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Analytical results for multifractal properties of spectra of quasiperiodic Hamiltonians near the periodic chain

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Abstract. The multifractal properties of the electronic spectrum of a general quasiperiodic chain are studied in first order in the quasiperiodic potential strength. Analytical expressions for the generalized dimensions are found and are in good agreement with numerical simulations. These first-order results do not depend on the irrational incommensurability.

1. Introduction

Quasicrystals are characterized by remarkable transport properties (e.g. low conductivities *increasing* with T or disorder) which are generally attributed to the complicated interplay between the electrons and the peculiar atomic structure [1]. Some of these have been related to the electronic properties found in 2D or 3D theoretical models (critical states, spiky singular density of states, anomalous transport etc) [1]. One-dimensional models of quasiperiodic structures share all these features, in addition to other properties such as the occurrence of a zero measure spectrum. Thus, despite their lack of direct physical interest, they are worth studying since properties which can only be illustrated numerically in higher dimensions, and thus sometimes lack a direct justification, can be calculated very precisely in 1D.

A frequently studied one-dimensional quasiperiodic tight-binding Hamiltonian is given by

$$H = \sum_i t_{i+1}|i\rangle\langle i+1| + v_i|i\rangle\langle i| + t_i|i\rangle\langle i-1| \tag{1}$$

where the $t_i \in \{1, \rho\}$ and $v_i \in \{-\lambda, \lambda\}$ follow quasiperiodic sequences to be specified below. The spectra of this kind of Hamiltonian have been proven to be Cantor sets of zero Lebesgue measure for all values of the potential $1 - \rho \neq 0$, respectively $\lambda \neq 0$ [2, 3]. Furthermore, the density of states (DOS) is purely singular continuous [2, 3]. In order to characterize the intricate nature of these spectra, a multifractal analysis of the measure can be elaborated, yielding a multifractal spectrum $f(\alpha)$. More precisely, $f(\alpha)$ is the Hausdorff dimension of the set of energies in the spectrum with local scaling exponent α, where α characterizes the DOS singularities ($D(E + \Delta E) - D(E) \sim \Delta E^{\alpha}$). The existence of the

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generalization of such exponents to 2D and 3D can be shown to affect the transport properties directly, and a phenomenological transport theory of quasicrystals involves the distribution of scaling exponents [1]. In the thermodynamic formalism, introduced by Halsey *et al*, generalized dimensions D_q can be defined [4, 5]. These also play an important role for the understanding of anomalous diffusion properties and the decay of the autocorrelation function encountered in quantum dynamics of quasiperiodic systems [6–9]. In the case of a quasiperiodic chain with the golden mean as incommensurability, a renormalization analysis based on the trace map approach leads to the exact minimal and maximal scaling exponents $\alpha_{\min}$ and $\alpha_{\max}$ for all values of the quasiperiodic potential, while the fractal dimensions $f(\alpha)$, $\alpha_{\min} < \alpha < \alpha_{\max}$, remain unknown [10–13]. In the limit of large potential ($|1-\rho| \gg 1$, $|\lambda| \gg 1$) the renormalization approach of Niu and Nori [14] has been used to obtain $f(\alpha)$ [15, 16] for this Fibonacci chain.

In the present paper we discuss the opposite limit ($|1-\rho| \ll 1$, $|\lambda| \ll 1$), for which a perturbation theory approach has been introduced in [17] for *any* quasiperiodic chain. We begin by reporting briefly on this approach (section 2), exploit the results in order to calculate the multifractal properties of the energy spectrum (section 3) and finally compare our theoretical relations with numerical data (section 4).

2. Perturbation theory for small potential

We consider the tight binding model,

$$t_{i+1}\psi_{i+1} + v_i\psi_i + t_i\psi_{i-1} = E\psi_i \tag{2}$$

with the hopping elements t_i arranged in a quasiperiodic manner:

$$t_i = \begin{cases} \rho & \text{for} \quad 0 < \{\omega i\} < 1-\omega \\ 1 & \text{for} \quad 1-\omega < \{\omega i\} < 1 \end{cases} \tag{3}$$

where $\{\cdot\}$ denotes the fractional part and $\omega \in (0,1)$ is an irrational number. The on-site potentials are $v_i = \lambda$ if the site i is surrounded by two different bonds, and $-\lambda$ otherwise. In the following we will consider rational approximants with p_l hopping elements of strength ρ and q_l ones of strength 1 (i.e. $\omega_l = 1/(1+p_l/q_l)$) and eventually take the limit $l \to \infty$. For these approximants with period $n_l = p_l + q_l$ Bloch theorem can be applied, and one obtains n_l energy bands.

For small $|\lambda|$ and $|1-\rho|$ perturbation theory is used, taking as a starting point the non-modulated chain ($\lambda = 1-\rho = 0$) with its eigenvalues,

$$E_j^{(0)}(k) = 2\cos\left(\frac{2\pi j + k}{n_l}\right) \qquad j = 0, \ldots, n_l - 1 \tag{4}$$

where k represents the Bloch vector. If the quasiperiodic potential is switched on, gaps open at the energies $E_j^{(0)}(0)$ ($j \neq 0$, $j \neq \frac{n_l}{2}$ (for n_l even)) and $E_j^{(0)}(\pi)$ ($j \neq \frac{n_l+1}{2}$ (for n_l odd)). For odd values of n_l these energies can be renumbered in a compact form:

$$E_{j,0} = \pm 2\cos\left(\frac{\pi j}{n_l}\right) \qquad j = 1, \ldots, \frac{n_l - 1}{2}\,. \tag{5}$$

Since in the limit of large system size, the spectral properties will not depend on whether n_l is even or odd, we will restrict ourselves, for sake of simplicity, to odd values of n_l.

In order to facilitate perturbation theory and to index the gaps roughly according to their width, Sire and Mosseri [17] introduced a new numbering, where the atoms of the quasiperiodic chain are numbered with respect to their location in perpendicular space rather

than with respect to their position in physical space. In this basis the originally tridiagonal Hamiltonian with quasiperiodic entries becomes a multidiagonal Hamiltonian with identical entries in each secondary diagonal, except for the two Bloch entries.

By applying perturbation theory for degenerate states to this Hamiltonian it can be shown that the band edges read in first order [17]†:

$$E_j \pm \Delta E_j = 2\epsilon \cos(\pi j \beta_l)(1-(1-\rho)\beta_l) + \lambda(4\beta_l - 1) \pm \frac{2}{\pi j}((1-\rho)\sin(\pi j \beta_l) - \epsilon\lambda \sin(2\pi j \beta_l)) \tag{6}$$

with $j \in [1, \ldots, (n_l - 1)/2]$, $\epsilon = \pm 1$ and $\beta_l = p_l/n_l = 1 - \omega_l$. In principle, this expression correctly describes the opening of gaps with index $j < \pi^2/(|\lambda| + |1-\rho|)$. For $\lambda = 1 - \rho = 0$ all gaps are closed and $E_j = 2\epsilon \cos(\pi j p_l/n_l)$, which is a mere renumbering of equation (5). Equation (6) is the starting point for our calculation for the multifractal properties.

3. Multifractal properties of the energy spectra

In the thermodynamic formalism the multifractal scaling function $\tau(q)$ is obtained by requiring that the partition function,

$$\Gamma(\tau, q) = \frac{1}{n_l^q} \sum_{j=1}^{n_l} \frac{1}{\Delta_j^\tau} \tag{7}$$

be constant for $n_l \to \infty$, where Δ_j denotes the widths of the individual (non-overlapping) bands. For a periodic chain it is straightforward to obtain that

$$q^{(0)}(\tau) = \begin{cases} \tau + 1 & \text{for} \quad \tau < 1 \\ 2\tau & \text{for} \quad \tau \geqslant 1 \end{cases} \tag{8}$$

so that the multifractal spectrum $f^{(0)}(\alpha)$, which is the Legendre transform of $\tau^{(0)}(q)$, consists of two parts: $f^{(0)}(1) = 1$, corresponding to the absolutely continuous component of the DOS, and $f^{(0)}\left(\frac{1}{2}\right) = 0$, reflecting the presence of van Hove singularities at the edge of the spectrum.

In the following, our aim is to calculate the corrections to $q^{(0)}(\tau)$, respectively $f^{(0)}(\alpha)$, in first order of the quasiperiodic potential. We will separately consider two cases: the on-site model ($\rho = 1, \lambda \neq 0$) and the off-diagonal model ($\rho \neq 1, \lambda = 0$). We begin by treating the former model, which is, as we will see, the more interesting one. In order to calculate the multifractal properties by means of perturbation theory, we will interpret changes in the scaling exponent as logarithmic corrections in the size of the system n_l for $q(\tau)$, in the limit of small perturbation ($n_l^q \sim n_l^{q^{(0)} + \lambda q^{(1)} + \cdots} \sim n_l^{q^{(0)}}(1 + \lambda q^{(1)} \ln n_l + \cdots)$). This method is reminiscent of what is achieved in the field of critical phenomena in order to calculate critical exponents in perturbation theory (e.g. ε expansion).

The bandwidths Δ_j of the modulated chain can be expressed by

$$\Delta_j = \Delta_{j,0} - \delta\Delta_j \tag{9}$$

where $\Delta_{j,0}$ stands for the corresponding width for the periodic chain:

$$\Delta_{j,0} = 2\left|\cos\left(\frac{\pi j p_l}{n_l}\right) - \cos\left(\frac{\pi(jp_l + 1)}{n_l}\right)\right| = \frac{2\pi}{n_l}\left|\sin\left(\frac{\pi j p_l}{n_l}\right)\right| + \mathcal{O}\left(\frac{1}{n_l^2}\right) \tag{10}$$

† Strictly speaking perturbation theory yields $n_l \sin(\pi j/n_l)$ instead of πj in the denominator of equation (6) (cf equation (10) in [17]). Our equation (6) corresponds to equation (17) in [17]; it can be shown that the scaling behaviour, in which we are interested, is not affected by the approximation employed.

and $\delta\Delta_j > 0$ denotes the decrease of the bandwidth due to the quasiperiodic potential, which can be expanded in a formal series,

$$\delta\Delta_j = \sum_{l=1}^{\infty} \lambda^l \delta\Delta_j^{(l)} . \tag{11}$$

For simplicity we take $\lambda > 0$, so that $\delta\Delta_j^{(1)} > 0$; the final result only depends on $|\lambda|$, which can be easily checked. Inserting equation (11) in (9) and (7) we find the partition function in first order in λ:

$$\Gamma(\tau, q) = \frac{1}{n_l^q} \sum_j \frac{1}{\Delta_j^\tau} = \Gamma_0(\tau, q)\left(1 + \lambda\tau \frac{\sum_j \Delta_{j,0}^{-1-\tau} \delta\Delta_j^{(1)}}{\sum_j \Delta_{j,0}^{-\tau}}\right) \tag{12}$$

where $\Gamma_0(\tau, q)$ is the partition function of the periodic chain. On the other hand, inserting $q(\tau) = \sum \lambda^l q^{(l)}(\tau)$ into the asymptotic relation $\Gamma(\tau, q) = n_l^{q(\tau)-q}$ yields in first order

$$\Gamma(\tau, q) = \Gamma_0(\tau, q)(1 + \lambda q^{(1)}(\tau) \ln n_l) . \tag{13}$$

Thus the first-order correction $q^{(1)}(\tau)$ reads

$$q^{(1)}(\tau) = \tau \lim_{n_l \to \infty} \frac{1}{\ln n_l} \frac{\sum_j \Delta_{j,0}^{-1-\tau} \delta\Delta_j^{(1)}}{\sum_j \Delta_{j,0}^{-\tau}} . \tag{14}$$

In order to evaluate this expression we remark that the decrease $\delta\Delta_j = \Delta_{j,0} - \Delta_j$ of each bandwidth is the sum of the half-widths of the two adjoining gaps, i.e. in first order:

$$\lambda\delta\Delta_j^{(1)} = \Delta E_{j_1} + \Delta E_{j_2} . \tag{15}$$

Since $\Delta_{j,0}$ depends smoothly on the location of the band, the sum in the numerator of equation (14) can be rearranged:

$$\sum_j \Delta_{j,0}^{-1-\tau} \delta\Delta_j^{(1)} = \sum_j \Delta_{j,0}^{-1-\tau} \frac{2}{\lambda} |\Delta E_j| . \tag{16}$$

In the diagonal case the half-width of the gap is given by $|\Delta E_j| = \frac{2}{\pi j}|\lambda \sin(2\pi j\beta_l)|$, so that we obtain

$$q^{(1)}(\tau) = \frac{8\tau}{\pi^2} \lim_{n_l \to \infty} \frac{1}{\ln n_l} \frac{\sum_{j=1}^{(n_l-1)/2} \frac{1}{j} |\sin(\pi j\beta_l)|^{-\tau} |\cos(\pi j\beta_l)|}{\frac{2}{n_l} \sum_{j=1}^{(n_l-1)/2} |\sin(\pi j\beta_l)|^{-\tau}} . \tag{17}$$

To proceed further we have to distinguish between $\tau < 1$ and $\tau > 1$. For the first case, and provided $\beta = \lim_{l \to +\infty} \beta_l$ is a generic irrational number (not too well approximated by rationals [3]), we can use the Euler–MacLaurin formula to convert the sum in the numerator into

$$\int_{\beta_l}^{\frac{n_l-1}{2}\beta_l} \frac{|\sin(\pi x)|^{-\tau} |\cos(\pi x)|}{x} \, \mathrm{d}x + C + \mathcal{O}\left(\frac{1}{n_l}\right) \tag{18}$$

where C is a constant.

Splitting this integral according to the periodicity of its numerator and replacing the sum in the denominator of equation (17) by the corresponding integral, we finally arrive at the following expression for $q^{(1)}(\tau)$:

$$q^{(1)}(\tau) = \frac{8\tau}{\pi^2} \frac{\int_0^1 |\sin(\pi x)|^{-\tau} |\cos(\pi x)| \, \mathrm{d}x}{\int_0^1 |\sin(\pi x)|^{-\tau} \, \mathrm{d}x} \qquad \tau < 1 \tag{19}$$

which yields

$$q^{(1)}(\tau) = \frac{16}{\pi^{5/2}} \frac{\tau \Gamma\left(\frac{-\tau+2}{2}\right)}{(-\tau+1)\Gamma\left(\frac{-\tau+1}{2}\right)} \qquad \tau < 1\,. \tag{20}$$

Therefore we find the following relation for $\tau(q)$ in first order in λ:

$$\tau + \frac{16}{\pi^{5/2}}|\lambda| \frac{\tau \Gamma\left(\frac{-\tau+2}{2}\right)}{(-\tau+1)\Gamma\left(\frac{-\tau+1}{2}\right)} = q - 1 \qquad \tau < 1\,. \tag{21}$$

Using $\tau(q) = (q-1)D_q$ one obtains for the generalized dimensions

$$D_q = 1 - |\lambda| \frac{16}{\pi^{5/2}} \frac{\Gamma\left(\frac{3-q}{2}\right)}{(2-q)\Gamma\left(\frac{2-q}{2}\right)} \qquad q < 2 \tag{22}$$

which remains valid for $q \to 2$, yielding $D_2 = 1 - 8\pi^{-2}|\lambda|$. The limit $\tau \to 1$ corresponds to a limiting point of the graph $f(\alpha)$, which is given by

$$\alpha_c = 1 - \frac{8}{\pi^2}|\lambda|\left(1 + \frac{1}{2}\left(\Gamma'(1) - \frac{\Gamma'(1/2)}{\sqrt{\pi}}\right)\right) \tag{23}$$

$$f(\alpha_c) = 1 - \frac{8}{\pi^2}|\lambda|\left(1 + \Gamma'(1) - \frac{\Gamma'(1/2)}{\sqrt{\pi}}\right). \tag{24}$$

The exponent γ describing the vanishing of the Lebesgue measure or total bandwidth ($W \sim n_l^{-\gamma}$) satisfies $D_{-\gamma} = (1+\gamma)^{-1}$, and is found to be $\gamma = 1 - D_0 = 4\pi^{-2}|\lambda|$, in agreement with the result given in [17]. As we have made the assumption that $\lambda q^{(1)}(\tau)$ is small, the results for $\tau(q)$ and D_q are not valid for large negative values of τ or q, where $q^{(1)}(\tau)$ scales as $\sqrt{-\tau}$. Therefore it is not possible to obtain $\alpha_{\max} = D_{-\infty}$ within this approximation. To check self-consistency of our results, however, we can set $\alpha_{\max}$ equal to the value where $f(\alpha) = 0$. This yields $\alpha_{\max} = 1 - 32\pi^{-5}\lambda^2$, which shows that the decrease of $\alpha_{\max} < 1$ is a second-order effect in λ, in agreement with the results obtained by the trace map for the Fibonacci chain [10–13], and we cannot expect to obtain an exact result for it in this first-order calculation. We also notice that our result is independent of the irrational number β. In the case $\tau > 1$, we find that the limit in equation (17) vanishes as $1/\ln n_l$ for $n_l \to \infty$, thus yielding $q^{(1)}(\tau) = 0$. Therefore the point ($\alpha_{\min} = \frac{1}{2}$, $f(\alpha_{\min}) = 0$), which corresponds to the van Hove singularities, does not move in first order of the potential. This is also consistent with results based on the trace map for the Fibonacci chain.

We have seen that perturbation theory in first order of the quasiperiodic potential leads to multifractal properties for the on-site model ($\rho = 1, \lambda \neq 0$). For the off-diagonal model ($\rho \neq 1, \lambda = 0$), however, the half-widths of the gaps $|\Delta E_j| = \frac{2}{\pi j}|1-\rho||\sin(\pi j \beta_l)|$ correlate strongly with the corresponding bandwidth of the periodic chain $\Delta_{j,0} = \frac{2\pi}{n_l}|\sin(\pi j \beta_l)|$. Following the same line of calculations as for the off-diagonal model, this uniform shrinking of the bandwidths leads to

$$q^{(1)}(\tau) = \frac{4}{\pi^2}\tau \qquad \tau < 1\,. \tag{25}$$

Therefore, the corresponding spectrum is a monofractal with all generalized dimensions equal to $D_0 = 1 - 4\pi^{-2}|1-\rho|$.

We conclude this paragraph with the remark that it is not the feature diagonal/off-diagonal that leads to the different behaviour of the two models. Indeed, for the diagonal model $\psi_{i+1} + v_i\psi_i + \psi_{i-1} = E\psi_i$ with on-site potentials,

$$v_i = \begin{cases} -\lambda & \text{for} \quad 0 < \{\omega i\} < 1-\omega \\ \lambda & \text{for} \quad 1-\omega < \{\omega i\} < 1 \end{cases} \tag{26}$$

the band edges are given by [17]

$$E_j \pm \Delta E_j = 2\epsilon \cos(\pi j \beta_l) + \lambda(2\beta_l - 1) \pm \frac{2\lambda}{\pi j} \sin(\pi j \beta_l)\,. \tag{27}$$

The same argument as above shows that in this case the spectrum is monofractal in first order in λ.

4. Comparison to numerical data and conclusion

Numerical calculations have been performed to determine the multifractal spectrum. In order to speed up the convergence of the numerical data, we calculate the multifractal scaling function $\tau(q)$ by using the more efficient condition,

$$\frac{\Gamma^{(l)}(\tau, q)}{\Gamma^{(l')}(\tau, q)} = 1 \tag{28}$$

rather than by using $\Gamma^{(l)}(\tau, q) = 1$ [18]. Furthermore, we correct the systematic error due to the finite size of the chains by setting

$$\left.\frac{\Gamma^{(l)}(\tau, q)}{\Gamma^{(l')}(\tau, q)}\right|_{\text{cor}} = \left.\frac{\Gamma^{(l)}(\tau, q)}{\Gamma^{(l')}(\tau, q)}\right|_{\text{num}} \left.\frac{\Gamma_0^{(l)}(\tau, q)}{\Gamma_0^{(l')}(\tau, q)}\right|_{\text{ex}} \left.\frac{\Gamma_0^{(l')}(\tau, q)}{\Gamma_0^{(l)}(\tau, q)}\right|_{\text{num}} \tag{29}$$

where the subscript 'num' refers to the data obtained by numerical diagonalization and $\left(\Gamma_0^{(l)}/\Gamma_0^{(l')}\right)_{\text{ex}}$ is the asymptotically exact value for the undisturbed system:

$$\left.\frac{\Gamma_0^{(l)}(\tau, q)}{\Gamma_0^{(l')}(\tau, q)}\right|_{\text{ex}} = \left(\frac{n_l}{n_{l'}}\right)^{q^{(0)}(\tau)-q}. \tag{30}$$

This correction procedure is also intended to eliminate the logarithmic contribution to the ideal power law (30) expected near ($\tau \approx 1, q \approx 2$), which is already present for the periodic chain case [19], and which can strongly affect the numerical determinations of scaling exponents [19]. As we are interested in calculating the first-order effects of the quasiperiodic potential, we can evaluate $\Gamma^{(l)}(\tau, q)|_{\text{num}}$ according to equation (12), where, of course, $\delta\Delta_j^{(1)}$ has to be replaced by the value $\Delta_{j,0} - \Delta_j|_{\text{num}}$.

Finally, the corrected value $(\Gamma^{(l)}/\Gamma^{(l')})|_{\text{cor}}$ is inserted into equation (28) for calculating $\tau(q)$, and, afterwards, $f(\alpha)$ by Legendre transformation.

In figure 1 the numerical curves $f(\alpha)$ are compared with the theoretical expression for the on-site model and two different values of λ ($\lambda = 0.001$, $\lambda = 0.002$). The limiting points at the left-hand side correspond to $\tau \to 1$ and are given by the expressions (23) and (24). The points calculated from the numerical data are in good agreement with the theoretical result. The difficulty of approaching the limiting point $(\alpha_c, f(\alpha_c))$ is due to the very slow convergence of the limit of equation (17), when τ approaches 1. As we have seen, $q^{(1)}(\tau)$ shows a discontinuity for $\tau = 1$, thus preventing good convergence for a finite system even quite far from the critical value. This explains why the numerical points end before reaching $\alpha = \alpha_c$. However, the numerically accessible α_c systematically approaches the theoretical value as the system size increases.

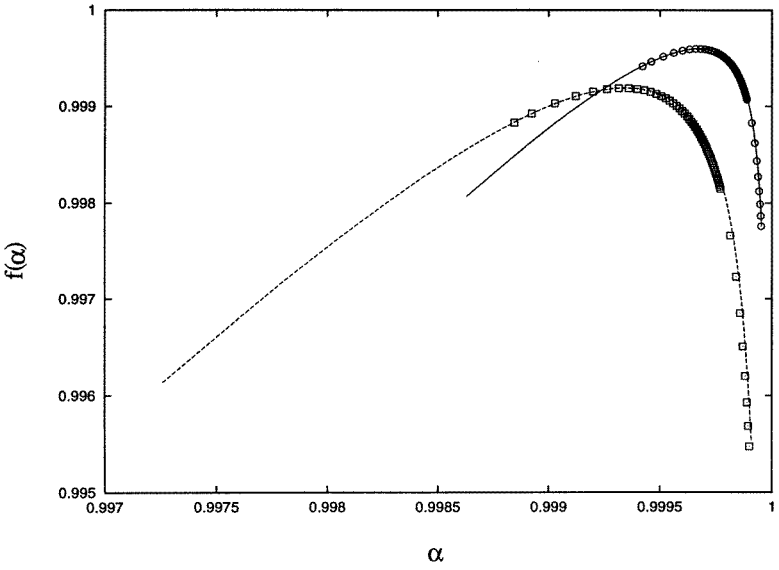

Figure 1. The theoretical multifractal spectrum $f(\alpha)$ for the on-site model ($\rho = 1$) is plotted for $\lambda = 0.001$ (full curve) and $\lambda = 0.002$ (broken curve) and compared to numerical data for the Fibonacci chain with $n_l = 987$ and $n_{l'} = 233$ (symbols). The theoretical curves are obtained by Legendre transformation of equation (21) in the range $\tau \in (1, 50]$. For the numerical data we have chosen $\Delta\tau = 0.2$ for $\tau < 10$ and $\Delta\tau = 5$ for $\tau \geqslant 10$ for the sake of clarity.

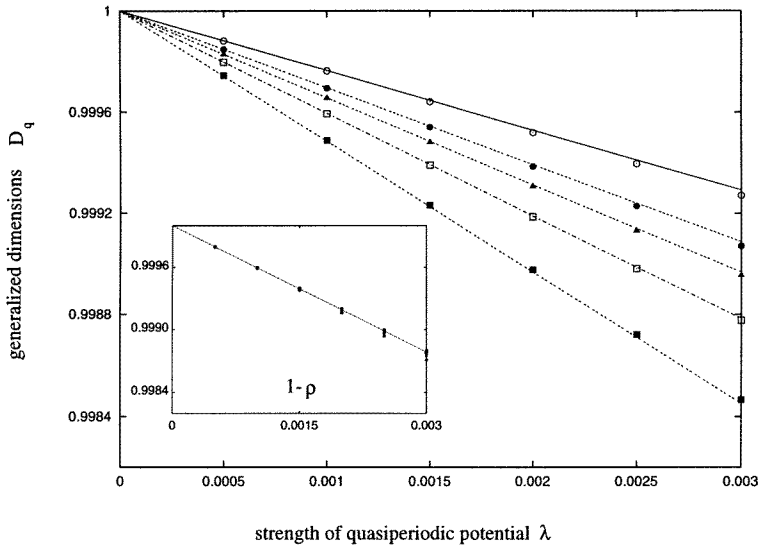

Figure 2. The theoretical dependence of the generalized dimensions D_q on the quasiperiodic potential λ for the on-site model, for $q = -5, -2, -1, 0, 1$ (broken lines from top to bottom) is compared to numerical data (symbols). Insert: same as before for the off-diagonal model ($\lambda = 0$).

Figure 2 shows the dependence of the generalized dimensions D_q ($q = -5, -2, -1, 0, 1$) on the quasiperiodic potential λ for the on-site model. The lines are the

theoretical expressions (equation (22)). Comparison with the insert, where the corresponding data are plotted for the off-diagonal model, shows that the different behaviour of the two models that has been found theoretically is confirmed by the numerical calculations.

In conclusion, we have calculated the multifractal spectrum for a general quasiperiodic chain in first order in the quasiperiodic potential. We have found analytical expressions for the generalized dimensions which are in good agreement with numerical calculations. The two models under investigation display qualitatively different behaviour, the on-site model showing multifractal behaviour, the off-diagonal being monofractal. For both models the multifractal properties do not depend on the irrational slope in first order in the potential.

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