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Spectral density correlations and eigenfunction fluctuations in one-dimensional quasi-periodic systems

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Abstract. We study the scaling and correlation–fluctuation properties for the spectra and wavefunctions of a simple one-dimensional quasi-periodic system that displays an Anderson metal–insulator transition. This system and its extensions are models for studying localization phenomena, and their usefulness for the description of the Anderson transition as well as insulating and metallic phases in disordered systems is exploited. We present numerical work on the critical behaviour of the spectrum and wavefunctions, which display multifractal fluctuations. Appropriate probability densities are studied, and it is demonstrated that: (i) the subband energy width statistics, which may express spectral correlations, is consistent with linear level repulsion at the critical point and a Poisson distribution in the insulating regime; and (ii) the critical wavefunction probability amplitude distributions approach a universal function as the system size increases. It is concluded that certain critical properties of quasi-periodic models are similar to what is expected for electronic states in weakly disordered metals, and others show a striking similarity to mobility edge behaviour in three dimensions.

1. Introduction

New features have emerged in the non-interacting electron band theory for two-dimensional systems under a sufficiently strong magnetic field and a periodic potential [1]. This behaviour is linked with the quantum Hall effect [2], which, together with the experimental design of new structures with a periodic modulation incommensurate with the underlying lattice and the experimental discovery of the quasi-crystalline phase in metallic alloys [3], initiated the study of quasi-periodic systems. The electron properties and lattice dynamics of such modulated structures and quasi-crystals are believed to be intermediate between periodic and random. The pertinent theoretical question concerns the nature of their electron states in connection with the phenomenon of Anderson localization and the associated metal–insulator transition, which are common in random systems [4]. In this context Aubrey and Andre [5] introduced and studied a one-dimensional equation, better known as the discrete Harper’s equation, originally used to describe the quantum theory of an electron confined in a plane with a periodic potential in the plane and a uniform magnetic field perpendicular to the plane. Of course,

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disordered electronic systems always show localization in one dimension and the quasi-periodic model, even if not disordered, might be expected to conform to this rule. Actually, the model of [5] and its extensions [6] mimic the real three-dimensional situation since they can show localized, extended as well as critical states. From a duality property it can be shown that an Anderson transition with a rich complex scaling behaviour [7–9] occurs for the one-dimensional self-dual system [5] at a critical value for the strength of the incommensurate potential, corresponding precisely to the magnetic field problem. This metal–insulator transition is thought to be rather simpler than that in the presence of a random potential [4]. The reason is that in quasi-periodic models when approaching the critical point from the metallic phase we do not encounter the quantum coherence phenomena that are known to exist in the diffusive regime of disordered metals. This implies that their extended states are not chaotic as in disordered metals but analytic, carrying a finite momentum corresponding to ballistic transport with infinite elastic mean free path. The Anderson transition from extended to localized states in quasi-periodic systems is regarded as due to breaking of analyticity [5].

In disordered systems the Anderson transition is defined at the point in the energy spectrum, known as the mobility edge, where the averaged wavefunction amplitude changes sharply from being constant in the metal to an exponential decaying function for the insulator. In the metallic phase close to the mobility edge the wavefunction amplitude fluctuations are large and the states are chaotic. Recently [10–12], a lot of attention has been focused on spectral correlation properties in this regime related to the physics of mesoscopic systems. As we approach even closer to the mobility edge the fluctuations increase dramatically and become very large indeed for the insulator. On the other hand, the averaged value of the spectral density clearly does not carry any information on the transition. But again its fluctuations, i.e. the higher statistical moments of the density of states, ‘feel’ the transition [10]. The nature of the spectrum changes drastically when crossing the mobility edge from being smooth and rigid in the metallic phase to a highly fluctuating spectrum for the insulating phase. The difference is assigned to the fact that the chaotic extended states overlap significantly, causing repulsion between the energy levels and a correlated spectrum. On the other hand, localized states that are close in energy are expected to be spatially largely separated so that the corresponding spectrum becomes uncorrelated. This picture for the spectral fluctuations is confirmed by eigenvalue statistical studies of random tight-binding matrix ensembles appropriate to describe disordered electronic systems [10–12]. In the limit of very strong diagonal disorder the role of the off-diagonal matrix elements diminishes and the energy levels are essentially similar to the input random diagonal matrix elements, leading to Poisson statistics. When the disorder decreases, the off-diagonal matrix elements instead contribute significantly and the eigenvalues begin to correlate, repelling their closest neighbours. This change of behaviour may also be seen by varying the hopping range in statistical random matrix ensembles [13]. For long-range hopping the Wigner–Dyson Gaussian ensembles [14] (or equivalently the infinite-dimensional tight-binding matrix ensembles) become appropriate, producing level repulsion and spectral rigidity. By shortening the matrix band range, a crossover to the uncorrelated spectrum occurs. The presence of the spectral correlations and of the corresponding wavefunction amplitude fluctuations should somehow be responsible for the fluctuations of a quantity that is of central interest in quantum transport, namely the conductance G . It has become clear over recent years that the full distribution function of $P(G)$, which incorporates all its fluctuations, must be studied [15] rather than just its averaged value $\langle G \rangle$. It is well known that $\langle G \rangle$ serves as the unique relevant variable in the one-parameter scaling theory of the Anderson transition [16].

In quasi-periodic systems the critical point is characterized by exotic scaling effects, which allow a multifractal description [17] for both the spectra [7] and the wavefunctions [8, 9]. It is still not clear to what extent these results are also relevant for understanding the Anderson transition in disordered systems. However, first Wegner [18] pointed out that such anomalous scaling for averaged moments of local quantities is not unlikely to occur in disordered systems. He computed the multifractal scaling exponents for the critical wavefunction amplitude probability distributions in $d = 2 + \varepsilon$ dimensions, and rather consistent numerical results were later shown in three dimensions [19]. For the quasi-periodic model, quantum-dynamic diffusion studies [20], which are intimately related to the spectral properties, have also been performed. It was found that the asymptotic long-time evolution of an electronic wavepacket put on a single site at time $t = 0$ has a mean-square-root spatial extend described at the critical point by the power law

$$\langle(\Delta x)^2\rangle^{1/2} \propto t^{\alpha_c} \quad \text{as } t \rightarrow \infty \quad (1)$$

where the exponent α_c is a little less than $1/2$. Equation (1) describes a dynamic evolution process close to ordinary diffusion, which is commonly observed in the diffusive metallic regime of disordered metals in three dimensions. The result of equation (1) is not incompatible with what the electron 'sees' at long times. Depending on the original choice made at $t = 0$ it should reflect the scaling of the spectral density versus energy. We must use the fact that the underlying band structure is of the well known Cantor set type characterized by a continuous spectrum of multifractal dimensions ranging from $D_{+z} = \alpha_{\min} = 0.421$ to $D_{-z} = \alpha_{\max} = 0.547$, while the most probable dimension is $D_0 \approx 1/2$ [7]. Therefore, the exponent α_c with the given starting condition should be equal to one of the fractal dimensions α , which corresponds to scaling near a specific energy. Below the critical point the asymptotic behaviour of $\langle(\Delta x)^2\rangle^{1/2}$ as $t \rightarrow \infty$ is described by the trivial exponent $\alpha = 1$, referring to ballistic electronic motion. In the insulating regime $\alpha = 0$ and $\langle(\Delta x)^2\rangle^{1/2}$ tends to a finite localization length as $t \rightarrow \infty$. Two important differences of the quasi-periodic model when compared to disordered systems have already been pointed out [20]: in the extended phase the electronic motion is always ballistic and the localized phase is characterized by long transient behaviour until the asymptotic localization length is reached. Both these features are usually not characteristic of real three-dimensional disordered systems.

Although the quasi-periodic model has been extensively studied and certain analogies have been implied in previous studies, it has not been seriously compared before with the real complicated problem of electrons in dirty systems. The purpose of this paper is to exploit further the model and to establish the essential connections between the two problems. We also report new results by focusing directly on the density-of-states correlations and the wavefunction amplitude fluctuations. In fact, in accord with the dynamic diffusion studies [20], we propose that the critical regime of the quasi-periodic model is indeed close to being diffusive-like and one encounters spectral density fluctuation phenomena similar to the mesoscopic fluctuation phenomena expected in the quantum coherent regime of three-dimensional disordered systems. But this does not hold for other properties, such as the wavefunction probability amplitude distributions, which seem to be exclusive to the mobility edge as we know it from studies in disordered systems.

We present a complete study of a one-dimensional quasi-periodic system mainly at the mobility edge. Most solutions for this model can be obtained via numerical techniques, without much difficulty, since the dimensionality is low and true randomness

is absent. Our emphasis is focused on the following three questions. (i) What are the fluctuations of the density of states as revealed from the statistics of the energy level spacings and what are the wavefunction amplitude fluctuations at the critical point? (ii) What are the corresponding distributions away from criticality? (iii) What do we learn from the solutions of the quasi-periodic model that is relevant and useful in order to elucidate the difficult problem of the corresponding behaviour at the Anderson transition in higher-dimensional disordered systems? In order to achieve our purpose, i.e. clarifying the previous questions, we exploit the multifractal scaling properties [9] for the fluctuating measures of the spectra and wavefunctions at the critical point. Our results also aim towards an interpretation of previously obtained data for the statistics of the density of states at the critical point [21–23] and reveal the true nature of the fluctuations.

2. The quasi-periodic model and the method of study

We studied the so-called Harper's equation brought to notice in [5]. In one dimension it is described by a tight-binding finite-difference equation with a cosine modulation of strength λ incommensurate with the underlying lattice. The ratio of the modulation period to the lattice constant ($a = 1$) is expressed by an irrational number σ . The linear chain is written as

$$\Psi_{n+1} + \Psi_{n-1} + \lambda \cos(2\pi\sigma n^\nu + \varphi)\Psi_n = E\Psi_n \quad (2)$$

where E is the energy, Ψ_n is the wavefunction amplitude at the n th site and φ is a phase factor. The case of $\nu \neq 1$ offers an interesting extension of the model, which is further discussed in section 4. For other extensions see [24]. The one-dimensional Fibonacci quasi-crystal [25, 26] also belongs to the same class of models at criticality. The well known duality argument of [5] goes as follows: When $\nu = 1$ and $\lambda = 2$, equation (2) is identical with its corresponding Fourier transform and we expect that the localized states in real space will be extended states in k -space and vice versa. Using also an assumption that the domains of localized and extended states are separated by a single point leads to the conclusion that for all energies a transition should occur at the self-dual point $\lambda = 2$. The nature of the spectrum similarly changes at $\lambda = 2$. For small λ , and almost every σ and φ , all states lie in smooth bands of finite measure. As λ approaches 2, the total measure of the bands goes to zero and the spectrum is said to be singular continuous. In [7] it was shown that the spectrum has an integrated density of states that is a Devil's staircase at the critical point (see figure 1) and multifractal. For values of λ larger than 2 the spectrum is point-like, corresponding to exponentially localized states.

In order to achieve a numerical solution of equation (2) we consider systematic approximations of the irrational number σ by a series of rational approximants obtained by truncating its continued fraction expansion. For well behaved quadratic irrationals, such as the inverse of the golden mean $\sigma_G^{-1} = (\sqrt{5} - 1)/2$ or the silver mean $\sigma_S = \sqrt{2} - 1$, the series of approximants are particularly simple. For σ_G^{-1} these are the rational numbers $F_{n-1}/F_n = \{1/2, 2/3, 3/5, 5/8, \dots\}$, where F_n is a Fibonacci number defined recursively from $F_{-1} = F_0 = 1$ and $F_{n+1} = F_n + F_{n-1}$; and for σ_S the sequence is $\{2/5, 5/12, 12/29, 29/70, 70/169, 169/408, 408/985, \dots\}$. For other irrationals the corresponding approximants may define irregular periodicities, which are not good for numerical studies. This is particularly distressing in view of encountering more complicated spectral hierarchies [1] than for σ_G^{-1} and σ_S . At the n th level of approximation, from the Bloch condition we have to solve an eigenvalue equation for each value

of the wavenumber k . From the periodic continuation of the lattice, a complex matrix of order $N = F_n$ is defined, which is written as

$$\begin{pmatrix} \lambda & \exp(ik) & 0 & 0 & \dots & \exp(-ik) \\ \exp(-ik) & \lambda \cos(2\pi\sigma^\nu 1) & \exp(ik) & 0 & \dots & 0 \\ 0 & \exp(-ik) & \lambda \cos(2\pi\sigma^\nu 2) & \exp(ik) & \dots & 0 \\ 0 & 0 & \exp(-ik) & \lambda \cos(2\pi\sigma^\nu 3) & \dots & 0 \\ 0 & 0 & 0 & \exp(-ik) & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \exp(ik) & 0 & 0 & 0 & \dots & \lambda \cos[2\pi\sigma^\nu(N-1)] \end{pmatrix} \quad (3)$$

and is studied for $\nu = 1, 2, 3$.

First, we focus our interest on the band structure of the model. From the eigen-solutions of equation (3) we find, as a function of k , N bands with widths S_i ($i = 1, 2, \dots, N$) and $N - 1$ gaps of widths Δ_i . N is our scaling length and the incommensurate limit is attained only when $N \rightarrow \infty$. The appropriate spectral density measure can be defined as the number of states contained in each band. We have also been interested in certain wavefunctions, which can be accurately computed from equation (3) for successive periodicities N . At special energies, such as at the band centre or the band edges, this can be done very efficiently [9], so that their scaling and fluctuation properties can be explored with a high degree of numerical accuracy.

In the rest of the paper, we shall be concerned with the study of the distributions whose statistical moments give rise to the multifractal exponents at the mobility edge. The multifractal formalism describes globally the singular character of a probability measure p . This is a positive quantity, which can be the density of states or the wavefunction amplitude, distributed on a set that defines the support of the measure. We may introduce a partitioning of the set, which consists of linear boxes of equal sizes l_i , with a probability measure p_i associated with each box. In order to obtain the scaling properties of the spectrum, p_i is defined as the number of states within an energy band of width l_i and for simplicity all bandwidths l_i can be chosen to be equal. A more natural partitioning arises if the boxes are chosen to coincide with the sub-bands that sustain a non-zero measure p_i , that is if $l_i = S_i$. In this case we have constant p_i in every sub-band but a distribution of the bandwidths l_i . In order to study the scaling properties of the normalized wavefunction amplitude we partition the lattice into equal boxes and choose as the measure p_i the squared wavefunction amplitude summed up on each box. Clearly, in this case we have, instead, a constant box size l_i and a distribution for the p_i .

The computation of the scaling exponents is conveniently achieved via a statistical formalism. At the n th stage of approximation a partition function

$$\Gamma_n(q) = \sum_i p_i^q l_i^{-\tau(q)}$$

is introduced where the summation is defined on all non-empty boxes, $i = 1, 2, \dots, N$. In the large- n limit the generalized dimensions (Renyi entropies) $D_q = \tau(q)/(q - 1)$ are computed by requiring that $\Gamma_n(q) = 1$. Via a Legendre transform the exponents D_q can be cast into an upward convex curve $f(\alpha)$ characterizing the spectrum of singularities α (or D_q). For $q = 0$, the partition function $\Gamma(0)$ just counts the number of non-empty

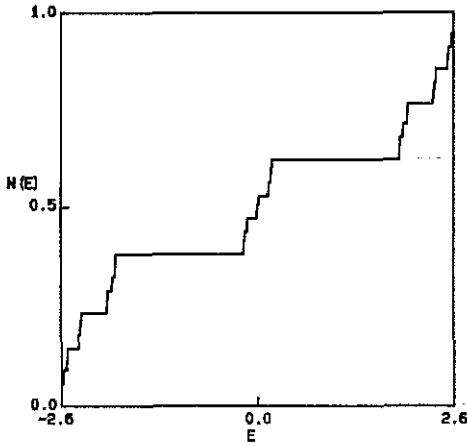


Figure 1. The calculated integrated density of states function for $\nu = 1, \lambda = 2$ computed for $N = 1597$.

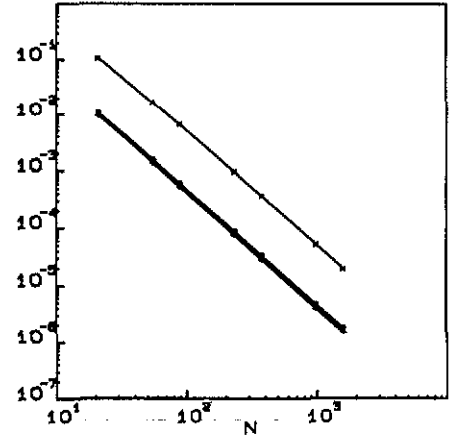


Figure 2. The arithmetic and geometric mean bandwidths $\langle S(N) \rangle$ (\circ) and $\langle S(N) \rangle_G$ ($+$) as a function of N for $\nu = 1, \lambda = 2$ (see equations (7) and (8)). The geometric mean gapwidth $\langle \Delta(N) \rangle_G$ (\times) is also shown. The least-squares fits are the expressions described by equations (8) and (9), respectively.

boxes and gives D_0 , which is the fractal dimension of the support of the measure. For the spectrum at the critical point $D_0 \approx 1/2$, and for the critical wavefunctions the corresponding $D_0 = 1$, since the wavefunctions have compact support, i.e. in this case D_0 equals the space dimension. The other dimensions D_q explore different regions of energy and space for the spectrum and wavefunctions, respectively. D_1 is usually referred to as the information dimension and D_2 as the correlation dimension. For normalized wavefunctions D_1 refers to the scaling of the information entropy, defined by $-\sum_i p_i \ln p_i$ and D_2 to the inverse participation ratio $\sum_i p_i^2$, often used to characterize localization [4].

3. Scaling and fluctuation statistics of the eigensolutions

3.1. For the energy spectrum

The band structure for $\nu = 1$ and any σ, λ has originally been understood via simple empirical rules [1], subsequently analytically confirmed [27], describing the hierarchical subdivision of the spectra. For $\sigma = \sigma_G^{-1}$ and $\sigma = \sigma_S$ each band is composed of two side sub-bands and one central sub-band, which follow roughly the same gap sequence as the full band itself. At the critical point ($\lambda = 2$) of the self-dual model the spectrum becomes a self-similar Cantor set. The numerically computed critical integrated density of states is shown in figure 1. The density of states is known to define a multifractal measure characterized by a α - $f(\alpha)$ curve of scaling exponents [7].

Before we attempt to characterize the distributions of fluctuations at this point we may exploit the approximate hierarchical structure of the spectrum. We immediately notice the two dominant band gaps in figure 1, which repeat indefinitely, leading to the self-similar band structure. The reduction of the total mother band to two left and right

equal sub-bands plus a smaller central band is achieved by the ratios a and b , respectively. We accurately compute the asymptotic ratios and the results are $a \approx 1/7.182$ and $b \approx 1/13.739$, which may be compared with the perturbation theory estimates and the computations of [27]. Naturally the previous considerations from the simple three-scale Cantor set lead to a binomial multifractal formula for the corresponding bandwidth distribution. At the n th stage of this approximate hierarchical construction of the spectrum the total number of bands is $N = 3^n$ and $(n + 1)$ different band sizes exist. The occurrence probability for a given band size is, therefore, given by

$$P(m) = \binom{n}{m} \left(\frac{2a}{2a+b} \right)^m \left(\frac{b}{2a+b} \right)^{n-m} \quad m = 0, 1, \dots, n \quad (4)$$

and the set may be generated via the partition function

$$\Gamma_1(q) = 2(1/3)^q a^{-\tau(q)} + (1/3)^q b^{-\tau(q)}. \quad (5)$$

In order to determine the exponents $\tau(q)$ the equation $\Gamma_1(q) = 1$ has to be solved. The corresponding α - $f(\alpha)$ spectra are obtained accordingly [17]. For the maximal and minimal scaling, corresponding to the most rarefied (largest intervals S_i) and the densest parts (the smallest S_i) of the density, from equation (5) we obtain

$$D_{-\infty} = \alpha_{\max} = \ln(1/3)/\ln a \approx 0.557 \quad (6a)$$

$$D_{+\infty} = \alpha_{\min} = \ln(1/3)/\ln b \approx 0.419 \quad (6b)$$

respectively. These values compare reasonably well with the corresponding numerical estimates $D_{-\infty} \approx 0.547$ and $D_{+\infty} \approx 0.421$, respectively [7]. For $\lambda < 2$ we have $\alpha = 1$ with $f = 1$ and $\alpha = 1/2$ with $f = 0$ due to the one-dimensional square-root Van Hove singularities; while for $\lambda > 2$ all the fractal measures are zero ($\alpha = 0$). We obtain the result $D_0 \approx 0.51$ for the Hausdorff dimension concerning the spectral support, which agrees with the expected almost universal value [7, 27] of $D_0 \approx 1/2$.

We now consider the corresponding statistical bandwidth and gapwidth distributions whose moments are responsible for the multifractal exponents of the density of states. It turns out that they cannot be understood as easily as the exponents themselves. For the successive approximants defining the periodicities described by the scale N we analysed numerically the distribution of the bandwidths $S_i(N)$ and the gapwidths $\Delta_i(N)$. The average bandwidth is found for $\lambda \leq 2$ to scale (see figure 2) as

$$\langle S(N) \rangle = AN^{-(1+\delta)} \quad (7)$$

where the exponent δ is precisely zero for $\lambda < 2$, $\delta = 1$ for $\lambda = 2$ and $\langle S(N) \rangle$ decays exponentially with N for $\lambda > 2$. From a least-squares fit of the data of figure 2 we find for the constant $A \approx 4.65$, in close agreement with the scaling law of the total bandwidth $B(N) = N\langle S(N) \rangle$ as considered in [28]. The exponent $\delta = 1$ at $\lambda = 2$ is connected with the Cantor set fractal support of the density of states by the relation $D_0 = 1/(1 + \delta)$ [25]. We have also computed the geometric mean of S_i , which is found (see figure 2) to be very close to the arithmetic mean of equation (7) but with a slightly different constant $A \approx 4.40$, indicating that the distribution is not broad. The corresponding distribution of the gapwidths Δ_i is instead much broader. It is described by an inverse power-law-type function [21, 22]. In this case we have computed a typical value defined by the geometric mean gapwidth $\langle \Delta(N) \rangle_G$. It is found (see figure 2) that for $\lambda \leq 2$ it scales with

N similarly to equation (7), that is

$$\langle \Delta(N) \rangle_G = BN^{-(1+\delta')} \quad (8)$$

but with a new exponent δ' and a different constant $B = 46.06$ at $\lambda = 2$. The corresponding exponent δ' increases with λ for $\lambda < 2$, becomes $\delta' = \delta = 1$ for $\lambda = 2$. For $\lambda > 2$ $\langle \Delta(N) \rangle_G$ decays exponentially, slower than $\langle S(N) \rangle$. The widths of the energy bands S_i can be related to the shifts of the energy levels due to changes in the boundary conditions from periodic to antiperiodic [4]. The conductance $G(N)$ in units of e^2/\hbar can be empirically defined for the finite system *à la* Thouless from the density of allowed bands near the Fermi energy. Its averaged value should, therefore, be proportional to the total bandwidth $B(N) = N\langle S(N) \rangle$. In the delocalized regime ($\lambda < 2$) it is finite and proportional to $2|\lambda - 2|$, while in the localized regime ($\lambda > 2$) it decays as $\exp(-N/\xi)$, where ξ is the appropriate localization length; exactly at the critical point ($\lambda = 2$) from (7) it must decay as A/N . The conductivity should be $N\langle G(N) \rangle$; for the infinite system it becomes infinite for $\lambda < 2$, is constant for $\lambda = 2$ and vanishes for $\lambda > 2$. Our results suggest that an alternative definition of $\langle G(N) \rangle$ may also be possible via the dimensionless ratio $\langle S(N) \rangle / \langle \Delta(N) \rangle_G$, where the arithmetic mean bandwidth $\langle S(N) \rangle$ and the geometric mean gapwidth $\langle \Delta(N) \rangle_G$ are used. This definition gives a different N -dependence of $\langle G(N) \rangle$ but a finite-size scaling analysis for the averaged conductance naturally arises. The log-log plots of $\langle G(N) \rangle$ versus N are characterized, from equations (7) and (8), by the difference of exponents $\delta' - \delta$ for $\lambda \leq 2$. In the extended phase $\langle G(N) \rangle$ increases versus N , leading eventually to infinite conductance, while in the localized phase it decreases and tends to zero. The fixed-point value (at $\lambda = 2$) is constant here

$$\langle G(N) \rangle_c = (A/B)(e^2/\hbar) = 0.1(e^2/\hbar) \quad (9)$$

while most available data for three-dimensional disordered systems suggest a value of $\langle G(N) \rangle_c = 0.03(e^2/\hbar)$ [10]. The critical fluctuations around $\langle G(N) \rangle$ can also be studied in this approach. They are very large, mostly due to the distribution of the gapwidths Δ_i .

In order to understand the conductance fluctuations we are now concerned with the nearest energy level spacing distribution $P(S)$, which describes first-order density correlations. This is the most common spectral fluctuation measure, which is expected in the metallic phase of disordered systems to follow the Wigner surmise while in the insulating limit to approach the Poisson distribution [10–12]. Previous results for the quasi-periodic model [21–23] have shown that $P(S)$ is trivial for $\lambda < 2$ and it follows the expected Poisson law for $\lambda > 2$. At the critical point they find [21, 22] an inverse power-law distribution function, $P(S) \propto S^{-3/2}$, as the nearest level spacing $S \rightarrow 0$, which implies a strong clustering of levels. In subsequent attempts [23] a cumulative level spacing distribution was computed, and it was correctly suggested that the spacings between adjacent levels had to be multiplied by the density of states, which amounts to the removal of the energy scale. This is equivalent to what is known as a deconvolution [29] of the spectrum, i.e. scaling it down by a smooth function so that the averaged density of states remains constant and is equivalent to studying, instead of the distribution of $E_i - E_{i-1}$, the distribution of $\langle N(E_i) \rangle \times \langle N(E_{i-1}) \rangle = (E_i - E_{i-1}) \cdot dN(E)/dE$ where $\langle N(E) \rangle$ is the averaged integrated density of states at energy E . In order to elucidate the question of the critical level statistics we distinguish large and small energy scales by separating the distributions of the bandwidths from the gapwidths. In our interpretation

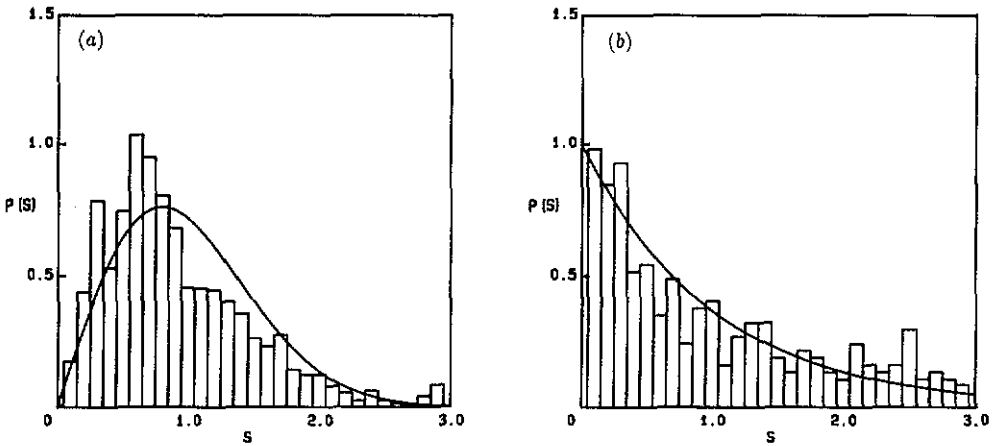


Figure 3. (a) The calculated level spacing distribution function at the mobility edge in histogram form for $\nu = 1$, $\lambda = 2$ from the subband width statistics. The horizontal axis is in units of the local mean level spacing and the full curve is the Wigner–Dyson formula $P(S) = S(\pi/2) \exp(-\pi S^2/4)$ [14] for the orthogonal ensemble, which implies linear level repulsion. (b) As in (a) but for the insulating regime ($\lambda = 3$). The full curve is the formula $P(S) = \exp(-S)$ (Poisson).

we rely on the fact that for a given N the number of energy levels per sub-band ($\propto 1/N$) is fixed and the corresponding eigenstates should have spacings S_i divided by a constant factor in order to retain a constant density of states in every band. Therefore, as it turns out, it is sufficient for the level statistics, coming from states in every sub-band, to consider only the statistics of bandwidths and $P(S)$ can be replaced from the distribution of the S_i . The result obtained for the normalized critical distribution function $P(S)$ is shown in figure 3(a) together with the corresponding Wigner surmise fit. It can be seen that the histogram follows, at least approximately, the Wigner–Dyson surmise at the mobility edge with $P(S) \propto S$ as $S \rightarrow 0$ being in sharp contrast with the inverse power law $P(S) \propto S^{-3/2}$ obtained in [21, 22]. The result of figure 3(a) can be regarded as evidence for the approximate validity of the Wigner-like statistics with the presence of level repulsion at the mobility edge. This novel result arises, equivalently, by studying a chain of length L much larger than the periodicity N , in the limits where both L and N go to infinity.

If one instead considers the energy spacings as arising from the statistics of the gapwidths, then the level spacing statistics can be easily understood from the support of the Cantor set spectrum. This means that the relevant exponent is D_0 and the power is given by $1 + 1/D_0 = 2 + \delta$ [21, 22]. This result can also be understood by simplifying further the three-scale Cantor set of equation (4) discussed previously by replacing $a = b$. Then $D_0 = \ln(1/3)/\ln a$ and the number of gaps of width larger than Δ can be approximately shown to obey the scaling $\text{Num}(\Delta) \propto \Delta^{-D_0}$ [30]. This is because at the n th level of construction a total number of $3^n - 1$ gaps exists with $2 \times 3^{m-1}$ gaps of sizes $\Delta_m = a^{m-1}[(1 - 3a)/2]S_0$, for $m = 1, 2, \dots, n$ and S_0 being the original band. Then

$$\text{Num}(\Delta_n) = \sum_{m=1}^n 2 \times 3^{m-1} \approx 3^n$$

and by using $\Delta_n = a^{n-1}[(1 - 3a)/2]S_0$ we can eliminate n so that $\text{Num}(\Delta) \propto \Delta^{-1/D_0}$. Then

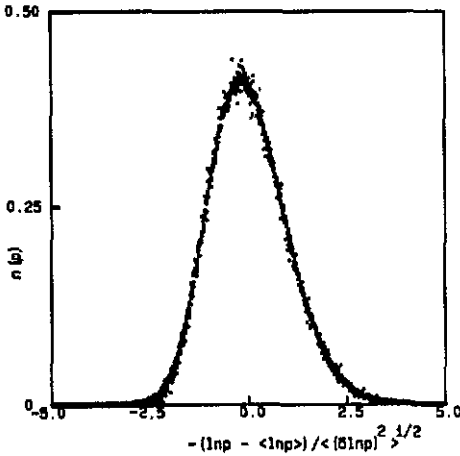


Figure 4. The calculated normalized distribution $n(p)$ for the critical wavefunction amplitude $p_i = |\Psi_i|^2$ at $E = 0$ for $\nu = 1, \lambda = 2$. The horizontal axis is in log scale. The wavefunction is computed for lattices of sizes: $N = F_{23} = 75\,025, F_{24} = 121\,393, F_{26} = 317\,811, F_{27} = 517\,229, F_{29} = 1\,346\,269$ and $F_{30} = 2\,178\,309$. It demonstrates the validity of an approximate two-parameter scaling of the distribution $n(p)$ for all different length periods N ranging from F_{23} to F_{30} .

by differentiating $P(\Delta) \propto |d\text{Num}(\Delta)/d\Delta| \propto \Delta^{-(1+D_0)}$ and relying on the assumption that the set mimics the critical situation ($D_0 \approx \frac{1}{2}$) we obtain $P(\Delta) \propto \Delta^{-3/2}$. This is the nearest level function $P(S)$ according to [21, 22]. We see that our results and the results of [21, 22] can both be understood as arising from the bandwidth and gapwidth distributions, respectively. It is clear that at least in one of the cases a deconvolution of the spectrum is essential. We also had to distinguish the statistics between small and large energy scales, guided by the intermediate Thouless energy scale $E_T = \langle S(N) \rangle$ from equation (7). In the former case a smoothing of the density of states within individual bands is employed and in the latter case smoothing for the whole of the density of states as a whole was required. For the insulating phase in both cases the simple Poisson law $P(S) = e^{-S}$ suffices as seen in figure 3(b).

3.2. For the wavefunction amplitude

The wavefunction is a more directly relevant measure of localization properties than the spectrum. At a particular level of approximation the system of size N is periodic and we may study the square of the wavefunction amplitude at every site as a local probability measure p_i that repeats indefinitely with period N . By normalizing it to unity for every N

$$\sum_i p_i = \sum_{i=1}^N |\Psi_i|^2 = 1 \tag{10}$$

we can study scaling. In the infinite- N limit the wavefunction amplitude may show singularities, which have been previously analysed in terms of generalized multifractal dimensions D_q and corresponding α - $f(\alpha)$ spectra of exponents. Extended wavefunctions are space filling and in the infinite- N limit $\alpha \approx 1$ with $f = 1$. The $f(\alpha)$ spectrum of exponents consists only of two points for localized wavefunctions: $f = 0$ at $\alpha = 0$ and $f =$

1 at $\alpha = \infty$. The former is due to sites having finite p , obviously of zero measure in the infinite- N limit; and the latter to the rest of the sites. The critical wavefunctions are characterized by a set of critical exponents converging to a continuous set D_q ranging from α_{\min} to α_{\max} and having a non-zero probability density $f(\alpha)$. They are defined from the scaling of all the moments

$$\sum_{i=1}^N p_i^q = \sum_{i=1}^N |\Psi_i|^{2q} = \sum_p n(p) p^q \sim N^{(q-1)D_q} \quad (11)$$

where $n(p)$ is the full probability distribution function of the fluctuating amplitude p . It has been found that states at the mobility edge in three-dimensional disordered electronic systems [19] are also multifractals, at least for the averaged positive moments. In this respect the spatial fluctuations of the wavefunction amplitude show similar critical behaviour in quasi-periodic and disordered systems.

Our calculations have been restricted to special energies. For odd $N = F_n$ there is always an eigenstate with energy $F = 0$ and we have concentrated mostly on this eigenstate, for which the wavefunction can be computed recursively [9]. The most prominent scaling exponents for this eigenstate (not to be confused with the exponents describing the spectrum) are $D_0 = 1$ and $D_1 \approx 0.7627$, $D_2 \approx 0.6123$ and $D_x \approx 0.3528$, respectively. D_2 is analogous to the correlation fractal dimension D first proposed to describe wavefunctions in [31]. For the quasi-periodic model at the critical point ($\lambda = 2$) it was found that $D \approx 0.80$ with error bars of about 15% [32]. Our value of D_2 may be compared with D and the reasonably close value of 0.82 reported in [8].

In order to understand better the nature of critical wavefunctions we choose to plot the full distribution function $n(p)$ for many systems of successive periods N . This distribution is very broad and resembles closely those obtained in disordered systems [19]. In figure 4 we display the full $n(p)$ distribution function for many different very large N values. It can be seen that, if all the data for various N are plotted versus $\ln p$ by subtracting the mean $\langle \ln p \rangle$ and dividing by the corresponding standard deviation $\delta \ln p = \ln p - \langle \ln p \rangle$, a single universal scaling function is obtained. This can be approximated by a Gaussian for the log, which implies the approximate validity of a two-parameter scaling at the mobility edge. We have also attempted to fit the data onto a one-parameter scaling curve. By assuming an inherent multiplicative process we may approximate $n(p)$ by a log-normal distribution but with mean \propto variance $\propto \ln N$. Such a one-parameter scaling fit does work only very approximately and we find that the variance is roughly 1.5 times the mean. However, a fit with at least two or even more parameters seems to be necessary to describe scaling of the wavefunction amplitude distributions. We cannot numerically distinguish the tails of the distribution, which must be responsible for the anomalous scaling of the higher-order moments. It must be pointed out that if one relied on the validity of a Wigner–Dyson theory [14] one might have expected that the eigenstates would be chaotic. Accordingly, in the limit of $N \rightarrow \infty$ the function $n(p)$ should become a χ^2 distribution, i.e. the distribution of a squared Gaussian variable [33]. Such chaotic eigenvectors would further imply that $D_q = 1$ for all q , which is clearly not the case for the computed critical wavefunctions. We obviously cannot fit $n(p)$ by a χ^2 distribution despite the results on the spectral statistics in the previous section. Our critical $n(p)$ function is much broader than χ^2 , if we note the log scale on the x axis of figure 4.

4. Extended quasi-periodic models

We have also considered a more general one-dimensional quasi-periodic version of equation (2) with $\nu = 2$ and 3. This extension was first proposed in [34] and it is believed

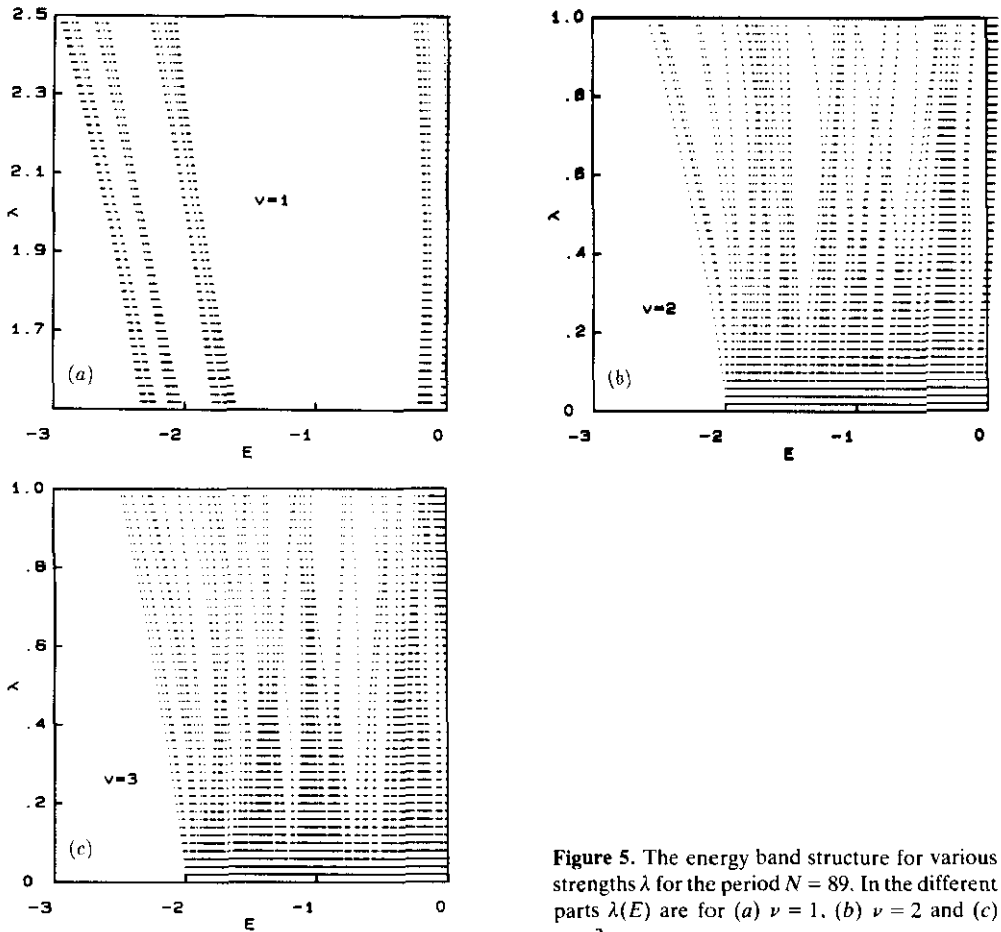


Figure 5. The energy band structure for various strengths λ for the period $N = 89$. In the different parts $\lambda(E)$ are for (a) $\nu = 1$, (b) $\nu = 2$ and (c) $\nu = 3$.

that, as a consequence of the non-linearity of the argument in the cosine in equation (2) for $\nu > 1$, no mobility edges exist for any λ [35]. The behaviour found for this model is essentially indistinguishable from that of a random system of the same variance for random input numbers. We have applied the same method in the case of $\nu = 2, 3$ and our results can be compared with the results obtained for the self-dual model of $\nu = 1$. In figure 5 the band structure is displayed for the three versions ($\nu = 1, 2, 3$) of equation (2) and every λ . It can be seen in the figures that $\nu = 2, 3$ have a different band structure from that of $\nu = 1$. The trend for the spectrum is to become more point-like as ν increases. This becomes clearer if we follow every band by increasing N (see also figure 6 for $\nu = 3$). In figure 7 the total bandwidth is plotted versus N for the values $\nu = 1, 2, 3$. If extended states exist, according to equation (7) $\delta = 0$ and it should reach a constant value for large N . This can be seen to occur only for $\nu = 1$ and $\lambda < 2$. The corresponding behaviour of a true one-dimensional random system with the same variance should not differ.

Therefore, it can be concluded that we may easily devise models that mimic strongly disordered systems. It is sufficient just to consider a simple non-linear mapping giving

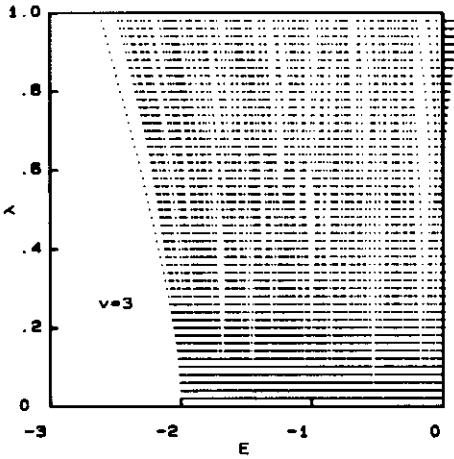


Figure 6. The same as figure 5(c) but for $N = 377$.

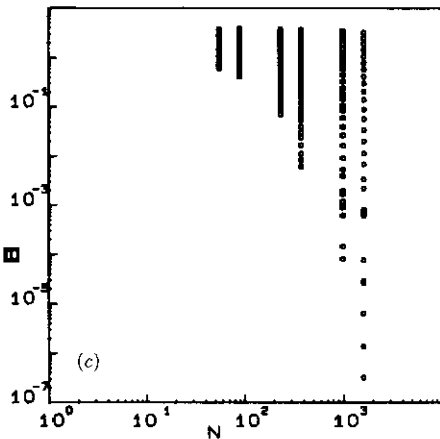
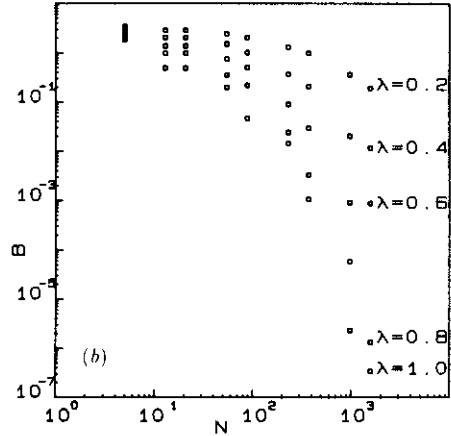
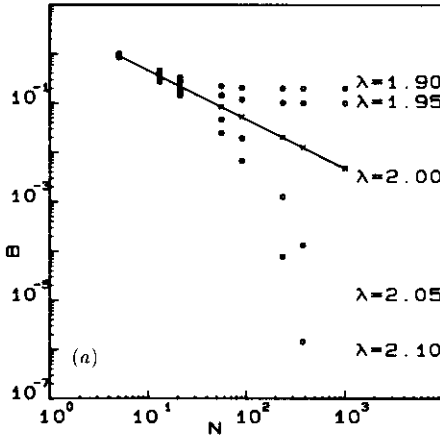


Figure 7. Log-log plots of the total bandwidth $B(N) = N\langle S(N) \rangle$ versus the period N for various quasi-periodic potential strengths λ marked in the figures. The different parts are for (a) $\nu = 1$, (b) $\nu = 2$ and (c) $\nu = 3$.

rise to a chaotic site potential, which essentially acts as a random site energy. For the spectral fluctuations of such models ordinary (Poisson) nearest level statistics are expected. The phenomenon is also familiar [36] in quantum models whose classical analogue exhibits chaotic behaviour. In this case the common signs of quantum chaotic behaviour, such as the Wigner–Dyson statistics, do not appear due to the presence of localization [13].

5. Discussion

There are not many examples where the Anderson transition can be studied without innumerable difficulties already present even in the simplest kind of numerical simulations. A rather tractable model is that of electronic systems in one-dimensional quasi-periodic lattices, which is studied in this article. We presented a complete numerical study focused on the most interesting questions concerning the energy spectrum and the nature of the eigenstates, in connection with the phenomenon of Anderson localization. We give numerical evidence supporting an important novel conjecture that the critical behaviour for such model systems is close, in some respects, to the diffusive metallic phase in random systems. This is verified from our findings of an almost Wigner–Dyson statistical description for the critical spectral bandwidth fluctuations. Although the quasi-periodic systems do not have a mesoscopic regime, we found that traces exist at the critical point. Other properties, such as the gap statistics, are also found to be power-law distributed confirming previous studies and our description of the spectral fluctuations can be further linked to the conductance fluctuations.

The properties of the normalized critical wavefunction amplitude distributions are also considered by scaling with the system size the moments of the associated probability density. This leads to a continuous set of fractal exponents D_q and α - $f(\alpha)$ spectra. Attention is focused again on the corresponding critical distributions, which are approximately described by a single limiting scaling function. On the other hand we find no obvious differences in the asymptotic limit between localized states in quasi-periodic and disordered chains. This is confirmed by studying models with pseudo-random potentials which display only localized states due to loss of the quasi-periodicity because of non-linearity.

In summary, our study, in connection with previous works, answers the questions (i) and (ii) of the introduction. Referring to question (iii) we have given here further evidence that the Anderson transition studied in these simple models shows a lot of similarities with the corresponding transition in disordered systems, both for the averaged values and the fluctuations of the quantities of interest. This suggests that the models can be used as a laboratory for studying the real transition. Our results also point towards a connection of experimental significance between these models, mesoscopic systems and quantum dynamics in classically chaotic systems. The key feature in our work is the presence of the complicated scaling of the moments at the transition. We showed that the distributions themselves can be understood too and it remains a future question to see the critical conductance distribution by the Kubo formula [15]. Recent considerations [37–39] relate the multifractal critical phenomena to field theories with high powers of gradients in appropriate non-linear σ models, a subject of current debate.

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