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1992 J. Phys. A: Math. Gen. 25 2483

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J. Phys. A: Math. Gen. **25** (1992) 2483–2488. Printed in the UK

Phase transition of quantum Ising spin models on *g*-letter generalized Thue–Morse aperiodic chains

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Received 18 October 1991

Abstract. The quantum Ising spin model in a transverse field with couplings ordered according to the *g*-letter generalized Thue–Morse sequence is considered. Exact analytical results for the critical line, energy gap and dispersion relation of the low-energy excitations are obtained. It is shown that the quantum Ising spin models can undergo a magnetic phase transition with the critical behaviour the same as in the periodic case.

In recent years, the phase transition of one-dimensional (1D) quantum Ising spin models (QIMs) with the nearest-neighbour couplings ordered according to different aperiodic sequences has been a focus of much attention [1–7] since these systems are interesting in conjunction with magnetic properties of aperiodic superlattices [8, 9]. In their earliest numerical work [1], Doria and Satija showed that the 1D Fibonacci quasiperiodic (QP) QIM exhibits an Ising-like critical point in the thermal sector with the correlation length exponent $\nu = 1$. The result was subsequently confirmed independently by the analytical studies of Ceccatto, Iglói and Benza [2–4]. The analytical investigations also showed that the QIM on the Fibonacci QP chain develops the usual logarithmic singularity in the ground state energy and the specific heat at the critical point. Recent work [6] showed numerical evidence that a phase transition could exist in copper- and nickel-mean generalized Fibonacci QIMs. On the basis of numerical analysis, Tracy [5] conjectured that, for the 1D ferromagnetic aperiodic QIM, the Ising-like phase transition is preserved on quasicrystals with the corresponding substitution rules satisfying the Pisot–Vijayaraghavan (PV) property, i.e. only one root of the characteristic polynomial associated with the substitution rule is in absolute value greater than one. This conjecture has recently been confirmed analytically by Benza and coworkers [7] on QIMs constructed with arbitrary two-letter substitution rules. Their results showed that the copper- and nickel-mean generalized Fibonacci QIMs do not exhibit a phase transition and the behaviour is similar to the random Ising case. Moreover, Benza *et al* also showed that although some two-letter substitution rules do not generate genuine quasicrystals, by which we mean that their Fourier transforms contain δ-function peaks, the corresponding QIMs can undergo a phase transition with critical behaviour the same as in the periodic case if the substitution rules satisfy the PV property. A famous example, which has been studied both numerically and analytically [10, 11], is the Thue–Morse (TM) aperiodic QIM. Up to now, most of the previous work in this line has been focused on the aperiodic QIMs constructed with two-letter

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0305-4470/92/092483+06$04.50 © 1992 IOP Publishing Ltd

substitution rules, in which there are only two kinds of couplings. On the other hand, a majority of the known quasicrystals are ternary alloys. It has been recently claimed [12] that in some cases the 1D two-letter Fibonacci sequence is no longer appropriate for the description of the quasicrystal model, and should be replaced by a multiletter sequence in order to represent greater reality. Hence, it is also necessary to study the physical properties of the multiletter aperiodic sequence, which has received relatively little attention. In this article we consider the phase transition problem of the QIM on g-letter generalized Thue-Morse (GTM) chains (see substitution rule (1) below). We will show that the g-letter GTM QIMs can undergo an Ising-like phase transition, independent of the value of g.

The study of the physical properties of the TM chain is motivated by the fact that this deterministic structure is believed to be more 'disordered' than the QP one. The experimental realization of a TM GaAs-AlAs superlattice due to Merlin *et al* further stimulates interest. Among many studies of this lattice, the phase transition problem of the TM QIM has been investigated both numerically and analytically by Doria *et al* and Lin and Tao [10, 11]. Recently, Kolár *et al* made an extensive study of the physical properties of the TM chain and its two-letter generalization [13]. The QIMs on the two-letter GTM chains show no essential difference, as far as their critical behaviour is concerned, from that on the ordinary TM chain. Kolár's two-letter GTM sequence is generated by the substitution rule [13] $A_{l+1}=A_l^mB_l^n$; $B_{l+1}=B_l^nA_l^m$, where m and n are positive integers. With $m=n=1$ the substitution rule will produce the ordinary TM sequence. Note that the substitution rule is indeed a direct analogue of that for the generalized Fibonacci lattice [14]. The g-letter GTM sequence studied in this article is, on the other hand, generated by the following substitution rule:

$$A_1\to A_1A_2A_3\ldots A_g \qquad A_2\to A_2A_3\ldots A_gA_1,\ldots \qquad A_g\to A_gA_1\ldots A_{g-1} \tag{1}$$

where the A_i's with $i=1,2,\ldots,g$ correspond to g letters. When $g=2$ the substitution rule (1) gives the ordinary TM lattice. Analogously to the ordinary TM case, the g-letter GTM lattice cannot be characterized by a finite set of irrational numbers and their Fourier spectra are singular continuous, i.e. the g-letter GTM systems have a degree of ordering intermediate between the QP and random ones. Will these multiletter aperiodic QIMs exhibit an Ising-like critical point? To be specific let us focus on the $g=3$ case first.

Before writing down the Hamiltonian, we would like to point out that if we represent the non-negative integers

$$0,1,2,3,4,5,6,7,8,9,\ldots$$

by the ternary code

$$00,01,02,10,11,12,20,21,22,100,\ldots$$

and then sum the digits in each number modulo 3, we also obtain the three-letter GTM sequence composed of three symbols, 0, 1 and 2, or, equivalently, A_1, A_2 and A_3. In what follows we will refer to this generating method as the 'ternary code method'. It will be useful in deriving the dispersion relation for the low excited states.

The QIM is defined by the Hamiltonian

$$H=-\sum_{i=1}^{M}\lambda(i)\sigma_i^x\sigma_{i+1}^x-h\sum_{i=1}^{M}\sigma_i^z \tag{2}$$

where σ_i^x and σ_i^z are Pauli matrices at site i and h is a constant transverse magnetic field. The coupling parameters $\lambda(i)$ form a three-letter GTM sequence with three values λr_1, λr_2 and λr_3 associated, respectively, with elements A_1, A_2 and A_3, whereas $M=3^N$

is the number of elements in an N-order GTM chain. For simplicity and without loss of generality, in what follows we set $r_1 = 1$ and $h = 1$.

To solve (2) we proceed with the well known Jordan-Wigner transformation [15] and rewrite (2) as

$$H = c^\dagger A c + \tfrac{1}{2}(c^\dagger B c^\dagger + \text{HC}) \tag{3}$$

where $c = (c_1, c_2, \ldots, c_M)$ and the c_j's are anticommuting fermionic operators. The matrices A and B are simply given by [1]

$$\begin{aligned} A_{i,j} &= -\lambda(j)\delta_{i,j+1} - \lambda(i)\delta_{i,j-1} - 2\delta_{i,j} \\ B_{i,j} &= \lambda(j)\delta_{i,j+1} - \lambda(i)\delta_{i,j-1}. \end{aligned} \tag{4}$$

Since we are interested in the properties of the infinite aperiodic system, here we can work with the so-called 'c-cyclic' problem [2, 10, 15] with an antiperiodic boundary condition for (3). The infinite aperiodic system is approached by setting the size of the unit cell $M = 3^N \to \infty$. The spin model displays long-range magnetic order above a certain critical coupling λ_c. The quantum-mechanical transition is driven by the zero mode of the Hamiltonian (3), which is given by $(A_c - B_c)\phi_0 = 0$ and $(A_c + B_c)\psi_0 = 0$, where A_c and B_c are the matrices A and B calculated at the critical line $\lambda_c = \lambda_c(r_2, r_3)$. The solutions to these equations are given straightforwardly by

$$\phi_{0,j} = (-1)^{j-1}\phi_{0,1}\prod_{i=1}^{j-1}\lambda_c(i) \qquad \psi_{0,j} = (-1)^{j-1}\psi_{0,1}\prod_{i=1}^{j-1}\frac{1}{\lambda_c(i)} \tag{5}$$

where $\phi_{0,1}$ and $\psi_{0,1}$ are normalized constants and $\lambda_c(i)$ assumes one of the three values λ_c, $\lambda_c r_2$ or $\lambda_c r_3$, depending on the site i in the GTM chain. The antiperiodic boundary condition requires $\Pi_{i=1}^{M}\lambda_c(i) = 1$, which immediately gives the critical line

$$\lambda_c = \frac{1}{(r_2 r_3)^{1/3}}. \tag{6}$$

We should note that the critical condition (6) does not definitely ensure a phase transition. It may only lead to the maximum but finite correlation length with a behaviour similar to the random Ising case [6, 7]. To establish whether the system can undergo a phase transition in the strict sense and develop the usual logarithmic singularity at the critical point, in what follows we will calculate the energy gap ΔE between the first excited and the ground state energies and the dispersion relation for the low-energy excitations near the critical point.

The model with the Hamiltonian in a general bilinear fermionic form like (3) has been completely studied by Ceccatto [2]. The energy gap ΔE is given by

$$\Delta E = 2\tau\frac{|\phi_0 H'\psi_0|}{|\phi_0|\,|\psi_0|} + o(\tau^{3/2}) \tag{7}$$

where $\tau = |\lambda - \lambda_c|/\lambda_c$ and the matrix $H'_{i,j} = \lambda_c(i)\delta_{i,j-1}$. If the prefactor

$$\eta = \frac{|\phi_0 H'\psi_0|}{|\phi_0|\,|\psi_0|} \neq 0$$

then, with the use of Floquet's theorem, Ceccatto gives the dispersion relation for the low-energy excitations close to the critical point [2]

$$\Delta E_{k'} = 2\eta(\tau^2 + k'^2)^{1/2} \tag{8}$$

where k' is the pseudo-wavenumber. From the dispersion relation (8) it is straightforward to deduce that the correlation length exponent $\nu=1$ and the system possesses the expected logarithmic singularity in the ground state energy and the specific heat at the critical point. In other words, the system undergoes a phase transition which falls into the two-dimensional (2D) classical Ising universality class.

To evaluate the value of η, we have to compute

$$|\phi_0|^2=\sum_{j=1}^{M}\phi_{0,j}^2=\phi_{0,1}^2\sum_{j=0}^{3^N-1}Q_j \tag{9}$$

where $Q_j=\Pi_{i=1}^{j}\lambda_c^2(i)$. Taking into account the fact that the three-letter GTM sequence satisfies the property that the sub-sequence from the first to the $(3m)$th element consists of m A_1's, m A_2's and m A_3's, and paying attention to the critical condition (6), we have $Q_{3m}=1$. Since the 'ternary code method' we described above is to start with non-negative integers, i.e. the first number is zero, corresponding to the fact that the first element in the N-order GTM sequence is A_1 with the ternary code

$$\underbrace{00\ldots0}_{N}$$

the corresponding ternary code for the $(3m)$th element should be

$$X_NX_{N-1}\ldots X_22$$

where X_i $(i=2,\ldots,N)$ may be 0, 1 or 2 whereas $X_1\equiv 2$. Let l and n denote the number of 1's and 2's, respectively, in the set $\{X_i, i=2,\ldots,N\}$. Obviously, we need to distinguish three cases with, respectively, $l+2n=3k$, $3k+1$ and $3k+2$ to evaluate Q_{3m-1} and Q_{3m-2}. For instance, if $l+2n=3k$, the $(3m)$th element should be A_3, the $(3m-1)$th one A_2 and the $(3m-2)$th one A_1. It follows that $Q_{3m-2}=\lambda_c^2$ and $Q_{3m-1}=\lambda_c^4r_2^2$. Applying a similar consideration to the other two cases with $l+2n=3k+1$ and $3k+2$, we have

$$Q_{3m-2}=\begin{cases}u_1 & l+2n=3k\\ u_2 & l+2n=3k+1\\ u_3 & l+2n=3k+2\end{cases}\qquad Q_{3m-1}=\begin{cases}1/u_3 & l+2n=3k\\ 1/u_1 & l+2n=3k+1\\ 1/u_2 & l+2n=3k+2\end{cases} \tag{10}$$

where $u_i=\lambda_c^2r_i^2$ with $i=1$, 2, 3 and $r_1\equiv 1$. On the basis of the above discussion, it follows that

$$\begin{aligned}|\phi_0|^2=\tfrac{2}{3}\phi_{0,1}^2\Re\Bigg(\sum_{l=0}^{N-1}\sum_{n=0}^{N-1-l}C_l^{N-1}C_n^{N-l-1}[(\tfrac{1}{2}+\theta^{l+2n})(u_1+u_3^{-1}+1)\\ +(\tfrac{1}{2}+\theta^{l+2n-1})(u_2+u_1^{-1}+1)+(\tfrac{1}{2}+\theta^{l+2n-2})(u_3+u_2^{-1}+1)]\Bigg)\end{aligned} \tag{11}$$

where $C_q^p=p!/[q!(p-q)!]$, $\theta=\exp(\mathrm{i}2\pi/3)$ and $\Re$ denotes the real part. The first (respectively, the second and third) term on the right-hand side of (11) corresponds to $l+2n=3k$ (respectively, $l+2n=3k+1$ and $3k+2$). After some algebra, we have

$$|\phi_0|^2=3^{N-2}U_3\phi_{0,1}^2 \tag{12}$$

where

$$U_3=3+\sum_{i=1}^{3}\lambda_c^2r_i^2+\sum_{i=1}^{3}\lambda_c^4r_i^2r_{i+1}^2$$

with $r_{i+3} \equiv r_i$. In a similar way we obtain

$$|\psi_0|^2 = 3^{N-2} U_3 \psi_{0,1}^2. \tag{13}$$

With these results and $|\phi_0 H' \psi_0| = 3^N \phi_{0,1} \psi_{0,1}$ it is not difficult to derive

$$\eta = 9/U_3 \neq 0. \tag{14}$$

Thus, the dispersion relation for the low-energy excitations is

$$\Delta E_{k'} = 2\eta(\tau^2 + k'^2)^{1/2} \tag{15}$$

which will produce a phase transition belonging to the 2D classical Ising universality class. So the three-letter GTM quantum spin system preserves the usual logarithmic singularity in both the ground state energy and the specific heat at criticality.

For general g-letter GTM spin models, where the couplings take g possible values $\{\lambda r_i, i = 1, 2, \ldots, g\}$ according to the g-letter GTM sequence, the prefactor η_g can be calculated analogously by taking advantage of the 'g-nary code method'. The calculation yields

$$\eta_g = g^2/U_g \tag{16}$$

where

$$U_g = g + \sum_{i=1}^{g} \lambda_c^2 r_i^2 + \sum_{i=1}^{g} \lambda_c^4 r_i^2 r_{i+1}^2 + \ldots + \sum_{i=1}^{g} \lambda_c^{2(g-1)} r_i^2 r_{i+1}^2 \ldots r_{i+g-2}^2 \tag{17}$$

with the critical condition

$$\lambda_c = \frac{1}{(\prod_{i=1}^{g} r_i)^{1/g}}$$

and $r_{i+g} \equiv r_i$. Thus, we observe that the QIM on the g-letter GTM lattice can exhibit an Ising-like phase transition with the critical behaviour the same as in the periodic case.

To summarize, we have studied quantum Ising spin models on a family of multiletter GTM lattices and obtained the analytical results for the critical line and the dispersion relation for the low-energy excitations close to the critical point. Our results show that the g-letter GTM quantum Ising spin models can undergo an Ising-like phase transition and develop the usual logarithmic singularity in the specific heat at the critical point.

Acknowledgments

The authors would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Center for Theoretical Physics, Trieste.

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