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On the dimensions of the spectral measure of symmetric binary substitutions

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Abstract
Substitution rules defined on the binary alphabet and invariant under the interchange of both participating symbols are considered. Typically, the resulting symbolic sequences are weakly disordered, and their Fourier spectra are singular continuous. Exact relations are derived which express the correlation dimension of the multifractal spectral measure in terms of the entries in the substitution pattern. Recurrence relations are obtained for the finite-length spectral sums and for the autocorrelation function.

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1. Introduction

Although our models of the surrounding world are based on continuous spatio-temporal coordinates, the presence of physical patterns which appear to be discrete in space and/or in time, can be recognized in almost every natural phenomenon. Since the relevant set of such patterns is in most cases finite, the description can often be reduced to strings of symbols from a finite alphabet. A symbolic description is often helpful in understanding critical or nearly critical phenomena which possess the property of scaling invariance. As a consequence, the corresponding symbolic sequences are self-similar: invariant with respect to replacement of certain blocks of several symbols by single symbols. Inversely, infinite self-similar symbolic codes can be generated from a single initial symbol by means of repeated substitutions (inflations): replacements of each symbol of the alphabet by the prescribed word (substitution pattern). Due to the simplicity of description, substitution sequences are widely employed for the studies of different aspects of complexity [1, 2].

Along with examples of well-correlated regular structures, substitutions can produce aperiodic symbolic sequences. The degree of disorder in such sequences is, in some sense, weak: dynamical systems arising from deterministic substitution rules are not mixing [3]. It is convenient to characterize substitution sequences in terms of an autocorrelation function and a Fourier spectrum. These characteristics vary widely among the aperiodic substitution patterns: thus, for the Fibonacci sequence the Fourier spectrum is discrete (atomic) and the autocorrelation displays peaks at Fibonacci numbers, whereas for the Rudin–Shapiro sequence the spectrum is absolutely continuous, and the autocorrelation vanishes identically [2]. An example of intermediate dynamics is delivered by the Thue–Morse binary substitution $A \rightarrow AB, B \rightarrow BA$ [4, 5] whose Fourier spectrum is neither discrete nor absolutely continuous [6], but singular continuous: it is supported by the dense disjoint continuum.

In this paper we describe the properties of the spectral measure for the natural extension of the Thue–Morse substitution rule: symmetric binary substitutions. Let the substitution rule be $A \rightarrow W_1$, $B \rightarrow W_2$, where W_1 and W_2 are two words of the same length which contain only A and B. Then the substitution is symmetric if W_2 can be obtained from W_1 by simultaneous replacement of all A by B and all B by A. An example is $A \rightarrow ABBAB$, $B \rightarrow BAABA$. An equivalent definition: let symbols be 0 and 1, and their substitution patterns, respectively, two words w_0 and w_1 of the same length L. Read these words as binary numbers. The substitution is symmetric if $w_0 + w_1 = 2^L - 1$. By explicit computation, we demonstrate that the Fourier spectrum of a non-trivial symmetric substitution is singular continuous; for a class of such substitutions it is shown that the generalized dimensions of the spectral measure are bounded away from zero.

Symmetric substitutions can be employed in the traditional domain of mathematical physics: studies of localization and disorder in terms of spectral properties of one-dimensional discrete Schrödinger operators for potentials which take finitely many values. Situations in which the latter values are supplied by various substitution sequences have been extensively treated [7–10]. It has been established that the singular continuous character of the spectrum is closely related to the abundance in the substitution sequence of arbitrarily long ‘palindromes’ (words which read backwards the same way as forwards, such as *ABBA*) [11, 12]. Being by construction rich in palindromes, symmetric substitution sequences can provide material for further advances in this direction.

Another physical context in which symmetric substitutions play an important role, arises in studies of scenarios of homoclinic bifurcations in continuous dissipative systems with saddle points and Lorenz-like mirror symmetries. Such scenarios, proposed in [13], were found in dynamical systems modelling chemical turbulence [14], thermal convection in a modulated gravity field [15], fluid motions in the magnetic field [16], thermocapillary flows [17], optical phenomena in nematic liquid crystals [18], etc. In short, this bifurcation sequence can be described as follows. Let the symmetry transformation leave the saddle point invariant but interchange two components of the one-dimensional unstable manifold of this point. In such systems, homoclinic orbits to the saddle point arise in pairs. The return mapping on the appropriate Poincaré plane can be reduced to a discontinuous one-dimensional map of the kind $x_{i+1} = (-\mu + |x_i|^\nu + \text{h.o.t.})\text{sign}(x_i)$, where μ is the parameter and $\nu > 1$ is the so-called ‘saddle index’: the ratio of the two leading eigenvalues of the flow linearized near the saddle point. It is natural to encode each turn of the orbit in the phase space by one of two letters (say, R and L), depending on the sign of x_i. The increase of μ is accompanied by the alternation of homoclinic bifurcations with symmetry-breaking bifurcations of more and more complicated periodic states. During the primary transition from order to chaos, transformation of the symbolic code of the attracting orbit follows the Thue–Morse substitution $R \rightarrow RL, L \rightarrow LR$. It has been found that the fractality of the Fourier spectrum of the Thue–Morse sequence is largely reproduced by power spectra of both the Poincaré map and the continuous-time flow variables [19] (in the latter case the slowdown of the motion near the saddle causes additional effects [20]). Beyond the onset of chaos, one finds on the parameter axis a countable set of further accumulation points; they correspond to bifurcation scenarios with symbolic dynamics different from the Thue–Morse substitution. Many (not all!) of the symmetric binary substitutions can be found among these scenarios; the next shortest example is $R \to RLL$, $L \to LRR$. Therefore, knowledge of the spectral characteristics of symmetric substitution rules can shed additional light on corresponding bifurcation sequences in families of mappings and differential equations.

In section 2 we discuss the properties of symmetric substitution rules, derive recursion relations which describe the growth of finite spectral sums, and introduce a multifractal formalism for the spectral measure. In section 3 we show how computation of the correlation dimension of this measure is reduced to solving the quadratic equation whose coefficients are explicitly expressed through the elements of the substitution pattern. As an illustration, this algorithm is applied to all substitutions with length of the substitution pattern $L \leqslant 16$. In section 4 the analysis is performed for the particular family of substitutions. Finally, the results are re-cast in terms of the autocorrelation function.

2. Inflation rule and spectral measure

Let the substitution rule be

$$\begin{aligned} A &\to C \\ B &\to \overline{C} \end{aligned} \tag{1}$$

where C is some string of L symbols A and B, and $\overline{C}$ denotes the 'negation' of C produced from it by replacement of each A by B and each B by A. Without restrictions of generality we assume that the first symbol in the substitution pattern C is A; if it is B, we obtain the string which begins with A by applying the substitution rule twice. Starting with the single symbol and performing the substitution n times, the sequence with length $l_n = L^n$ is created; for $n \to \infty$ this yields the fixed point of the substitution: (semi-)infinite symbolic sequence $\{\zeta_j\}$, $j = 1, 2, 3, \ldots$.

The same sequence $\{\zeta_j\}$ can be generated from the initial symbol by using repeated concatenations instead of substitutions. Each such concatenation abuts onto the already existing sequence a set consisting of $L - 1$ copies and 'negations': out of a sequence $\{x_j\}$ it builds the sequence of L consecutive blocks in which the kth block is $\{x_j\}$ if the kth entry in the pattern C is A, and $\{\overline{x_j}\}$ if this letter is B.

When the substitution rule is viewed as a dynamical system, the sequence $\{\zeta_j\}$ becomes the record of states of this system, and the index j plays the role of discrete time. Since the alphabet consists of two symbols, a generic observable in this dynamics has only two values. It is convenient to assign numerical values to symbols: $A = 1$ and $B = -1$, and take for an observable the value of ζ_j itself. By this, the substitution pattern C is associated with the sequence of integers $\{\xi_i\}$, $i = 1, \ldots, L$ where $\xi_i = 1$ if the ith symbol in C is A, and $\xi_i = -1$ if the ith symbol in C is B.

Symmetric substitution rules cannot have a purely discrete spectrum. According to theorem VI.24 from [1], the necessary and sufficient condition for this is the existence of such i and j that, after i iterations of the substitution, the jth symbol in the sequence obtained from A coincides with the jth symbol in the sequence obtained from B. Since, due to symmetry, the sequence obtained from B is always complementary to the sequence obtained from A, this condition cannot be fulfilled.

As a quantitative characteristic of the degree of disorder in the symbolic string generated by the substitution sequence, let us determine the structure of its Fourier spectrum. Take a real ω ($0 \leqslant \omega < 1$) and consider dynamics of finite-length Fourier sums under the application of transformation (1). For the first l_n symbols of $\{\zeta_j\}$ this sum is defined as $\sigma_n(\omega) = \sum_{j=1}^{l_n} \zeta_j \exp(2\pi \mathrm{i} j\omega)$, and the corresponding finite-length approximation to the power spectrum is $S_n(\omega) = |\sigma_n(\omega)|^2/l_n$. Obviously, $\sigma_0(\omega) = S_0(\omega) = 1$. Performing one concatenation, we proceed to l_{n+1} and obtain recurrent relations for the Fourier sums:

$$\sigma_{n+1}(\omega) = \sigma_n(\omega) \sum_{j=1}^{L} \xi_j \exp(2\pi\omega \mathrm{i}(j-1)L^n) \tag{2}$$

and

$$S_{n+1}(\omega) = S_n(\omega) \sum_{j=1}^{L} g_j \cos(2\pi\omega(j-1)L^n) \tag{3}$$

where the coefficients g_i are sums of pairwise products of elements of the substitution pattern:

$$g_i = \frac{2-\delta_{i,1}}{L} \sum_{j=1}^{L+1-i} \xi_j \xi_{i+j-1}. \tag{4}$$

It is straightforward to see that $g_1 = 1$.

The limit of large n in (3) characterizes the local nature of the power spectrum at each given point ω and yields the global distribution of the spectral measure μ:

$$\mu(\omega) = \lim_{n\to\infty} S_n(\omega) = \lim_{n\to\infty} \prod_{k=0}^{n-1} \left(1 + \sum_{j=2}^{L} g_j \cos(2\pi\omega(j-1)L^k)\right). \tag{5}$$

The properties of this infinite product can be inferred with the help of approximations $S_n(\omega)$. Vanishing of $S_n(\omega)$ for some n implies $\mu(\omega) = 0$. For those rational numbers $\omega = p/q$ for which finite spectral sums do not vanish, the ratio $\rho(n) = S_{n+1}(\omega)/S_n(\omega)$ oscillates as a function of n with period $\tau \leqslant q-1$. If L divides q, these oscillations are preceded by a transient whose length equals the multiplicity of L in the factorization of q. 'On average', finite-length approximations to the power spectrum evolve according to $S_m \sim (\overline{\rho})^m$ with $\overline{\rho}$ being the geometric mean of $\rho(n)$ over the period τ of oscillations. In terms of the length l of the symbolic string, this growth or decay is proportional to l^κ where the exponent κ equals $\log \overline{\rho}/\log L$ (accordingly, the Fourier sums $|\sigma_n|$ evolve proportionally to l^γ, with $\kappa = 2\gamma - 1$ [21]). Obviously, for the values of ω with negative κ the spectral sums vanish in the limit $l \to \infty$, which results in $\mu(\omega) = 0$. The values of ω with positive κ correspond to the singularities (peaks) of the power spectrum. It can be shown that the maximal possible value $\kappa = 1$, required for δ-peaks, can be reached only in two cases:

(a) by trivial substitutions where all L symbols in C are the same ($C = AA\cdots AA$); here $g_j = 2 - 2(j-1)/L$, $j = 2, \ldots, L$, and the only δ-peak is located at $\omega = 0$;
(b) by patterns of odd length L in which the symbols in C alternate ($C = ABA\cdots BA$); in this case a sequence with period 2 is generated, and the only δ-peak sits at $\omega = 1/2$.

For all other substitutions, the inequality $\kappa < 1$ holds for all rational values of ω; accordingly, the singularities of the spectral measure are weaker than δ-peaks, and the discrete (atomic) component is absent in the spectral measure of these substitutions.

Equation (3) describes evolution of the spectral sum under concatenation. Alternatively, we can follow the transformation of spectral sums under inflation; this results in the 'non-local' recurrent relation

$$S_{n+1}(\omega) = S_n(L\omega) \left(1 + \sum_{j=2}^{L} g_j \cos 2\pi(j-1)\omega\right). \tag{6}$$

The limit of this expression at $n \to \infty$ yields the functional equation for the spectral measure $\mu(\omega)$:

$$\mu(\omega) = \mu(L\omega)\left(1 + \sum_{j=2}^{L} g_j \cos 2\pi(j-1)\omega\right). \tag{7}$$

In order to evaluate the multifractal characteristics of the spectral measure, we follow the approach of [21] and divide the interval of ω between 0 and 1 into N segments of length $\varepsilon = 1/N$; the probability to locate the spectral measure in the kth segment is $p_k = \int_{(k-1)\varepsilon}^{k\varepsilon} \mu(\omega)\,\mathrm{d}\omega$. For a real number q the partition function is introduced as $Z(q) = \sum_{k=1}^{N} p_k^q$. Since the spectral measure $\mu(\omega)$ is not directly available, the approximations $S_n(\omega)$ are used for the estimates of the local density of the probability p_k/ε. In this way we get a sequence of approximations $Z(q, n)$ to the partition function; as N tends to infinity, summation in these approximations can be replaced by integration: $Z(q, n) = \varepsilon^{q-1} \int_0^1 S_n^q(\omega)\,\mathrm{d}\omega$. On the other hand, the spectral sums $S_n(\omega)$, being computed over the first L^n symbols of the sequence, enable only finite resolution in the frequency domain; therefore there is no sense in infinite refinement of the partition without the simultaneous increase of n. Usage of S_{n+1} instead of S_n improves the resolution by the factor L; hence the partition segments of the length ε can be replaced by segments of length ε/L. This interrelates the order of the approximation n and the length ε_n of the box of the corresponding partition: $\varepsilon_n \propto L^{-n}$.

The usual scaling assumption $Z(q, n) \sim \varepsilon^{\tau(q)}$ leads to the generalized (Rényi) dimensions: $D_q = \tau(q)/(q-1)$. Substituting here the relation $\varepsilon_n \propto L^{-n}$, we arrive at

$$D_q = \frac{\tau(q)}{q-1} = 1 - \frac{\log \lambda(q)}{(q-1)\log L} \tag{8}$$

where λ is defined as

$$\lambda(q) = \lim_{n\to\infty} \frac{\int_0^1 S_{n+1}^q(\omega)\,\mathrm{d}\omega}{\int_0^1 S_n^q(\omega)\,\mathrm{d}\omega} = \lim_{n\to\infty} \frac{\int_0^1 \prod_{k=0}^{n} \left(\sum_{j=1}^{L} g_j \cos(2\pi\omega(j-1)L^k)\right)^q \mathrm{d}\omega}{\int_0^1 \prod_{k=0}^{n-1} \left(\sum_{j=1}^{L} g_j \cos(2\pi\omega(j-1)L^k)\right)^q \mathrm{d}\omega}. \tag{9}$$

The value of D_0 (box-counting dimension, capacity) equals 1. This results from the fact that the values of ω with positive 'growth rates' κ are dense on the interval: it is enough to find just a single rational value of ω for which the spectral sums grow, in order to establish the existence of the countable dense set of such values. For $0 < q \ll 1$ the leading term in the expansion of (9) describes the decrease of generalized fractal dimension from 1 as a function of q:

$$D_q \cong 1 + q\frac{\int_0^1 \log\left(1 + \sum_{j=1}^{L-1} g_{j+1} \cos 2\pi j\omega\right)\mathrm{d}\omega}{\log L} + O(q^2). \tag{10}$$

In several cases integration in (10) can be performed explicitly. Thus, for the Thue–Morse substitution $A \to AB$ this yields $D_q \cong 1 - q + O(q^2)$; for the pattern $A \to ABB$ (and equivalent pattern $A \to AAB$) we get $D_q \cong 1 + q(\log(3+\sqrt{5}) - \log 6)/\log 3 + O(q^2) = 1 - 0.12396q + O(q^2)$, etc.

In general, evaluation of $\lambda(q)$ from (9) requires numerical integration of finite spectral sums and extrapolation to the limit $n \to \infty$. However, as shown in [22], for integer $q \geqslant 2$ the explicit relation between $S_{n+1}(\omega)$ and $S_n(\omega)$ in terms of trigonometric series (akin to equation (3)) can be used for reducing the problem to the computation of the largest eigenvalue of the $q \times q$ matrix. Below, we will mostly concentrate on the case $q = 2$ which yields the correlation dimension of the spectral measure.

3. Correlation dimension of spectral measure: general results

For positive integer values of q, the integrands in equation (9) turn into trigonometric polynomials. Let us denote in the cos-expansion of $S_n^2(\omega)$ the ω-independent term by P_n and the coefficient at $\cos(2\pi\omega l_n)$ by Q_n. The evolution of P and Q under the increase of n is governed by linear recursion

$$P_{n+1} = a_{11}P_n + a_{12}Q_n \qquad Q_{n+1} = a_{21}P_n + a_{22}Q_n \tag{11}$$

with matrix elements given by the expressions:

$$\begin{aligned} a_{11} &= \frac{1}{2}\left(1 + \sum_{j=1}^{L} g_j^2\right) & a_{12} &= \frac{1}{2}\left(g_2 + \sum_{j=1}^{L-1} g_j g_{j+1}\right) \\ a_{21} &= \frac{1}{2}\left(\sum_{j=2}^{L} g_j g_{L+2-j}\right) & a_{22} &= \frac{1}{4}\left(2g_1 g_L + \sum_{j=1}^{L} g_j g_{L+1-j} + \sum_{j=3}^{L} g_j g_{L+3-j}\right) \end{aligned} \tag{12}$$

where the coefficients g_j are recovered from the substitution pattern C by means of equation (4).

Since only the ω-independent term P_n contributes to the integral $\int_0^1 S_n^2(\omega)\,\mathrm{d}\omega$, the value of $\lambda(2)$ in equation (9) equals the growth rate of P, i.e. the largest eigenvalue of the matrix (12). Thus, computation of the correlation dimension D_2 has been reduced to solving the quadratic equation whose coefficients can be easily determined from the substitution pattern. In figure 1 the values of D_2 are plotted for all possible non-trivial substitutions of the length $L \leqslant 16$.

Notably, almost all of the values of D_2 plotted in figure 1 correspond to several different substitution patterns. This is a consequence of various internal symmetries within the set of all possible patterns of the given length; the most obvious of these is the symmetry between the 'right' and the 'left': naturally, properties of spectral measure are independent of the direction in which the substituted word is read, and $A \to ABAA$ is equivalent to $A \to AABA$.

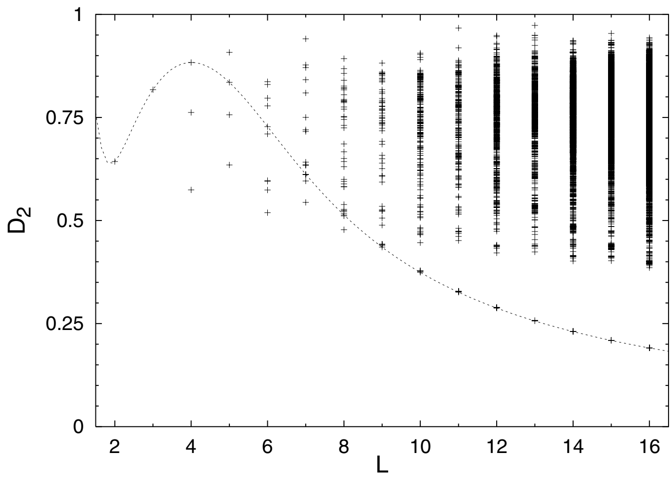

Figure 1. Correlation dimension for the spectral measure of symmetric binary substitutions of length L. Dashed line: family $A \to ABB\cdots BB$.

4. The 'least disordered' substitutions

Of all possible substitutions with given length L the 'least continuous' spectral measure (measure with the value of D_2 closest to zero) belongs to those whose substitution pattern is the least disordered. For $L > 8$ these are the 'nearly trivial' substitutions: those which have in the substitution pattern $L-1$ consecutive identical symbols preceded (or followed) by one complementary symbol: $A\,\underbrace{BB\cdots BB}$ or $\underbrace{AA\cdots AA}\,B$.

For this family of substitutions the above expressions can be substantially simplified. The coefficients g_j in the recurrent relation (3) for spectral sums are $g_j = 2 - 2(j+1)/L$, $j = 2, \ldots, L$. Substituting this into (12) we see that the values of λ for this family are the larger roots of the quadratic equation:

$$\lambda^2 - \lambda\frac{L^3 - 8L^2 + 25L - 24}{L^2} + \frac{(L-8)(3L^2 - 8L + 8)}{3L^3} = 0. \tag{13}$$

The corresponding values of $D_2 = 1 - \log\lambda/\log L$ are shown by the dashed line in figure 1. It can be seen that for $L > 10$ they lie distinctly lower than the values for all other families of substitutions. The asymptotic expression for $L \to \infty$ is

$$D_2 = \frac{8}{\log L}\left(\frac{L+1}{L^2} + O(L^{-4})\right). \tag{14}$$

Another important observation for this family of substitutions is that for $L > 5$ the peak of $S_n(w)$ which is the highest and grows the fastest, is located at $\omega = 0$, with $S_{n+1}(0) = S_n(0) \times (L-2)^2/L$. Knowledge of this growth rate allows us to estimate the asymptotics of fractal dimensions D_q at $q \to \infty$: for large q the dominating contribution to the partition sum is made by the segments containing the peaks which grow the fastest; these peaks sit at the dense set of values of ω whose expansion in the L-adic system ends with the infinite string of zeros. On proceeding to the next value of n, the height of such peaks grows by the factor $\left((L-2)^2/L\right)^q$, whereas their width decreases by the factor L. Accordingly, equation (9) yields $\lambda \approx (L-2)^{2q}L^{-1-q}$. Thereby

$$D_q = 1 - \frac{\log\lambda}{(q-1)\log L} \approx \frac{2q}{q-1}\left(1 - \frac{\log(L-2)}{\log L}\right). \tag{15}$$

This gives the lower bound for generalized dimensions: $D_q > D_\infty = 2 - 2\log(L-2)/\log L$; for large L it turns into

$$D_\infty = \frac{4}{\log L}\left(\frac{1}{L} + \frac{1}{L^2} + O(L^{-3})\right) \approx \frac{D_2}{2}. \tag{16}$$

Thus we see that for finite L the range of generalized fractal dimensions of the spectral measure is bounded away from zero.

5. Recurrent relations for the autocorrelation

A similar analysis can be pursued for any integer $q > 1$: presentation of $S_n^q(\omega)$ in the form of finite trigonometric series shows that from all $1 + qn(L-1)$ terms of this expansion only q terms contribute to the ω-independent term of $S_{n+1}^q(\omega)$. Evolution of these terms is governed by q linear recursion relations; accordingly, the growth rate $\lambda(q)$ turns out to be the largest eigenvalue of the $q \times q$ matrix whose elements are polynomial combinations of the entries g_j of the substitution pattern.

A power spectrum characterizes a substitution sequence in the frequency domain; in the 'spatial' domain the sequence is characterized by the autocorrelation function $C(j)$,

$j = 1, 2, \ldots$. In our case, if the numerical values assigned to symbols are $\zeta_j = \pm 1$, this function is given by $C(j) = \langle \zeta_k \zeta_{k+j} \rangle$, where averaging is performed over the position k. The autocorrelation function is the Fourier transform of the power spectrum: if the spectral measure is presented in the form $\mu(\omega) = 1 + \sum_{j=1}^{\infty} c_j \cos(2\pi j \omega)$, then $C(m) = c_m/2$. On substituting this trigonometric expansion into equation (7), we derive L recursions which relate the values of $C(Lk + j)$, $j = 0, 1, \ldots, L - 1$ to the values of $C(k)$ and $C(k + 1)$:

$$C(Lk) = C(k) \tag{17}$$

$$C(Lk + j) = \tfrac{1}{2}(C(k)g_{j+1} + C(k+1)g_{L-j+1}) \qquad j = 1, \ldots, L - 1. \tag{18}$$

This permits us to begin with $C(0) = 1$ and compute $C(m)$ recursively for each m, starting with $C(1) = g_2/(2 - g_L)$. For even values of L, $g_2 \neq 0$, and, hence, $C(1)$ cannot vanish; for L odd, it can, in principle, vanish, but in this case $C(2) = g_3/2 \neq 0$. Thereby, owing to equation (17), $C(j)$ does not decay completely at $j \to \infty$. Accordingly, the spectral measure of the substitution sequence cannot be absolutely continuous with respect to the Lebesgue measure.

As seen from equation (17), the values of arguments corresponding to the highest peaks of $C(k)$ form the geometric progression, and the whole pattern of the autocorrelation function is approximately log-periodic.

Autocorrelation can be used as a tool which provides information on the fractal characteristics of the spectral measure without constructing this measure itself. Thus, the asymptotic decay rate of the integrated autocorrelation $C_{\text{int}}(k) \equiv k^{-1} \sum_{j=1}^{k} C(j)^2$ yields the correlation dimension: $C_{\text{int}}(k) \sim k^{-D_2}$ [23, 24]. Evaluation of this decay rate in our case, leads, naturally, to the computation of the largest eigenvalue of the matrix (12). The values of generalized dimensions D_q for integer $q > 2$ can be found from the growth rates of sums of products $\prod_{j=1}^{j=q} C(k_j)$, $k_q = k_1 + k_2 + \cdots + k_{q-1}$ [22]; this approach is equivalent to the aforementioned reduction to the $q \times q$ matrix.

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