Critical properties of a two-dimensional Ising magnet with quasiperiodic interactions

G. A. Alves, M. S. Vasconcelos, and T. F. A. Alves

1Departamento de Física, Universidade Estadual do Piauí, 59078-900, Teresina - PI, Brazil
2Escola de Ciências e Tecnologia, Universidade Federal do Rio Grande do Norte, 59078-900, Natal - RN, Brazil
3Departamento de Física, Universidade Federal do Piauí, 57072-970, Teresina - PI, Brazil

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We address the study of quasiperiodic interactions on a square lattice by using an Ising model with ferromagnetic and antiferromagnetic exchange interactions following a quasiperiodic Fibonacci sequence in both directions of a square lattice. We applied the Monte Carlo method, together with the Metropolis algorithm, to calculate the thermodynamic quantities of the system. We obtained the Edwards–Anderson order parameter $q_{EA}$, the magnetic susceptibility $\chi$, and the specific heat $c$ in order to characterize the universality class of the phase transition. We also use the finite size scaling method to obtain the critical temperature of the system and the critical exponents $\beta$, $\gamma$, and $\nu$. In the low-temperature limit we obtained a spin-glass phase with critical temperature around $T_c \approx 2.274$, and the critical exponents $\beta$, $\gamma$, and $\nu$, indicating that the quasiperiodic order induces a change in the universality class of the system. Also, we discovered a spin-glass ordering in a two-dimensional system which is rare and, as far as we know, the unique example is an under-frustrated Ising model.

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I. INTRODUCTION

Since the discovery of quasicrystals by Shechtman et al. [1], awarded with the Nobel Prize, and the pioneering work of Merlin et al. [2] on the nonperiodic Fibonacci and Thue–Morse GaAs-AlAs superlattices, these quasiperiodic systems have attracted interest and hundreds of quasicrystals have been reported and confirmed. Quasicrystals are a particular type of solid that have a discrete point-group symmetry not present in Bravais lattices like a Cs symmetry in two dimensions or icosahedral symmetry in three dimensions [3,4]. These systems can be viewed as intermediate between full translational symmetric systems and random amorphous solid systems [1] and possess a long-range structural order called quasiperiodicity. Some examples of such quasiperiodic systems are metallic alloys [5,6], soft-matter systems [7], supramolecular dendritic systems [8,9], and copolymers [10,11]. Quasiperiodic crystals have some unique properties, such as fractal spectra (in the case of exact solvable models) and localization of electronic [12,13] and photonic [14–16] states. Also, a model was proposed with localized spins [17] as an alternative way to simulate disorder.

In the last 30 years since their discovery, the study of quasicrystals significantly advanced our knowledge about the atomic scale structure [18,19], but many questions regarding the consequences of quasiperiodicity on physical properties, such as electronic and magnetic properties, remain open. One of the most interesting questions regarding magnetism in quasicrystals, yet unanswered, is whether long-range antiferromagnetic (AFM) order can be sustained in real quasicrystals, yet unanswered, is whether long-range antiferromagnetic (AFM) order can be sustained in real quasicrystals, and localization of electronic [12,13] and photonic [14–16] states. Also, a model was proposed with localized spins [17] as an alternative way to simulate disorder.

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II. MODEL AND SIMULATIONS

The most widely used model in the description of magnetic systems is the Ising model [30] which is given by the Hamiltonian

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j. \quad (1)$$

Here, $S_i$ and $S_j$ are the spin on sites $i$ and $j$, respectively and their values can be $\pm 1$. $J_{ij}$ is the exchange interaction.
impurities diluted in Cu and Au, inducing an effective coupling giving origin to the Ruderman–Kittel–Kasuya–Yosida interaction [9].

Theoretically, these systems with competitive interactions were investigated by using the Edwards–Anderson (EA) model [29]. It is worth mentioning that the EA model originally considered a Gaussian distribution of strengths \( J_{ij} \) in a \( d \)-dimensional lattice with nearest-neighbor interactions similar to the Ising model. The most important result of this model is the presence of a spontaneous symmetry breaking leading to an ordered phase in the low-temperature limit, called the spin-glass phase. In a spin-glass phase the spin at a particular site has a nonzero mean value \( m_i = \langle S_i \rangle \); however, the total magnetization is zero.

We generated an initial random spin configuration \( S_i = \pm 1 \) in a square lattice and used the Metropolis algorithm for the Monte Carlo method (MCM) [31] to generate the steady-state configurations. In this way, we determined the EA order parameter \( \langle q_{EA} \rangle \) [29], the susceptibility \( \chi \), the specific heat \( c \), and Binder cumulant \( g_L \) [32], defined by the following relations:

\[
q_{EA} = \frac{1}{N} \sum_{i,j} S_{ij}^2,
\]

\[
\chi = N \left( \langle q_{EA}^2 \rangle - \langle q_{EA} \rangle^2 \right) / T,
\]

\[
c = N \left( \langle H^2 \rangle - \langle H \rangle^2 \right) / T^2,
\]

\[
g_L = \frac{1}{2} \left( 3 - \frac{\langle q_{EA}^4 \rangle}{\langle q_{EA}^2 \rangle} \right),
\]

respectively. Here \( \langle \cdots \rangle \) stands for a thermal average over sufficiently many independent steady-state-system configurations and \( L \) and \( T \) are the lattice size and the absolute temperature, respectively. We used the following values of the lattice size \( L: 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, \) and 610, which are the first Fibonacci numbers. The total number of spins for each lattice size is \( L^2 \).

The thermodynamic properties are functions of the temperature \( T \) and they obey the following finite size scaling (FSS) relations [33]:

\[
q_{EA} = L^{-\beta/\nu} f_\beta(\vartheta),
\]

\[
\chi = L^{\gamma/\nu} f_\chi(\vartheta),
\]

\[
c = L^{\nu/\nu} f_c(\vartheta),
\]

where \( \beta, \gamma, \nu, \) and \( \alpha \) are the usual critical exponents and \( f_i(\vartheta) \) are the FSS functions with

\[
\vartheta = L^{1/\nu} \left| T - T_c \right|
\]

being the scaling variable. Therefore, from the lattice-size dependence of the EA parameter \( q_{EA} \) and the susceptibility \( \chi \) we obtained the critical-exponent ratios \( \beta/\nu \) and \( \gamma/\nu \), respectively. Following the scaling-variable dependence, we expect that the susceptibility maxima \( T_\chi \) scales with the system size \( L \) as

\[
T_\chi = T_c + bL^{-1/\nu}.
\]
where $b \approx 1$. Therefore, the susceptibility maxima $T_x$ as a function of system size $L$ can be used to evaluate the exponent $-1/\nu$.

We used $1 \times 10^6$ MCM steps to make the system reach the steady state and the independent steady-state system configurations are estimated in the next $1 \times 10^5$ MCM steps. One MCM step is accomplished when all $N$ spins are investigated if they flip or not. We carried out $10^5$ independent steady-state configurations to calculate the needed thermodynamic averages.

III. RESULTS AND DISCUSSION

We investigated first the influence of lattice boundary conditions on thermodynamic properties. We show the EA order parameter $q_{EA}$ given by Eq. (2) as a function of temperature $T$ in Fig. 2 for periodic boundary conditions. We observe the presence of plateaux on $q_{EA}$ which are a finite-size effect. These plateaux are absent in open boundary conditions.

We estimated the critical temperature $T_c$ for different lattice sizes $L$ as in Fig. 3. The critical temperature $T_c$ is estimated as the point where the curves for different size lattices intercept each other. We obtained $T_c \approx 2.274$.

The correspondent behavior of the EA parameter $q_{EA}$ versus temperature $T$ is presented in Fig. 4. The $q_{EA}$ dependence suggests the presence of a second-order phase transition in the system. The phase transition occurs at the critical temperature $T_c \approx 2.274$. The critical behavior given by Eq. (6) of the EA order parameter is shown in Fig. 5. The slope of the curve corresponds to the exponent ratio $\beta/\nu = 0.40$ (2). The exponent ratio differs from the pure model and this change of the universality class is induced by the quasi-periodic order.

It is well known that, if the model has a continuous transition in its full translational symmetric version, the influence of random interactions on their critical behavior is summarized by the Harris criterion [34], which establishes that, if $2 - d\nu < 0$ where $d$ is the spatial dimensionality, the quenched disorder will not change the critical behavior of the system and it is said to be irrelevant. However, the Harris criterion is not valid at the random system criticality [35] where $\phi \neq \alpha$ for the random model, as known from perturbative expansions where $\phi = 2 - d\nu$ is the crossover exponent. For the pure model, the equality $\phi = \alpha$ is restored.

By the inequality involving $\alpha$ and $\phi$, it is possible, at least in theory, to have a model with $\alpha$ positive and $\phi$ negative, in a way the random system will have the same critical behavior as the pure model. However, there are no systems reported with such behavior as far as we know. In our case, we have $\phi = 0$, as we show later. In this way, we can expect a different critical behavior and different exponents from the Ising 2D exponents.

The Luck criterion for the quasi-periodic ordered model, analogous to the Harris criterion for the random disordered model, establishes that, if the $\phi$ exponent is positive, the critical behavior of the quasi-periodic model differs from the fully translational symmetric model and the disorder is called relevant. Conversely, if $\phi$ is negative, the critical behavior is the
same of the pure model and the disorder is called irrelevant. On the marginal case \( \phi = 0 \) we obtained a change of the universality class of the model as observed, for example, in mean-field results for an Ising model in a hypercubic lattice [28].

To obtain an explicit expression for the crossover exponent, we can follow Refs. [36–38] to express the total number of exchange interactions and the fluctuations between the frequencies of the ferromagnetic and antiferromagnetic interactions between the \( n \)-esimal generation of the lattice and the semi-infinite lattice scales with the total length of the system \( L \) as

\[
J \propto N \propto L, \quad (11)
\]

\[
\Delta J \propto \Delta N \propto L^\omega, \quad (12)
\]

where \( \omega \) and \( J \) are, respectively, the geometrical wandering exponent of the lattice and the total exchange strength. The critical temperature \( T_c \) is proportional to \( J \), so we can write

\[
\delta t = \frac{\Delta J}{J} \sim L^{\omega - 1}, \quad (13)
\]

where \( t = (T - T_c)/T_c \) is the reduced temperature and \( \delta t \) stands for the fluctuations on the reduced temperature when we introduce the aperiodicity. Combining Eq. (13) with the scaling form \( L \sim \varepsilon \sim t^{-\nu} \) for the pure model (\( \varepsilon \) is the correlation length), we have

\[
\frac{\delta t}{t} = t^{-1-\nu(\omega - 1)}, \quad (14)
\]

and by using the expression \( \frac{\delta t}{t} \sim t^{-\phi} \), we obtain the crossover exponent

\[
\phi = 1 + \nu(\omega - 1), \quad (15)
\]

which is the same expression obtained in Ref. [36]. In our case, \( \nu = 1 \) for the uniform model.

To evaluate the crossover exponent, we need the wandering exponent for our lattice. To accomplish this task we note that the 2D lattice showed in Fig. 1 can be generated by the geometric recursive substitutions of the lattice monomers shown in Fig. 6. Starting from the lattice monomer in panel (a), we can obtain the successive generations of the lattice in Fig. 1 by applying the recursive geometrical substitutions presented in panels (a)–(d) which are formally equivalent to the respective substitution rules \( (AA) \rightarrow (AA)(AB)(BA)(BB) \), \( (AB) \rightarrow (AA)(BA) \), \( (BA) \rightarrow (AA)(AB) \), and \( (BB) \rightarrow (AA) \). In panel (e) we show the first three generations of our lattice by applying the geometrical substitution rules presented in panels (a)–(d).

![FIG. 5. Critical behavior of \( q_{EA} \) at \( T = T_c \) as a function of lattice size \( L \) obtained from Eq. (6). Alongside the \( q_{EA} \) points we show the error bars on the same scale. The curve slope gives the exponent ratio \( \beta/\nu = 0.40(2) \). This exponent ratio differs from that of the pure model and this change in universality class is induced by the quasiperiodic order.](image)

![FIG. 6. Starting from the lattice monomer in panel (a), we can obtain the successive generations of the lattice in Fig. 1 by applying the recursive geometrical substitutions presented in panels (a)–(d) which are formally equivalent to the respective substitution rules (AA) \( \rightarrow (AA)(AB)(BA)(BB) \), (AB) \( \rightarrow (AA)(BA) \), (BA) \( \rightarrow (AA)(AB) \), and (BB) \( \rightarrow (AA) \). In panel (e) we show the first three generations of our lattice by applying the geometrical substitution rules presented in panels (a)–(d).](image)

![FIG. 7. The susceptibility \( \chi \) as function of temperature \( T \) for different lattice sizes \( L \). The values of \( L \) obey the Fibonacci sequence. The susceptibility diverges at \( T_c \) in the large-lattice-size limit, suggesting a second-order phase transition.](image)
in Fig. 6, starting with the monomer shown in Fig. 6(a). The recursive geometrical substitutions are formally equivalent to the substitution rules (AA) → (AA)(AB)(BA)(BB), (AB) → (A A)(BA), (BA) → (AA)(AB), and (BB) → (AA). Therefore, we can write the following substitution matrix for the substitution rules:

\[
\mathcal{M} = \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 0 & 1 & 0 \\
1 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}.
\]

The substitution matrix connects the number of the four possible letter pairs between the \(n+1\) and \(n\)-esimal generations of the lattice. The above substitution rules are analogous to four-letter inflation rules. The eigenvalues of \(\mathcal{M}\) are given by \(\lambda_1 = \varphi^2\), \(\lambda_2 = \lambda_3 = -1\), and \(\lambda_4 = 1/\varphi^2\), where \(\varphi = \frac{1 + \sqrt{5}}{2}\) is the golden ratio. The wandering exponent is given by the following expression [37]:

\[
\omega = \frac{\ln |\lambda_2|}{\ln (\lambda_1)},
\]

where \(\lambda_1\) and \(\lambda_2\) are the leading and the next-to-leading eigenvalues (in moduli) of the substitution matrix \(\mathcal{M}\). By using the eigenvalues of \(\mathcal{M}\) we evaluated \(\omega = 0\) and from Eq. (15) we obtained \(\phi = 0\). Therefore, our lattice has marginal fluctuations according to the Harris–Luck criterion [37] and we can expect a change in the universality class.

To obtain the critical exponent \(1/\nu\), we investigated the critical behavior of the temperatures \(T_{\chi}\) for which the susceptibility is maximal. We show the critical behavior of \(T_{\chi}\) in Fig. 9. The critical behavior obeys Eq. (10) and from the slope of the curve we obtain the value of the exponent \(1/\nu = 0.84(2)\), which differs from the pure Ising 2D case. The quasi-periodic order induces a change in the universality class of the system.

We show the specific heat \(c\), given by Eq. (4), in Fig. 10. The curves suggest a critical behavior as a function of \(T\). When increasing the lattice size we observe a crescent maxima, suggesting a logarithmic divergence or a negative-exponent divergence at the critical temperature \(T_c \approx 2.274\).

FIG. 8. Critical behavior of \(\chi\) at \(T = T_c\) as a function of lattice size \(L\) obtained from Eq. (7). Alongside the \(\chi\) points we show the error bars on the same scale. The curve slope gives the exponent ratio \(\gamma/\nu = 1.25(2)\), differing from the pure Ising 2D case.

FIG. 9. Critical behavior of susceptibility maxima temperatures \(T_{\chi}\) as function of lattice size \(L\) obtained from Eq. (10). The curve slope gives the exponent \(1/\nu = 0.84(2)\), differing from the pure Ising 2D case.

FIG. 10. Specific heat \(c\) as function of temperature \(T\) for different lattice sizes \(L\). The values of \(L\) obey the Fibonacci sequence. When increasing the lattice size we observe a crescent maxima, suggesting a logarithmic divergence or a negative-exponent divergence at the critical temperature \(T_c \approx 2.274\).

FIG. 11. Data collapse of specific heat \(c\) for different lattice sizes \(L\). The best data collapsing gives us the estimate \(\alpha/\nu \approx -0.40\).
correspondent scale forms given in Eq. (6) for a second-order phase transition. We have for this system a second-order phase transition from a paramagnetic phase to a spin-glass phase by decreasing the temperature. We would like to emphasize that the exponent ratios obtained differ from the Ising 2D ones, changing the universality class of the system.

IV. CONCLUSIONS

We presented a simple model with quasiperiodic long-range order with competing interactions and obtained the critical behavior of a second-order transition in the Edwards–Anderson parameter driven by temperature. In the low-temperature limit we obtained a spin-glass phase with critical temperature $T_c \approx 2.274$. The spin-glass ordering in a two-dimensional system is rare and, as far as we know, the only other example is an under-frustrated Ising model [39].

We obtained the critical exponents $\beta$, $\gamma$, and $\nu$ in the case of equal antiferromagnetic and ferromagnetic strengths. The values of the exponents $\beta/\nu$, $\gamma/\nu$, and $1/\nu$ are $0.40(2)$, $1.25(2)$, and $0.84(2)$ respectively. Our result for $\beta = 0.48(2)$ is interesting because it is the same for the Landau classic theory of second-order phase transitions. The exponents obtained differ from Ising 2D exponents so the quasiperiodic order can change the universality class of the model. Therefore, the quasiperiodic ordering changes the critical behavior in the 2D case.

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