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Global scaling properties of the spectrum for a quasiperiodic Schrödinger equation

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A tight-binding model in one dimension with an incommensurate potential $V_n = \lambda\cos(2\pi\sigma n)$ is investigated. It is found that at the critical point of the localization transition $\lambda = 2$, there is a finite range of scaling indices $\alpha_{\min} \leq \alpha \leq \alpha_{\max}$ each of which is associated with a fractal dimension $f(\alpha)$. In the extended region $0 < \lambda < 2$, scaling is "trivial" with a single index $\alpha = 1$ almost everywhere in the spectrum, while in the localized region $\lambda > 2$, there is no scaling.

One-dimensional Schrödinger equations with quasiperiodic potentials have attracted the attention of physicists and mathematicians for many years.[1-12] Besides their intrinsic interests, these equations also provide simple cases in which we can understand the crossover between periodic and random potentials. The nonlinear coupling of the two incommensurate competing periods in the equation usually leads to a very rich behavior and structure of the system, e.g., metal-insulator transition.[1,8] This problem is also closely related to some other problems, such as two-dimensional (2D) periodic crystals in magnetic fields,[13,14] superconducting lattices in magnetic fields,[15] incommensurate superlattices,[16] and 1D quasicrystals.[17]

In this paper, we study the 1D discrete Schrödinger equation

$$\psi_{n+1} + \psi_{n-1} + \lambda\cos(2\pi\sigma n + \theta)\psi_n = E\psi_n \ . \qquad (1)$$

The two competing periods are 1, the lattice spacing, and σ^{-1}, the period of the potential. Equation (1) is called Harper's equation,[18] or the "almost Mathieu" equation[2] because of the analogy to the continuous Mathieu equation. Here we list some of the known properties of Eq. (1). (a) (Aubry duality) If we substitute[1]

$$\psi_n = e^{ikn}\sum_m f_m e^{im(2\pi\sigma n + \theta)}$$

in (1), we obtain the dual equation

$$f_{m+1} + f_{m-1} + \frac{4}{\lambda}\cos(2\pi\sigma m + k) f_m = \frac{2E}{\lambda} f_m \ . \qquad (2)$$

Note that $\lambda < 2$ and $\lambda > 2$ are dual and $\lambda = 2$ is the self-dual point. (b) If σ is an irrational number, (1) has a Cantor spectrum.[2] (c) It is believed[1,2,8,11] that, if σ is an irrational number,[19] for $0 < \lambda < 2$, the spectrum is absolutely continuous and all the eigenstates are extended, while for $\lambda > 2$, the spectrum is pointlike and all the states are localized. At the transition point $\lambda = 2$, the spectrum is singular continuous and the states are "critical" (neither extended nor localized in the usual sense).

The goal of this paper is to understand the scaling behavior of the spectrum in the three different regions. Specifically, we take σ to be the inverse of the golden mean, $\sigma = [(5)^{1/2} - 1]/2 \equiv \sigma_G$ and set the phase θ to be zero. This paper is an extension of an earlier Letter by Kohmoto.[8]

Local scaling of a spectrum can be defined as follows. Let E and $E + \Delta E$ both be in the spectrum. If the integrated density of states, $D(E)$, behaves as

$$D(E + \Delta E) - D(E) \sim (\Delta E)^{\alpha}, \ (\Delta E \to 0) \ , \qquad (3)$$

we say that the spectrum has scaling at E with a scaling index α. Kohmoto[8] and Ostlund and Pandit[11] studied local scaling at $E = 0$ for Eq. (1) with $\sigma = \sigma_G$. They found that $\alpha = 1$ for $0 < \lambda < 2$ and $\alpha = 0.547\ldots$ for $\lambda = 2$. Now the questions are the following. (a) Are there different scalings at different parts of the spectrum? (b) If so, what is the distribution of α's in the spectrum? The remainder of this paper is an answer to these questions.

In order to obtain knowledge of the spectrum for an irrational $\sigma = \sigma_G$, we study a series of spectra S_l for $\sigma = \sigma_l$, where σ_l is a rational approximant of σ_G with $\lim_{l\to\infty}\sigma_l = \sigma_G$. The natural way of choosing σ_l is successive truncations of the continued-fraction expansion of σ_G. This gives $\sigma_l = F_{l-1}/F_l$, where F_l is the lth Fibonacci number defined by a recursion relation $F_{l+1} = F_l + F_{l-1}$ with $F_0 = F_1 = 1$.

For a rational $\sigma = \sigma_l = F_{l-1}/F_l$, (1) is periodic with a period F_l and can be solved with the help of the Bloch theorem. The spectrum S_l consists of F_l bands and $F_l - 1$ gaps. In Fig. 1, S_l for $l = 3$, 4, 5, and 6 are shown. By using the Bloch condition $\psi_{n+F_l} = e^{ikF_l}\psi_n$, where k is the Block index, (1) can be written in a matrix eigenvalue problem form

$$H_l\Psi = E\Psi \ , \qquad (4)$$

with

$$H_l = \begin{pmatrix} V_1 & 1 & & & & e^{-ikF_l} \\ 1 & V_2 & 1 & 0 & & \\ & 1 & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & 0 & & \cdot & \cdot & 1 \\ e^{ikF_l} & & & & 1 & V_{F_l} \end{pmatrix} \qquad (5)$$

and the vector Ψ is the transpose of $(\psi_1, \psi_2, \ldots, \psi_{F_l})$. For a fixed value of k, the matrix H_l has F_l eigenvalues. These eigenvalues form F_l energy bands as k is varied in the first Brillouin zone $[-\pi/F_l, \pi/F_l]$, and $k = 0$ and $\pm\pi/F_l$ correspond to the band edges. If the total number of states in S_l is normalized to 1, the number of states in each band is $1/F_l$, since each band has the same number of states. The

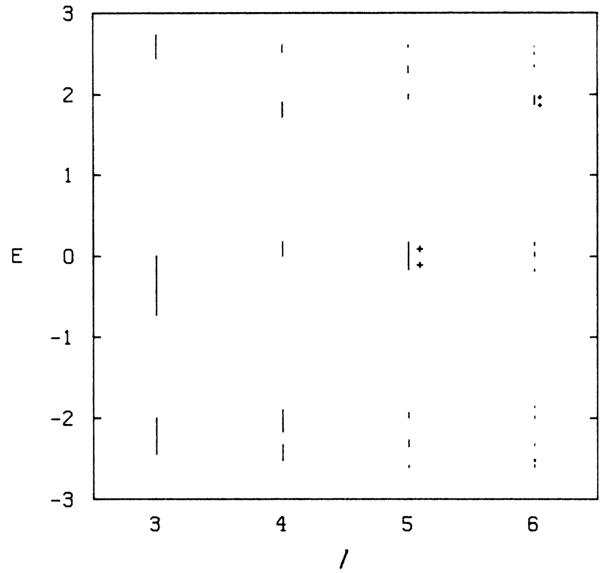

FIG. 1. The series of spectra S_l for $l=3$, 4, 5, and 6. Double + denotes that there are actually two bands there.

spectrum S_l is a better and better partition of $S_\infty \equiv S$, the spectrum for $\sigma=\sigma_G$, as l becomes larger and larger.

We can study local scaling numerically from the series of spectra S_l. Let us choose an E such that it is in the spectra of S_{L+mp}, $m=1,2,3,\ldots$, where L and p are integers. Denote the width of the band to which E belongs by W_{L+mp}. We know that the number of states in each band of S_l is $\Delta D_l = 1/F_l \sim (\sigma_G)^l$. So if W_{L+mp} behaves like

$$W_{L+mp} \sim A^m, \quad (m \to \infty) , \tag{6}$$

with some constant A, then the spectrum S has a scaling property at E with an index

$$\alpha = \frac{p \ln \sigma_G}{\ln A} . \tag{7}$$

It is hard, of course, to find all the indices α and their distributions in this way. But this approach can give some information about what kind of scaling behaviors the spectrum would have. If there are interesting scaling properties in the spectrum, one can then use a newly developed powerful technique[20] to understand the global scaling properties.

Let us first consider the case $\lambda=2$. We find, via (6) and (7), that there are many different values of α in the spectrum S. Particularly, we find that $\alpha_1 = 0.54688 \pm 0.00002$ with $p=3$ at $E=0$ and $\alpha_2 = 0.42123 \pm 0.00003$ with $p=1$ at $E=\pm E_0$ ($\pm E_0$ being the upper and lower bounds of the spectrum). Since $E=0$ and $E=\pm E_0$ are the most ramified and the most dense regions in the spectrum, respectively (see Fig. 1), α_1 and α_2 set the upper and lower bounds for the scaling indices in the spectrum.

We now use the algorithm developed in Ref. 20 to calculate the global properties of the spectrum. Consider the F_l bands of S_l as the partition of S and take the number of states (normalized to 1) as the measure. So the measure of each band is $1/F_l$. Define the partition function

$$\Gamma_l(q,\tau,\{S_l\}) = \sum_{i=1}^{F_l} \frac{(F_l)^{-q}}{(w_i)^{\tau}} , \tag{8}$$

where w_i is the width of the ith band and F_l^{-1} the measure of it. The condition

$$\Gamma(q,\tau) \equiv \lim_{l\to\infty} \Gamma_l(q,\tau,\{S_l\}) = 1 \tag{9}$$

gives a function $\tau(q)$. Then the scaling indices α and $f(\alpha)$, the fractal dimension of the subset of S consisting of all the points with the scaling index α, are given by a Legendre transformation

$$\alpha(q) = \frac{d\tau(q)}{dq} , \qquad f(q) = q\alpha(q) - \tau(q) . \tag{10}$$

Much information about the global properties of the spectrum is contained in the function $f(\alpha)$. The Hausdorff dimension D_H of the spectrum S is just the maximum value of $f(\alpha)$. In order to speed up the convergence, we ask,[20] instead of Eq. (9), that $\Gamma_l/\Gamma_{l'}=1$. The f-α curve obtained from the condition $\Gamma_{12}/\Gamma_{15}=1$ is shown in Fig. 2. As one can see, it is a continuous curve and exists for a range of α values $[\alpha_{\min},\alpha_{\max}]$. Note that the two end points of the curve converge to previously obtained α_1 and α_2, respectively. The most probable scaling index (i.e., the one with the maximum f) is $\alpha_0 = 0.5 \pm 0.003$, with the maximum being $f(\alpha_0) = D_H = 0.498 \pm 0.004$. We now discuss the consequence of singular α for the low-temperature specific heat. If each lattice site contributes one electron, the Fermi energy lies at the center of the spectrum, namely, at $E=0$. At temperature T, the number of states available in thermal excitation scales as $(k_B T)^{\alpha_1}$, where k_B is the

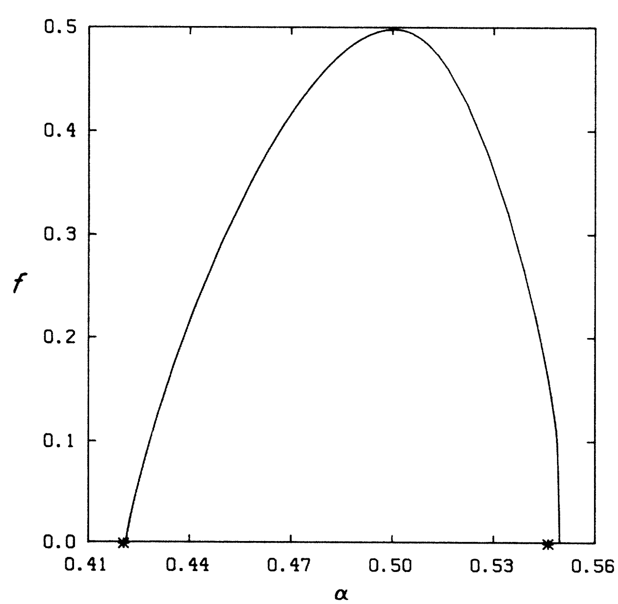

FIG. 2. The f-α curve of the spectrum for $\lambda=2$ and $\sigma=\sigma_G$. It is calculated from $\Gamma_{12}/\Gamma_{15}=1$. $*$'s indicate the values of α_1 and α_2.

Boltzmann constant. Each excitation gains an amount of energy of the order $k_B T$. So the total thermal energy scales as $(k_B T)^{\alpha_1+1}$. Hence the temperature dependence of the low-temperature specific heat will be T^{α_1}.

Next, let us consider the subcritical region $0<\lambda<2$. We find, via (6) and (7), that $\alpha=1$ with $p=1$ for almost all the points in the spectrum except at large gap edges where we have $\alpha=0.5$. These singularities are remnants of the van Hove singularities in the periodic case. For $\lambda=0$, (1) has only one period and the van Hove singularities at the band edges have a index $\alpha=0.5$. For small but nonzero λ, S_l has F_l bands, $2F_l$ van Hove singularities. The function $\tau(q)$ calculated by the method described above is

$$\tau=\begin{cases} q-1 & \text{for } q\le 2\ , \\ \dfrac{q}{2} & \text{for } q>2\ . \end{cases} \qquad (11)$$

This gives a two-point f-α "curve": $\alpha=1, f=1$ and $\alpha=0.5, f=0$. The fractal dimension f is zero for the set of van Hove-type singularities $\alpha=0.5$. This is because the number of "edges" where singularities of this type exist is infinite, but only countable. The scaling of the spectrum is dominated by the "trivial" index $\alpha=1$ with $f=1$ and there is no set of singularities with α other than 0.5. The spectrum is uniformly scaled. Moreover, this result is independent of λ as long as $0<\lambda<2$. Ostlund and Pandit[11] showed that in this region $\lambda=0$ is the trivial fixed point and the energy E is the only relevant parameter. Our result is consistent with their renormalization-group analysis.

For $\lambda>2$, we find that W_{L+mp} (defined previously) goes to zero faster than the exponential of m for all the points in the spectrum. This we attribute to a pure point spectrum for an irrational σ. There is no scaling property of the type (3) in the spectrum. The Hausdorff dimension of the spectrum is, by duality, the same as that of $\lambda<2$, namely, 1.

We performed the same analysis for $\sigma=\sqrt{2}-1\equiv\sigma_S$, the "silver mean," and $\sigma=(\pi-3)\sqrt{3}$. All the results are qualitatively the same. Only the $f(\alpha)$ curve (particularly the two bounds of the scaling indices α_1 and α_2) at $\lambda=2$ appears to be σ dependent. However, the most probable scaling index α_0 is 0.5 in all the cases. Furthermore, the maximum of f, the Hausdorff dimension of the spectrum, seems to be independent of σ within the numerical accuracy.

In conclusion, we have studied Harper's equation (1). The scaling properties of the spectrum are drastically different in subcritical, critical, and supercritical regions. We believe that these are rather general results in the localization problems. In fact, recently we, together with Sutherland,[21] studied a model of a 1D quasicrystal[17] using the present technique of analyzing spectra. The work confirmed an earlier conjecture[6-8,12,22] that models of this class have a purely singular continuous spectrum.

Based on the analysis for the particular model presented here, we make a conjecture about the following unique relation between a spectral type and scaling properties of the spectrum for a general Schrödinger operator: (a) An absolutely continuous spectrum (extended states)— it is dominated by points with "trivial" scaling index $\alpha=1$ and a fractal dimension $f=1$. It can contain a finite or a countably infinite number of singularities with $\alpha\neq 1$, perhaps van Hove singularities. (b) Singular continuous spectrum (critical states)—each point has a scaling index α which can take a value in a range $[\alpha_{\min},\alpha_{\max}]$. A fractal dimension $f(\alpha)$ of a set of points with α is a smooth function of α. (c) Point spectrum (localized states)—has stronger singularities than the type of (3).

The technique developed in the present paper to analyze energy spectra for the localization problem would have many applications to the problems which are less understood, e.g., quasicrystals in two and three dimensions.[23-27]

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[1]G. Andre and S. Aubry, Ann. Isr. Phys. Soc. **3**, 133 (1980).

[2]B. Simon, Adv. Appl. Math. **3**, 463 (1982), and references therein.

[3]J. B. Sokoloff, Phys. Rep. **126**, 189 (1985).

[4]D. R. Grempel, S. Fishman, and R. E. Prange, Phys. Rev. Lett. **49**, 833 (1982).

[5]J. Bellisard, D. Bessis, and P. Moussa, Phys. Rev. Lett. **49**, 701 (1982).

[6]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).

[7]S. Ostlund, R. Pandit, D. Rand, H. Schellnhuber, and E. D. Siggia, Phys. Rev. Lett. **50**, 1873 (1983).

[8]M. Kohmoto, Phys. Rev. Lett. **51**, 1198 (1983).

[9]R. E. Prange, D. R. Grempel, and S. Fishman, Phys. Rev. B **28**, 7370 (1983).

[10]J. Bellisard, R. Lima, and D. Testard, Commun. Math. Phys. **88**, 207 (1983).

[11]S. Ostlund and R. Pandit, Phys. Rev. B **29**, 1394 (1984).

[12]M. Kohmoto and Y. Oono, Phys. Lett. **102A**, 145 (1984).

[13]D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976).

[14]D. J. Thouless, M. Kohmoto, P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).

[15]R. Rammal, T. C. Lubensky, and G. Toulouse, Phys. Rev. B **27**, 2820 (1983); S. Alexander, *ibid.* **27**, 1541 (1983).

[16]R. Merlin, K. Bajema, R. Clarke, F.-T. Juang, and P. K. Bhattacharya, Phys. Rev. Lett. **55**, 1768 (1985).

[17]M. Kohmoto and J. R. Banavar, Phys. Rev. B (to be published).

[18]P. G. Harper, Proc. Phys. Soc. London, Sect. A **68**, 874 (1955).

[19]By irrational number, we mean those which have typical Diophantine properties. An irrational number σ has Diophantine properties if and only if for some c,k and all p,q, we have $|\sigma-p/q|\geq cq^{-k-1}$. The set of these irrationals has full measure in R. For the case of Liouville number, see J. Avron and B. Simon, Bull. Am. Math. Soc. **6**, 81 (1982).

[20]T. C. Halsey, M. H. Jensen, L. P. Kadanoff, I. Procaccia, and B. I. Shraiman, Phys. Rev. A **33**, 1141 (1986).

[21]M. Kohmoto, B. Sutherland, and C. Tang (unpublished).

[22]F. Delyon and D. Petritis, Commun. Math. Phys. **103**, 441 (1986).

[23]T. C. Choi, Phys. Rev. Lett. **55**, 2915 (1985).

[24]T. Odagaki and D. Nguyen, Phys. Rev. B **33**, 2184 (1986).

[25]M. Kohmoto and B. Sutherland, Phys. Rev. Lett. **56**, 2240 (1986).

[26]M. Kohmoto and B. Sutherland, Phys. Rev. B (to be published).

[27]H. Psunepsugu, P. Fujiwara, K. Ueda, and P. Tokihiro, J. Phys. Soc. Jpn. **55**, 1420 (1986).