# Quasiperiodicity and Long-Range Order in a Magnetic System

Mauro M. Doria and Indubala I. Satija[(a)]

*Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*

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We study the 1D quasiperiodic quantum Ising model in a transverse field, which exhibits long-range order above a critical coupling and describes the phase diagram of the 2D classical Ising model quasiperiodic in one direction. We numerically determine the correlation length, magnetization, and energy spectrum of this system. The site dependency of the magnetization is described by a new order parameter, the width of the magnetization. The scalings $\delta$ and $f(\alpha)$ associated with the Cantor spectrum are found to exhibit special features at the onset of long-range order.

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The investigation of systems displaying quasiperiodicity (QP) has acquired direct experimental relevance since the recent construction of Fibonacci superlattices.[1] The many studies carried out for the one-dimensional tight-binding[2,3] and phonon[4] models have shown that quasiperiodicity does introduce a whole new set of properties for such systems. In this Letter we study a model of direct importance for magnetic superlattices as the two-dimensional Ising model is relevant to magnetism. This model is the one-dimensional QP *quantum* Ising model in transverse magnetic field (1D QPIM) and is equivalent to the following Hamiltonian, up to a similarity transformation:

$$H=-\sum_j \lambda(j)\sigma_x(j)\sigma_x(j+1)+\sigma_z(j). \tag{1}$$

Here the $\sigma_a(j)$ are Pauli matrices and the couplings $\lambda(j)$ form a QP sequence with two values $\lambda$ and $\lambda'=r\lambda$. In our study QP is characterized by the golden mean ratio $\sigma_g=(\sqrt{5}+1)/2$.[5] We found that similarly to the pure Ising case $(r=1)$, the model undergoes a phase transition for a critical value of the coupling $(\lambda=\lambda_c)$ above which there exists long-range order (LRO). Hence the novel feature of this model not present in the QP systems studied in the past[2-4] is the existence of LRO. The interest in study of the 1D QPIM is twofold. (i) At zero temperature this theory describes the phase diagram, and so the critical region, of the two-dimensional *classical* Ising model having QP in one of the directions (2D QPIM). Hence the following question is addressed here: How does the absence of translational invariance modify the LRO features and affect the scaling properties of the 2D QPIM? (ii) The energy spectrum of the 1D QPIM forms a Cantor set. Then the main question under investigation is the following: How do the scaling properties of this spectrum change as the model undergoes a phase transition in the coupling constant and acquires LRO?

We study the 1D QPIM by first expressing it as a one-dimensional fermionic model. The model is quadratic in the fermionic fields and displays a feature not seen in all the previous studies of QP models.[2-4,6] The fermionic number is not conserved and the model cannot be expressed in position space as a single-fermion problem. Therefore to the best of our knowledge this is the first time a QP model exhibiting LRO is investigated. To analyze the 1D QPIM we have used a special method developed by Lieb, Schultz, and Mattis[7] long ago.

We now summarize our results for the zero-temperature properties of (1) in two parts. *All* the results of this paper are numerically obtained. The first part of the results also concerns the thermodynamics of the 2D QPIM. The second one addresses the energy spectrum of the 1D QPIM.

(i) The 1D QPIM exhibits LRO above the critical coupling. We deduce from our numerical analysis done on finite chains that the critical coupling depends upon $r$ for the infinite chain as $\lambda_c(r)=1/|r|^{1/\sigma_g^2}$. The correlation length of the 2D QPIM diverges with $\nu=1$ exactly like in the pure Ising model. QP results in local magnetization varying from site to site (Fig. 1). To characterize such variation we introduce a new order parameter called the width, $w(\lambda,r)$, defined as the difference between the maximum and the minimum magnetization at

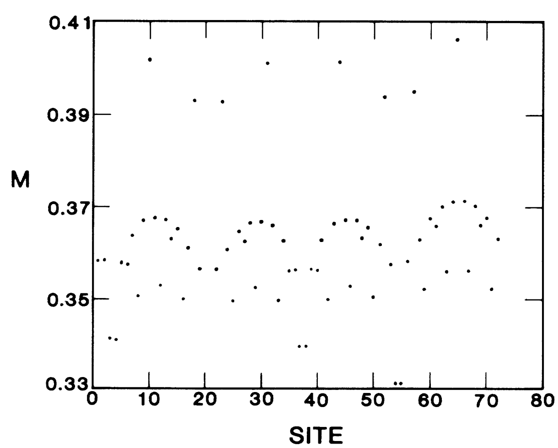


FIG. 1. Magnetization vs site at criticality for a chain of 144 sites, $r=0.5$.

 

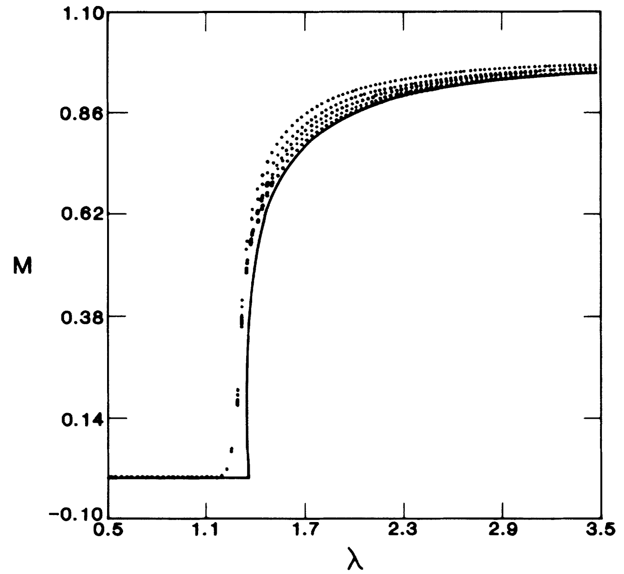


FIG. 2. Magnetization of all sites vs coupling (chain of 89 sites, $r=0.5$). The solid line plots the function $M(\lambda)=0$, $\lambda\le\lambda_c$; $M(\lambda)=(1-1/\lambda^2)^{1/4}$, $\lambda>\lambda_c$, which is the pure Ising magnetization for an infinite chain.

given values of λ and $r$ (Fig. 2). We claim that for an infinite system the width should vanish for $\lambda<\lambda_c$ and decay exponentially to zero for $\lambda\gg\lambda_c$, attaining its maximum value at $\lambda_c$. We also find that in the neighborhood of the pure Ising case ($r\approx1$), the critical width has the linear dependency $w(\lambda_c,r)\propto 1-r$.

(ii) Analogous to previous studies,[8] the energy spectrum is found to be a Cantor set for all couplings including the critical one. The index $\delta$,[2] which describes the scaling of the total allowed energies with the size of the system, has linear dependence on λ (Fig. 3). Numerical evidence indicates that this dependence becomes nonanalytic at the critical point, where $\delta$ attains its minimum value. We also computed the global scaling properties of the Cantor-set spectrum using the so-called $f(\alpha)$ curve[9,10] (Fig. 4). This function shows a characteristic shape change as $\lambda\to\lambda_c$. The Hausdorff and the other higher moments of dimension were found to attain their maximum values at criticality.

In our numerical study, the QP system is approximated by a sequence of periodic systems with progressively larger unit cells of size $F_n$. The $F_n$'s are the Fibonacci numbers obtained by optimal rational approximants to $\sigma_g$, $\sigma_g=F_n/F_{n-1}$; $F_n=F_{n-1}+F_{n-2}$ with $F_1=F_2=1$. The 1D QPIM corresponds to the so-called $\tau$ continuum Hamiltonian[11] of the 2D QPIM. The latter model has couplings $J_x$ and $J_x'$ that alternate in, say, the $x$ direction according to the prescription in Ref. 5. In the $y$ direction all couplings are equal to $J_y$. The transfer matrix for the 2D QPIM is given by

$$T=\exp\left\{\beta J_y^*\textstyle\sum_j\sigma_x(j)\right\}\times\exp\left\{\beta\textstyle\sum_j J_x(j)\sigma_z(j)\sigma_z(j+1)\right\},\qquad(2)$$

where $\beta J_y^*=-(\ln\tanh\beta J_y)/2$. To define a smooth $\tau$ continuum limit, $J_y$ must grow large while the couplings $J_x(j)$ become weaker so that the following proportionality holds for each site: $\beta J_x(j)=\lambda(j)\exp(-\beta J_y)$. Therefore the parameter $r$ previously defined is *temperature independent,* $r=J_x'/J_x$, and λ plays the role of inverse of temperature for the 2D QPIM. To describe the phase diagram of the 2D QPIM by means of $r$ and λ, we studied two quantities of the quantum chain (1). The first is the mass gap, $E_0(\lambda,r)$, defined as the difference between the first excited- and ground-state energies. The second one is the long-range correlation,

$$\rho_x(j,\lambda,r)=\langle G|\sigma_x(j)\sigma_x(j+N)|G\rangle,\qquad(3)$$

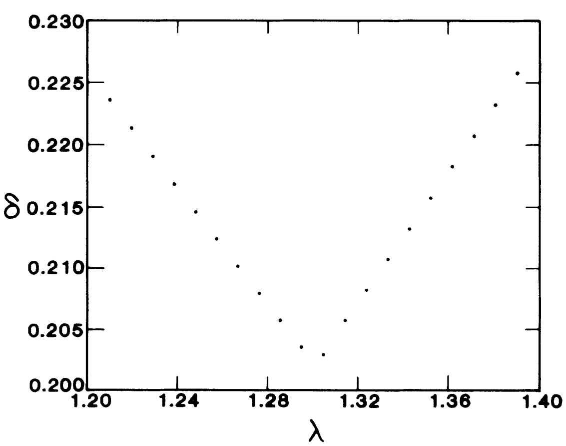


FIG. 3. Plot of $\delta$ vs λ for $r=0.5$ and the chain sizes ranging from 13 to 610 sites.

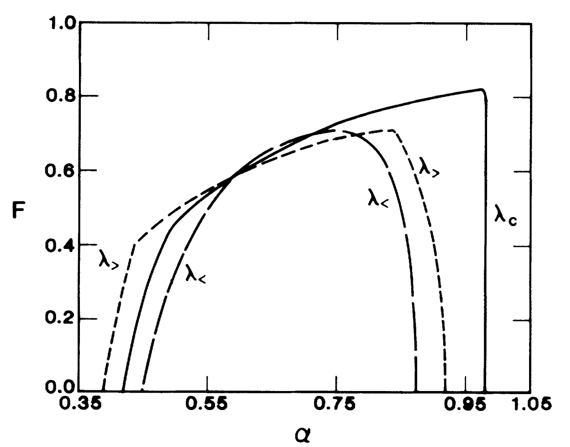


FIG. 4. $F(\alpha)$ curve for three different couplings for $r=0.5$ for chain sizes ranging from 13 to 610 sites.

where $|G\rangle$ is the ground state of (1) and $N$ is the halfway point of the periodic chain, equal to $F_n/2$ and $(F_n+1)/2$ for even and odd sites, respectively. $E_0(\lambda,r)$ is the inverse of the correlation length for the 2D QPIM. The relation $E_0(\lambda,r)=2c|\lambda-\lambda_c(r)|$ is true for all values of $\lambda$ ($r\neq 0$ or $\infty$) in the neighborhood of $\lambda_c$; hence, $\nu=1$. The constant $c$ is found to be equal to $1/\lambda_c(r)$ in the neighborhood of the pure Ising case ($r\approx 1$). The fact that the exponent $\nu$ is identical to that in the pure Ising model implies that some of the characteristics of the model become insensitive to the QP in the critical regime. It is well known[7,12] that $\rho_x(j,\lambda,r)$ describes the magnetization of the Ising model at all temperatures. Above $\lambda_c$ the correlation $\rho_x(j,\lambda,r)$ drastically changes from site to site (see Fig. 1). Our numerical results show that for a finite chain the width goes as

$$w(\lambda,r)\approx(\lambda/\lambda_c)^{N/2},\quad \lambda<\lambda_c, \tag{4a}$$

$$w(\lambda,r)\approx\exp(-K\lambda),\quad \lambda\gg\lambda_c, \tag{4b}$$

where $K$ is a function of $r$ (see Fig. 2). Therefore for the infinite system we conclude that $w(\lambda,r)\to 0$ for $\lambda<\lambda_c$.

We have studied the eigenvalues of Hamiltonian (1) as a function of $\lambda$. Like other QP systems, this model has a Cantor spectrum in this case with nontrivial scaling for all values of $\lambda$. For an infinite chain, periodic every $F_n$ sites, the spectrum consists of $F_n$ bands and $F_n-1$ gaps. In the limit of large $n$, the width of allowed bands becomes narrower. So in this limit the sum of all band widths, denoted by $B_n$, has measure zero and scales with the size of the system as $B_n\propto F_n^{-\delta}$, the exponent $\delta$ being a function of $\lambda$ and $r$. Our numerical results give the following linear dependency:

$$\begin{aligned}\delta(\lambda)-\delta(\lambda_c)&=b_-(\lambda_c-\lambda),\quad \lambda<\lambda_c,\\ \delta(\lambda)-\delta(\lambda_c)&=b_+(\lambda-\lambda_c),\quad \lambda>\lambda_c,\end{aligned} \tag{5}$$

where $b_\pm$ are positive functions of $r$ (see Fig. 3).

We have also studied the global scaling properties of the Cantor-set spectrum by computing the $f(\alpha)$ curve using a kind of partition-function formalism recently proposed by Halsey *et al.*[9] For each $\lambda$, this function is a continuous curve existing for a range of $\alpha$ values, $[\alpha_{\min},\alpha_{\max}]$. The exponent $\alpha$ is a local scaling exponent characterizing the scaling associated with the integrated density of states for a given energy. In general, this exponent is different in distinct parts of the spectrum. Hence the curve $f(\alpha)$ describes the distribution of $\alpha$'s in the whole spectrum. This curve acquires its maximum value at the most probable scaling $\alpha_0$. The value $f(\alpha_0)$ is equal to the Hausdorff dimension $D_{\rm H}$ of the spectrum. For the pure Ising model ($r=1$) the energy spectrum is continuous and the $f(\alpha)$ curve consists of just two points: $f(1)=1$ and $f(0.5)=0$. The latter point corresponds to the scaling exponent of the Van Hove singularities at the band edge. Figure 4 shows the $f(\alpha)$ function for three different couplings, $\lambda_<$, $\lambda_c$, and $\lambda_>$ corresponding respectively to below, at, and above the critical coupling for a given value of $r$. $D_{\rm H}$ along with other higher-order dimensions $D_q$ have their maximum values at the critical point $\lambda=\lambda_c$ and then slowly drop to zero as $\lambda\to 0$ or $\lambda\to\infty$. At criticality, $D_{\rm H}$ is equal to $0.84\pm 0.01$ ($r=0.5$) and $D_{-\infty}$, the dimension characterizing the most ramified part of the spectrum, becomes unity. Also $\alpha_{\max}$ achieves its maximum value of unity at criticality. As Fig. 4 shows, the shape of the function undergoes a characteristic change near the critical coupling without any further drastic changes in its shape in the LRO phase. However, our numerical results indicate that the smoothness of this function, clearly present for $\lambda\ll\lambda_c$, may disappear at criticality. This nonsmoothness around $\alpha=0.5$ may be partly related to the remnants of the Van Hove singularities. Also, it should be noticed that whereas the $f_<(\alpha)$ corresponding to $\lambda_<$ always lies inside $f_c(\alpha)$, $f_>(\alpha)$ corresponding to $\lambda_>$ intersects $f_c(\alpha)$ with $\alpha_{\min}\to 0$ as $\lambda\to\infty$.

Finally we describe the fermionic representation employed to study Eq. (1). By means of the Jordan-Wigner transformation one rewrites (1) as

$$H=c^+Ac+(c^+Bc^++\text{H.c.})/2, \tag{6}$$

where $c$ is the vector $(c_1,c_2,\ldots,c_{Fn})$ and the $c_j$'s are anticommuting fermionic operators. The nonzero elements of the matrices $A$ ($A^t=A$) and $B$ ($B^t=-B$) are defined as follows: $A_{jj}=-2$, $A_{j,j+1}=-\lambda(j)$, $A_{1,Fn}=-\lambda(F_n)$; $B_{j,j+1}=-\lambda(j)$, $B_{1,Fn}=\lambda(F_n)$. Because of lack of translational invariance, the usual method of Bogoliubov transformation does not work here. This is because not just momenta $k$ and $-k$ are mixed together but many others as well. Hence to solve (6) one needs the method of Lieb, Schultz, and Mattis.[7] All our calculations are numerical *exact* and have been done in position space with periodic boundary conditions on the fermionic model. Hamiltonians (1) and (6) are only equivalent up to a boundary term. However, the effects of this term are of order $1/F_n$ as shown in Ref. 7. The method requires the diagonalization of matrix $D=(A+B)(A-B)$ which should be seen as a tight-binding model associated with this problem. This matrix is also the initial point for renormalization-group studies of the 1D QPIM. Our numerical approach consisted of finding eigenvalues and eigenvectors of the matrix $D$ of various chain sizes of maximum size 610. To determine $\rho_x$, Wick's theorem is used to express Eq. (3) in terms of Green's functions which are directly evaluated from the eigenvalues and eigenvectors of $D$.[7] Most of our results were obtained for $0.5\le r\le 1.5$. It should be pointed out that for $r=0$ or $r=\infty$, the model (1) becomes zero dimensional and hence falls into a different universality class. In this limit the gap vanishes exponentially with $\lambda$. The crossover to the regions $r\to 0$ and $r\to\infty$ will be described elsewhere. Our study indicates that at $r=-1$ the model shows no width in the magnetization. The renormalization-group approach to this problem will shed light on this peculiar result. At this point we found that $\lambda_c = 1$ thus agreeing with our formula for $\lambda_c(r)$.

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[a]Present address: Department of Physics, George Mason University, 4400 University Drive, Fairfax, VA 22030.

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[5]Let $\sigma = F_n/(F_n+1)$ be a rational approximation to the golden mean. Consider the sequence defined by

$$dx(j) = 1 + [j/\sigma]/\sigma - [(j-1)/\sigma]/\sigma,$$

for any integer $j \geq 1$. The symbol $[X]$ stands for the largest number contained in $X$. This sequence has periodicity $F_n$ and only contains two distinct elements. To the values 1 and $1+1/\sigma$ obtained from this sequence, we associate $\lambda$ and $\lambda'$, respectively, to the site function $\lambda(j)$ at Hamiltonian (1).

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