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LETTER TO THE EDITOR

Level statistics in a quasiperiodic system

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Abstract. We examine the level statistics of Harper's equation, a simple model of a one-dimensional quasiperiodic system, through the distribution of the spacings between adjacent eigenvalues, each normalised by the average local density of states.

We present exact results for the distribution for both small and large amplitude α of the incommensurate potential, showing it has a simple form in each of these limits. We show numerically that these distributions are preserved as α approaches its critical value 2 from each side, and also that at the critical point the distribution of the normalised spacings has a distinct but simple form.

Harper's equation defines a simple model which shows some of the novel properties of the quasiperiodic systems that have aroused much interest, both theoretical and experimental, in recent years. Such systems are intermediate between periodic crystal structures, characterised by Bloch states extended throughout the system, and disordered systems, which in one and two dimensions have exponentially localised states; quasiperiodic systems may have localised or extended states and there may exist critical points at which the states are neither strictly localised nor extended. The localisation properties of the eigenstates of disordered systems in the infinite-volume limit are known to have direct consequences on the form of the spectrum for finite specimens; when the states are extended there is a large degree of overlap between states of similar energies and hence level repulsion occurs, while for localised states this does not happen and the energy levels are essentially uncorrelated, giving a level spacing distribution of Poisson form (Molchanov 1981). A pertinent question is therefore whether such a correspondence holds for quasiperiodic systems. In addition, a novel feature of quasiperiodic systems is that their spectra in general show fractal behaviour, in that structures in the spectrum found on a given energy scale are repeated on smaller and smaller scales, and the integrated density of states is a 'devil's staircase'.

Harper's equation describes a tight-binding system in one dimension with a site energy which takes the form of a cosine whose period has irrational ratio β to the lattice constant, and whose amplitude α and phase δ are parameters of the system. If the eigenfunction with energy E at the nth site of a chain of length N sites is $u_n^{(i)}$, then Harper's equation can be written as

$$u_{n-1}^{(i)} + u_{n+1}^{(i)} + [\alpha \cos(2\pi\beta n + \delta) - E_i]u_n^{(i)} = 0. \tag{1}$$

It is known (Aubry and Andre 1980) that for $\alpha < 2$ all the states are extended; for $\alpha > 2$ the states are exponentially localised with inverse localisation length $L^{-1} = \ln(\alpha/2)$, while at the critical point $\alpha = 2$ the states are neither extended nor localised

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and the spectrum is a Cantor set with a hierarchical band structure which is related to the continued-fraction representation of β (Hofstadter 1976, Simon 1982, Sokoloff 1985). Thouless and Niu (1983), Ostlund and Pandit (1984), Wilkinson (1984, 1987) and others have investigated the form of the spectrum through renormalisation group approaches, while Tang and Kohmoto (1986) introduce a local fractal dimensionality for the spectrum. Machida and Fujita (1986) have studied the level spacing statistics and found the expected Poisson distribution for $\alpha > 2$ and an inverse power law distribution at the critical point. Prange *et al* (1984a, b) calculated the density of states, the localisation properties of the wavefunctions and the frequency-dependent conductivity for the related problem where the cosine in equation (1) is replaced by a tangent.

Examination of the spectrum through the distribution of level spacings provides a valuable comparison with the corresponding results for disordered systems, but we shall show in this letter that simpler results may be obtained if the spacing between adjacent levels is normalised by the average of the local density of states and the distribution of the resulting quantities calculated. A single level spacing can be seen as the product of two distinct factors; the behaviour we are interested in (for example, possible level repulsion), represented by some function $\phi(E)$, is multiplied by the inverse density of states, so that where the density of states is not independent of the energy the statistics of the raw level spacings does not yield directly the information we want (in one-dimensional systems, such as the one discussed here, a band edge in the spectrum corresponds to a singularity in the density of states, so the problem becomes acute). Using our normalised spacings, however, each level spacing is individually compared with the local average before the statistics are evaluated, so that we expect that, as the spectrum fills out with increasing system size, features such as the fractal nature of the spectrum at the critical point should show up in the distribution of the normalised spacings.

We define the normalised level spacing Δ_j by

$$\Delta_j = \overline{(\rho(E))}_j \Delta E_j \tag{2}$$

where $\overline{(\rho(E))}_j$ is the average local density of states per site of a chain of length $N_D \gg N$ over an energy range ΔE_j between adjacent levels E_j and E_{j+1}. We rewrite this for convenience as

$$\Delta_j = K(E_j) - K(E_{j-1}) \tag{3}$$

where $K(E)$ is the integrated density of states per site of a 'long chain' of N_D sites; $K(E)$ is well defined for an infinite chain and is also more straightforward to evaluate numerically than $\rho(E)$. With this definition the typical value of Δ_j for a chain of length N is $1/N$. We define the cumulative distribution $f(\Delta)$ as the fraction of the total number of Δ_j having values less than or equal to a given Δ; the cumulative distribution will provide a clearer comparison between exact and numerical results than the simple density of values per unit interval.

In a system where the spectrum fills out uniformly as the size of the system increases (for example, a single particle in a square well) it follows that the Δ_j have the same value, $1/N$, everywhere and hence $f(\Delta)$ is a unit step function at $\Delta = 1/N$. By contrast, let us consider a simple Cantor set which has a fractal structure analogous to—although much simpler than—that of the spectrum of Harper's equation at the critical point. If we start with a spectrum of two levels, we can recursively double the number of levels of a system with $N = 2^n$ levels by placing two new levels between alternate pairs of levels, and none in the other half of the gaps. With this prescription it is clear that

only half of the gaps of the spectrum at any stage subsequently have levels inserted in them, so we obtain the result that Δ_j can have one of two values, zero and $2/N$, and hence $f(\Delta)$ has the value $\frac{1}{2}$ for $0<\Delta<2/N$ and unity for $2/N<\Delta$. It should be noted at this point that this result depends only on the relative ordering of levels in the recursion scheme and not on any specification of the size of the gaps at each recursion step.

We know that the structure of the spectrum depends on the continued-fraction expansion of β; we therefore choose to compare results for β, a quadratic irrational (those numbers which have all the terms in their continued fraction equal), with those for a more general irrational, with no special pattern in the continued fraction. We use the reciprocal of the golden mean, $\sigma_G^{-1}=(\sqrt{5}-1)/2=1/(1+1/(1+1/(1+\ \ldots)))$ as an example of the former, and the natural logarithm of 2, $\ln 2=1/(1+1/(2+1/(3+1/(1+1/(6\ \ldots)))))$. To minimise boundary effects we set the size of the system equal to the denominator of one of the series of rational approximants to the appropriate β: for $\beta=\sigma_G^{-1}$ these are $\{1, \frac{1}{2}, \frac{2}{3}, \frac{3}{5}, \frac{5}{8}, \frac{8}{13}, \ldots\}$, while for $\beta=\ln 2$ they are $\{1, \frac{2}{3}, \frac{7}{10}, \frac{9}{13}, \frac{61}{88}, \frac{192}{277}, \frac{253}{365}, \ldots\}$. In figure 1 we illustrate the spectrum of equation (1) as a function of α, in the case $\beta=\sigma_G^{-1}$.

Equation (1) can be written as a matrix equation; with the boundary conditions $u_0=u_{N+1}=0$ the problem reduces to the diagonalisation of a symmetric tridiagonal matrix. The integrated density of states $K(E)$ is found by counting the zero crossings of u_n per unit length as (1) is iterated at energy E from one end of a long chain of length $N_D \gg N$. We found that using $N_D=1000N$ gave adequate resolution in $f(\Delta)$; increasing N_D beyond this changed $f(\Delta)$ negligibly even for $N_D=10^7$. In the following our analytic results are derived with the phase δ equal to zero, so for consistency the comparable numerical results were also calculated with $\delta=0$. Except at the critical point, the numerical results presented here suggest that large enough systems are being treated for the limiting behaviour to be evident, but at $\alpha=2$ finite-size effects still appear to be significant. The effects of boundary conditions are therefore reduced by the alternative method of averaging the distributions over many evenly spaced phases in the range $0<\delta<2\pi$.

We derive exact results for the cases $\alpha=0$ and $\alpha\to\infty$ and present numerical results for α just below, at and above the critical point, $\alpha=2$.

(*a*) $\alpha=0$. With the boundary conditions as given, the eigenvalues of (1) for a chain of N sites are

$$E_k=2\cos\left(\frac{\pi k}{N+1}\right) \qquad k=1, \ldots, N.$$

Hence for a long system of length $N_D\to\infty$, the density of states is

$$\rho(E)=\frac{N_D}{\pi(4-E^2)^{1/2}}$$

and

$$K(E)=\frac{N-k}{N}. \tag{4}$$

Since the energy E_k is a monotonic function of k, the difference in $K(E)$ between adjacent eigenvalues is

$$\Delta=1/N$$

and hence $f(\Delta)$ is a unit step function at $\Delta=1/N$.

(*b*) $\alpha \to \infty$. By redefining the energy, $E \to E_k/\alpha$, we find

$$\begin{aligned} K(E_k) &= 1 - \frac{1}{\pi}\cos^{-1}[\cos 2\pi(\beta k+\delta)] \\ &= 1 - 2\{\beta k+\delta\}_{\text{mod }1} \qquad \text{if} \qquad \{\beta k+\delta\}_{\text{mod }1} \leqslant \tfrac{1}{2} \\ &= 2\{\beta k+\delta\}_{\text{mod }1} - 1 \qquad \text{if} \qquad \{\beta k+\delta\}_{\text{mod }1} \geqslant \tfrac{1}{2}. \end{aligned} \tag{5}$$

With $\beta = \sigma_G^{-1}$, $\delta = 0$ and $N = F_l$, the lth Fibonacci number, this expression gives three possible values of $\Delta: 2\beta^{l+1}$, $2\beta^l$ and $2\beta^{l-1}$, with weights which tend as $N \to \infty$ to the values $\frac{1}{2}N\beta^2$, $\frac{1}{2}N$ and $\frac{1}{2}N\beta$, respectively. With $\delta \neq 0$ it was found numerically that more than three different values of Δ appear and that they are displaced in a non-trivial way as δ is varied.

With other values of β, and with N equal to the denominator q_j of a rational approximant to β, a small number of values of Δ_k are again obtained. In general, these values and their relative weights depend on N, and a scaling limit like that observed above for $\beta = \sigma_G^{-1}$ results only when all the terms in the continued fraction are the same, as is the case for the quadratic irrationals. Changing N away from one of the q_j or introducing a non-zero phase δ has a similar effect to that described above.

Numerical results with $\beta = \sigma_G^{-1}$, $N = 377$, for both $\alpha = 0$ and $\alpha = 50$ are shown (figures 2 and 3), together with the appropriate exact results; these demonstrate the accuracy of the numerical procedure.

Figure 4 shows numerical results for $\beta = \sigma_G^{-1}$, $\alpha = 1.8$, together with the exact $f(\Delta)$ for the same length chains with $\alpha = 0$, while figure 5 shows the results for $\alpha = 2.2$, with

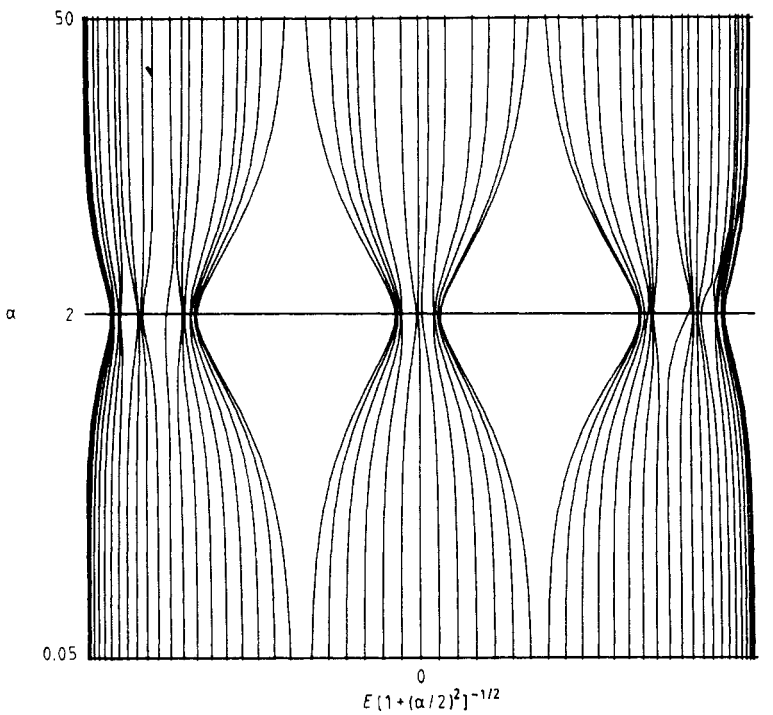

Figure 1. The spectrum of equation (1) for $\beta = \sigma_G^{-1}$, $N = 55$ and $\delta = 0$ for varying α, scaled by $[1+(\alpha/2)^2]^{-1/2}$.

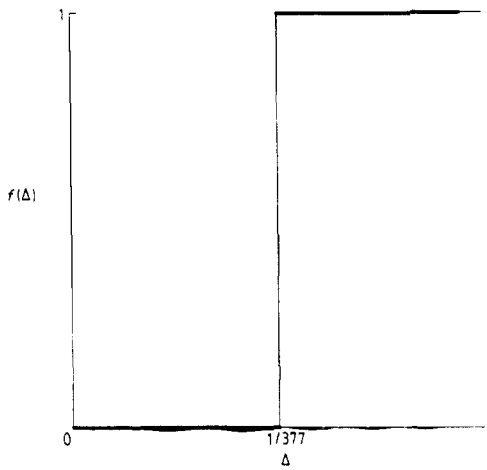

Figure 2. Numerical result for $f(\Delta)$ with $\beta = \sigma_G^{-1}$, $N = 377$ and $\alpha = 0$, with the exact result for $\alpha = 0$ (full line).

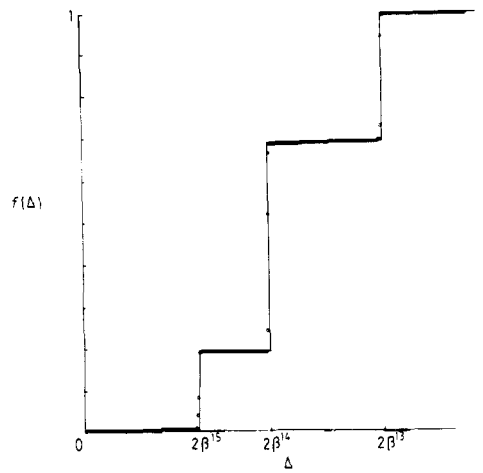

Figure 3. Numerical result for $f(\Delta)$ with $\beta = \sigma_G^{-1}$, $N = 377$ and $\alpha = 50$, with the exact result for $\alpha \to \infty$.

those for $\alpha \to \infty$ for comparison. It can be seen immediately that the forms of $f(\Delta)$ for these chains close to the critical point increasingly resemble those in the respective limiting regime as their length increases. This is remarkable since the spectrum close to the critical point (figure 1) is very different from that obtained in either $\alpha = 0$ or $\alpha \to \infty$. The distributions for $\alpha < 2$ were found to be independent both of the phase δ and the incommensuration parameter β, while phase averaging for $\alpha > 2$ gave a continuous range of Δ.

For other non-quadratic irrational β, $f(\Delta)$ in large systems is close to its $\alpha \to \infty$ form throughout the localised regime (figure 6). Since this form depends on system length there is no simple scaling limit as for quadratic irrationals, but neither does the behaviour resemble that in random systems.

In the case of $\alpha = 2$ and $\beta = \sigma_G^{-1}$ (figure 7) short chains give a rather complicated $f(\Delta)$ with many large sharp steps at integer powers of β and elsewhere. For longer

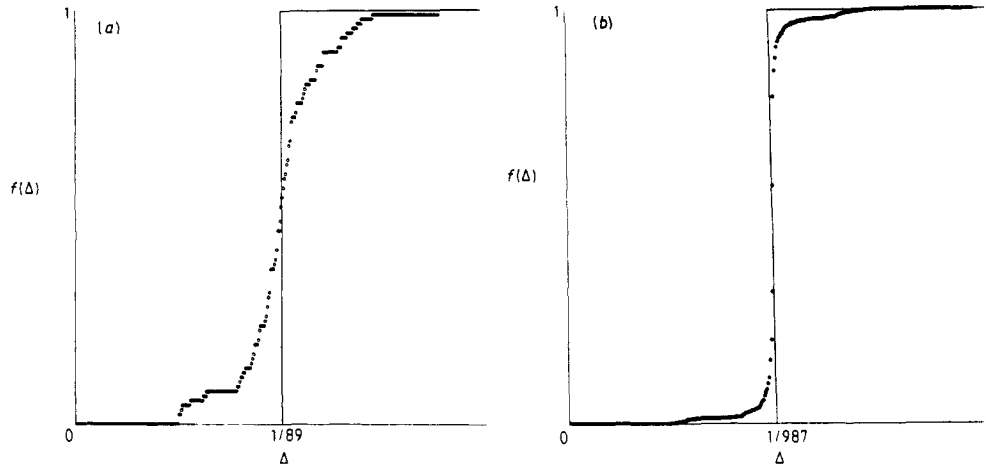

Figure 4. Numerical results for $\beta = \sigma_G^{-1}$, $\alpha = 1.8$, with the exact results for $\alpha = 0$. (*a*) $N = 89$, (*b*) $N = 610$.

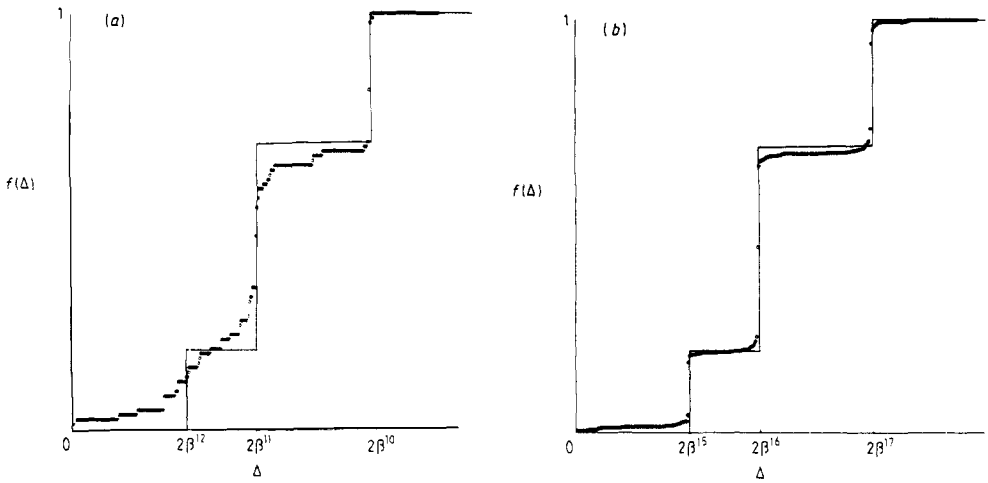

Figure 5. Numerical results for $\beta = \sigma_G^{-1}$, $\alpha = 2.2$, with exact results for $\alpha \to \infty$. (*a*) $N = 89$, (*b*) $N = 610$.

chains, or if phase averaging is used, the two steps at β^{l-1} and β^l become more dominant, with the remaining weight (less than 30%) divided between many steps (figure 8(*a*)). For general β it was observed that the positions of these sharp steps may be fitted very well by the allowed values of Δ_k given by

$$K(E_k) = \{\beta k\}_{\text{mod } 1}$$

(figure 8(*b*)).

We have therefore demonstrated that the normalised level spacing Δ for the Harper equation in the cases $\alpha = 0$ and $\alpha \to \infty$ has distribution functions $f(\Delta)$ with simple forms which differ from those in random systems. Our results indicate in addition that, for long enough chains, the trivial distribution of Δ at $\alpha = 0$ is maintained as α is brought up to the critical point from below, and similarly the distribution in the

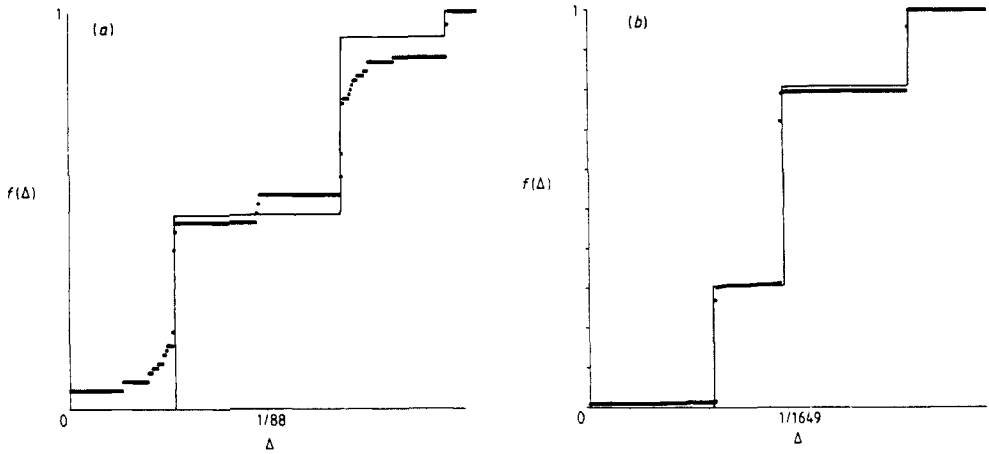

Figure 6. As figure 5 but with $\beta = \ln 2$. (*a*) $N = 88$, (*b*) $N = 1649$.

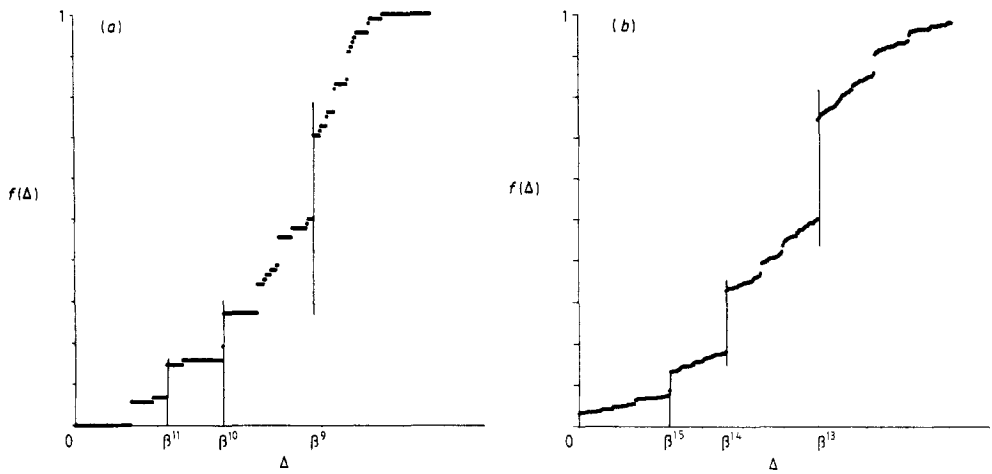

Figure 7. Numerical results for $f(\Delta)$ at $\beta = \sigma_G^{-1}$, $\alpha = 2$. (*a*) $N = 89$, (*b*) $N = 610$.

limit $\alpha \to \infty$ is preserved as α approaches 2 from above, despite the fact that the form of the spectrum itself near the critical point is very different from its appearance for α far from 2. Our results are consistent with the level repulsion one might expect for $\alpha < 2$, since the latter would favour maximising the level spacing in any energy range to give a spacing which is directly proportional to the inverse density of states, while in the case of $\alpha > 2$ the spacings vary about a local average on a scale of the order of $1/N$ compared with the bandwidth of the spectrum (see figure 1). Our numerical results suggest that, at $\alpha = 2$ and with $\beta = \sigma_G^{-1}$ for long enough chains, $f(\Delta)$ has a scaling limit with two values of Δ dominant, but we have no analytic result to confirm this.

Our normalisation of the level spacings removes much of the structure of the distributions obtained by Machida and Fujita (1986), which appear to be superpositions of distributions of more than one functional form. Our results, in contrast, are simple in form and, in addition, indicate trivial behaviour for all α in the extended regime

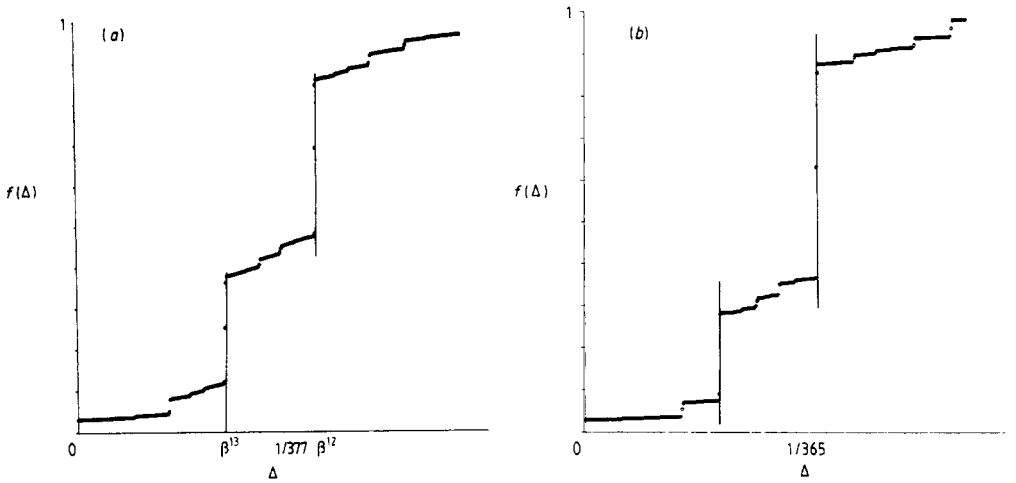

Figure 8. Numerical results at $\alpha = 2$ averaged over 100 phases. (*a*) $\beta = \sigma_G^{-1}$, $N = 377$, (*b*) $\beta = \ln 2$, $N = 365$. The full lines indicate the allowed values for Δ_k given by $K(E_k) = \{\beta k\}_{\text{mod } 1}$.

($\alpha < 2$), which is not shown by the distribution of the raw spacings. There is a distinct contrast to the disordered case, where the Poisson distribution is maintained for the normalised level spacings. Our results are not directly comparable with those of Tang and Kohmoto (1986), since the latter authors study how the number of states in an energy interval scales with the size of the interval; by contrast, in our approach the normalisation by the density of states removes the energy scale throughout the spectrum and so we treat the filling of gaps between levels with increasing system size independent of the size of the gaps. Our results for $\alpha < 2$ are broadly compatible with theirs, however, in that our 'trivial' $f(\Delta)$ over the whole of this regime corresponds to the trivial Hausdorff dimensionality of unity. A complete description of a recursion scheme for filling in a fractal spectrum would lead to a prediction of $f(\Delta)$ at the critical point but so far such an exact result has not been found for this system.

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