

Fractal character of wave functions in one-dimensional incommensurate systems

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The electronic wave functions of simple one-dimensional systems with a modulation potential incommensurate with that of the underlying lattice are determined by a direct diagonalization method. The existence of the metal-insulator transition is also obtained by a renormalization-group method. Numerical evidence for a fractal character of the wave functions is obtained and the fractal dimensionality D is calculated as a function of the strength of the modulation potential V_0 . At the critical point $V_0 = 2t$, we find that $D = 0.80 \pm 0.15$. The wave functions can also be characterized by the localization length l_c and the amplitude correlation length ξ .

In recent years, there has been much interest in crystalline solids with incommensurate lattice potentials.¹⁻¹⁰ These systems lead to rich spectra and wave functions because they are, in some sense, intermediate between periodic and random. Periodic potentials lead to extended eigenstates, whereas random potentials lead to localized eigenstates in one dimension (1D). Although there is no rigorous proofs, the general belief is that almost periodic potentials lead in 1D to a metal-insulator transition (Anderson transition) at a critical value of the potential strength. Such a transition in the nature of the eigenstates—which may be induced experimentally in the same sample by, for example, external pressure—presents a very interesting theoretical possibility that is worth investigating experimentally.

Within the subject of localization in disordered systems the question of how to characterize the wave functions has been under intense discussion.^{11,12} A new way for characterizing the wave functions of disordered systems by their fractal dimensionality has lately been suggested¹¹ and has been used to determine the mobility edge separating localized and extended states. The almost periodic potential in one dimension with its Anderson localization transition is a very interesting system to study the fractal behavior of the wave function at the mobility edge where the upper cutoff length is infinite. The behavior of the localization length in the localized regime as well as the behavior of the correlation length in the extended regime is worth investigating.

In the present paper we show results of numerical experiments on one-dimensional incommensurate systems which produce a metal-insulator transition as the strength of the incommensurate potential increases. We are able to assign a fractal dimensionality to the eigenstates, and through the fractal dimensionality we obtain the position of the mobility edge.

The model we consider is

$$\epsilon_n C_n + t(C_{n+1} + C_{n-1}) = EC_n, \quad (1)$$

where the energy at site n is $\epsilon_n = V_0 \cos(Qn)$, C_n is the amplitude at site n , t is the hopping matrix element, V_0 is the modulation potential strength, Q is the wave vector of

the modulation, and the lattice constant is taken to be 1. We also impose rigid boundary conditions to simplify diagonalization of Eq. (1).

To decide the nature of the eigenstates of the model in Eq. (1), we first accurately calculated the density of states (DOS) so the positions and widths of bands and gaps are known. With the DOS known, by direct diagonalization of Eq. (1) we obtained the eigenstates, and from its spatial behavior one can decide their nature, i.e., whether they are localized or extended. We also study the transmission coefficient of the system as the size of the system N increases for a given energy E , modulation strength V_0 , and wave vector Q . For localized states the transmission coefficient approaches zero as $n \rightarrow \infty$, while for extended states the transmission coefficient is nonzero as $n \rightarrow \infty$. Special care is required, for some extremely narrow bands, in order to avoid calculating the transmission coefficient at the gap and erroneously interpreting the result as showing the existence of localized eigenstates. Finally, we have shown numerically,⁴ and Suslov⁹ has demonstrated subsequently but independently, that there is a real-space renormalization transformation which maps the Hamiltonian to itself and allows important conclusions to be reached. It is indeed the consistency of the three complementary techniques which allowed us to decide with confidence about the nature of eigenstates.⁴

We have found that for the case where $\epsilon_n = V_0 \cos(Qn)$ and Q is an irrational multiple of π , $V_{0c}/t = 2$ is the critical modulation strength independent of E and Q . For $V_0 > 2t$ all the states are localized, while for $V_0 < 2t$ all the states are extended. For more complicated modulations⁴ such as

$$\epsilon_n = V_0 [\cos Qn + V_1 \cos(2Qn)],$$

mobility edges have been found even in one dimension. For a given value of V_0 and V_1 eigenstates corresponding to high energies are easier to localize than those for low energies. Of course, for high values of V_0 and V_1 , all eigenstates are localized.

The most successful technique in deciding about the nature of eigenstates is the real-space renormalization or block method that was introduced in Ref. 4. One can ap-

proximate Q by $2\pi N_1/M_1$ (N_1 and M_1 are integers without a common factor) so that after M_1 sites the potential almost repeats. Consider the n th group of M_1 consecutive sites (n th block). Within this group one can define $\epsilon_n^{(1)}$ as the eigenvalue closer to the energy under consideration and $t^{(1)}$ as the effective hopping-matrix element between the corresponding wave functions of neighboring blocks. We define $t^{(1)} = \langle \psi_n | H | \psi_{n+1} \rangle$ where ψ_n is the wave function of the n th block belonging to the eigenenergy closer to the energy under consideration. Since $\psi_n = \sum_i C_{ni} | i \rangle$, where the i th summation is over the sites of the n th block, one obtains $t^{(1)} = t C_{nM}^\dagger C_{(n+1)M}$. $C_{(n+1)M}$ is the amplitude at the first site of the $(n+1)$ th block. In all the cases we examined $\epsilon_n^{(1)}$ is, within numerical uncertainties, of the form $V_0^{(1)} \cos(Q^{(1)}n + \phi)$. This shows that under this transformation the original Hamiltonian maps into itself with transformed values of the parameters $y^{(1)} \equiv V_0^{(1)}/2t^{(1)}$ and $Q^{(1)}$. In Fig. 1 we show our numerical results for the model with $\epsilon_n = V_0 \cos(Qn)$ and $Q=0.7$. For this value of Q we have that the first period is $M_1=9$. Therefore we diagonalize the 9×9 matrix and find all the eigenvalues and eigenvectors. Within this group we define $\epsilon_n^{(1)}$ as the eigenvalue closer to the energy under consideration. In the results shown in Fig. 1 we used $E=2.0t$ as the energy under consideration. We continue diagonalizing the next 9×9 matrix and so on. As we discussed before, $t^{(1)} = t C_{nM}^\dagger C_{(n+1)M}$, where C_{nM} is the eigenvector at the last site of the n th block and $C_{(n+1)M}$ is the amplitude of the eigenvector at the first site of the $(n+1)$ th block. By plotting $\epsilon_n^{(1)}$ versus the index n of the block, we obtain

$$\epsilon_n^{(1)} = V_0^{(1)} \cos(Q^{(1)}n + \phi).$$

Thus, after the block transformation, the Hamiltonian was indeed mapped into itself. Using the new value of

$Q^{(1)}$, we can repeat the transformation by introducing second-level blocks consisting of consecutive first-level blocks. After the second transformation our unit of length is $L_2 = M_1 M_2$. In the case of $Q=0.7$, we find that $Q^{(1)} \approx 2\pi(4/36)$, and consequently, $M_2=36$. Suslov⁹ has demonstrated that the numbers M_1, M_2, \dots are obtained by a continued fraction expansion of $Q/2\pi$, where M_n is essentially determined as the integer part of the inverse of the difference $1/\beta_{n-1} - [1/\beta_{n-1}]$, where β_{n-1} is the terminating part of the continued fraction and $[1/\beta_{n-1}] = M_{n-1}$ is the integer part of $1/\beta_{n-1}$. From Fig. 1, note that $V_0^{(1)}/t^{(1)}$ versus V_0/t increases very quickly for $V_0 > 2t$ and decreases very quickly for $V_0 < 2t$. For $V_0=2t$, we have $V_0^{(1)}=2t^{(1)}$, i.e., $V_0=2t$ is a critical point. It is very encouraging that even with the first level of approximation of $Q/2\pi$ by the ratio of two integers without a common factor gives a simple law for the transformation of the coefficient V_0 . Our numerical results showed that for all the values $V_0/2t > 1$, $V_0^{(1)}/2t^{(1)} > V_0/2t$, while for all the values $V_0/2t < 1$ and $V_0^{(1)}/2t^{(1)} < V_0/2t$ independent of the values of E and Q . Hence, by repeating this transformation it follows that for $V_0 > 2t$ ($V_0 < 2t$) the Hamiltonian maps finally into

$$\lim_{n \rightarrow \infty} V_0^{(n)}/2t^{(n)} \rightarrow \infty(0),$$

which physically means that in the first case the states are localized and in the second case they are extended. To find the exact form of the transformation of the coefficient V_0 , we plot in Fig. 2 $\ln(V_0^{(1)}/2t^{(1)})$ versus $\ln(V_0/2t)$. All the numerical results lie on a straight line, and therefore we have that

$$V_0^{(1)}/2t^{(1)} = (V_0/2t)^{S_1}. \quad (2)$$

The exponent S_1 is just 9, i.e., the first period one obtains by approximating $Q/2\pi$ as the ratio of two integers without a common factor: $S_1 = M_1$. Note from Fig. 2 that the transformation law given by Eq. (2) is obeyed for $V_0 > 2t$ and for $V_0 < 2t$ as well. This transformation law

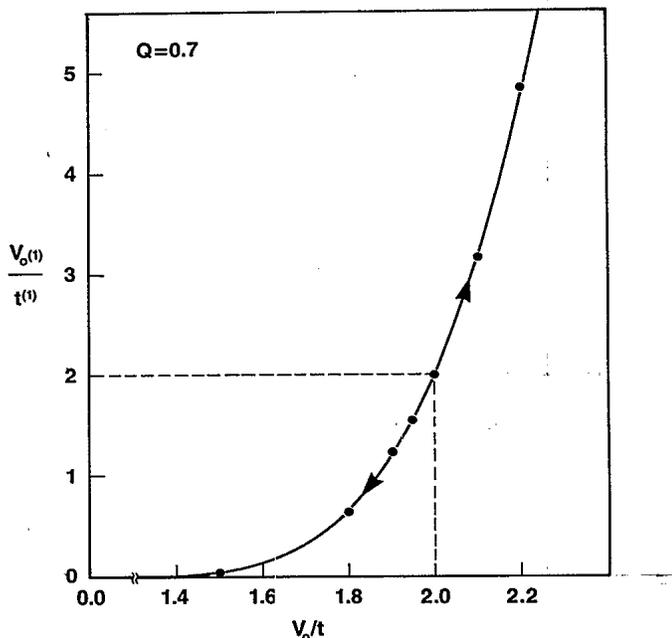


FIG. 1. $V_0^{(1)}/t^{(1)}$ versus V_0/t for $Q=0.7$ and $E=2.0t$. $V_0=2t$ is a critical point.

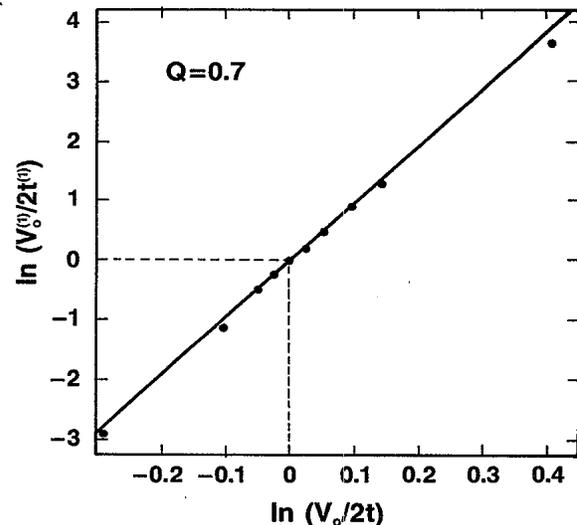


FIG. 2. Logarithm of $V_0^{(1)}/2t^{(1)}$ versus logarithm of $V_0/2t$ for $Q=0.7$ and $E=2.0t$. The straight line through the points gives $V_0^{(1)}/2t^{(1)} \sim (V_0/2t)^9$.

is in agreement with the analytical results of Suslov,⁹ which also finds that $y^{(n)} = (y^{(n-1)})^{S_n}$ with $S_n = M_n$. Thus for the simple case of $\epsilon_n = V_0 \cos(Qn)$ we obtained a metal-insulator transition as V_0 crosses $2t$. Aubry has suggested that the localization length l_c is given by

$$l_c = 1/\ln(V_0/2t) \rightarrow \frac{2t}{V_0 - 2t} \text{ as } V_0 \rightarrow 2t, \quad (3)$$

$$\equiv \frac{1}{y^{(0)} - 1}.$$

Suslov,⁹ using renormalization group ideas, found that the localization length diverges near the transition in accord with a power law, with a universal critical exponent equal to unity. Note from the second part of Eq. (3) that same law is obtained by expanding Aubry's result for l_c near the transition $V_0 = 2t$. The block transformation allows an easy derivation of Eq. (3). Indeed after the n th transformation we have [using Eq. (2)]

$$\ln y^{(n)} = M_n \ln y^{(n-1)} = M_n M_{n-1} \cdots M_1 \ln y^{(0)} \\ = L_n \ln y^{(0)}. \quad (4)$$

However, for $y^{(n)}$ much larger than unity one can use perturbation theory to obtain the localization length which then is simply equal to $1/\ln(y^{(n)})$ in units of L_n . Combining this with Eq. (4), we obtain Eq. (3). We have numerically calculated the localization length l_c and find that it agrees very well with the form given by Eq. (3). Very close to the critical point special care has to be taken in order to correctly calculate l_c . In particular, for $1/(V_0 - 2t) > 1000$, we had problems calculating l_c correctly. Very close to the critical point we always have new periods of larger and larger lengths, and as we increase the size of the system to better calculate l_c , we obtain large fluctuations for the value of l_c . In the three-dimensional disordered systems where we have a metal-insulator transition in the extended regime, one usually defines a correlation length ξ , which describes the maximum distance scale on which the amplitudes of the wave functions fluctuate appreciably. For the disordered systems ξ , as well as l_c , diverges near the mobility edge¹³ with a power law and with a universal critical exponent believed to be equal to unity. For the incommensurate modulation in one dimension in the extended regime, it is very tempting to define a correlation length ξ also.

The transformation (4) allows us to show the existence of a correlation length ξ in the extended regime and to obtain its dependence of $V_0/2t$ for $V_0/2t < 1$. Indeed, when $y^{(n)}$, for large enough n , reaches a value y_c , which is much smaller than unity, the perturbation $V_0^{(n)}$ is practically negligible, and from then on the wave function is essentially uniform. Thus the largest length for which there are still appreciable fluctuations in L_n corresponds to $\ln y^{(n)} = \ln y_c$. It follows then that $\xi = L_n$, or using Eq. (4), that

$$\xi = L_n = \frac{|\ln y_c|}{\ln(2t/V_0)}. \quad (5)$$

The way ξ was defined does not fix a multiplicative factor of order unity. This is reflected in the appearance of the

quantity y_c in Eq. (5). One way to define y_c is as the point, where the tangent at the critical value in Fig. 1 crosses the horizontal axis. If we further assume that the quantities β_n are uniformly distributed over their range $[0,1]$ as Q varies, we obtain for the average value of $|\ln y_c|$, $\langle |\ln y_c| \rangle \approx 0.5$. Our numerical data are inconclusive regarding the value of ξ . This is due to the broad crossover character of ξ and to the Q dependence of the proportionality factor. However, our data are not inconsistent with a value of $|\ln y_c| \approx 1$. From Eq. (5) it follows that

$$\xi \approx |\ln y_c| \frac{2t}{2t - V_0} \quad (6)$$

for $2t - V_0 \ll 2$.

It has recently been suggested that the fractal dimension is a new way of characterizing the wave functions in disordered systems.¹¹ The quantity D can be defined if

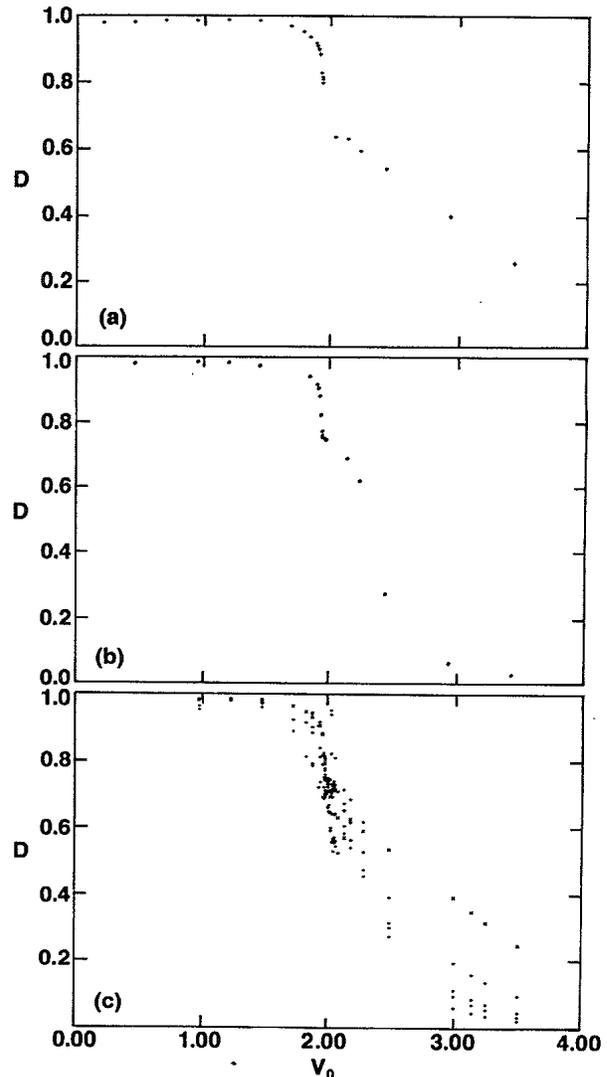


FIG. 3. Fractal dimensionality D versus V_0/t for different values of Q and $E=0$: (a) $Q=0.3$; (b) $Q=0.7$; (c) superimposed results for five different values of Q (0.3, 0.4, 0.5, 0.6, and 0.7).

the integral of the probability density $|\psi(r)|^2$ within a sphere of radius L is proportional to L^D with D independent of L . $\psi(r)$ is the normalized wave function of the disordered system under consideration. For a disordered eigenfunction the result depends strongly on where the center of the sphere is placed. To avoid this difficulty a weighted average over all positions of the center is taken. The weight is the probability density of finding the particle at each point. Thus the fractal dimensionality was defined as the L -independent exponent in the relation $A(L) = \text{const}L^D$, where $A(L)$ is the density correlation function

$$A(L) = \int dr |\psi(r)|^2 \int_0^L dr' |\psi(r'+r)|^2. \quad (7)$$

For uniform extended states, the fractal dimensionality coincides with the Euclidean dimensionality $D=d$. Thus for extended states and $L \gg \xi$, $D=d$; as a result a non-trivial fractal dimensionality can be defined only for $L \ll \xi$. For localized states, a fractal dimensionality can only be defined for lengths less than the effective extent of the eigenfunction, beyond this length $A(L)$ saturates approaching asymptotically one. Recently, Soukoulis and Economou¹¹ have calculated numerically the density correlation function $A(L)$ defined by Eq. (7) in order to check whether a fractal dimensionality can be defined for an eigenfunction in a disordered system. Their numerical results strongly suggest that D is well defined for length scales $L \ll \xi, l_c$. The most interesting case is for $d=3$ at the mobility edge, where both l_c and ξ are infinite. The fractal dimensionality at the mobility edge was estimated to be 1.7 ± 0.3 . Using these fractal ideas, Schreiber¹² calculated the whole mobility edge trajectory for a three-dimensional disordered tight-binding model with diagonal

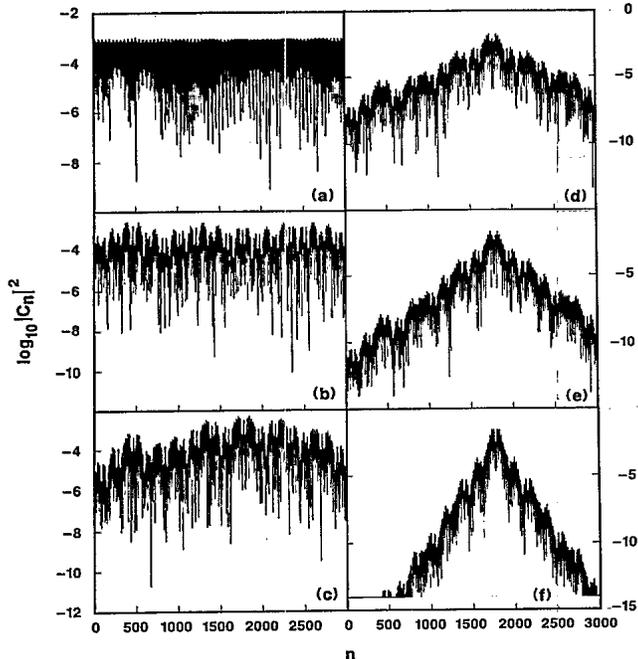


FIG. 4. Logarithm of the square of the wave functions versus length n at $E \approx 0$ and $Q = 0.3$ for (a) $V_0 = 1.50t$, (b) $V_0 = 1.99t$, (c) $V_0 = 2.00t$, (d) $V_0 = 2.005t$, (e) $V_0 = 2.01t$, and (f) $V_0 = 2.02t$.

disorder of Gaussian type.

For the one-dimensional incommensurate system given by Eq. (1), we calculate the fractal dimensionality D as a function of V_0 for a constant energy E . (We took $E=0$ as the energy under consideration in our numerical work.) Figure 3 shows the fractal dimensionality D as a function of V_0 . For $V_0 < 1.95t$, $D=1$, while for $V_0 > 2.05t$, D drops below 0.5. At the critical point $V_0 = 2t$, we estimate that $D = 0.80 \pm 0.15$ independent of E and Q . A very interesting feature of the fractal dimensionality D versus V_0 as can be seen from Fig. 3 is that D stays constant very close to 1 all the way to the critical point $V_0 = 2t$, and then just above the critical point, D drops rather abruptly and approaches zero.

The fluctuations in the value of D for different Q 's permits doubts as to whether the fractal dimensionality D is a rigorous concept in the present system, where there are infinite but *discrete* scales of fluctuation. Nevertheless, even if D is only an approximate concept, its systematic

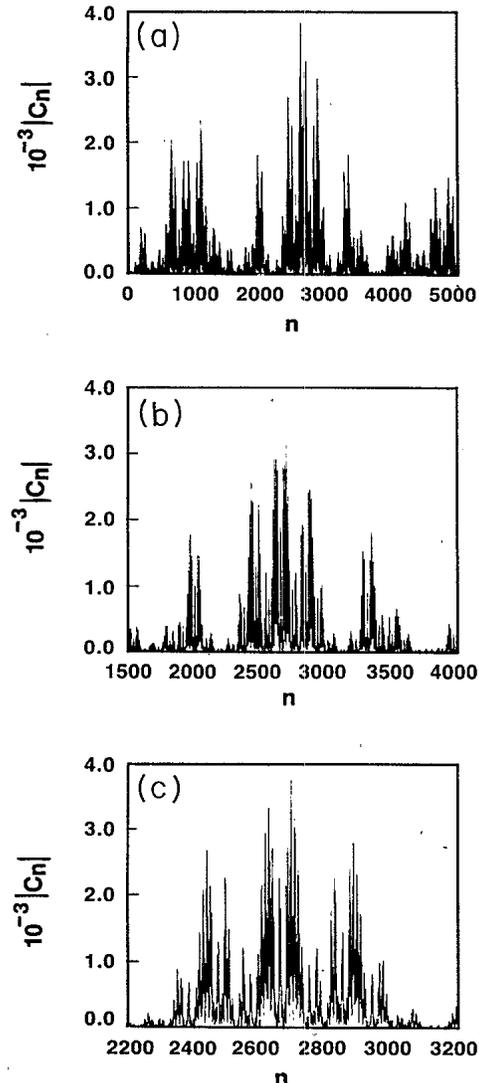


FIG. 5. Square of the wave function versus length n for $E \approx 0.0$, $Q = 0.3$, and $V_0 = 2.0t$. The display of different portions of the same wave function illustrate the self-similarity.

rather abrupt drop at the critical point provides an easy and convenient way to determine the position of the mobility edge very accurately. It must be pointed out that the narrowness of the critical region can be easily understood from Eqs. (3) and (6). Indeed, in order to observe even approximately a fractal behavior, a sufficient number of length scales (let us say four) must be present within the upper cutoff lengths ξ or l_c . In order for that to happen we must have $L_4 < \xi, l_c$, which implies (since each M_n is on the average equal to e) that

$$|1 - V_0/2t| \lesssim e^{-4} \approx 0.02, \quad (8)$$

which is consistent with our numerical results. This abrupt behavior of D can be used as another easy way to find critical points (mobility edges).

In Fig. 4 we plot the logarithm of the square of the wave functions versus the lattice sites for different values of V_0 for $E=0.0$ and $Q=0.3$. Note that even for $V_0=1.99t$ [Fig. 4(b)] the wave function is clearly extended. The only difference from the corresponding wave function at $V_0=1.5$ [Fig. 4(a)] is the absence of fluctuations in the latter. At $V_0=2t$ [Fig. 4(c)] we see that the fluctuations are more violent. We will study further the wave function at the critical point below. As we increase V_0 to $2.005t$ [Fig. 4(d)] we obtain a localized wave function which has strong amplitude fluctuations, but there is an overall exponential decrease. For $V_0=2.01t$ and $2.02t$ [Figs. 4(e) and 4(f)] we have clearly localized states. Now, exactly at the critical point the wave function is self-similar. In order to make the self-similarity clear, we plot in Fig. 5(a) the amplitude of the wave function for 5000 sites; in Fig. 5(b) we plot the amplitude of the wave function for 2500 sites, and in Fig. 5(c) for 1000 sites. Note that to a very good approximation the three figures are the same, which illustrate the approximate scale invariance.

CONCLUSIONS

We presented results based on the scaling theory that was developed⁴ by two of us by considering blocks whose size is equal to, or close to, the approximate periods of the system. Each successive transformation maps the problem into itself, with $y^{(n)} = (y^{(n-1)})^{M_n}$. This law, which was obtained numerically in Ref. 4, was derived analytically later by Suslov.⁹ From our experience with work in disordered systems, we feel that this renormalization group (or block method) is one of the most accurate and convenient methods for obtaining critical points (mobility edges).

We have been able to assign, at least approximately, a fractal character to the wave function of a one-dimensional incommensurate system. The fractal dimensionality D was obtained for different values of V_0 for $E=0$. Our results suggest that D stays close to 1 almost all the way to the critical point ($V_0=2t$) and then drops rather abruptly to small values. At the critical point, $V_0=2t$, $D=0.80 \pm 0.15$. It will be very interesting to calculate analytically D at $V_0=2t$. We have computed the localization length l_c , and this agrees reasonably well with Aubry's result, $l_c = 1/\ln(V_0/2t)$. We have also obtained a formula for the correlation length ξ in the extended states regime, and we have thus explained why the transition region around the critical point is so narrow. Finally, the self-similar character of the wave function at $V_0=2t$ was illustrated by the spatial behavior of the wave functions.

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