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# Thue-Morse quantum Ising model

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We study the one-dimensional quantum Ising model in a transverse magnetic field where the exchange couplings are ordered according to the Thue-Morse (TM) sequence. At zero temperature, this model is equivalent to a two-dimensional classical Ising model in a magnetic field with TM aperiodicity along one direction. We compute the order parameter (magnetization) of the chain and the scaling behavior of the energy spectrum when the system undergoes a phase transition. Analogous to the quasiperiodic (QP) quantum Ising chain, the onset of long-range order is signaled by a *nonanaliticity* in the exponent $\delta$ which describes the scaling of the total bandwidth with the size of the chain. The critical spin-coupling can be computed analytically and it is found to be lower than the QP case. Furthermore, the energy bands are found to be narrower than the corresponding QP chain. The former and latter results are consistent with the fact that the present structure has a degree of ordering intermediate between QP and random.

## I. INTRODUCTION

Recently, new magnetic structures have been produced artificially by depositing rare-earth based materials on a crystalline substrate.[1] This epitaxial-growth technique allows the introduction of new periodicities (or aperiodicities) on the atomic scale. Merlin *et al.*[2] pioneered the use of aperiodicity in nonmagnetic superlattices. More recently, quasiperiodic (QP) ordering of layers and multilayers of magnetic materials have produced very complicated spin arrangements.[3] So far, the only experimental realization of the Thue-Morse[4,5] (TM) sequence has been produced by Merlin and collaborators.[5] However, the physics involved there is entirely different from the one considered here, since their multilayers are nonmagnetic.

By considering here the magnetic properties of an aperiodic *quantum* spin Hamiltonian, we are only attempting to gain some insight into the complicated behavior of magnetic chains with a varying degree of aperiodicity (this statement will be made more precise in a moment). Our results concerning the Thue-Morse quantum spin chain, will be presented in comparison with the more familiar quasiperiodic case. Recall that at zero temperature, the one-dimensional (1D) quantum TM Ising model is equivalent to a two-dimensional (2D) *classical* Ising model having TM ordering of bonds only in one direction. Furthermore, the study of the magnetic behavior of quantum spins on the Thue-Morse sequence is motivated by the fact that this deterministic structure is more "disordered" than the QP one. In other words, this system has a degree of aperiodicity intermediate between QP and random. More precisely: the Fourier spectrum of the TM sequence does *not* have $\delta$-function peaks. On the other hand, the Fourier spectrum of any QP structure is only composed of $\delta$-function peaks (like in the periodic case). In the mathematical lore, neither singular nor absolutely continuous components are present in the Fourier spectra of the QP and periodic chain, while the spectrum of the TM sequence has only a singular continuous component.[6]

Two specific questions will be raised in this paper. The first one is concerned with thermodynamics, namely, how does the lack of translational invariance, in general, and the TM ordering (with its Fourier spectra without delta functions), in particular, affects the long-range ordered phase? The second question is concerned with the energy spectrum of the quantum TM Ising model. When the coupling constant increases, the model undergoes a phase transition into a phase with long-range order. We want to know the scaling properties of this spectrum when the system crosses the critical region. The related questions in QP magnetic systems were raised in Ref. 7.

When the coupling among spins is weak, the aperiodic quantum spin chain does not exhibit long-range order *in* the $x$ direction. For large values of the interspin coupling energy, long-range order is present in this ($x$) direction. At which value of lambda, say $\lambda_c$, the system undergoes its phase transition? The expression for $\lambda_c$ can be computed analytically and it turns out to be independent of the ordering of the couplings. Instead, $\lambda_c$ depends only on the relative population of strong and weak bonds.

As the reader will see in the following pages, we will present evidence supporting the conjecture of the *nonanaliticity* of the scaling exponent $\delta$ at the *onset* of long-range magnetic order. The exponent $\delta$ describes the scaling of the total bandwidth with the size of the system. We conjecture that the basic ingredients needed in order to obtain the nonanaliticity of the scaling exponent $\delta$, close to the critical region, are aperiodicity and self-similarity in the increasingly large unit cell present in the periodic approximants to the aperiodic infinite chain. Both, the TM and QP (Ref. 7) cases satisfy this condition. On the other hand, the exact values of the critical coupling are different from each other.

## II. MODEL

In this paper, we study the quantum Ising model in a transverse magnetic field with two distinct nearest-

 

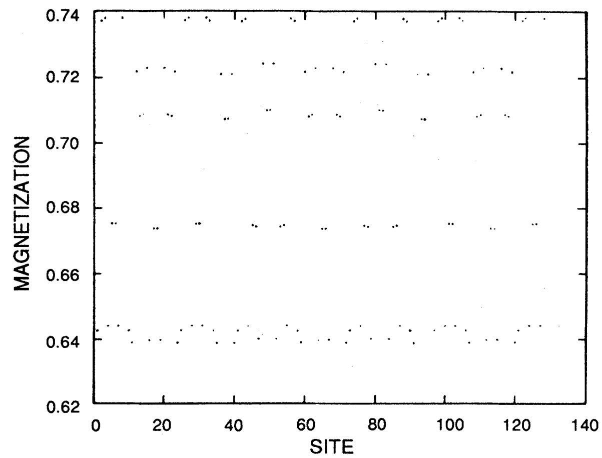


FIG. 1. Magnetization, $M$ vs position along the chain (i.e., $M$ at each site) for the TM sequence at $\lambda=\frac{8}{5}=1.6$ and $r=\frac{1}{2}$. The chain has $256=2^8$ sites. However, because of the periodic boundary conditions only half of the points are displayed.

neighbor spin couplings, $J(n)$, arranged according to the Thue-Morse (TM) sequence (to be defined herein)

$$H=-\sum_n J(n)\sigma^x(n)\sigma^x(n+1)+\sigma^z(n) . \tag{1}$$

The $\sigma^a(n)$ are the Pauli matrices, and the transverse magnetic field has been absorbed in the $J$'s. In order to study this model we express it, using the Jordan-Wigner transformation, as a 1D fermionic model which is quadratic in the fermionic fields,

$$H_{\rm JW}=c^\dagger \underline{A} c+(c^\dagger \underline{B} c^\dagger+\text{H.c.})/2 , \tag{2}$$

where $c=(c_1, c_2, \ldots, c_{2^n})$ and $c_j$ are anticommuting fermionic operators. The nonzero elements of the matrices $\underline{A}$ ($\underline{A}^t=\underline{A}$) and $\underline{B}$ ($\underline{B}^t=-\underline{B}$) are defined by

$$\begin{aligned} &A_{j,j}=-2,\quad A_{j,j+1}=-\lambda(j),\quad A_{1,2^n}=-\lambda(2^n) ,\\ &B_{j,j+1}=-\lambda(j),\quad B_{1,2^n}=\lambda(2^n) . \end{aligned} \tag{3}$$

This model cannot be expressed in position space as a single-fermion problem since the fermionic number is not conserved. The usual Bogoliubov transformation does not work here because of the aperiodicity (i.e., the states with momenta $k$ and $-k$ are not the only ones which have nonzero matrix elements). Therefore, in order to solve Eq. (1) we need to employ the method developed by Lieb, Schultz, and Mattis[8] which requires the diagonalization of the matrix

$$\underline{D}=(\underline{A}+\underline{B})(\underline{A}-\underline{B}) .$$

As this matrix defines a generalized tight-binding problem, the renormalization group approach for aperiodic systems, as in Ref. 9, can provide further insight into this

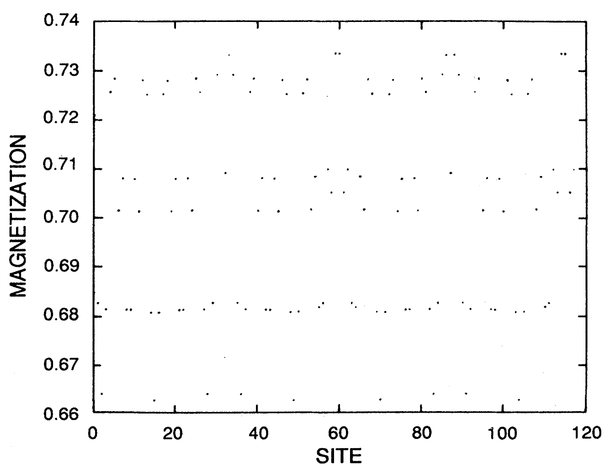


FIG. 2. Magnetization at each site for the Fibonacci sequence at $\lambda=1.489$ and $r=\frac{1}{2}$. The chain has 233 sites. Also, notice that the $\lambda$ value was chosen at the same distance from criticality as in the TM case.

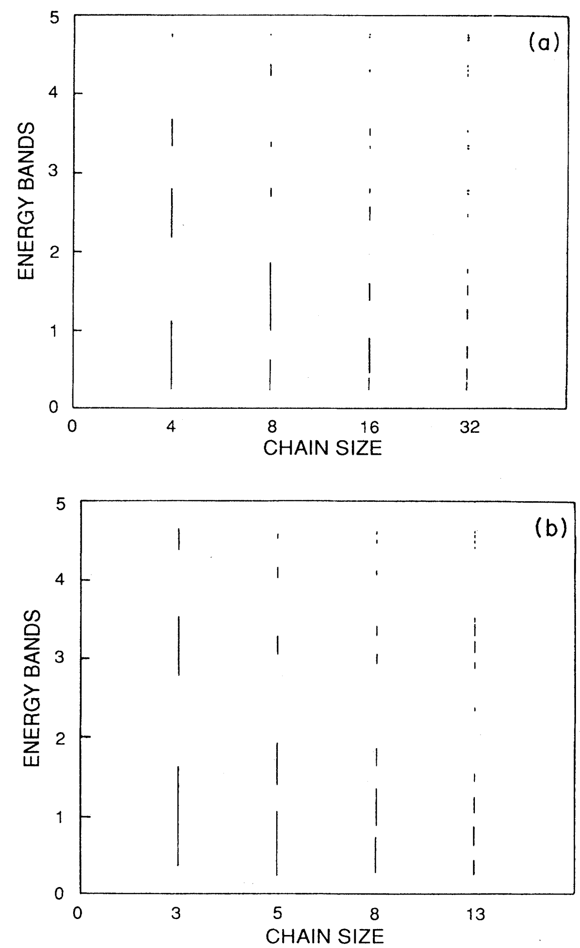


FIG. 3. (a) The energy bands for chain sizes from 4 to 32 are displayed here for the TM sequence. $\lambda$ is taken to be $\frac{8}{5}$ and $r$ equal to $\frac{1}{2}$; (b) The energy bands for chain sizes from 3 to 13 are displayed here for the Fibonacci sequence. $\lambda$ is taken to be 1.489 and $r$ equal to $\frac{1}{2}$.

problem. The Jordan-Wigner-transformed Hamiltonian, $H_{JW}$, and the original one, Eq. (1), are equal up to a boundary term which produces effects of the order $2^{-n}$. On the other hand, by recalling that the 1D quantum TM Ising model is the $\tau$-continuum Hamiltonian (see Ref. 10) of the 2D classical Ising model, it can be proved that the strongest spin-coupling constant plays the role of the inverse temperature in the 2D classical TM Ising model. This result indicates that the phase diagram of the 2D classical TM spin model can be described in terms of both spin couplings.

The TM sequence of order $N$ has $M=2^N$ elements composed of two symbols, 0 and 1, defined recursively as follows:

$$\epsilon_0=0,\quad \epsilon_{2n}=\epsilon_n,\quad \epsilon_{2n+1}=1-\epsilon_n\ . \tag{4}$$

The preceding equations generate an infinite string of digits which never repeats itself. In spite of this aperiodicity, the TM sequence is self-similar. Furthermore, and unlike the quasiperiodic (QP) case, the TM chain cannot be characterized by a finite set of irrational numbers. Alternatively, this sequence can be defined by considering the positive integer numbers and writing them in binary form. Afterwards, one sums the digits of every integer modulo 2 and obtains the TM sequence. The periodic approximants ($2^n$ sites and periodic boundary conditions) to the aperiodic limit do exhibit mirror symmetry.

The sequence of couplings, $\lambda(n)$, in the TM Ising model is obtained by associating to every 1 and 0 of the above sequence, the exchange couplings $\lambda_1=\lambda$ and $\lambda_2=r\lambda$, respectively. Therefore, the deviation of $r$ from unity describes the lack of translational invariance in the system. In our numerical computations, the aperiodic TM model is approximated by a sequence of chains with progressively larger unit cells of sizes $2^n$ and periodic boundary conditions.

TABLE I. For a given chain size, and for a given band index associated for that chain size, $E(k=0)$ represents the bottom of the band and $E(k=\pi)$ the top of the band for an aperiodic (TM) quantum Ising model. Surprisingly, some bands overlap. No other aperiodic structure exhibits this kind of degeneracy. The only symmetry left into the system, mirror symmetry, is responsible for such degeneracies (in pairs). Without periodic boundary conditions, the mirror symmetry appears only in every other sequence. Once periodic boundary conditions are imposed, all periodic approximants to the aperiodic sequence do have mirror symmetry. The backslash, \, and the slash, /, right next to the bottom-band energies, $E(k=0)$, indicate which bands are degenerate. Notice that the bands located at the edges of the spectrum and at the center are the only ones which are not degenerate. Therefore, the number of effective "bands" [continuous lines in Fig. 3(b)] which denote either a nondegenerate band or the union of two degenerate ones is given by $(M+4)/2$ were $M$ denotes the total number of bands (distinct sites in the periodic-approximant chain). The same type of results were also obtained for larger chains.

| Chain size | Band index | $E(K=0)$ | $E(k=\pi)$ |
|---|---|---|---|
| 4 | 1 | 0.23044 | 1.1287 |
| 4 | 2 | 2.8 | 2.1633 |
| 4 | 3 | 3.3272 | 3.6725 |
| 4 | 4 | 4.7577 | 4.7072 |
| 8 | 1 | 0.2304 | 0.6274 |
| 8 | 2 | 1.5097 \ | 1.0040 |
| 8 | 3 | 1.5097 / | 1.8641 |
| 8 | 4 | 2.8 | 2.7039 |
| 8 | 5 | 3.3272 | 3.3816 |
| 8 | 6 | 4.3035 \ | 4.2200 |
| 8 | 7 | 4.3035 / | 4.3769 |
| 8 | 8 | 4.7577 | 4.7549 |
| 16 | 1 | 0.23044 | 0.3995 |
| 16 | 2 | 0.74030 \ | 0.4664 |
| 16 | 3 | 0.74030 / | 0.9190 |
| 16 | 4 | 1.50973 \ | 1.3817 |
| 16 | 5 | 1.50973 / | 1.6139 |
| 16 | 6 | 2.47888 \ | 2.3938 |
| 16 | 7 | 2.47888 / | 2.5804 |
| 16 | 8 | 2.8 | 2.7724 |
| 16 | 9 | 3.32729 | 3.3435 |
| 16 | 10 | 3.53528 \ | 3.4903 |
| 16 | 11 | 3.53528 / | 3.5682 |
| 16 | 12 | 4.30356 \ | 4.2973 |
| 16 | 13 | 4.30356 / | 4.3097 |
| 16 | 14 | 4.73380 \ | 4.7294 |
| 16 | 15 | 4.73380 / | 4.7388 |
| 16 | 16 | 4.75773 | 4.7570 |

## III. LONG-RANGE MAGNETIC ORDER

The model considered here displays long-range magnetic order above a certain critical coupling $\lambda_c$. The critical coupling is easily obtained from the equation[8]

$$\prod_{n=1}^{2^n} J(n)=1 \ . \tag{5}$$

This condition corresponds to the vanishing of the gap at the onset of criticality. This gives, for the TM case,

$$\lambda_c(r)=1/\sqrt{r} \ . \tag{6}$$

This value of $\lambda_c$ is the same critical coupling of a random system where, for any given site $n$, the probabilities of $\lambda(n)$ being either $\lambda_1$ or $\lambda_2$ are equal. The analog result for the Fibonacci chain is[7]

$$\lambda_c(r)=r^{-(\sigma_g)^{-2}} \ ,$$

where $\sigma_g=(1+\sqrt{5})/2$, which, for any given $r$ is higher than the critical coupling for the TM case. These results imply that it is easier to destroy long range magnetic order in the TM case then the Fibonacci case.

Figure 1 shows the magnetization at each site of the TM system for fixed values of $r$ and $\lambda$. Similarly, and for the sake of comparison, the QP modulation is displayed in Fig. 2 for the same value of $r$ and for a value of $\lambda$ that is at the same distance from criticality as in the TM case. Hence this modulation in magnetization characterizes the underlying sequence in the couplings of the spin chain.

The Figs. 3(a) and 3(b), respectively, show the energy bands for the TM and QP Fibonacci spin chains. We find that the total band width i.e., the total Lebesque measure of the energy spectrum scales with size of the system as $M^{-\delta}$, analogous to the corresponding results of Ref. 7 for the Fibonacci chain. Unlike the Fibonacci case, in the TM model the energy bands *overlap* (see Table I). In fact, the number of continuous lines in Fig. 3(b) is $(M+4)/2$ where $M$ is the number of bands (distinct sites in the periodic chain). The TM spectrum for some values of Bloch vector **k** are found to be twofold degenerate, except for the states of lowest, highest and middle two energies. It is interesting to note that although the TM is more "disordered" than the QP sequence, this fact does *not* lift the degeneracies of the periodic system completely. We believe that this degeneracy is due to the *mirror symmetry* that exists in the TM sequence when periodic boundary conditions are imposed on it.

Figure 4 shows the exponent $\delta$ for a fixed value of $r$ and varying $\lambda$. As seen in the figure, the exponent $\delta$ for the TM chain is *larger* than the corresponding QP case, consistent with the fact that the TM structure is more disordered. Analogous to the QP case,[6] we find that in the TM chain $\delta$ displays a linear behavior at both sides of the phase transition leading us to conjecture the *nonanalyticity at criticality.* This "$V$" shaped behavior for $\delta$ has also been seen in the anisotropic $XY$ model with a Fibonacci sequence.[6]

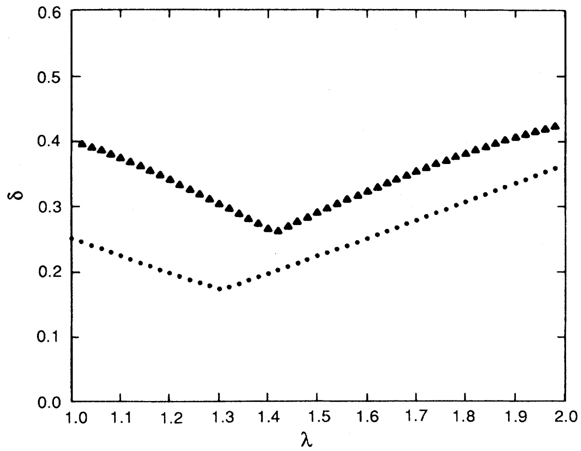


FIG. 4. The scaling exponent delta is plotted for both the TM (triangles) and Fibonacci (circles) systems. $r$ is taken to be $\frac{1}{2}$ in both cases and the chain sizes are 128 and 144, respectively. The delta value at each coupling is obtained by taking chain sizes of 32, 64, and 128 for the TM and 55, 89, and 144 for the Fibonacci quantum Ising models.

## IV. CONCLUSIONS

We have computed the following quantities for the TM quantum Ising model: magnetization, critical spin coupling, energy spectra, and its scaling behavior on and around the critical region. Moreover, we have compared every one of these results with the more familiar ones corresponding to the QP geometry. The former one has a higher value of the critical coupling and larger spreading of the values of the magnetization versus position along the chain. Also, in spite of the fact that the TM structure is more "disordered" than the QP one, the energy spectrum of the former has degeneracies which are absent in the latter.

In translationally-invariant systems, the onset to long-range order is signaled by a nonvanishing value of the magnetization of the system. The lack of translational invariance preserves this behavior. However, it adds two new features: (1) a modulating magnetization as a function of position along the chain, and (2) an additional singularity at criticality. Our studies of aperiodic magnetic chains indicate that the conjectured nonanalyticity of the scaling exponent $\delta$ is a clear signal of the onset of a phase transition. Therefore, a new critical exponent which does not exist in periodic systems is required here. It describes the way $\delta$ approaches its critical value in each side of the transition. It is possible that this exponent (here found equal to one) characterizes a new type of universality class. The renormalization-group approach for aperiodic systems as, in Ref. 9, will provide further insight into this problem.

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