Static critical behavior of a weakly frustrated Ising model on the octagonal tiling

D. Ledue
LMA URA CNRS 808, Faculté des Sciences de l'Université de Rouen, 76821 Mont-Saint-Aignan Cédex, France
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The static critical behavior of a weakly frustrated ferromagnetic Ising model on the two-dimensional (2D) quasiperiodic octagonal tiling is studied by means of Monte Carlo simulations and finite-size scaling analysis. Our results strongly suggest that this frustrated Ising model on the octagonal tiling belongs to the same universality class as the ferromagnetic Ising model on 2D periodic lattices. The infinite tiling critical temperature, $kT_c/J=1.49\pm0.02$, agrees with previous studies indicating that tendency to ferromagnetic ordering is higher in quasiperiodic tilings than in periodic lattices.

I. INTRODUCTION

The discovery of quasicrystals in 1984 is responsible for studies about quasiperiodic tilings.[1,2] In particular, numerical simulations about the nonfrustrated ferromagnetic Ising model on the two-dimensional (2D) Penrose tiling and the 2D octagonal tiling have been performed in order to study the static critical behavior.[3–5] For the Penrose tiling, finite-size scaling analysis of a phenomenological Monte Carlo renormalization group using periodic approximants with periodic boundary conditions provided the critical temperature $kT_c/J=2.392\pm0.004$.[3] Another Monte Carlo investigation on periodic approximants with periodic boundary conditions leaded to a consistent value $kT_c/J=2.401\pm0.005$.[4] More recently, a study of the ferromagnetic Ising model on the octagonal tiling with free boundary conditions provided $kT_c/J=2.39\pm0.01$.[5] Since the mean number of interacting spins in the Penrose tiling and in the octagonal tiling are equal to 4, as in the square lattice, these results indicate that tendency to ferromagnetic ordering is higher in quasiperiodic tilings than in periodic lattices ($kT_c/J=2.269$ in the square lattice[6]). Moreover, calculated critical exponents for the Penrose tiling and for the octagonal tiling are in reasonable agreement ($\eta\approx1/4$ and $\nu\approx1$) and strongly suggest that the nonfrustrated ferromagnetic Ising model on 2D quasiperiodic tilings belongs to the same universality class as the ferromagnetic Ising model on 2D periodic lattices.

On the other hand, very few studies have been devoted to frustrated spin systems on quasiperiodic tilings. For example, numerical simulations about the *XY* model on the Penrose tiling have indicated a Kosterlitz-Thouless transition as in 2D periodic lattices.[7] For the frustrated antiferromagnetic Ising model on the Penrose tiling, numerical studies allowed to determine a complex phase diagram.[8] As far as we know, no study about the effects of the combination of quasiperiodicity and frustration on the critical behavior has been carried out. In this paper, we investigate the static critical behavior of a weakly frustrated ferromagnetic Ising model on the octagonal tiling which is a 2D quasiperiodic tiling with an eightfold orientational symmetry (Fig. 1).[5,9,10] Because of the topological properties of the octagonal tiling, the nearest-neighbor interaction (J_1), which corresponds to the short diagonal of the rhombuses, is a nonpercolating interaction. More precisely, it can only connect the spins into very small clusters (maximum size: eight spins).[11] The aim of this work is to study the effects on the critical behavior of such an unusually frustrating interaction which cannot exist in periodic lattices. Moreover, we shall test the validity of the finite-size scaling theory on frustrated quasiperiodic Ising spin systems with free boundary conditions.

With this aim in view, J_1 was taken to be antiferromagnetic, while the next-nearest-neighbor interaction (J_2), which corresponds to the edges of the squares and the rhombuses is ferromagnetic. It should be noted that since all octagonal tilings are locally isomorphic, the ground states, the critical temperature, and the static critical exponents do not depend on the special tiling on which numerical simulations are performed.[5,12] Here, we have considered the octagonal tiling with a perfect eightfold symmetry around its center (Fig. 1). Before starting our investigation, we checked, by Monte Carlo simulation, that the ground state of our frustrated system ($J_1=-J_2<0$) is ferromagnetic. Then, the suitable order parameter is still the spontaneous magnetization per spin.

The models, simulation techniques, and finite-size scaling

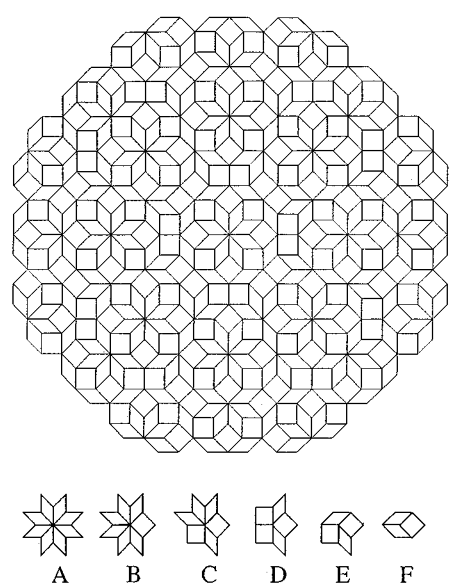

FIG. 1. The octagonal tiling and the six local environments.

analysis are described in Sec. II. Results and discussion are presented in Sec. III and a summary is given in Sec. IV.

II. BACKGROUND

A. Spin Hamiltonian

We have considered the frustrated Ising model with the Hamiltonian

$$H=J\sum_{\langle i,j\rangle} S_iS_j-J\sum_{\langle i,k\rangle} S_iS_k \qquad (J>0),$$

where the spins, which take on the values ± 1, are located at the vertices of the octagonal tiling. S_j, S_k are, respectively, the nearest and the next-nearest neighbors of a given spin S_i. The mean numbers of interacting neighbors in the infinite tiling are, respectively, $\langle z_1\rangle=2\sqrt{2}/(1+\sqrt{2})$ for the nearest neighbors and $\langle z_2\rangle=4$ for the next-nearest neighbors.[11]

B. Numerical simulation

Numerical simulations were carried out on finite octagonal tilings of size $N=185$, 481, 1169, 2481, 3801, and 5497 with free boundary conditions. The procedure is the Monte Carlo simulated annealing method.[13] In our procedure, the temperature is slowly decreased or slowly increased according to a geometric law ($T_{n+1}=\tau T_n$) with a rate τ=0.99 or $\tau=0.99^{-1}$. At each temperature, thermal equilibrium is achieved after few thousands Monte Carlo steps (MCS) per spin following the Metropolis algorithm.[14] The first 20 000 MCS per spin were discarded before averaging over the next 80 000 MCS per spin ($N=185$) up to 480 000 MCS per spin ($N=5497$).

All simulations were done using the CRIHAN high-performance computer consisting of a CONVEX C 3420 vector computer. The speed of the program is roughly 325 000 spin-flip trials per second.

C. Finite-size scaling theory

The static critical behavior of an infinite system may be deduced from the size dependence of several thermodynamic quantities such as the specific heat,

$$C(T,L)=L^{-d}\frac{\langle E^2\rangle-\langle E\rangle^2}{kT^2},$$

the spontaneous magnetization per spin,

$$m(T,L)=\langle|m|\rangle=L^{-d}\left\langle\left|\sum_{i=1}^{N} S_i\right|\right\rangle,$$

and the true susceptibility,

$$\chi(T,L)=L^{d}\frac{\langle m^2\rangle-\langle m\rangle^2}{kT}$$

(d is the dimensionality of the system, $L^d=N$ is the number of spins, E is the total energy and $\langle\ \rangle$ means thermal average at temperature T). According to this theory,[15,16] for a sufficiently large system at temperature T close enough to the infinite critical temperature T_c:

$$C(T,L)\sim L^{\alpha/\nu}C^0(tL^{1/\nu}),$$

$$m(T,L)\sim L^{-\beta/\nu}m^0(tL^{1/\nu}),$$

$$\chi(T,L)T\sim L^{\gamma/\nu}\chi^0(tL^{1/\nu}),$$

where

$$t=|T-T_c|/T_c$$

and α, β, γ, and ν are the static critical exponents of the infinite system.[17]

The critical exponent ν can be estimated without knowing T_c from the logarithmic derivatives of $\langle|m|^n\rangle$, $\phi_n(T,L)=(1/k)(\langle E\rangle-\langle|m|^nE\rangle/\langle|m|^n\rangle)$.[18] Since $\phi_n^{\max}\sim L^{1/\nu}$, the slope of the log-log plot of size dependence of $\phi_n^{\max}$ is ν^{-1}. In our analysis, we have considered ϕ_1 and ϕ_2.

With ν, the infinite tiling critical temperature can be deduced from the "effective transition temperatures," $T_c(L)$, corresponding to the location of the maxima in the specific heat, the finite tiling susceptibility,

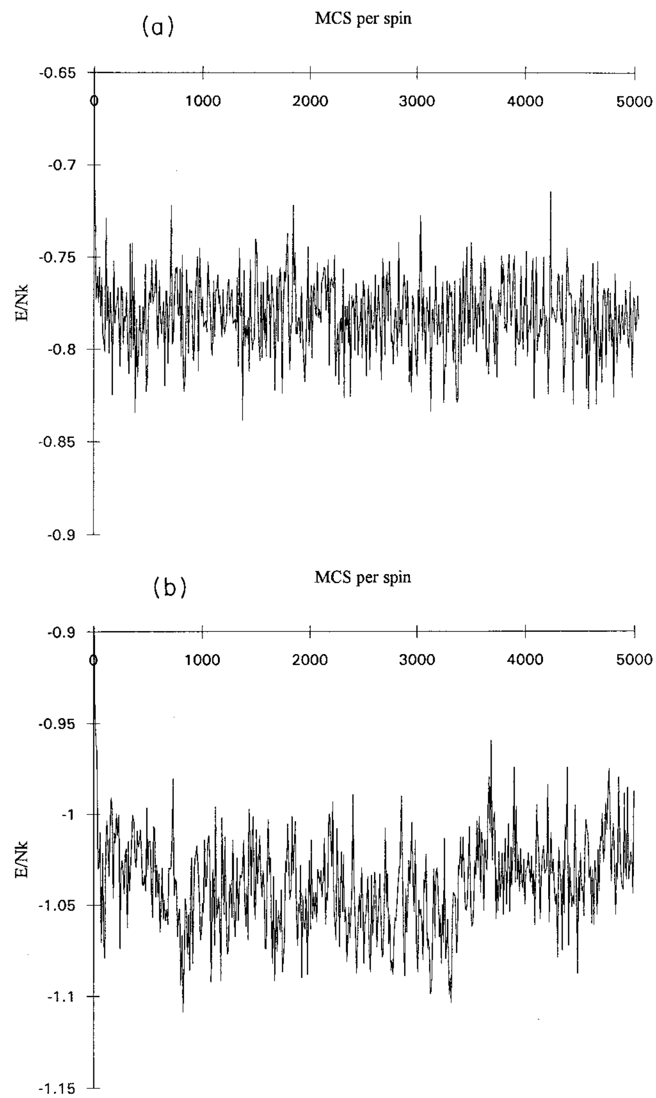

FIG. 2. Time dependence of the energy per spin for the first 5000 MCS per spin at $kT/J=2$ (a) and $kT/J=1.45$ (b) ($N=2481$).

$$\chi'(T,L)=L^d\frac{\langle m^2\rangle-\langle|m|\rangle^2}{kT},$$

and the derivative of the spontaneous magnetization per spin, $\partial m/\partial T^{-1}=(1/k)(\langle|m|\rangle\langle E\rangle-\langle|m|E\rangle)$. The "effective transition temperatures," $T_c(L)$, vary with the system size, asymptotically, as[19]

$$\frac{kT_c(L)}{J}=\frac{kT_c}{J}+aL^{-1/\nu},$$

where a is a quantity-dependent constant.

At the critical point ($t=0$), the spontaneous magnetization per spin has the scaling behavior $m(T_c,L)\sim L^{-\beta/\nu}$ and the true susceptibility satisfies $\chi(T_c,L)\sim L^{\gamma/\nu}$. Moreover, some studies which have shown that χ' diverges with the same critical exponent γ as χ does[20,21] provided the scaling form $\chi'_{\max}\sim L^{\gamma/\nu}$. Thus, the log-log plot of size dependence of $m(T_c,L)$ and the log-log plot of size dependence of $\chi(T_c,L)$ and $\chi'_{\max}$ are straight lines with slopes $-\beta/\nu$ and γ/ν, respectively.

III. RESULTS

For each size, a run with $\tau=0.99$ (cooling) and a run with $\tau=0.99^{-1}$ (annealing) were performed. The final thermodynamic quantities have been obtained by averaging over the two runs. For each plot, three different linear fits were performed using system sizes $N_{\min}\leqslant N\leqslant 5497$ with $N_{\min}=185$, 481, or 1169.

The time dependence of the internal energy per spin for the first 5000 MCS per spin at $kT/J=2$ and $kT/J=1.45$ is shown in Fig. 2. It can be seen that the magnitude of the fluctuations is slightly larger at $kT/J=1.45$ indicating that the critical point is closer to 1.45 than 2.

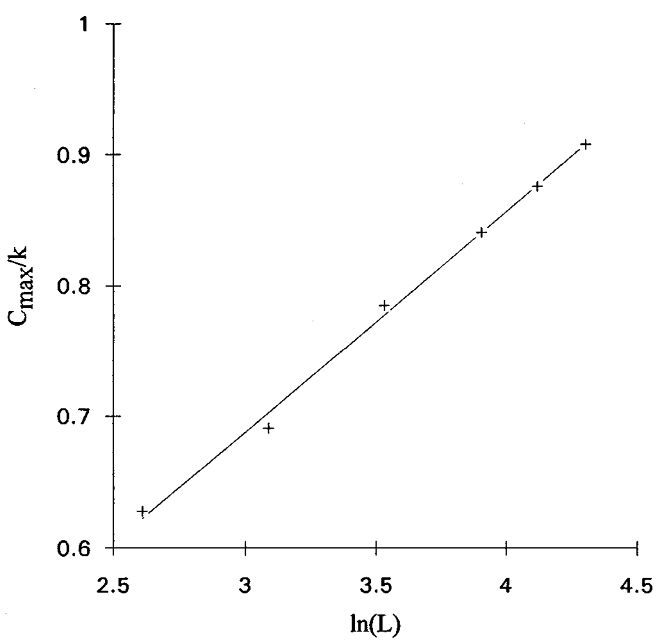

FIG. 3. Semilogarithmic plot of the size dependence of the maximum value of the specific heat.

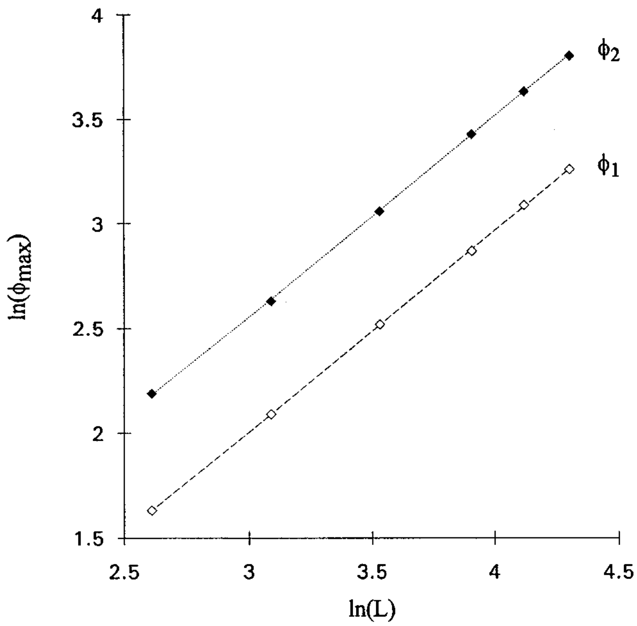

FIG. 4. Log-log plot of the size dependence of the maximum value of ϕ_1 and ϕ_2.

A. Evidence for a second-order phase transition

In order to check that the transition is second order, we plotted in Fig. 3 the maximum of the specific heat as a function of system size on a semilogarithmic scale [$C_{\max}(L)\sim\ln(L)$ if the transition is second order with $\alpha=0$, while $C_{\max}(L)\sim L^d$ if the transition is first order]. This plot indicates that the data are well described by a linear fit as for the 2D Ising model on periodic lattices. No significant deviation to the asymptotic linear regime has been noticed. This result agrees with the energy histograms which exhibit only one maximum at all temperatures.

B. Determination of ν and T_c

In Fig. 4, we plot the maximum value of the thermodynamic quantities ϕ_1 and ϕ_2 as a function of system size on a log-log scale. For each quantity, the three linear fits evidence that the asymptotic finite-size scaling regime is already reached by $N=185$ as for the nonfrustrated ferromagnetic Ising model.[5] The two estimates of ν deduced from ϕ_1 and ϕ_2 (linear fits with $N_{\min}=185$) are, respectively, 1.04 ± 0.02 and 1.04 ± 0.01. Combining these two estimates, we find $\nu=1.04\pm0.01$ which is in reasonable agreement with the 2D nonfrustrated Ising value ($\nu=1$).

The size dependence of the "effective transition temperatures" extracted from C, χ', and $\partial\langle m\rangle/\partial T^{-1}$ is plotted in Fig. 5. Since no significant deviation to the asymptotic linear regime was noticed for the data from C and χ', we considered the two linear fits with $N_{\min}=185$ which provided the same value $kT_c/J=1.49\pm0.02$. On the other hand, $T_c(N=185)$ obtained from the derivative of the magnetization seems to be out of the asymptotic linear behavior. So, we estimated the critical point $kT_c/J=1.48\pm0.01$ from the fit with $N_{\min}=481$. Since the data from the specific heat seem more reliable, we estimate the infinite tiling critical point at $kT_c/J=1.49\pm0.02$. The slope of the linear fits extracted from C, χ', and $\partial\langle m\rangle/\partial T^{-1}$ is, respectively, -2.38 ± 0.15,

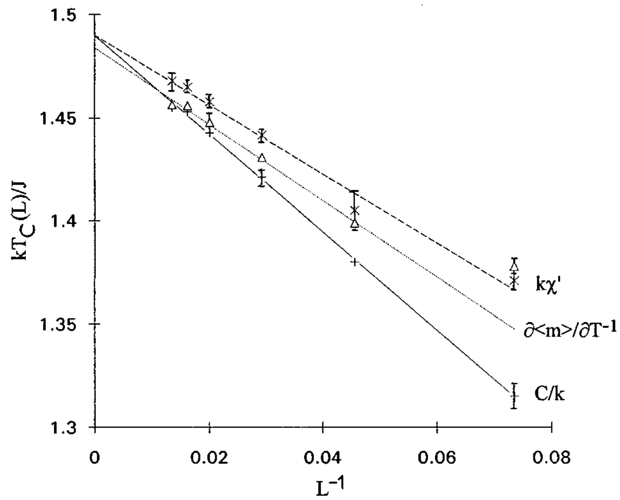

FIG. 5. Size dependence of the "effective transition temperatures" (where not shown, error bars are smaller than the symbols).

-1.68 ± 0.14, and -1.85 ± 0.19. For comparison, we note that the absolute value of the slope of the size dependence of $T_c(L)$ for the specific heat and the finite tiling susceptibility are lower than the values of the nonfrustrated ferromagnetic Ising model: $a\approx-3.16$ and $a\approx-2.09$.[5]

In order to analyze the effects of quasiperiodicity and frustration on ferromagnetic ordering, we have estimated the critical temperature of a frustrated ferromagnetic Ising spin system on the square lattice[22,23] ($J_1^{\mathrm{sq}}>0$ and $J_2^{\mathrm{sq}}<0$ with $J_2^{\mathrm{sq}}/J_1^{\mathrm{sq}}>-1/2$) which exhibits the same ground-state energy as our frustrated quasiperiodic spin system:

$$z_1J_1^{\mathrm{sq}}+z_2J_2^{\mathrm{sq}}=\langle z_1\rangle J_1+\langle z_2\rangle J_2.$$

Setting down $\lambda=J_2^{\mathrm{sq}}/J_1^{\mathrm{sq}}$ and replacing each term by its numerical value, we obtain the relation $(4+4\lambda)J=[4-2\sqrt{2}/(1+\sqrt{2})]J$, that is $\lambda=-0.292\,89$, which provides the critical temperature $kT_c/J\approx1.32$ for the square lattice.

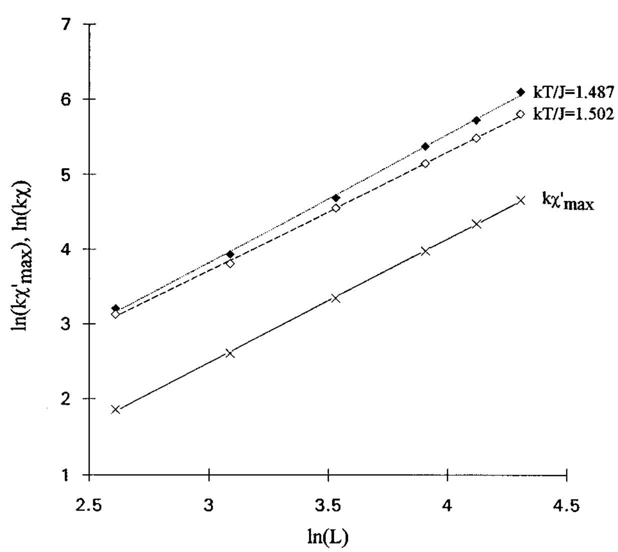

FIG. 6. Log-log plot of the size dependence of the maximum value of the finite quasilattice susceptibility and the true susceptibility at $kT/J=1.487$ and $kT/J=1.502$.

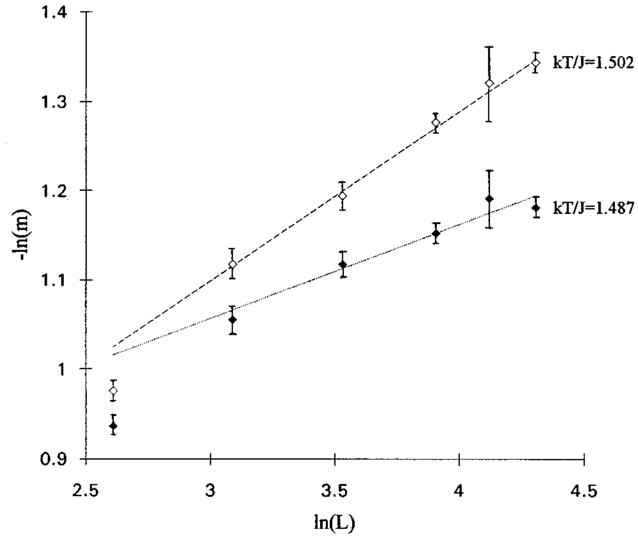

FIG. 7. Log-log plot of the size dependence of the spontaneous magnetization per spin at $kT/J=1.487$ and $kT/J=1.502$ (the straight lines are linear fits with $N_{\mathrm{min}}=481$).

Then, it is interesting to compare the ratio $(kT_c/J)_{\mathrm{octagonal}}/(kT_c/J)_{\mathrm{square}}$ without and with frustration. We find $2.39/2.269\approx1.053$ for nonfrustrated system[5] and $1.49/1.32\approx1.129$ for frustrated systems. It should be noted that the ratio is greater than 1 in the two cases indicating that tendency to ferromagnetic ordering is higher in quasiperiodic tilings than in periodic lattices.[3–5] Moreover, the difference between the octagonal tiling and the square lattice is bigger for frustrated systems. This can be explained by the different nature of the frustrating interaction in the octagonal tiling (J_1) and in the square lattice (J_2^{sq}): J_1 is a nonpercolating interaction in the octagonal tiling which only induces local frustration, while J_2^{sq} is a percolating interaction in the square lattice.

C. Determination of β and γ

In order to determine γ, we plot in Fig. 6 the size dependence of the maximum in the finite quasilattice susceptibility and the size dependence of the true susceptibility at $kT/J=1.487(\approx kT_c/J)$ on a log-log scale. For each plot, no significant deviation to the asymptotic linear regime has been noticed and the quality of the fits is roughly independent of N_{min}. The estimates of γ from the fits with $N_{\mathrm{min}}=185$ are, respectively, 1.66 ± 0.08 and 1.71 ± 0.04. Combining these two estimates, we obtain a final value $\gamma=1.69\pm0.06$ which is in reasonable agreement with the 2D periodic value $\gamma=1.75$. For comparison, we also plot in Fig. 6 the size dependence of the true susceptibility at $kT/J=1.502$. The

TABLE I. Slopes of the linear fits of the magnetization per spin vs system size at $kT/J=1.487$ and $kT/J=1.502$.

N_{min}	$s(kT/J=1.487)$	$s(kT/J=1.502)$
185	0.14 ± 0.01	0.21 ± 0.01
481	0.11 ± 0.02	0.19 ± 0.02
1169	0.089 ± 0.035	0.198 ± 0.037

data are well described by a linear fit but the slope is lower than the slope of the size dependence at $kT/J=1.487$ (1.58 ±0.03 from the fit with $N_{\rm min}=185$).

The size dependence of the spontaneous magnetization per spin at $kT/J=1.487$ and $kT/J=1.502$ is plotted on a log-log scale in Fig. 7. The slope s of the three linear fits at each temperature are reported in Table I.

As can be seen in Table I, it is difficult to estimate β from the linear fits at $kT/J=1.487$ with good accuracy $[(\Delta s/\langle s\rangle)(1.487)=(0.14-0.089)/\langle s\rangle\approx0.45]$. On the other hand, the quality of the fits at $kT/J=1.502$ are better (whatever is $N_{\rm min}$) and $(\Delta s/\langle s\rangle)(1.502)\approx0.1$ is lower than $(\Delta s/\langle s\rangle)(1.487)$. However, although the estimate of β from the scaling behavior of the spontaneous magnetization at the critical point seems to be very difficult, the values of the slope $s(1.487)$ are consistent with the expected value $\beta=0.5(d\nu-\gamma)$.[24]

IV. CONCLUSION

Our investigation of a weakly frustrated ferromagnetic Ising model on the octagonal tiling has been carried out using a finite-size scaling analysis of quasilattices with free boundary conditions. Our results indicate a second-order transition with the 2D periodic Ising critical exponents and show that weak local frustration induced by the nonpercolating nearest-neighbor interaction J_1 has no influence on the nature of the transition. As for the nonfrustrated ferromagnetic Ising model on the octagonal tiling,[5] the critical exponents ν and γ can be determined with reasonable accuracy. On the other hand, one should note that it is very difficult to calculate the critical exponent β. The different estimates of the infinite tiling critical temperature which have been determined from several thermodynamic quantities are clearly consistent. However, because of frustration, the use of the fourth-order magnetization cumulant[20] would require more MCS per spin at each temperature. In agreement with previous works on quasiperiodic tilings,[3–5] the infinite tiling critical temperature has been found slightly higher than the critical temperature of an ''equivalent'' frustrated Ising spin system on the square lattice. In the near future, it is planned to investigate the critical behavior of some more frustrated Ising spin systems on the octagonal tiling for which the ground state is still unknown.

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