New Localization in a Quasiperiodic System

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We present a new type of localization phenomenon in a one-dimensional tight-binding model with a quasiperiodic potential $V_n = \lambda \tanh[A\cos(2\pi\omega n)]/\tanh A$, where ω is an irrational number. When A is small, the localization starts from the *center* of the spectrum at a value of λ; then the mobility edges move towards the edges of the spectrum with increasing λ; finally all the states become localized. This behavior is in contrast to the Anderson localization in three-dimensional random systems. When A is large, a more complicated behavior is found.

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A one-dimensional quasiperiodic tight-binding model (or discrete Schrödinger equation) is written as

$$-\psi_{n+1} - \psi_{n-1} + \lambda V(n\omega)\psi_n = E\psi_n\,, \qquad (1)$$

where ω is an irrational number and $V(x)$ is a periodic function, i.e., $V(x+1)=V(x)$. When the potential part is random, it represents the Anderson model of localization. The random electronic (or phonon) system is known to be always localized for one dimension (rigorous) and for two dimensions. Therefore one has to go to three dimensions to study the transition between the localized and the extended states.[1]

It is known that the quasiperiodic systems can have localized states.[2] In fact, they can have both extended and localized states even in one dimension for which one can apply many analytical or numerical techniques.

The quasiperiodic models studied well so far are (A) $V(x)=\cos(2\pi x)$,[3] (B) $V(x)=\tan(2\pi x)$,[4] and (C) $V(n\omega)$ having two values 1 and -1 which are arranged in the Fibonacci seuqence.[5,6] In model (A), all the states are extended for $\lambda < 2$ (purely absolutely continuous spectrum) and all the states are localized for $\lambda > 2$ (purely dense point spectrum). At the critical coupling $\lambda_c = 2$, all the states are critical (purely singular continuous spectrum). All the states are localized for model (B) and all the states are critical for model (C). All the above examples have a pure spectrum (absolutely continuous, singular continuous, or dense point). However, these are special cases and the pure spectrum is not a general feature of the one-dimensional quasiperiodic systems. For example, if we add one more frequency to (A) it appears that the localization starts from the edges of the spectrum as λ is increased and we have mobility edges.[7,8] This behavior of having localized states near the edges of the spectrum and extended states near the center of the spectrum is similar to that of the disordered systems,[1] and also it is natural from the mathematical point of view.[9] However, even the last case may be a special case since $V(x)$ contains only two Fourier components and it has a rather special form.

In this Letter we study a model

$$V(x) = \tanh[A\cos(2\pi x)]/\tanh A \qquad (2)$$

in order to understand the general localization phenomena in the quasiperiodic systems. Note that $V(x)$ takes only two values 1 and -1 when A goes to infinity and it is similar to model (C). When A approaches 0 it reduces to model (A), and for small A it is a smooth modification of model (A) since it contains all the higher Fourier components in $V(x)$. All the states are localized for a sufficiently large coupling $\lambda > \lambda_c$.[10] One expects the existence of mobility edges for $\lambda < \lambda_c$. One of the possibilities of the mobility-edge structure is that there would be infinitely many mobility edges. The remarkable feature of the one-dimensional quasiperiodic systems is the tendency for having a Cantor-set-like spectrum. There are infinitely many gaps and it is topologically self-similar. Therefore "subbands" may have mobility edges and there are an infinite hierarchical structure of subbands in the Cantor set. We find that this is not the case. Instead there are a finite number of mobility edges which behave in an unusual manner.

In order to distinguish localized, extended, and critical states we use two methods: One is to measure the bandwidths of the periodic systems where the irrational number ω is replaced by rational approximants;[5,10] the other is the multifractal analysis of the wave function itself.[11-13] In both methods, it is essential to take an appropriate series of rational approximants which converges to the irrational number ω. This corresponds to a finite-size scaling analysis. In the following calculation, we take ω to be $\sigma = (\sqrt{5}-1)/2$, the inverse of the "golden mean." Then the rational approximants are F_{n-1}/F_n, where F_n is the nth Fibonacci number defined by F_n

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$=F_{n-1}+F_{n-2}$ and $F_0=F_1=1$. In this case, each band is divided into three subbands as n is increased. Therefore each point in the spectrum for the irrational limit ($n\rightarrow\infty$) is identified by an infinite sequence of 1, 0, and -1, which represent the upper, middle, and lower subbands, respectively. This situation is the same as model (C).[14] The behavior of the bandwidth and wave function along the sequence is traced to distinguish localized, extended, and critical states.

The spectra of Eqs. (1) and (2) are shown in Fig. 1(a) for $A=1.0$ and Fig. 1(b) for $A=3.0$. Only the lower halves of the spectra ($E<0$) are displayed since the spectra are symmetric with respect to $E=0$. In region I, the spectra are dense point (localized state), while in region II the spectra are absolutely continuous (extended state). The concrete data to distinguish them will be presented in the latter part of this Letter. One of the most remarkable features we find in these figures is that localization of the wave functions does not always start from the edge of the spectrum.

At small values of λ, all the states are extended for both $A=1.0$ and $A=3.0$. For $A=1.0$, localization takes place first at the center of the spectrum as λ is increased; the boundary between the localized and the extended states (mobility edge) moves from the center towards the edge of the spectrum with increasing λ; finally all the states become localized at a value of λ ($=2.526$) as pointed out by one of us previously.[10] For $A=3.0$ a more complicated behavior is found. Localization from the edge of the spectrum occurs in addition to that from the center, and two mobility edges (in $E<0$) exist in a range of λ. For larger λ, however, the localized states near the edge of the spectrum disappear. On the other hand, the region of the localized states around the center gradually extends towards the edge, and finally at $\lambda=7.28$ all the states become localized.

The global dependence of this transition between localized and extended states on A and λ is shown in Fig. 2. In the area below the dashed line, the states near the center of the spectrum are extended; above the dashed line the localized region around the center appears; above the solid line all the states become localized. In the area to the right of the dash-dotted line, the localized region starting from the edge appears, and there are two mobility edges in $E<0$.

Now let us show examples of the analysis to distinguish localized and extended states numerically. First we show the approach from the bandwidth measurement. If we want to decide whether a state specified by a code $\{C_1,C_2,C_3,\ C_4,\dots\}$ ($C_m=-1$, 0, or 1) is extended, localized, or critical, we measure the width of the subband pointed to by a finite part of the sequence $\{C_1,C_2,C_3,C_4,\dots,C_p\}$. This subband is a band of a periodic system with a rational approximant F_{n-1}/F_n. The asymptotic behavior of the bandwidth B_n for large F_n determines the type of state. If the state is localized, B_n

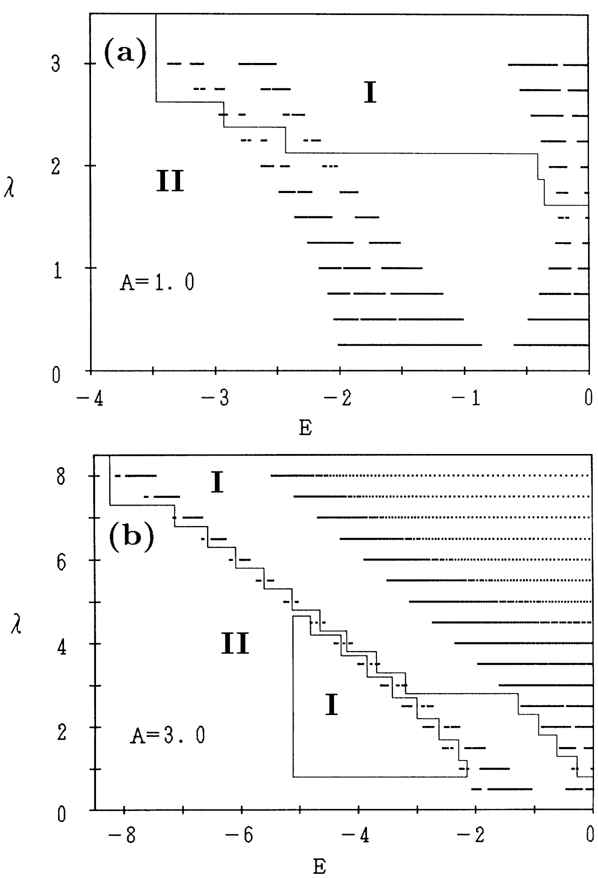

FIG. 1. Energy spectra of the model defined by Eqs. (1) and (2) with (a) $A=1.0$ and (b) $A=3.0$ for various values of λ. The wave functions are localized in region I, and are extended in region II.

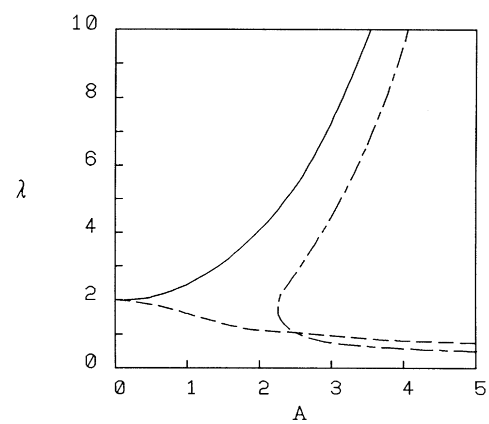

FIG. 2. The phase diagram on the A-λ plane. Above the solid line all the states are localized. The state at the center of the spectrum is localized (extended) above (below) the dashed line. In the area to the right of the dash-dotted line, localized states appear near the edges of the spectrum.

should decrease exponentially as a function of F_n. If the state is extended, B_n should behave as $B_n \sim 1/F_n$ unless the state coincides with an "edge state" which is identified by the codes $\{C_1,C_2,C_3,\ldots,1,1,1,1,1,1,\ldots\}$ or $\{C_1,C_2,C_3,\ldots,-1,-1,-1,-1,-1\ -1,\ldots\}$. For edge states, B_n should behave as $B_n \sim 1/F_n^2$ as a result of the Van Hove singularity. If the state is critical, B_n is expected to decrease with an arbitrary power (>1) of $1/F_n$. This method was successful in other quasiperiodic problems.[5,10] In fact, it is related to the idea of Thouless[15] who relates the energy change due to the periodic and antiperiodic boundary conditions of random systems to the electronic conductivity.

Figure 3 is a plot of n [$\simeq \log F_n/\log(1/\sigma)$] vs F_nB_n for the states with the code $\{0,-1,1,\ldots\}$ when $A=3.0$ and $\lambda=1.0$. The states specified by $\{0,-1,1,-1,1,1,1,1,1,1,\ldots\}$ and $\{0,-1,1,-1,-1,-1,-1,-1,-1,-1,\ldots\}$ (edge states) are extended because $B_n \sim 1/F_n^2$. The state specified by $\{0,-1,1,-1,0,0,0,0,0,0,\ldots\}$ is extended as well because $B_n \sim 1/F_n$. On the other hand, the state specified by $\{0,-1,1,0,-1,-1,-1,-1,\ -1,-1,\ldots\}$ is localized because B_n decrease exponentially. Therefore, there is a mobility edge located between the two states $\{0,-1,1,0,-1,-1,-1,-1,-1,\ldots\}$ and $\{0,-1,1,-1,1,1,1,1,1,1,\ldots\}$, which are next to each other. Therefore, it is concluded that a mobility edge is located in the energy gap between the two states.

By applying the same analysis to other states, it is concluded that all states from $\{0,0,0,0,0,\ldots\}$ to $\{0,-1,1,0,-1,-1,-1,-1,-1,-1,-1,\ldots\}$ are localized, and all the states from $\{0,-1,1,-1,1,1,1,1,\ldots\}$ to $\{-1,-1,1,-1,0,-1,-1,-1,-1,-1,\ldots\}$ are extended, and all the states from $\{-1,-1,1,-1,-1\ 1,1,1,1,1,1,\ldots\}$ to $\{-1,-1,-1,\ -1,-1,\ldots\}$ are localized. Thus there are two mobility edges for $E<0$ (i.e., four mobility edges on the whole spectrum) when $A=3.0$ and $\lambda=1.0$.

Next we show an analysis to study wave functions themselves from the multifractal point of view. We study the singular spectrum $f(\alpha)$[11] or equivalently the entropy function $S(\alpha)$[12,13] of the scaling index α defined by $p_j=|\psi_j|^2 \sim (1/F_n)^{\alpha_j}$ $(\sum_{j=1}^{F_n} p_j=1)$. An extended wave function does not have a singular probability measure and $p_j \sim 1/F_{n'}$ so $f(\alpha)$ is defined at a single point by $f(\alpha=1)=1$. On the other hand, a localized wave function has nonvanishing probability only on a finite number of lattice points (measure $=0$). These points have $\alpha=0$ and the other lattice points with zero probability have $\alpha=\infty$. So one has $f(\alpha=0)=0$ and $f(\alpha=\infty)=1$. A critical wave function with a distribution of α has a smooth $f(\alpha)$ defined on a finite interval $[\alpha_{\min},\alpha_{\max}]$. We calculate $f(\alpha)$ numerically in a finite system (a periodic approximation) according to the method of Refs. 12 and 13. However, in the analysis, we must be deliberate, because the numerical calculation in a finite system always gives a smooth $f(\alpha)$. Therefore a careful extrapolation is required to distinguish extended, localized, and critical states.[8]

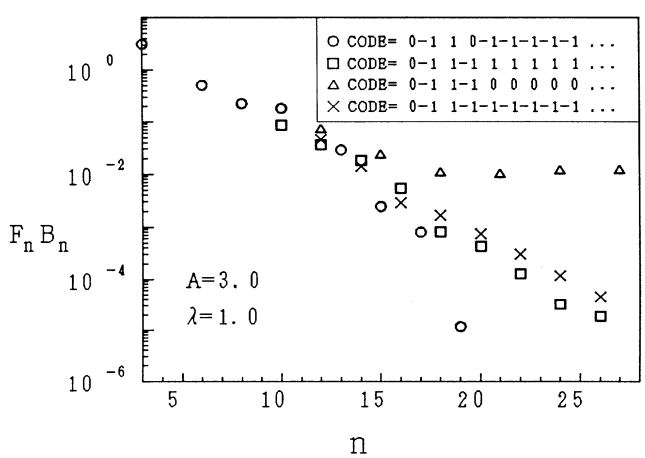

FIG. 3. Plot of F_nB_n vs n for $A=3.0$ and $\lambda=1.0$. The states specified by $\{0,-1,1,-1,\ldots\}$ are extended, while the state specified by $\{0,-1,1,0,-1,-1,-1,-1,\ldots\}$ is localized.

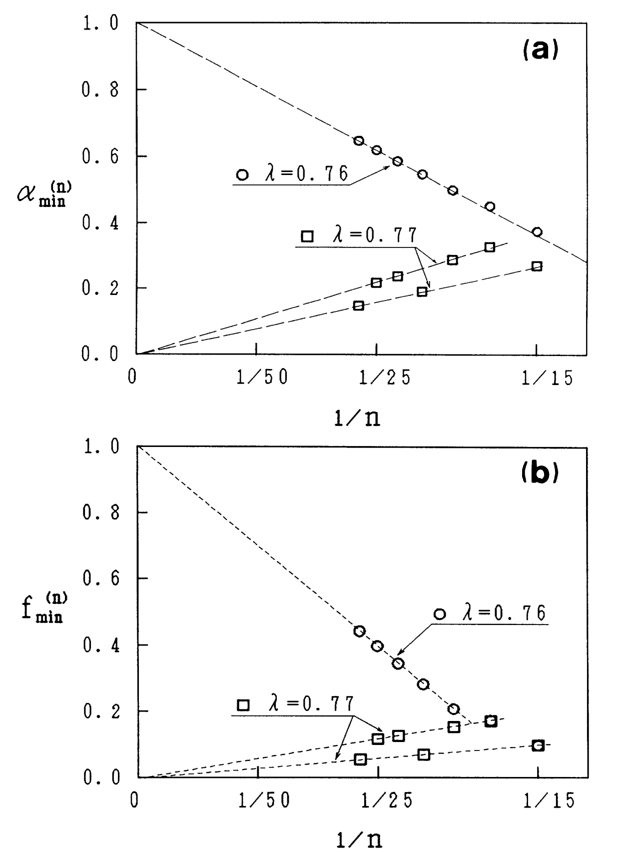

FIG. 4. Plots of (a) $\alpha_{\min}^{(n)}$ and (b) $f_{\min}^{(n)}$ as a function of $1/n$ at $\lambda=0.76$ and $\lambda=0.77$ with $A=3.0$ for the state $\{-1,-1,-1,-1,-1,\ldots\}$. A sharp transition is observed between $\lambda=0.76$ and $\lambda=0.77$.

Figures 4(a) and 4(b) are plots of $\alpha_{\min}^{(n)}$ and $f_{\min}^{(n)}$ [$\alpha_{\min}$ and $f(\alpha_{\min})$ calculated for F_n] against $1/n$ for the state $\{-1,-1,-1,-1,-1,-1,\ldots\}$ at $\lambda=0.76$ and $\lambda=0.77$ with $A=3.0$. $\alpha_{\min}^{(n)}$ and $f_{\min}^{(n)}$ turn out to be linear with respect to $1/n$. It is thus easy to extrapolate to n infinity and estimate $\alpha_{\min}$ and $f(\alpha_{\min})$. From these figures, it is found that $\alpha_{\min}=1$ and $f(\alpha_{\min})=1$ for $\lambda=0.76$, while $\alpha_{\min}=0$ and $f(\alpha_{\min})=0$ for $\lambda=0.77$. By a similar analysis, $\alpha_{\max}$ and $f(\alpha_{\max})$ can be estimated, and the result is that $\alpha_{\max}=1$ and $f(\alpha_{\max})=1$ for $\lambda=0.76$, while $\alpha_{\max}=\infty$ and $f(\alpha_{\max})=1$ for $\lambda=0.78$. Therefore it is concluded that the state $\{-1,-1,-1,-1,-1,\ldots\}$ is extended for $\lambda=0.76$ and is localized for $\lambda=0.77$.

These two methods (the bandwidth analysis of the spectrum and the multifractal analysis of the wave functions) were used to determine whether a state is extended or localized. The results of Figs. 1(a), 1(b), and 2 were consistently obtained. In the model studied here, critical states were not found.

A probable explanation of the localization starting from the center of the spectrum is as follows. In the present model, the probability to find a site with a potential energy near 0 ($\pm\lambda$) is smaller (larger) than that in model (A) in which all the states localize at once. Thus localization (delocalization) is encouraged around the center (edges). This model also exhibits localization from the edge of the spectrum when A is large. This behavior may appear to be natural from the experiences in the three-dimensional disordered systems. However, we found a surprising phenomenon that the states near the edge become extended and then localized reentrantly as λ is increased.

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