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Quasiperiodicity and magnetic phase transition of a class of one-dimensional aperiodic systems

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Abstract. It has been proven that the quasiperiodicity and magnetic phase transition of a one-dimensional aperiodic system depend on the characteristic values of the corresponding substitution rule. By means of the principle of the argument we have developed a general method to study the properties of the characteristic equations of any substitutional sequences, which relates to the study of one-dimensional quasiperiodic lattices. Particularly, a class of typical sequences, which consist of k letters and is given by the substitution rule $A_1 \rightarrow A_2, A_2 \rightarrow A_3, \dots, A_{k-1} \rightarrow A_k, A_k \rightarrow mA_k n A_1$ ($k = 2, 3, 4, \dots$ and $m, n = 1, 2, 3, \dots$) are systematically studied.

In recent years, substitutional structures (or deterministic aperiodic structures) have been studied in many respects [1-9]. The majority of these works have been focused on the Fibonacci lattices or superlattices [7, 8]. But other kinds of aperiodic systems, such as generalized Fibonacci systems [10, 11], Thue-Morse and generalized Thue-Morse aperiodic crystals [12-14], Rudin-Shapiro sequence [15], and three-tile SML quasiperiodic lattices [16, 17], have also attracted much attention of both physicists and mathematicians. Particularly, it is worth mentioning that the universal problems of trace maps for any substitution sequences have been taken into account [17, 18]. On the other hand, the characteristic equations of generating matrices for any substitution structures consisting of more than two building blocks have not yet been studied thoroughly [19]. The characteristic values are very important for the properties of substitutional structures. The largest eigenvalue of a substitution matrix is often referred to as its Perron-Frobenius eigenvalue. The absence of any other eigenvalue larger than unity in modulus is usually called the Pisot-Vijayaraghavan (PV) property and the quasiperiodicity of a one-dimensional substitution structure is determined by its PV property. In fact, it was first introduced by Bombieri and Taylor [20] as a definition of quasiperiodicity with Dirac delta peaks in the Fourier spectrum of an infinite deterministic structure. They have shown that, generally, a necessary and sufficient condition for the presence of atomic components (i.e. delta peaks) in the Fourier spectrum is that the characteristic equation of the generating matrix should have only

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one eigenvalue greater than unity in modulus. Godréche and Luck [21] have taken a multifractal analysis in reciprocal space for several kinds of self-similar substitutional structures. Their results are consistent with the definition of Bombieri and Taylor mentioned above. Severin and Riklund have used the Fourier spectrum to classify families of generalized Fibonacci lattices [22]. The results they found are in agreement with the definition of Bombieri and Taylor, even though their definition of Fourier transform is not the same as that of Bombieri and Taylor. In addition, some authors have studied the phase transition problems of the one-dimensional aperiodic quantum Ising model, in which the exchange couplings are arranged according to a relevant substitutional sequence with only two letters, such as the Fibonacci and generalized Fibonacci sequences [23–26]. The phase transition, in the strict sense, can occur only if there is a critical coupling for which the zero energy is allowed. This energy value corresponds to an infinite correlation length that is the necessary and sufficient condition for the existence of the phase transition on a one-dimensional quantum Ising model. Benza *et al* [26] have considered quantum Ising chains formed by distributing two coupling parameters according to the generalized Fibonacci sequences. They have shown that such models (and by a straightforward generalization all models obtained with arbitrary two-letter substitution rules) exhibit a magnetic phase transition only if the respective rules has the pv property. Following the lines of these authors, it can be directly proven that the necessary and sufficient condition for the occurrence of phase transition is that the product of all exchange couplings equals one for the infinite limit of chain. Benza *et al* [26] discussed a finite case in which this condition (i.e. the product of all exchange couplings equals one) can always be satisfied by a suitable choice of the values of the exchange couplings, but it seems that they have ignored the fact the above condition cannot be satisfied for the infinite limit in some one-dimensional quantum Ising models without a magnetic phase transition (for example, cases (ii) and (iii) in [26]). If the infinite limit of the chains is taken into account, the condition that the product of all (infinite) couplings equals one is necessary and sufficient to ensure a phase transition.

Returning to the substitution structures, the above condition is equivalent to the requirement that one or more eigenvalues of the characteristic equation is smaller than unity in modulus, and it is consistent with the results of previous works [23–26] for the quantum Ising models with two-letter substitution rules. In this paper, we will deal with the same problem of quantum Ising models with more than two kinds of coupling parameters and the quasiperiodicity of any substitutional sequences. In detail, we will investigate the quasiperiodicity and phase transition problem relating to a class of one-dimensional systems with typical substitution rules $A_1 \rightarrow A_2, A_2 \rightarrow A_3, \dots, A_{k-1} \rightarrow A_k, A_k \rightarrow mA_k nA_1$ ($k = 2, 3, 4, \dots$ and $m, n = 1, 2, 3, \dots$).

In the present paper, the general method for studying the characteristic value problem of substitutional sequences is based on *the principle of the argument* (and *Rouché's theorem*) from complex variable theory [28]. To explain our general method, we first study a specific case, then show how to apply this method to the general case. The specific case obeys the following substitution rules:

$$A_1 \rightarrow A_2, A_2 \rightarrow A_3, \dots, A_{k-1} \rightarrow A_k, A_k \rightarrow mA_k nA_1 \quad (1)$$

where $m A_k n A_1$ represent a string of $m A_k$ s and $n A_1$ s. Setting $k = 2$ gives the generalized Fibonacci sequence, in particular for the Fibonacci sequence $m = n = 1$. Similarly, the poly-tile aperiodic sequence [16, 17] can be obtained by setting $m = n = 1$ and $k = 3, 4, 5, \dots$. According to the definition of generating matrix [19, 20], we can obtain

the corresponding characteristic equations as:

$$\lambda^k = m\lambda^{k-1} + n. \tag{2}$$

By means of the substitution $Z = \lambda^{-1}$, we have

$$nZ^k + mZ - 1 = 0. \tag{3}$$

It is very complicated to calculate the k roots of this equation. Fortunately, the central problem considered here relates to only the distribution of the k characteristic values on the complex λ -plane, i.e. the distribution of the k roots of (3) on the regions $|Z| \leq 1$ and $|Z| > 1$ in the Z -plane shown in figure 1(a). It is obvious that the k roots of (3) are the k zeros of following functions:

$$G_{m,n}^k(Z) = Z^k + (m/n)Z - 1/n \quad \text{for } n \geq m + 1$$

and

$$F_{m,n}^k(Z) = Z + (n/m)Z^k - 1/m \quad \text{for } n \leq m - 1. \tag{4}$$

The principle of the argument [28] states that the sum of the orders of zeros of the function $G_{m,n}^k(Z)$ inside region A with bounding curve C in the Z -plane is determined by the argument increment of the function when the variable Z completes a cycle along the closed curve c , i.e.

$$[\text{Zeros}]_A = \frac{1}{2\pi} [\text{Arg } G_{mn}^k(Z)]_C = \int_C \frac{dZ}{2\pi i} \frac{G_{mn}^{k'}(Z)}{G_{mn}^k(Z)} \tag{5}$$

provided no zero actually lies on curve C . For example, figure 1(b) shows that for the well known Fibonacci sequence the argument increment of the function $F(Z)$ is 2π , therefore only one characteristic value is greater than unity in moduli since there is only one root with absolute value smaller than unity. This principle is an elementary

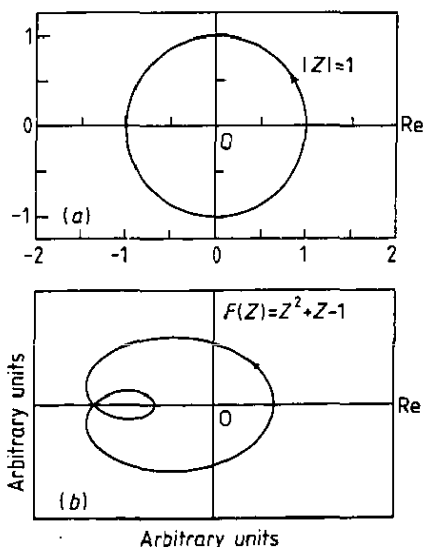


Figure 1. The application of the principle of the argument to characteristic value problem. (b) Shows the curve of the $F(Z) = Z^2 + Z - 1$ corresponding to the characteristic equation of the Fibonacci sequence while the complex variable Z is confined to the unit circle $|Z| = 1$ shown in (a).

consequence of the fundamental theorem of residues [28]. Noting that the function $G_{mn}^k(Z)$ we deal with here is a polynomial, the zeros of it must be the simple poles of the integrated function $G'(Z)/G(Z)$. Therefore the contour integral of (5) equals the number of zeros of $G_{mn}^k(Z)$ contained in the interior of bounding curve C , each zero being reckoned according to its degree of multiplicity. In the following, we will systematically study, by means of the principle of the argument, the distribution of characteristic values of the substitutional sequences defined by (1) for all possible values of the positive integers k, m and n .

(i) *The case $n \geq m + 1$*

To investigate the substitutional sequences of this case, Rouché’s theorem is most effective. Rouché’s theorem is a simple corollary of the principle of the argument [28]. It states that if the functions $f(Z)$ and $g(Z)$ are regular within and on a simple closed contour C and $|f(Z)| > |g(Z)|$ on C then $f(Z)$ and $f(Z) + g(Z)$ have the same number of zeros within C . In our problem, the functions $f(Z) = Z^k$ and $g(Z) = (m/n)Z - 1/n$ satisfy the prerequisite $|f(Z)| > |g(Z)|$ on the unit circle $|Z| = 1$ except at one point, $Z = -1$, for $n = m + 1$ and k being an even integer; it is easy to avoid this point by indenting our contour $|Z| = 1$ in a small enough neighbourhood of the point $Z = -1$. So it follows from Rouché’s theorem that the function $G_{m,n}^k(Z)$ has the same number of zeros of $f(Z) = Z^k$ within the region $|Z| \leq 1$. In other words, the substitutional sequences of this case ($n \geq m + 1$) have k characteristic values with amplitudes greater than or equal to unity. Figure 2(a-c) show the typical curves of the functions $G_{m,n}^k(Z)$. With the help of the principle of the argument, one can also see clearly from the figures that the results are consistent with the above general conclusion. Figure 2(a) shows that the substitutional sequence with $k = 4$ (even integer), $m = 3$ and $n = m + 1 = 4$ has one characteristic value with absolute value equal to unity and three characteristic values greater than unity in moduli. Figure 2(b) shows that the substitutional sequence with $k = 3$ (odd integer), $m = 1$ and $n = m + 1 = 2$ has three characteristic values greater than unity in moduli. Figure 2(c) shows that the substitutional sequence with $k = 2$ (even integer), $m = 2$ and $n = 5 \neq m + 1$ has two characteristic values with absolute values greater than unity.

(ii) *The case $n \leq m - 1$*

In exactly similar fashion we can, generally, prove that the substitutional sequences of this case have only one characteristic value with amplitude greater than unity, and no characteristic value equal to unity in modulus. Figure 3(a, b) depict the typical curves of the functions $F_{m,n}^k(Z)$, which show clearly that any of these sequences has one characteristic value with modulus greater than unity.

(iii) *The case $n = m$*

To deal with the substitutional sequences of this case, we define another kind of function:

$$D_k(Z) = Z^k + Z \tag{6}$$

and

$$D_{m,m}^k(Z) = Z^k + Z - 1/m. \tag{7}$$

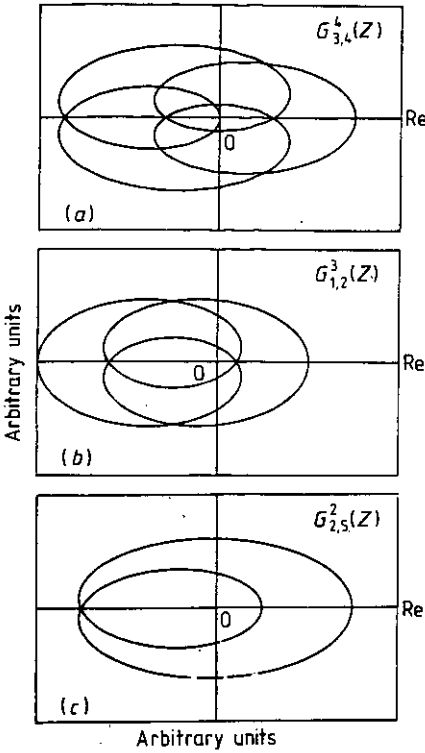


Figure 2. The curve of $G_{m,n}^k(Z)$ when $|Z|=1$ for three typical sequences with $n \geq m+1$. (a) $k=4$, $m=3$ and $n=m+1=4$; (b) $k=3$, $m=1$ and $n=m+1=2$; (c) $k=2$, $n=5 > m+1$.

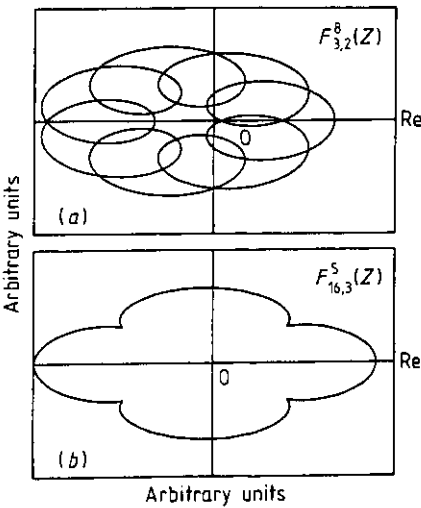


Figure 3. The curve of $F_{m,n}^k(Z)$ when $|Z|=1$ for two typical sequences with $n \leq m-1$. (a) $k=8$, $m=3$ and $n=m-1=2$. (b) $k=5$, $m=16$ and $n=3 < m-1$.

It is obvious that the curve of the function $D_{m,m}^k(Z)$ can be directly obtained by moving the curve of the function $D_k(Z)$ a distance $1/m$ along the negative direction of the real axis, or, the curve of $D_{m,n}^k(Z)$ is the same as curve $D_k(Z)$ except the origin O'_m is shifted to $1/m$. By using the principle of the argument, one can easily prove that, when the variable Z completes a cycle along the unit circle $|Z|=1$ shown in figure 1(a), the number of times that the curve of $D_{m,m}^k(Z)$ passes through the origin O'_m equals the number of zeros of $D_{m,m}^k(Z)$ lying on the contour $|Z|=1$, and the number of circuits surrounding the origin O'_m by the curve of $D_{m,m}^k(Z)$ equals the number of zeros of $D_{m,m}^k(Z)$ lying within the unit circle $|Z|=1$. Figure 4(a-c) show the curves of the function $D_k(Z)$ for $k=3, 5$ and 8 , respectively. One can see from figure 4(a) that any of the substitutional sequences with $k=3$ has, for all possible integers $m=1, 2, 3, \dots$, only one characteristic value greater than unity in modulus. Figure 4(b) shows us that the substitutional sequences with $k=5$ and $n=m=1$ has only one characteristic value with amplitude greater than unity and two characteristic values with amplitudes equal to unity, and that three characteristic values are greater than unity and no one equals unity in modulus when m becomes greater than one. It follows from figure 4(c) that any of the substitutional sequences with $k=8$ and small enough values of the integer m has three characteristic values with absolute values greater than unity, but when the integer m becomes great enough, i.e. the origin O'_m for $D_{m,m}^k(Z)$ lies to the left of the point O_2 , the sequences with such an integer m will have five characteristic values greater than unity in moduli. An example (for $k=11$) discussed below will illustrate how we apply the principle of the argument to finding

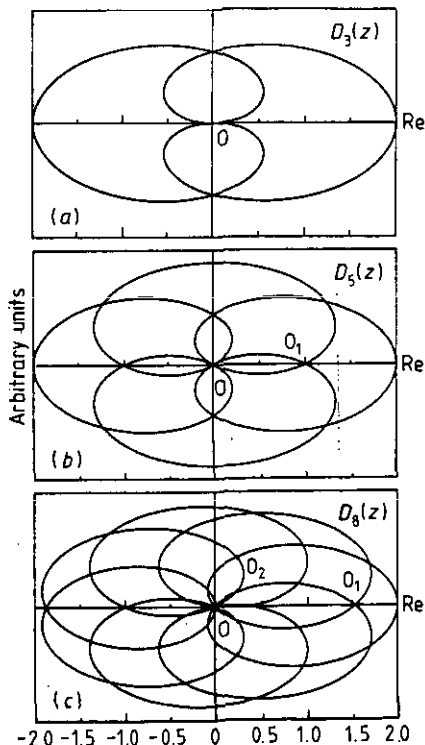


Figure 4. The curve of $D_k(Z)$ when $|Z|=1$ for three typical sequences with $n=m$. (a) $k=3$; (b) $k=5$; (c) $k=8$.

the general results about the characteristic values for the substitutional sequences with arbitrary integer k .

When the complex variable Z is confined to the unit circle $|Z| = 1$, equations (6) and (7) can be written as follows, by means of the substitution $Z = \exp(i\theta)$

$$D_k(\theta) = \exp(ik\theta) + \exp(i\theta) \tag{8}$$

and

$$D_{m,m}^k(\theta) = \exp(ik\theta) + \exp(i\theta) - 1/m. \tag{9}$$

It is easy to see that the real axis is an inversion axis of the closed curve of the functions $D_k(\theta)$ since $D_k(-\theta) = D_k^*(\theta)$. Figure 5(a) depicts the curve of $D_{11}(\theta)$. According to the principle of the argument, we know that, by carefully studying the curve of $D_{11}(\theta)$, the number of zeros of $D_{m,m}^k(Z)$ ($m = 1, 2, \dots$) is determined by the intersections $O_0, O_1,$ and O_2 of the closed curve lying on the positive real axis. These points O_0, O_1 and O_2 correspond to the intersections of the curve of $\cos(\theta)$ in first quadrant for the argument θ and the curve of $\cos(11\theta)$ in the fourth quadrant for the argument 11θ shown in figure 5(b). One can find that the function $D_{11}^k(Z)$ has two zeros with amplitudes equal to unity and three zeros with amplitudes smaller than unity, and the function $D_{m,m}^k(Z)$ with $m \geq 2$ has five zeros with amplitudes smaller than unity and no zero with amplitude equal to unity.

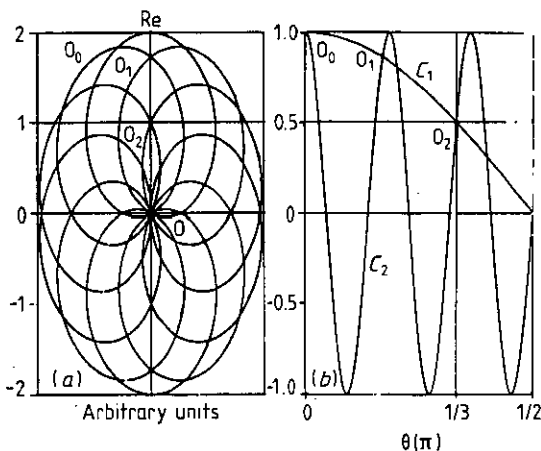


Figure 5. (a) The curve of $D_{11}(\theta)$, the real axis lies in the vertical direction. (b) The curve C_1 of $\cos(\theta)$ and the curve C_2 of $\cos(11\theta)$ for $0 \leq \theta \leq \pi/2$.

The above results can be generalized in a straightforward manner to the functions $D_{m,m}^k(Z)$ for any possible integers k and m . The number of intersections of the curve of $\cos(\theta)$ for $0 \leq \theta \leq \pi/3$ and the curve of $\cos(k\theta)$ in the fourth quadrant for the argument $k\theta$ is $2[(k+1)/6] + 1$ ($[]$ represents the greatest integer function), and these points $O_0, O_1, \dots, O_{p'}$ ($p' = [(k+1)/6]$) correspond to the intersections $O_0, O_1, \dots, O_{p'}$ of the closed curve of $D_k(\theta)$ lying to the right of the origin O' (if $[(k+1)/6] = (k+1)/6$ then $O_{p'}$ was on the point O'). Therefore, if $[(k+1)/6] = (k+1)/6$ then two zeros $Z_{1,2} = \exp(\pm i\pi/3)$ of $D_{m,m}^k(Z)$ has absolute values equal to unity, and $2[(k+1)/6] - 1$ zeros are smaller than unity in moduli; if $[(k+1)/6] \neq (k+1)/6$ then $2[(k+1)/6] + 1$ zeros of $D_{m,m}^k(Z)$ are smaller than unity in moduli, and

no zero equals unity in modulus. In addition, the total number of intersections of the curve of $\cos(k\theta)$ in the first quadrant for the argument θ and the curve of $\cos(k\theta)$ in the fourth quadrant for the argument $k\theta$ is $2[k/4]+1$. These points O_0, O_1, \dots, O_p ($p = [k/4]$) correspond to the intersections O_0, O_1, \dots, O_p of the closed curve of $D_k(\theta)$ lying on the positive real axis. Because the new origin O'_m moves to the origin O when the integer m increase continually, the number of zeros of $D_{m,m}^k(Z)$ lying on or within the unit circle $|Z|=1$ does not decrease with the increase of integer m for a given integer k . So we can make a conclusion that, for any substitutional sequence of case $m = n$, the total number of characteristics values with amplitudes greater than or equal to unity does not decrease with the increase of integer m for a given integer k . If $n = m = 1$ and $6p' - 1 < k < 6p' + 5$ ($p' = 0, 1, 2, \dots$) then $2p' + 1$ characteristic values are greater than unity in moduli; if $n = m = 1$ and $k = 6p - 1$ ($p = 0, 1, 2, \dots$) then $2p - 1$ characteristic values are greater than unity in moduli and two characteristic values have amplitudes equal to unity. If $4p \leq k < 4(p + 1)$ ($p = 0, 1, 2, \dots$) and $m = n$ being great enough then the number of characteristic values with amplitudes greater than or equal to unity gains the maximum $2p + 1$.

According to the above analytical results on characteristic values of substitutional sequences, we may draw conclusions concerning the quasiperiodicity of the deterministic aperiodic sequences and phase transition behaviour of the quantum Ising model related to the sequences. Because the characteristic equation of any substitutional sequence with $n \geq m + 1$ has no eigenvalue with amplitude smaller than unity, all of these substitutional sequences are not quasiperiodic sequences, and the corresponding one-dimensional aperiodic Ising model cannot undergo a magnetic phase transition. On the other hand, all of the substitutional sequences with $n \leq m - 1$ are quasiperiodic, and the corresponding one-dimensional quasiperiodic Ising models can undergo a magnetic phase transition since any of them has only one characteristic value greater than unity and none equal to unity in modulus. If $m = n$ then all of the substitutional sequences are non-quasiperiodic except a few particular cases $k = 2, 3$ and 4 , but all of the corresponding one-dimensional Ising models can undergo a magnetic phase transition.

The investigation of the Fourier spectrum is the first step in the study of the substitution structures. The characteristics of spectrum are related to other physical properties. Bombieri and Taylor [20] have shown that the PV property of a substitution structure and the quasiperiodicity of the corresponding aperiodic structure and the quasiperiodicity of the corresponding aperiodic structure generally come together. A series of works on the Fourier spectrum of the aperiodic structures is consistent with Bombieri and Taylor's rule [21, 22, 29]. The only known exception is the Thue-Morse sequence, of which the Fourier transform is singular continuous (i.e. neither Dirac peaks nor a smooth distribution in its spectrum) nevertheless this substitution has the PV property. But this paradox can be easily understood by the fact that a simple prefactor vanishes in the Fourier amplitude for the values of wavevector where a delta peak would be expected [22, 29]. On the other hand, Elser has provided a projection method to obtain a quasiperiodic structure [30]. It is obvious that the delta peaks must appear in the Fourier spectrum of such a projected structure [31]. Therefore we can conjecture that the substitution structures without PV property cannot be constructed by using the ordinary projection method, and that any attempt to calculate the diffraction pattern of them using this method [30, 31] would be in vain. For example, the substitution structure of $m = n = 1, k = 6$ cannot be obtained by projecting a set of points of the regular lattice of higher dimensional space onto an embedded line,

because the substitution matrix has three eigenvalues greater than unity in moduli, and the relevant Fourier spectrum should be singular continuous.

Doria and Satija [24] have numerically studied the one-dimensional Fibonacci quantum Ising model in transverse magnetic field. They have found a novel feature of this model: a phase transition occurs for a critical value of the couplings, above which there exists long-range order. Bentz *et al* [26] have studied the phase transition in the generalized Fibonacci quantum Ising models. They have confirmed that all models obtained with arbitrary two-letter substitution rules exhibit a magnetic phase transition only if the corresponding rules has the ν property. This result should be modified when being applied to models with more than two letters. Generally speaking, the sufficient and necessary condition for the existence of phase transition in a one-dimensional quantum Ising model is that one or more eigenvalues of the corresponding substitution matrix are smaller than unity in moduli. Following this line, we have proven in the present paper that all of the models of $n \leq m$ can undergo a phase transition, but those of $n \geq m + 1$ cannot. A detailed discussion with more numerical results will be presented in [27].

Finally, we would like to emphasize again that, for any k -letter substitutional sequence, the problem of how many characteristic values have amplitudes greater than unity and how many characteristic values equal unity in moduli can be solved by means of the principle of the argument. This extension is straightforward. So the quasiperiodicity of any substitutional sequences can be determined, and whether or not the corresponding one-dimensional aperiodic Ising model undergoes a magnetic phase transition can also be immediately resolved.

Acknowledgments

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