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A study of the structure factor of Thue–Morse and period-doubling chains by wavelet analysis

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Abstract. One-dimensional systems generated by deterministic rules show interesting properties, such as a structure factor with peaks whose amplitudes scale with the size of the system according to a power law, with a scaling exponent in general dependent on the wavevector. I apply a wavelet transform to the structure factor of the Thue–Morse and the period-doubling chains and show how this technique succeeds in computing the scaling exponents and in finding the wavevector associated with them. This example shows that wavelet analysis could become an efficient tool for studying the Fourier transform of aperiodic systems.

1. Introduction

In recent years much effort has been devoted to the analysis of one-dimensional tilings generated by substitutional rules operating on a finite alphabet [1]: in fact, since they present a long-range non-periodic order, their study is a first step toward the comprehension of the properties of two- and three-dimensional aperiodic structures. I concentrate here on two of these one-dimensional systems, the Thue–Morse and the period-doubling chains, and use the wavelet transform technique to study some of their properties. Following [2, 3], I define the structure factor of a chain as

$$S_N(q) = \frac{1}{N}|G_N(q)|^2 = \frac{1}{N}\left|\sum_{k=0}^{N-1} \mathrm{e}^{\mathrm{i}qx_k}\right|^2$$

where x_k is the position of the kth atom and N is the number of atoms. When the chain becomes infinite, a well-defined function is the integrated density $H(q)$ [4]

$$H(q) = \lim_{N\to\infty}\int_0^q S_N(q')\,\mathrm{d}q'$$

while the structure factor is formally defined by $\mathrm{d}H(q) = S(q)\,\mathrm{d}q$. The behaviour of these quantities reflects the nature of the order (disorder) shown by the chain: the averaged structure factor of an amorphous system is a smooth function, practically independent of N, whereas, when there is a long-range order, some sharp peaks appear, whose amplitudes depend on the size of the system according to a power law

$$G_N(\tilde{q}) \simeq C(\tilde{q})N^{\gamma(\tilde{q})}.$$

Bragg peaks, corresponding to $\gamma = 1$, characterize periodic, quasiperiodic and almost-periodic systems [5] (pure point spectrum), while in aperiodic structures the exponent γ takes a value intermediate between 1/2 and 1, depending on the point $\tilde{q}$ of the reciprocal space [4, 6] (singular continuous spectrum). The behaviour of the integrated density around these particular points may be expressed as [4, 7]

$$|H(q) - H(\tilde{q})| \simeq \pm C_{\pm}|q - \tilde{q}|^{\alpha(\tilde{q})} \tag{1}$$

where the scaling indices $\alpha = 2(1-\gamma)$, $0 < \alpha < 1$, for different $\tilde{q}$, are distributed according to a certain density function $f(\alpha)$ [4, 8]. The same description is used for an object with multifractal properties: in [8] the authors, using the technique of multifractal analysis [9, 10] in reciprocal space, have studied the global scaling properties of the Fourier transform of some self-similar structures (the period-doubling chain was not included). Although this kind of analysis is very powerful in detecting the scaling indices, it is not suitable for localizing the points in the reciprocal space with which they are associated. In order to get this information I use the wavelet transform analysis [11, 12, 13], which is able to detect local singularities because it is a scale-independent method based on localized functions. It was introduced by Morlet (see [14]) to analyse seismic data and it has since been applied to many different fields. In particular, the authors of [15, 16, 17] and, very recently, [18] have shown how to use it to describe uniform fractals and multifractals. Using as the analysing wavelet the so-called 'Mexican hat' [15]

$$h(x) = (1 - x^2)\mathrm{e}^{-x^2/2} \tag{2}$$

I apply the wavelet transform to the function $S_N(q)$ and obtain

$$T(s, u) = \lim_{N\to\infty} \frac{1}{s} \int_{-\infty}^{+\infty} h\left(\frac{q-u}{s}\right) S_N(q)\, \mathrm{d}q. \tag{3}$$

When $s \to 0^+$ (u constant), the Mexican hat becomes more and more localized at the point u, and if here the integrated density presents a singularity with scaling coefficient α, then [17]

$$T(\lambda s, u) \simeq \lambda^{\alpha(u)-1} T(s, u). \tag{4}$$

From this expression, we can see that the slope of $\ln\left|T(s, u)\right|$ as a function of $\ln s$ gives the coefficient $\beta = \alpha - 1$. A rigorous theorem about the wavelet transform of a measure and its local scaling exponents is given in [19], but for my purpose the relation (4) is sufficient.

2. The structure factor

2.1. The Thue–Morse chain

Let us consider the following constant length substitution acting on two letters A and B:

$$\sigma_{TM} = \begin{cases} \mathrm{A} \Rightarrow \mathrm{AB} \\ \mathrm{B} \Rightarrow \mathrm{BA}. \end{cases}$$

The word w obtained by iterating σ infinitely starting from A is the Thue–Morse sequence. It represents a fixed point of this substitution, since $\sigma(w) = w$. The one-dimensional geometrical structure associated with this abstract sequence is the Thue–Morse chain, whose properties have been extensively studied by several authors (see, for example, [20, 21, 22, 23]). The Fourier spectrum of the sequence is singular continuous and its peaks are characterized by a set of scaling exponents α ranging from α_{min} to ∞ [6, 21]. Since the structure factor of the Thue–Morse chain has already been described in [3], I report here only its main features. The nth-generation chain has $N = 2^n$ atoms, its length is $L_n = 2^{n-1}(a + b)$ and its Fourier transform is given by

$$G_n(q) = 2^{n-1}\mathrm{e}^{[\mathrm{i}(q/2)(a+b)(2^{n-1}-1)]}\left(\Pi_+ f_1 - (-\mathrm{i})^n \Pi_- f_2\right) \tag{5}$$

where

$$\Pi_+(q) = \prod_{j=0}^{n-2} \cos[2^{j-1} q(a+b)] \tag{6}$$

$$\Pi_-(q) = \prod_{j=0}^{n-2} \sin[2^{j-1} q(a+b)] \tag{7}$$

$$f_1(q) = e^{i(q/2)a} \cos\left(\frac{q}{2}a\right) + e^{i(q/2)b} \cos\left(\frac{q}{2}b\right) \tag{8}$$

$$f_2(q) = e^{i(q/2)a} \sin\left(\frac{q}{2}a\right) - e^{i(q/2)b} \sin\left(\frac{q}{2}b\right). \tag{9}$$

Equation (6) can be rewritten in the form

$$\Pi_+(q) = 2^{-(n-1)} \frac{\sin[2^{n-1}(q/2)(a+b)]}{\sin[(q/2)(a+b)]}$$

from which I can deduce that the points

$$q_M = \frac{2\pi}{a+b} M$$

where M is an integer correspond to Bragg peaks with

$$C(q_M) = (-1)^M \cos^2(\phi_M) \qquad \phi_M = \frac{\pi a}{a+b} M.$$

When N becomes large, the value of this product decreases rapidly and its contribution to the whole Fourier transform is important only at the points q_M. The other product, Π_-, is the same as the one which appears in the structure factor of the abstract Thue–Morse sequence and it is responsible for the singular continuous aspect of S_N. There are singular peaks at each rational, non-dyadic value of $q(a+b)$, in units of 2π. The smallest scaling exponent α_{min} is associated with the point $q_{min} = (2\pi/3)/(a+b)$:

$$\alpha_{min} = 2 - \frac{\ln 3}{\ln 2} \approx 0.415.$$

If at the wavevector $\tilde{q}$ there is a peak with scaling exponent $\tilde{\alpha}$, the same exponent is found at wavevectors $q = 2^{-P}(\tilde{q} + 2\pi Q)$, with P, Q integers.

2.2. *The period-doubling chain*

The period-doubling sequence is defined as the fixed point (starting from A) of the binary constant-length substitution:

$$\sigma_{PD} = \begin{cases} \mathrm{A} \Rightarrow \mathrm{AB} \\ \mathrm{B} \Rightarrow \mathrm{AA}. \end{cases}$$

This abstract sequence is almost periodic, as the calculation of its Fourier transform reported in [6] shows. In order to calculate the structure factor of the corresponding one-dimensional chain, I observe that for odd k

$$x_k = x_{k-1} + a \tag{10}$$

where x_k is the position of the kth atom on the line. Thus, the Fourier transform $G_n(q; a, b)$ of the nth generation ($N = 2^n$) of the period-doubling chain with periods a and b can be decomposed as follows:

$$G_n(q; a, b) = \sum_{k \text{ even}} e^{iqx_k} + \sum_{k \text{ odd}} e^{iqx_k} = (1 + e^{iqa}) G_{n-1}(q; a' = a+b, b' = 2a). \tag{11}$$

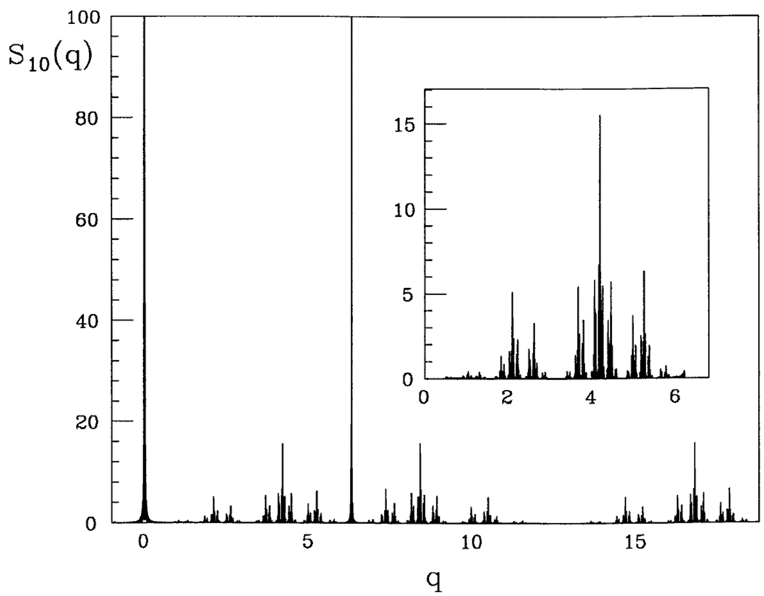

Figure 1. The structure factor of the 10th Thue–Morse generation with $a = 1/4$ and $b = 3/4$ as a function of the wavevector q. The inset shows the trifurcation structure of the peaks.

Iterating (11) gives

$$G_n(q; a, b) = \prod_{m=0}^{n-1} \left(1 + \mathrm{e}^{\mathrm{i}qy_m}\right) \tag{12}$$

with the definitions

$$\begin{cases} y_m = 2^m p_1 - (-1)^m p_2 \\ p_1 = (2a + b)/3 \\ p_2 = (b - a)/3. \end{cases}$$

The quantity p_1 represents the mean interatomic distance defined as [2]

$$\lim_{k\to\infty} \frac{x_k}{k}.$$

The quantity I have called y_m is simply the length of the mth period-doubling chain generation. It is easy to rewrite the expression (12) in a more opportune way and to obtain for the modulus of the Fourier transform

$$|G_n(q)| = 2^n \prod_{m=0}^{n-1} \left|\cos\left(\frac{q}{2} y_m\right)\right|. \tag{13}$$

The behaviour of this function when n tends to infinity is not trivial. For generic values of the wavevector q, I expect the Fourier transform to have a complex behaviour. I am interested in the presence of peaks in the structure factor, so I look for those wavevectors which realize a constructive interference among the factors of the product. There is a Bragg peak at the point $\tilde{q}$ (besides the trivial Bragg peak at $q = 0$) if

$$\frac{\tilde{q}}{2} y_m \to 0 \qquad (\mathrm{mod}\ \pi) \tag{14}$$

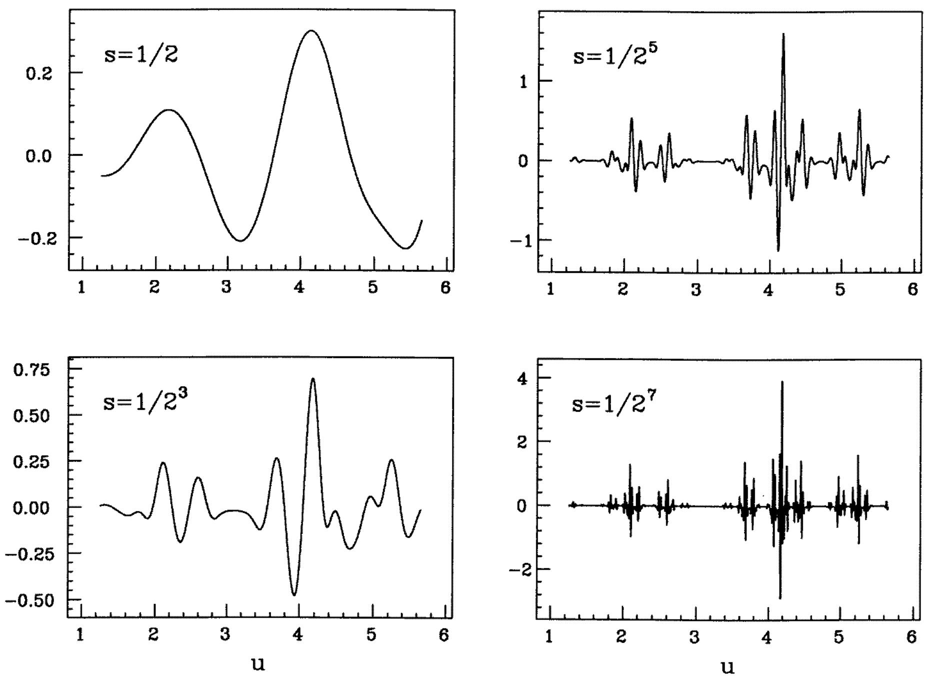

Figure 2. The wavelet transform of the structure factor of the 10th Thue–Morse generation, for four different values of the scale parameter s.

when $m \to \infty$. This is possible if the ratio a/b between the two main periods of the chain takes a rational value [3]. With regard to singular peaks the condition (14) becomes

$$\frac{\tilde{q}}{2} y_m \to \pm\delta \qquad (\mathrm{mod}\ \pi). \tag{15}$$

For instance, if

$$\left|\cos\left(\frac{\tilde{q}}{2} y_m\right)\right| = |\cos\delta| = K(\tilde{q})$$

(K independent of m) for every m larger than some integer $\tilde{m}$, then

$$S_n(\tilde{q}) \simeq (2K^2)^n \qquad (n \to \infty). \tag{16}$$

For $K = 1$ this reduces to (14), while if $1/\sqrt{2} < K < 1$ a singular peak results and the scaling exponent is given by

$$\gamma(\tilde{q}) = 1 + \frac{\ln K(\tilde{q})}{\ln 2}. \tag{17}$$

This happens, for example, at the points q (L and J integers, $L > 0$):

$$q = \frac{2\pi}{p_1} J 2^{-L}$$

where

$$\gamma_{L,J} = 1 + \frac{\ln(|\cos(\pi J p_2/2^L p_1|)}{\ln 2}.$$

If $a = 5$ and $b = 6$ ($p_1 = 16/3$ and $p_2 = 1/3$), I expect, besides the trivial Bragg peak at $q = 2\pi$, a singular peak for $q = \frac{3}{4}\pi$ with scaling index $\gamma_{0,2} \approx 0.886$ ($\alpha \approx 0.228$) and one for $q = \frac{3}{8}\pi$ with $\gamma_{0,1} \approx 0.972$ ($\alpha \approx 0.056$).

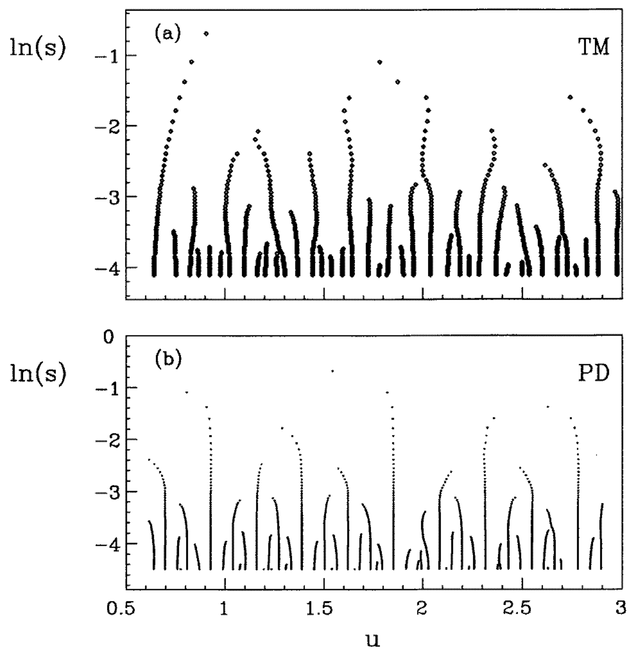

Figure 3. Maxima lines for the 12th Thue–Morse generation with $a = 1/4$ and $b = 3/4$ (a) and maxima lines for the 12th period-doubling generation with $a = 5$ and $b = 6$ (b).

3. The wavelet analysis

Figure 1 shows the structure factor of a 10th-generation Thue–Morse chain (for simplicity I have chosen the values of the intervals $a = 0.25$ and $b = 0.75$ so that $a + b = 1$). Besides the two Bragg peaks at the points $q = 0$ and $q = 2\pi$ (corresponding, respectively, to $M = 0$ and $M = 1$), there is a system of peaks densely distributed on the q-axis with an interesting trifurcation structure (see also the inset), which also appears in the study of other aspects of this chain [24, 25]. The wavelet transform of the structure factor is shown for four different values of the scale parameter in figure 2, where, in each box, s is kept constant: for $s = 1/2$ the wavelet transform possesses only two large maxima at the points $u \simeq 4.2$ and $u \simeq 2.2$. An increasing number of maxima appear when I investigate smaller values of the scaling parameter. In particular, the position of the local maxima of the wavelet modulus is of great interest, because, as shown in [26], each singular point of the measure corresponds to a maximum in the modulus of the wavelet transform [27] (there are, however, some extra maxima which do not correspond to any singular points). All the points $(u_{max}(s), s)$ lie on curves called maxima lines: by following these lines for $s \to 0$ I am able to locate the singularities. Figure 3(a) shows these maxima lines in the $(u, \ln s)$ half-plane for the Thue–Morse chain. When $s \to 0$, the centres of the two main maxima for $s = 1/2$ approach $u = 2\pi/3$ and $u = 4\pi/3$, which are singular points for the

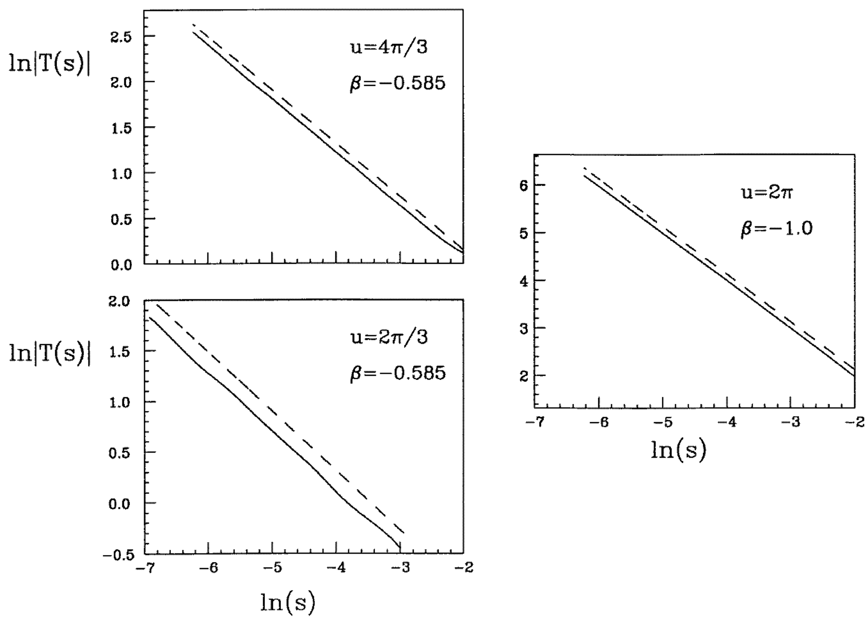

Figure 4. The log of the wavelet transform of the structure factor of the 12th Thue–Morse generation ($a = 1/4$ and $b = 3/4$) as a function of $\ln s$, for three different values of the translation parameter u. Full curve: wavelet transform; broken curve: theoretical prediction.

Thue–Morse chain structure factor. The corresponding scaling exponents can be compared with those obtained by a direct computation. The results, for $n = 12$, are presented in figure 4, where the continuous line corresponds to the wavelet transform, while the dashed line is the theoretical prediction

$$\alpha = 0.415 \rightarrow \beta = \alpha - 1 = -0.585.$$

A least-squares fit of the wavelet data gives $\beta \simeq -0.58$ for both $u = 4\pi/3$ and $u = 2\pi/3$. The wavelet transform displays a linear trend which follows the dashed line quite well and indicates a good correspondence between the wavelet results and those from theory. This proves the ability of our wavelet to provide a quantitative estimate of the scaling indices. The result is also shown for the Bragg peak at $q = 2\pi$, where the exponent α is zero and $\beta = -1$.

The same kind of computation has been made for the period-doubling chain. For $a = 5$, $b = 6$ and $n = 12$, figure 5 shows the graph of $\ln|T(s)|$ versus $\ln s$, when $u = 3\pi/8$ and $u = 3\pi/4$. In this case too, the wavelet result (continuous line) agrees with the theoretical analysis. Least-squares fitting gives $\beta \simeq -0.92$ and $\beta \simeq -0.76$, respectively, for $u = 3\pi/8$ and $u = 3\pi/4$. The maxima lines are shown in figure 3(b).

4. Conclusion

The main aim of this paper is to show that the wavelet transform can be used to study the multifractal properties of the structure factor of self-similar chains. This tool is able to give local information which cannot be obtained by classical multifractal analysis, because of the global nature of the latter. This work concentrates on two one-dimensional systems and

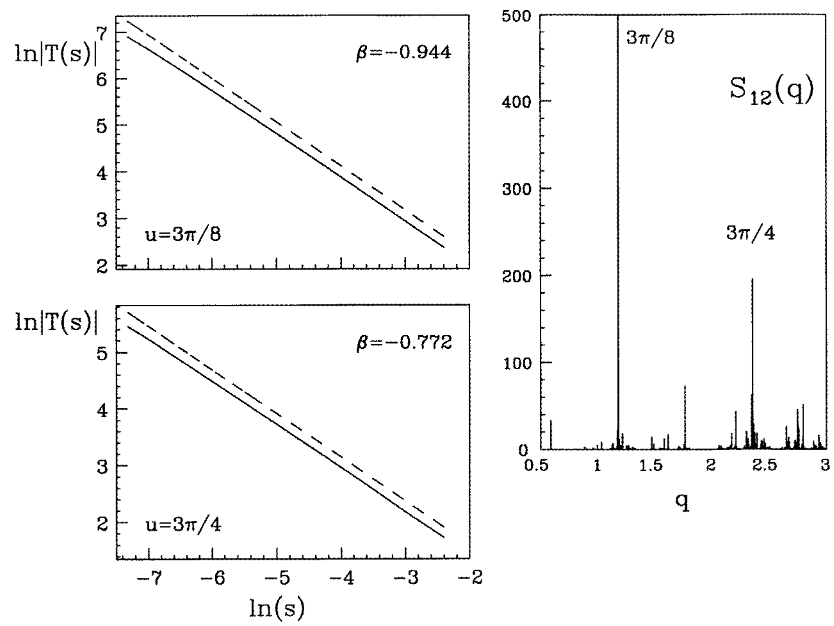

Figure 5. On the right: the structure factor of the 12th period-doubling generation with $a = 5$ and $b = 6$ as a function of the wavevector q. On the left: the log of the wavelet transform of the structure factor as a function of $\ln s$, for two different values of the translation parameter u. Full curve: wavelet transform; broken curve: theoretical prediction.

I have compared the analytical results with the performance of the wavelet transform. The Thue–Morse chain was chosen because of its remarkable self-similar structure and because it has been intensively studied by other authors [2, 3, 6, 8, 21] both analytically and by multifractal analysis. In particular, the lowest scaling exponent and the corresponding set of wavevectors are known, so this chain is a good example on which to test the predictions of the wavelet analysis.

The structure factor of the period-doubling chain has been calculated and some of its properties have been discussed. I have also calculated some scaling exponents corresponding to particular values of the wavevector q (to determine the whole range of scaling exponents needs multifractal analysis). The wavelet transform method in section 3 fully confirmed these calculations. Thus, in this second example, wavelet analysis has been found useful for verifying new theoretical predictions. Figures 4 and 5 show the power of this technique in giving local information.

It may be concluded that a fairly complete and exhaustive knowledge about the multifractal properties of the structure factor of one-dimensional aperiodic structures can be reached by using wavelet analysis to extract local features on the one hand, and multifractal analysis to obtain a global view on the other.

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