Self-similar ground-state wave function for electrons on a two-dimensional Penrose lattice

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I define a hopping Hamiltonian for independent electrons on a two-dimensional, infinite, quasiperiodic Penrose lattice with a particular on-site potential, depending upon a parameter r. I then find the exact ground-state wave function for this Hamiltonian. The wave function is shown numerically to have a power-law decay from the origin, and the exponent is determined numerically. The wave function may or may not be normalizable over the infinite lattice, depending upon the parameter r. The wave function is then demonstrated to be self-similar, in that the wave function for two identical regions of the lattice is the same, except for a scale factor. The scaling of the wave function is discussed, and a bound for the decay of the wave function established. Finally, I determine exactly the scaling distribution for the wave function, and thus calculate exactly the previously introduced decay exponent. The wave function is shown to have a critical value of the parameter r, above which the wave function is normalizable and thus localized, while below the wave function has a power-law decay but is not normalizable.

I. INTRODUCTION

With the experiments of Schechtman *et al.*,[1] which seem to show evidence for a quasicrystal structure in nature, there has been a great interest in the physics of materials with quasiperiodicity, which are intermediate between periodic and random structures. The theoretical understanding of these systems is usually based on generalizations of a nonperiodic tiling of the two-dimensional plane first introduced by Penrose,[2] and described by Gardner.[3] Important theorems are due to Conway,[4] and the papers of de Bruijn[5] contain the most recent discussion. At the same time, the one-dimensional quasiperiodic Fibonacci lattices have been treated theoretically by Kohmoto and Banavar,[6] and by others. The properties found for the zero-energy wave function by Kohmoto and Banavar are the same as we find in this paper, where we treat electrons on a two-dimensional Penrose lattice.

Other recent papers on electronic properties of a Penrose lattice are by Odagaki and Nguyen,[7] Choy,[8] and Kohmoto and Sutherland.[9,10] These papers, however, are largely concerned with the spectrum of the Hamiltonian, and except for some exact results for the strictly localized states in the peak, due to Kohmoto and Sutherland, have little to say about the wave functions.

In this paper I present the exact ground-state wave function for a tight-binding model for independent electrons hopping on a two-dimensional infinite Penrose lattice, with a particular on-site potential depending on a parameter. I was then able to give a rather complete description of the properties of this wave function. It is hoped that these properties are qualitatively the same for more general systems.

II. THE MODEL AND THE GROUND-STATE WAVE FUNCTION

I begin my investigation with the familiar two-dimensional quasiperiodic Penrose lattice derived from a tiling by fat and thin rhombuses. The vertices of the rhombuses are the sites of the lattice, and the edges are the bonds between nearest neighbors. I take the bond length to be unity. When tiling the plane by these Penrose tiles, there is a constraint on which edges can be adjacent. This is traditionally expressed by labeling the edges of the two tiles by either single arrows or double arrows as shown in Fig. 1. The constraint then consists of requiring the labels of adjacent edges to match. A portion of such a tiling of the plane, with arrows, is shown in Fig. 2.

These arrows can be considered as a vector field on the lattice. In fact, let $\mathbf{A}(\mathbf{y})$ be the vector field of single arrows on the lattice, and $\mathbf{B}(\mathbf{y})$ the vector field of double arrows on the lattice. The index $\mathbf{y}$ labels the bonds, and can be taken to be the coordinates of the midpoint of the bond. The values that the vector fields take are either zero, if there is no arrow of the proper type on the bond, or a unit vector pointing in the direction of the arrow, if the arrow is of the proper type.

I now note from Fig. 1 that if I walk around the perimeter of either tile, I meet exactly one arrow of each type going my way, and one arrow of each type going the opposite way. This means the circulation of either vector field around a tile is zero, or

$$\sum_{\text{tile}} \Delta \cdot \mathbf{A} = 0 ,$$

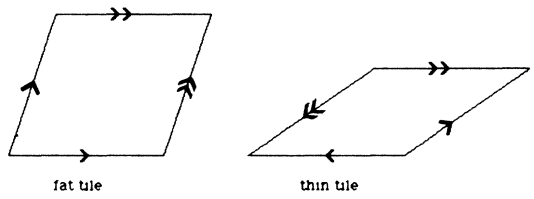

FIG. 1. The two basic Penrose tiles with edges labeled by arrows are shown. Note that this labeling differs by that of de Bruijn by exchanging single and double arrows, and then reversing the arrows.

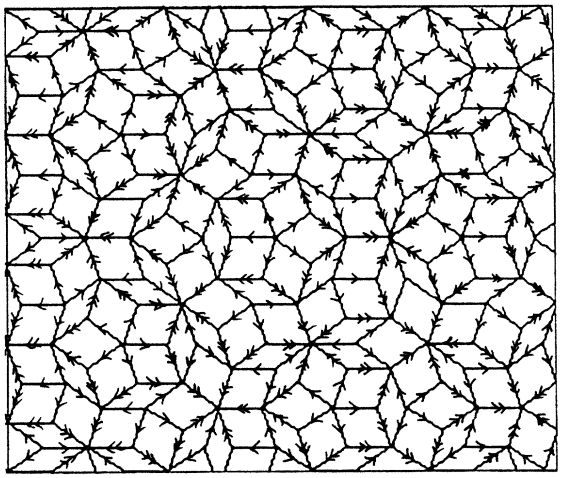

FIG. 2. A portion of the infinite Penrose lattice with arrows on the bonds is shown. The origin is at the center of the figure, and coincides with the absolute maximum of the wave function.

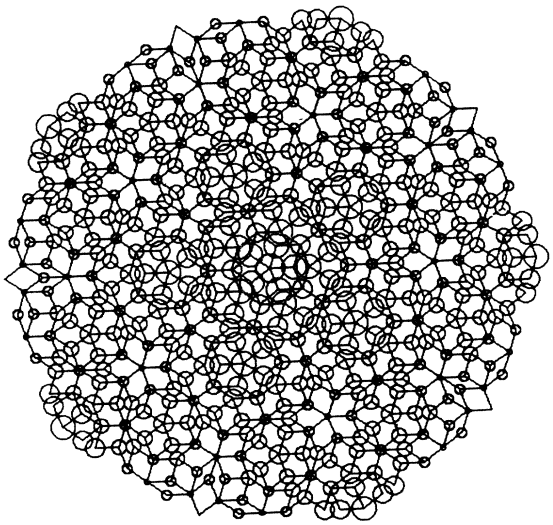

FIG. 3. A portion of the infinite Penrose lattice is shown. This is a dodecahedron of radius $R(5)=f^5$—the image of the seed after inflating four times. A circle is drawn centered on each site, with a radius proportional to the logarithm of the wave function at that site.

etc., for **B**, where Δ are a sequence of four unit vectors directed along the edges of the tile, pointing in the direction of the path. This is simply the discrete analogue of the line integral, and would be equivalent to curl $\mathbf{A}=0$ for a continuous system.

This condition then ensures that for any closed loop on the lattice,

$$\sum_{\text{loop}} \Delta\cdot\mathbf{A}=0 ,$$

etc., for **B**. Thus both **A** and **B** can be "integrated" to give single-valued scalar functions $m(\mathbf{x})$ and $n(\mathbf{x})$ of the lattice sites by

$$m(\mathbf{x})=\sum_{0}^{\mathbf{x}}\Delta\cdot\mathbf{A} ,$$

etc., for **B**, or

$$\Delta\cdot\mathbf{A}(\mathbf{x}+\Delta/2)=m(\mathbf{x}+\Delta)-m(\mathbf{x}) .$$

Examination of Fig. 2 shows that $m=0,1$ and $n\geq 0$.

With these preliminaries, I now introduce a tight-binding Hamiltonian for independent electrons, which sit on the sites with an on-site energy V, and hop along the bonds to neighboring sites. Thus, the Hamiltonian is to be of the form

$$H\Psi(\mathbf{x})=-\sum_{NN}\Psi(\mathbf{x}+\Delta)+V(\mathbf{x})\Psi(\mathbf{x})=E\Psi(\mathbf{x}) ,$$

where the summation is over all nearest-neighbor sites separated from **x** by a unit vector Δ. The eigenvalue equation can be rewritten as

$$\sum_{\text{NN}}\Psi(\mathbf{x}+\Delta)/\Psi(\mathbf{x})=V(\mathbf{x})-E .$$

I now try as an ansatz for an exact, unnormalized wave function the following form:

$$\Psi(\mathbf{x})=\exp\{-[rm(\mathbf{x})+sn(\mathbf{x})]\} .$$

Then the eigenvalue equation can be rewritten as

$$\sum_{\text{NN}}\exp[-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})]=V(\mathbf{x})-E .$$

This is a local potential, depending only on the nature of the local site at **x**. There are eight different sites, so the potential takes only eight different values.

Because the wave function is positive everywhere, it is the ground state, provided it does not increase too rapidly. This is the case, as will be demonstrated in Sec. V. In Figs. 3 and 4, I plot the logarithm of the wave function over the lattice, for a portion of the infinite lattice. I have chosen $r=s=1$.

In Fig. 5, I plot the wave function itself over the lattice, again with the choice $r=s=1$. If we denote the depen-

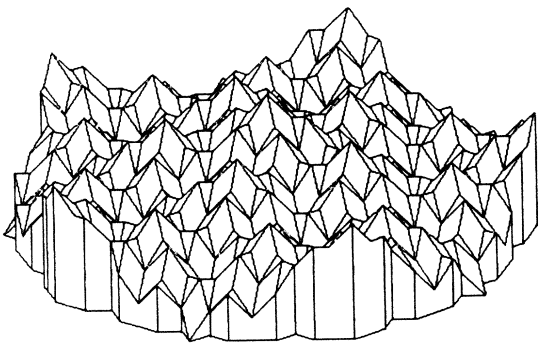

FIG. 4. Graph of the logarithm of the wave function over the previous portion of the Penrose lattice.

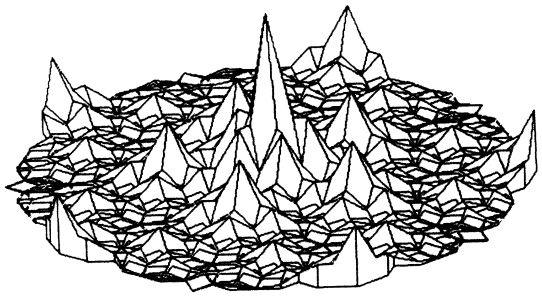

FIG. 5. Same figure as Fig. 4, except now I graph the wave function itself instead of the logarithm. The figure gives a better idea of the electronic density.

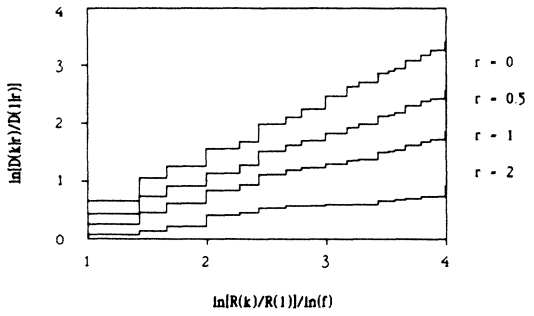

FIG. 6. Logarithm of the rth moment of the wave function versus the logarithm of the radius of the region. Specifically, I plot $\ln[D(k\,|\,r)/D(1\,|\,r)]$ as a function of $\ln[R(k)/R(1)]/\ln(f)$; all quantities are defined in the text. Note the approach to straight lines.

dence of the wave function on the parameters r,s by $\Psi(\mathbf{x}\,|\,r,s)$, then we note the relationship

$$\Psi^k(\mathbf{x}\,|\,r,s)=\Psi(\mathbf{x}\,|\,kr,ks)\ .$$

Thus we can relate different powers of the wave function to the wave function for different parameters. Figure 5 then is also the probability density for the wave function with $r=s=\frac{1}{2}$.

An interesting quantity to investigate is the integral of the wave function out to a given radius, for the growth of this quantity gives much information about the decay and localization of the wave function. Instead of the radius, I consider a slightly different variable R, defined to be the distance from the origin out to the vertex of a decagon centered on the origin, which I call the radius of the decagon. This decagon has the same orientation as the lattice itself. I then scale the radius R as $R(k)=f^k$, where $f=(\sqrt{5}+1)/2$ is the golden mean, so that whenever k takes integer values, the decagon is the same size as an inflated sample.

I now restrict myself to $r=s$, and define $D(k\,|\,r)$ to be the sum of the wave function $\Psi(\mathbf{x}\,|\,r,r)$ over all sites $\mathbf{x}$ within the decagon of radius $R(k)$. Equivalently,

$$D(k\,|\,r)=\sum_{|\mathbf{x}|<R(k)}\Psi(\mathbf{x}\,|\,r,r)=\sum_{|\mathbf{x}|<R(k)}\Psi^r(\mathbf{x}\,|\,1,1)\ .$$

Thus $D(k\,|\,r)$ might also be called the rth moment of the wave function $\Psi(\mathbf{x}\,|\,1,1)$, or the partial participation ratios.

If $r=0$, then $D(k\,|\,0)$ is just the number of sites in the decagon of size $R(k)$, so that it grows as $R^2(k)$. In Fig. 6, I show a plot of $\ln[D(k\,|\,r)/D(1\,|\,r)]$ versus $k=\ln[R(k)/R(1)]/\ln(f)$, for various values of r. [Once again, f is the golden mean $(\sqrt{5}+1)/2$.] The curves approximate straight lines for increasing k, so one defines an exponent $\alpha(r)$, where for large R,

$$D(k\,|\,r)\to D_0R^{\alpha(r)}(k)\ ,$$

with D_0 a more slowly varying factor. The exponent $\alpha(r)$ is given by the slope of the curve divided by the scale factor $\ln(f)$. I find the following values:

$$r=0,\quad \alpha(0)=2\ \text{(exact)}\ ,$$

$$r=0.5,\quad \alpha(0.5)=1.57\pm0.05\ ,$$

$$r=1,\quad \alpha(1)=1.1\pm0.1\ ,$$

$$r=2,\quad \alpha(2)=0.49\pm0.05\ .$$

III. THE SELF-SIMILARITY OF THE WAVE FUNCTION

I now demonstrate the self-similarity of the wave function. Consider two identical regions of the Penrose lattice of diameter D, located about points $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively. According to a theorem of Conway, quoted by Gardner, two such identical regions are never more than $2D$ apart, and are usually only D apart. Thus, identical regions are very common in a Penrose lattice.

Corresponding points in the two regions are $\mathbf{x}_1+\mathbf{x}$ and $\mathbf{x}_2+\mathbf{x}$. I write the wave function as

$$\Psi_1(\mathbf{x})=\Psi(\mathbf{x}_1+\mathbf{x})\ \text{ and }\ \Psi_2(\mathbf{x})=\Psi(\mathbf{x}_2+\mathbf{x})\ ,$$

and compare the two functions Ψ_1 and Ψ_2.

Note first, however, that the vector fields $\mathbf{A}$ and $\mathbf{B}$ are identical in the two regions, since they can be determined locally. Thus,

$$\mathbf{A}(\mathbf{x}_1+\mathbf{x})=\mathbf{A}(\mathbf{x}_2+\mathbf{x})\ ,$$

etc., for $\mathbf{B}$.

Now,

$$\Psi_2(\mathbf{x})=\Psi(\mathbf{x}_2+\mathbf{x})=\exp\left[\sum^{\mathbf{x}_2+\mathbf{x}}[-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})]\right]=\exp\left[\left[\sum^{\mathbf{x}_1}{}_0+\sum^{\mathbf{x}_2}{}_{\mathbf{x}_1}+\sum^{\mathbf{x}_2+\mathbf{x}}{}_{\mathbf{x}_2}\right][-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})]\right]\ .$$

But since the vector fields are identical in the two regions,

$$\sum^{x_2+x}{}_{x_2}[-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})] = \sum^{x_1+x}{}_{x_1}[-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})] .$$

Thus, I rewrite the equation as

$$\Psi_2(\mathbf{x})=\exp\left[\sum^{x_2}{}_{x_1}[-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})]\right] \times\exp\left[\sum^{x_1+x}[-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})]\right] =\Omega\Psi_1(\mathbf{x}) .$$

One finally arrives at the result that the wave functions in the two regions are multiples of one another, and differ only by a scale factor or normalization constant,

$$\frac{\Psi_2(\mathbf{x})}{\Psi_1(\mathbf{x})}=\Omega=\exp\left[\sum^{x_2}{}_{x_1}[-(r\Delta\cdot\mathbf{A}+s\Delta\cdot\mathbf{B})]\right] .$$

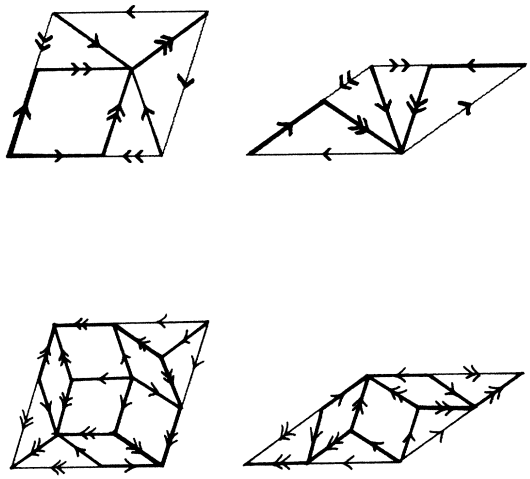

FIG. 7. (a) shows how the basic tiles are inflated to produce a larger pattern, here shown on a smaller scale by darker lines. (b) similarly shows the effect of a twofold inflation.

IV. SCALING PROPERTIES OF THE WAVE FUNCTION

The Penrose lattice itself is self-similar and the transformation which relates two lattices of different sizes is the inflation transformation. This transformation can be used in either direction. For instance, the finite portions of the infinite Penrose lattice in the figures were grown by the inflation transformation from a seed of ten tiles, which form a small decagon at the center of Fig. 2. This method also has the desirable effects of preserving the D_5 dihedral symmetry of the lattice, and ensuring that the maximum of the wave function is at the origin.

But the inflation transformation also can be used in the other direction, so that for a given Penrose lattice, one can find within it larger and larger Penrose patterns. In this case, these patterns will be the previous lattices in the growth process, suitably enlarged. The scale factor for this transformation is the golden mean $f=(\sqrt{5}+1)/2$. I now want to exploit this aspect of the inflation transformation.

First, I show the inflation transformation in Fig. 7(a), by showing the effect on the two basic Penrose tiles. However, because a single inflation reverses the arrows, it is actually more convenient to inflate twice. The result of such a twofold inflation is shown in Fig. 7(b).

After a twofold inflation, two vertices of a big rhombus that were previously connected by a single arrow, are now connected by a single arrow and two double arrows, while two vertices that were previously connected by a double arrow, are now still connected by a double arrow, because the two single arrows introduced have opposite orientation, and thus cancel.

Suppose I take the initial seed of ten tiles. The origin is the reference point, and the ten sites at the vertices of the perimeter alternate. Five of them (the fat vertices) are separated a single and a double arrow away from the origin, while the other five (the thin vertices) are separated only a double arrow away from the origin.

After I inflate $k-1$ times, k an odd integer, these vertices are still the vertices of a decagon, but a decagon of size $R(k)=f^k$. And the sites I called the thin vertices are still only separated a single double arrow away from the origin. Thus the wave function at this site is down from the value at the origin by a factor of only $\exp(-s)$, and does not decay at all with distance.

On the other hand, for the fat vertices, after I have inflated $k-2$ times suppose we have m single arrows and n double arrows. After a twofold inflation, we have $m'=m$ single arrows and $n'=n+2m$ double arrows. Thus for the fat vertices, I start with $(m,n)=(1,1)$, I get (1,3), then $(1,3+2)=(1,5),\ldots,(1,k)$. Assume that $r=s$, then the wave function on a fat site is down from the value at the origin by a factor of $\exp[-r(k+1)]$. Since this fat site is now located a distance $R(k)=f^k$ from the origin, this gives a power-law decay for the wave function on these sites of the form

$$\Psi(\mathbf{x}\mid r,r)=\exp(-r)R^{-r/\ln(f)} .$$

Examine the tiles in Fig. 1; the scalar functions m,n are larger on some vertices, smaller on others. Now examine the effect of a twofold inflation on the tiles as shown in Fig. 7(b). Of all the new sites in and on the perimeter of each tile, the scalar functions m,n are still either larger or smaller on the same sites as before inflation. Thus, the previously determined wave function on the fat site of a decagon is a lower bound for the wave function over the whole decagon.

V. LIMITING DISTRIBUTION OF THE WAVE FUNCTION

Let (m,n) denote the arrow coordinates of a site or tile from the origin, meaning that if $\mathbf{x}$ is the location of the site or of the labeled corner of a tile, then $m=m(\mathbf{x})$ and $n=n(\mathbf{x})$. (The labeled corner of a tile is the corner with both single arrows going out.) If I know the arrow coordinates of a site $\mathbf{x}$, then I immediately know the wave function at the site $\mathbf{x}$ to be $\Psi(\mathbf{x})=\exp[-(rm+sn)]$.

Thus if I know the number of sites with arrow coordinates (m,n), then I know the number of sites with wave function $\Psi=\exp[-(rm+sn)]$, and hence the moments of Ψ. This distribution I now determine.

First, if I examine Fig. 2, I see that the arrow coordinates of all tiles are of the form $(0,n)$. Let the distributions $F(n)$ and $T(n)$ denote the number of fat and thin tiles, respectively, in a given decagon of radius R. If I perform a twofold inflation, I obtain new numbers $F'(n)$ and $T'(n)$ in a decagon of radius $R'=f^2R$. I can easily find the relationship between the new and old distributions, and in this way generate distributions for larger and larger regions of the infinite Penrose lattice.

The initial seed has the distributions:

$$F(n\mid 1)=0\ ,\quad \text{except } F(0\mid 1)=5,$$

$$T(n\mid 1)=0,\quad \text{except } T(1\mid 1)=5\ .$$

After $(k-1)/2$ twofold inflations, k an odd integer, I obtain the new distributions $F(n\mid k)$ and $T(n\mid k)$ for a decagon of radius $R(k)=f^k$.

Since the arrow coordinates of a tile are $(0,n)$, the coordinates after inflation of the labeled vertex are unchanged, because the single-arrow coordinate is zero. If there is a fat tile with n, then I see from Fig. 7(b) that after a twofold inflation, there is a fat tile with n, three fat tiles and one thin tile with $n+1$, and one fat tile and two thin tiles with $n+2$. Likewise for a thin tile with n, I again see from Fig. 7(b) that after a twofold inflation there are two fat tiles with n, and one fat tile and two thin tiles with $n+1$.

Converting these observations into equations, I find the following recursion relations for the distribution functions:

$$F(n\mid k)=2F(n\mid k)+3F(n-1\mid k)+F(n-2\mid k)+2T(n\mid k)+T(n-1\mid k)\ ,$$

$$T(n\mid k+2)=2T(n-1\mid k)+F(n-1\mid k)+2F(n-2\mid k)\ .$$

Then from our initial conditions, the equations can easily be iterated, and in fact can be solved exactly.

One feature that can easily be seen from the equations, and which was determined previously, is that $F(n\mid k)=0$ for $n>k$, and etc. for T. This leads me to introduce the scaled variable $z\equiv n/k$. Then for large k, I find the scaling forms for $0\le z\le 1$,

$$F(n\mid k)\to F_0 f^{8kz(z-1)}\ ,$$

$$T(n\mid k)\to T_0 f^{8kz(z-1)}\ .$$

The coefficients F_0, T_0 are more slowly varying functions of k.

These forms then give us the scaling distribution $P(n\mid k)$, which is defined to be the limit as $k\to\infty$ of the number of sites in a decagon of radius f^k, with arrow coordinates (m',n'), where $m'+n'=n$. Thus, $P(n\mid k)$ is also the scaling distribution for $\ln[\Psi(x\mid 1,1)]=n$. The result is

$$P(n\mid k)\equiv P(z,k)=P_0 f^{8kz(1-z)},\quad 0\le z\le 1\ ,$$
$$=0,\quad z\ge 1\ ,$$

where $z=n/k$, and P_0 is determined by the overall normalization to the total number of sites as

$$P_0=20f^2[2k\ln(f)/\pi]^{1/2}\ .$$

This expression can now be used to evaluate the moments

$$D(k\mid r)=\sum_{|x|<R(k)}\Psi(x\mid r,r)=\sum_{|x|<R(k)}\Psi^r(x\mid 1,1)\to k\int_0^1 P(z,k)\exp(-rkz)dz\ .$$

For large k, this integral can be evaluated by the saddle-point method, and I find

$$D(k\mid r)\to\exp\{k[8\ln(f)z_0(1-z_0)-rz_0]\}\ ,$$

where z_0 is the value of z at which the exponent is a maximum, given by

$$z_0=\begin{cases}[1-r/8\ln(f)] & \text{if } r\le 8\ln(f)\ ,\\ 0 & \text{if } r\ge 8\ln(f)\ .\end{cases}$$

Substitution gives

$$D(k\mid r)\to\begin{cases}f^{2[1-r/8\ln(f)]^2} & \text{if } r\le 8\ln(f)\ ,\\ 1 & \text{if } r\ge 8\ln(f)\ .\end{cases}$$

Combining this result with the expression for the radius of the decagon, $R(k)=f^f$, the exponent $\alpha(r)$ can now be evaluated as

$$\alpha(r)=\begin{cases}2[1-r/8\ln(f)]^2, & r\le 8\ln(f)\ ,\\ 0, & r\ge 8\ln(f)\ .\end{cases}$$

The fit with the previous numerical data is excellent. Note that when the parameter r in the potential becomes greater than the critical value $r_c=4\ln(f)=1.9248\ldots$, the wave function becomes square integrable and hence localized.

VI. CONCLUSION

Since I knew the exact ground-state wave function—in fact, I started with the wave function and then constructed the Hamiltonian accordingly—I could evaluate the properties of this wave function in much greater detail than one could hope to do for a general system. Yet the properties I have found are qualitatively what one might expect for the general case. As I mentioned in the Introduction, the one-dimensional Fibonacci lattice can be treated by the same methods, and the self-similarity is the same for certain states in the spectrum. However, Kohmoto and Tang have found other states which are chaotic.[11] Thus I am led to conjecture that for at least some eigenstates of a more general quasiperiodic system: (1) the wave functions exhibit self-similarity, in that portions of a wave function over identical configurations

differ only by a scale and phase factor, and (2) the distribution of the wave function for larger and larger regions approaches a rather simple scaling function. Kohmoto would go further, and argues for a particular scaling relation between exponents for the wave function and the density of states.[11] Perhaps my conjecture is only based on hope, and on two exactly solved models, yet I see nothing pathological in the particular model I have solved, except possibly the fact that I could solve it.

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