau^{10}} \approx 1.316\times10^{-2}$
Type 6	$\frac{1}{\tau^{10}}-\frac{1}{\tau^{12}} \approx 5.025\times10^{-3}$
Total	$-50\tau+81 \approx 9.830\times10^{-2}$

IV. ANOTHER ESTIMATION OF THE FRACTION

In this section we estimate the fraction of confined states by another method. According to rule 1.1, a set of equations [Eq. (2.1)] can be separated into groups of finite-dimensional simultaneous equations. A set of simultaneous equations corresponds to a finite independent region divided by linear alignment of forbidden sites on strings. The number of variables is equal to that of allowed sites (N_a) in the region. The number of equations is equal to that of forbidden sites (N_f). Concerning the number of confined states (N_c) in this region, it is easily found that

$$N_c \geq N_a - N_f \ . \tag{4.1}$$

Total number of confined states is the sum of N_c in all regions. On the right-hand side of Eq. (4.1) there are neither double-counting nor missing sites, because there is no forbidden (allowed) site surrounded by forbidden (allowed) sites. Therefore the fraction of confined states, f_c, is

$$f_c \geq f_a - f_f \ , \tag{4.2}$$

where f_a (f_f) is the fraction of allowed (forbidden) sites, and

$$f_a + f_f = 1 \ . \tag{4.3}$$

From rule 2 we find

$$f_a = f(3) + f_{1S} + f_{0S5} \ , \tag{4.4}$$

where $f(3)$ is the fraction of three-edge vertices and f_{1S} (f_{0S5}) is that of first S (zeroth $S5$) strings. The $f(3)$ is the sum of the fraction of D vertices and Q vertices. The f_{0S5} is equal to the fraction of $S5$ vertices. Thus we obtain

$$f(3) = \frac{1}{\tau^2} + \frac{1}{\tau^4} \ , \tag{4.5}$$

$$f_{0S5} = \frac{1}{\tau^6(\tau^2+1)} \ , \tag{4.6}$$

where

$$\tau = \frac{1+\sqrt{5}}{2} \ .$$

The first S strings are generated by the twice deflation of zeroth S strings. The total number of vertices increases

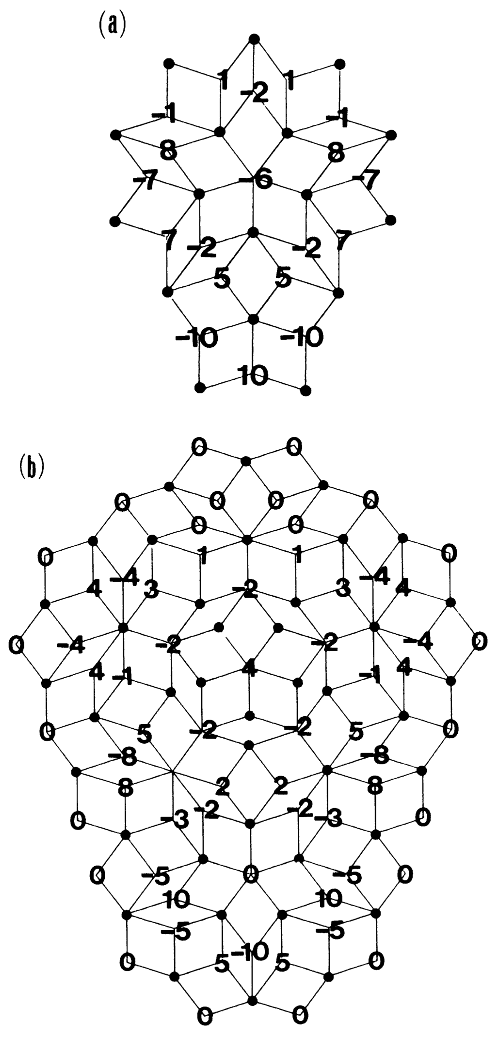

FIG. 6. The confined states which have amplitudes on non-three-edge vertices [(a) type 5 and (b) type 6]. Type 5 is the unique confined state which has an amplitude on an $S5$ vertex, and type 6 is that on an S vertex and J vertices around it. The meaning of the symbols on the vertices is identical with those in Fig. 1.

by factor τ^4 for the twice deflation. Thus we find

$$f_{1S} = \frac{1}{\tau^4} f_S = \frac{1}{\tau^8(\tau^2+1)} , \tag{4.7}$$

where f_S is the fraction of S vertices. As a result we get an exact lower bound,

$$\begin{aligned} f_c &\geq 2\left[\frac{1}{\tau^2}+\frac{1}{\tau^4}+\frac{1}{\tau^8}\right]-1 \\ &= -50\tau+81 \\ &\approx 9.830056\times 10^{-2} . \end{aligned} \tag{4.8}$$

Up to the extent shown in Fig. 2 the equality in Eq. (4.1) holds, and the right-hand side of Eq. (4.8) gives the same fraction as the one in Sec. III. Thus we guess that the right-hand side of Eq. (4.8) gives the exact fraction of confined states of the vertex model.

Finally, we consider the influence of a magnetic field. The effect of the magnetic field is included in the additional phase factors of transfer integrals. We can easily verify that theorems 1 and 2 are satisfied on the presence of the magnetic field. Thus the estimation of (4.8) is unchanged. This conclusion is consistent with previous numerical work.[21]

V. CONCLUSION

In this paper we studied the eigenstates with $E=0$ on the 2D Penrose lattice in the vertex model. These states are all confined in some finite region. We have shown that confined states have amplitudes on some specific vertices called allowed sites. The allowed sites are not restricted to three-edge vertices. The exact lower bound on their fraction is estimated as $-50\tau+81\approx 0.0983$.

ACKNOWLEDGMENTS

One of us (M.K.) was supported in part by the U.S. National Science Foundation under Grant No. PHY-82-17853 and by a grant from the Alfred P. Sloan Foundation.

[1]D. Shechtman, I. Bleck, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).
[2]D. Levine and P. J. Steinhardt, Phys. Rev. Lett. **53**, 2477 (1984).
[3]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).
[4]S. Ostlund, R. Pandit, H. J. Schellnhuber, and E. Siggia, Phys. Rev. Lett. **50**, 1873 (1983).
[5]M. Kohmoto, B. Sutherland, and C. Tang, Phys. Rev. B **35**, 1020 (1987).
[6]M. Casdagli, Commun. Math. Phys, **107**, 295 (1986).
[7]P. A. Kalugin, A. Yu. Kitaev, and L. S. Levitov, Zh. Eksp. Teor. Fiz. **91**, 692 (1986) [Sov. Phys.—JETP **64**, 410 (1986)].
[8]R. Penrose, Bull. Inst. Math. Appl. **10**, 266 (1974).
[9]M. Gardner, Sci. Am. **236(1)**, 110 (1977).
[10]N. G. de Bruijn, Indag. Math. Proc. Ser. A **84**, 39, 53 (1981).
[11]P. Kramer and R. Neri, Acta Crystallogr. Sect. A **40**, 580 (1984).
[12]H. Tsunetsugu, T. Fujiwara, K. Ueda, and T. Tokihiro, J. Phys. Soc. Jpn. **56**, 1420 (1986).
[13]B. Sutherland, Phys. Rev. B **34**, 3904 (1986).
[14]T. Tokihiro, T. Fujiwara, and M. Arai, Phys. Rev. B (to be published).
[15]T. Fujiwara, T. Tokihiro, and M. Arai, in *Proceedings of International Workshop of Quasicrystals, Beijing, 1987* (Trans Tech Publications, Zurich, 1988).
[16]K. Semba and T. Ninomiya (unpublished).
[17]M. Kohmoto and B. Sutherland, Phys. Rev. B **34**, 3849 (1986).
[18]T. Fujiwara, M. Arai, T. Tokihiro, and M. Kohmoto, Phys. Rev. B **37**, 2797 (1988).
[19]M. Arai (unpublished); B. Sutherland, Phys. Rev. B **34**, 5208 (1986).
[20]V. Kumar, D. Sahoo, and G. Athinthan, Phys. Rev. B **34**, 6924 (1986).
[21]T. Hatakeyama and H. Kamimura, Solid State Commun. **62**, 79 (1987).

(a)

(b)

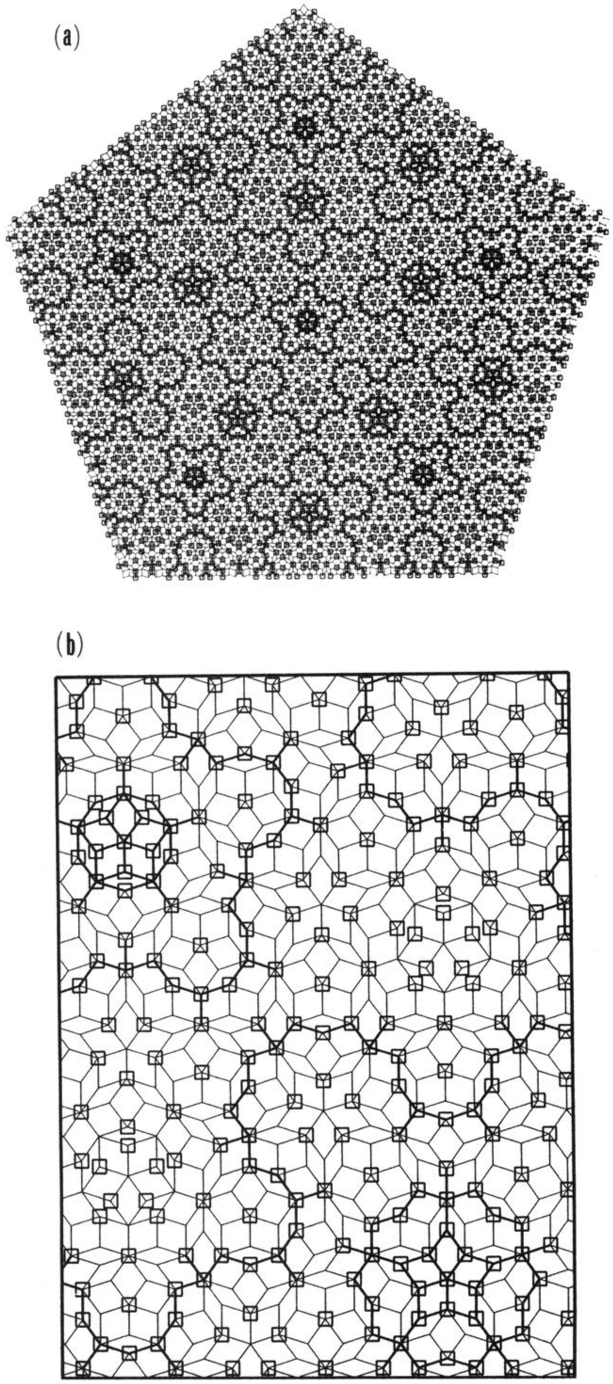

FIG. 2. (a) The results of numerical calculation. The forbidden sites are shown by squares. One-dimensional alignments of forbidden sites are shown by bold lines. (b) Enlarged part of (a). The central S vertex of the fivefold symmetry is located near the upper left-hand corner. The one sublattice consists of allowed sites and the other consists of forbidden sites. The sublattice of forbidden sites changes from one to the other on strings.

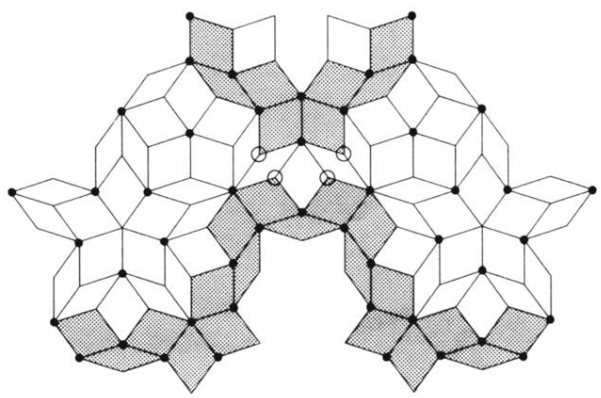

FIG. 5. An example of a bridge. The upper (lower) shaded rhombuses are a part of a third (second) S string. The solid-dotted sites are forbidden sites. The confined states which are independent of types 3 and 4 must vanish on the vertices shown by circles.