$q=5$ Potts model on the quenched anisotropically site-diluted Penrose lattice

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Anisotropic site dilution is introduced into the two-dimensional Penrose lattice by varying the seven-nearest-neighbor (7NN) site concentration p_7 from zero (no 7NN sites) to one (all 7NN sites present). A first-order phase transition line is found for the $q=5$ Potts model in the region $p_{7c}<p_7\leq 1$ which terminates at a critical point $p_{7c}=0.941(3)$, conjectured to be in a new universality class.

I. INTRODUCTION

One model for the underlying structure of recently discovered quasicrystalline systems[1] is the Penrose tiling,[2] made up of two rhombi, one with angles 36° and 144°, and the other with angles 72° and 108°. Although these lattice structures appear to lie somewhere between amorphous and periodic structures, the universality class of various models has been shown to be unaffected by quasiperiodicity.[3–6] This is an interesting result given that the coordination number of the sites varies throughout the lattice between a minimum of three and a maximum of seven (with an average coordination number per site equal to four).

The primary objective in this study is to investigate a new type of site dilution which we call "anisotropic dilution," unique to quasicrystalline systems, by selectively diluting only sites with a particular environment. Here we study, in particular, the quenched dilution of the most densely surrounded sites, those with seven nearest neighbors (7NN). These 7NN sites make up only about 5.5% of the total number of sites, yet they participate in over 19.5% of the Penrose lattice's bonds. To this end we introduce an anisotropic site dilution variable p_7, where $p_7=1$ represents the full, undiluted Penrose lattice, and $p_7=0$ represents the case where no 7NN sites are present in the lattice. This dilution is clearly different from isotropic site dilution where all sites may participate in dilution since the fully anisotropically diluted lattice is still connected, as seen in Fig. 1. No completely disconnected "islands" are found, but there are regions which are relatively isolated from the rest of the lattice, connected by only a few bonds. We have found that the $q=5$ Potts model[7] exhibits interesting behavior under anisotropic dilution and will present the results below.

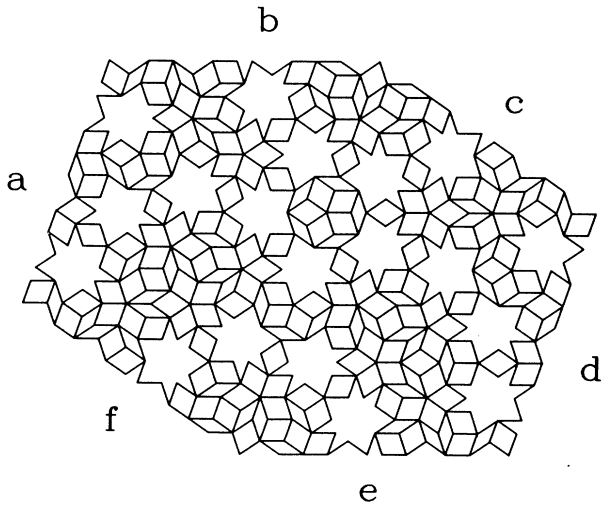

FIG. 1. A fully anisotropically diluted Penrose lattice is shown where all seven nearest-neighbor sites have been removed. Periodic boundary conditions are applied by joining sides *a*-*d*, *b*-*f*, and *c*-*e*, resulting in a lattice with 357 sites.

Random bond dilution of Potts models on periodic lattices has been studied under annealed and quenched conditions.[8,9] Although the exact phase diagram of the annealed bond-diluted system has been obtained,[8] little is known concerning quenched bond or site dilution in periodic lattices;[10,11] the phase diagrams of quenched systems are expected to be qualitatively different than for annealed systems.[8]

The q-state Potts model Hamiltonian[7] is given by

$$H=-J\sum_{\langle i,j\rangle}\delta(\sigma_i,\sigma_j)\ , \tag{1}$$

where $J>0$ is the ferromagnetic interaction, $\sigma_i,\sigma_j=1,2,\ldots,q$, are the spin variables, $\delta(\sigma_i,\sigma_j)$ is the Kronecker δ function, and the summation is made over nearest neighbors i,j. In two dimensions it is known that the phase transition changes from second order to first order as q changes from four to five for periodic lattices[12] and for the aperiodic Penrose lattice.[6]

II. METHODOLOGY

In our study we implement the microcanonical simulation,[13,14] based on the microcanonical ensemble in which a system's energy if held fixed while the temperature is calculated. One advantage this technique has over the traditional Monte Carlo approach[15] (based on the canonical ensemble) is that the van der Waals curve of an inhomogeneous finite-sized system indicative of a first-order phase transition in the infinite system can be obtained.

This curve enables the determination of the transition point via a Maxwell equal-area construction. The method as applied to this problem will be discussed only briefly here, with details of the general method published elsewhere.[6,13,14]

In the microcanonical simulation, the closed system is imagined to consist of two parts, the extensive spin system and an intensive "demon." The demon is simply an extra degree of freedom with a Hamiltonian $H_d = Jn$ ($n = 0, 1, 2, \ldots, 7$) which can be used as a small excess energy sack during the spin flipping process. This is needed since it is a difficult task to *exactly* conserve the spin system's energy while flipping a spin. The demon can be used to place excess energy into or take reserve energy out of when the spin flip does not exactly conserve the spin system's energy. In addition, the spin system acts as a reservoir to the demon, hence, the demon's states are canonically distributed, meaning the closed system's temperature can be determined from the measurement of the demon's average energy and the knowledge of its partition function.

The simulation begins by first reading a data file into the program that contained the relevant information for the full Penrose lattice, specifically each site's NN sites. We generate the lattices using the deflation method,[16] and apply "periodic" boundary conditions by joining the lattice edges *a*-*d*, *b*-*f*, and *c*-*e* together (Fig. 1). Our simulation algorithm allows for the simulation of 64 lattice systems simultaneously, or one lattice system for each bit position of the 64-bit Cray Research X-MP supercomputer word. A second file contains a "dilution array" which holds information regarding whether a particular lattice site is occupied by a spin or not. This array is N elements in length, where N is the total number of lattice sites in the undiluted system. Each bit position in the dilution array corresponds to the lattice at the same bit position in the array that holds the spins, with a particular bit set to 1 if the corresponding lattice site is occupied, or set to 0 if the site is vacant. Thus we are able to randomly dilute 7NN sites with a vacancy, and create an ensemble of 64 independent anisotropically site-diluted lattices. This provides us with a way to perform a quenched average for each value of p_7.

Next, the lattice systems are brought to the desired energy for the simulation. This is achieved by placing all of the energy into a large array, with the spin systems in a ground state, then dumping the energy into the spin systems as spins are flipped. In this energy dump, everything is randomized to avoid correlated starting configurations for the 64 lattices. Since the corresponding sites on each of the lattices must be visited simultaneously, energy is dumped at a site with only a one in 16 chance, otherwise the energy would be placed at identical positions for all 64 lattices, exactly correlating their initial configurations. When the energy array is depleted the lattices are considered initialized, and the simulation proceeds to the equilibrium period.

The purpose of equilibration is to bring the systems away from their initial configurations and allow correlations to grow to equilibrium values. We found in this study, as in the simulation on the undiluted lattice,[6] that the temperature relaxes very quickly to equilibrium values, but the order parameter relaxes very slowly. Thus, due to the vast amount of computer time that would be required to gain useful information regarding the order parameter, only the energy-temperature curve could be obtained in this study.

When a simulation run is completed, the results for each individual lattice are determined separately, then these results are averaged to give the reported values for a particular p_7 and energy per site ε (in units of J). The uncertainties are calculated as the standard deviation of the 64-lattice mean.

III. RESULTS

We examine systems with number of spins $N = 378$, 988, and 2585 in the undiluted limit, which in the fully diluted limit contain $N = 357$, 933, and 2441 spins, respectively. The simulation data of the reduced energy ε versus the reduced temperature $\tau = k_B T/J$ for the largest lattice are shown in Fig. 2(a) for selected values of p_7. The uncertainties in the data are on the temperature, and in all cases are much smaller than the size of the plotting symbol and are excluded. As can be seen from the data, the undiluted system displays a van der Waals curve indicating a first-order phase transition, whereas for small values of p_7 the phase transition appears "smeared." The more interesting region $p_7 > 0.9$ is expanded in Fig. 2(b), where it is observed that as p_7 is decreased from unity, the van der Waals curve disappears and gives way to a different behavior which we analyze below. We have applied a Maxwell equal-area construction for the incipient first-order phase transitions to determine the first-order phase transition points. This construction arises from the condition that the entropy change between two equilibrium points is independent of the path taken. Hence,

$$(\varepsilon_2 - \varepsilon_1)/\tau^* = \int_{\varepsilon_1}^{\varepsilon_2} d\varepsilon\, \tau^{-1} , \tag{2}$$

where ε_1 and ε_2 are the coexisting energies, τ^* is the transition temperature, and the integral is evaluated along the van der Waals curve. The transition energies and temperature are found by replacing the integral in (2) by a sum and adjusting ε_1, ε_2, and τ^* until the root of (2) is found. Standard error propagation provides estimates for the uncertainties in these quantities.

In the region of p_7 where there is no van der Waals curve, we have examined two possibilities. The first is a singular scaling form indicative of a second-order phase transition

$$t = A_{\pm} e^{1/(1-\alpha)} , \tag{3}$$

where $t = |\tau - \tau_c|/\tau_c$, $e = |\varepsilon - \varepsilon_c|/\varepsilon_c$, and $A_{\pm}$ is the critical amplitude above ($+$) and below ($-$) the transition, in order to obtain the universal specific-heat exponent α, the critical energy ε_c, and the critical temperature τ_c. The second is an analytic form

$$t = ae + be^2 + ce^3 \tag{4}$$

with a, b, and c constants, which is appropriate for a sys-

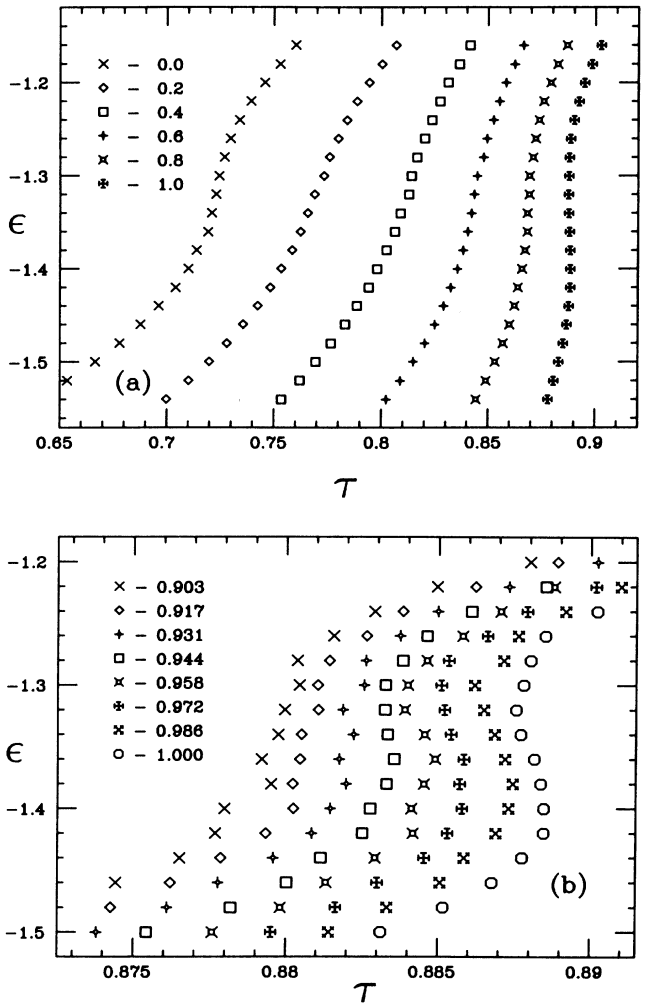

FIG. 2. The reduced energy vs the reduced temperature for the $N=2585$ Penrose lattice is shown for (a) $0 \le p_7 \le 1$, and for (b) $p_7 > 0.9$. The transition changes from first order to second order at $p_{7c}=0.941(3)$. The uncertainties are approximately the size of the plotting symbol and have been excluded.

tem with no true phase transition in the thermodynamic limit ("smeared").

The fits to the data of the largest fully anisotropically diluted lattice ($N=2441$) give reduced χ-squared values of $\chi^2=4.1$ with 29 degrees of freedom for the singular fit (3), and $\chi^2=2.9$ with 22 degrees of freedom for the analytic form (4). We regard both fits as poor and the functional forms to be unable to provide a quantitative characterization of the system at this stage of dilution. However, we find improvement in both fits upon increasing p_7 from zero, with the analytic form being favored over the singular fit for lower and intermediate values of p_7. For example, at $p_7=0.597$ ($N=2527$) the fit to (3) gives $\chi^2=1.51$ for 28 degrees of freedom, whereas the fit to (4) gives $\chi^2=1.17$ for 31 degrees of freedom. At $p_7=0.896$ ($N=2570$), both fits are very good with (3) giving $\chi^2=0.82$ for 31 degrees of freedom, and (4) giving $\chi^2=0.88$ for 30 degrees of freedom. Finally, for $p_7=0.938$ ($N=2576$), the fit to the singular form (3) gives $\chi^2=0.94$ for 25 degrees of freedom, compared with $\chi^2=1.46$ for 23 degrees of freedom for the fit to the analytic form (4). Thus, increasing p_7 from zero shows a trend of favoring (4) at intermediate values of p_7 giving way to near critical behavior in the region $p_7 \simeq 0.9$. On the other hand, as discussed above, upon decreasing p_7 from unity, the system exhibits first-order behavior which disappears upon diluting to $p_7 \simeq 0.94$. These results lead us to conclude that the line of first-order transitions (coexistence curve) terminates at a second-order transition (critical point) p_{7c}, and for $p_7 < p_{7c}$, there is no phase transition. The data in the region p_7 slightly below p_{7c} are revealing precritical behavior. An examination of the constant volume specific heats provides a more striking picture of the phase transition behavior for the lower values of p_7. Figure 3 displays the specific heats at various values of p_7 for the $N=2585$ lattice, obtained by differentiating the fits to the polynomial (4). A sharp decrease in the specific-heat maximum is observed as p_7 is decreased from p_{7c}.

We determined the critical value of p_{7c} in the following manner. For the largest lattices, the system with $p_7=0.944$ ($N=2577$) clearly indicates a first-order transition [see Fig. 2(b)], whereas the system with $p_7=0.938$ ($N=2576$, not shown) has no van der Waals curve and has an excellent fit with the singular form (3) as described previously. Hence, our estimation of p_{7c} involves the averaging of p_7 for these systems (they differ by only one site) which gives $p_{7c}=0.941(3)$. It is quite astonishing that the removal of only *nine* 7NN sites from the $N=2585$ Penrose lattice, only 0.35% of the total number of sites, is a large enough perturbation to change the transition from first order to second order.

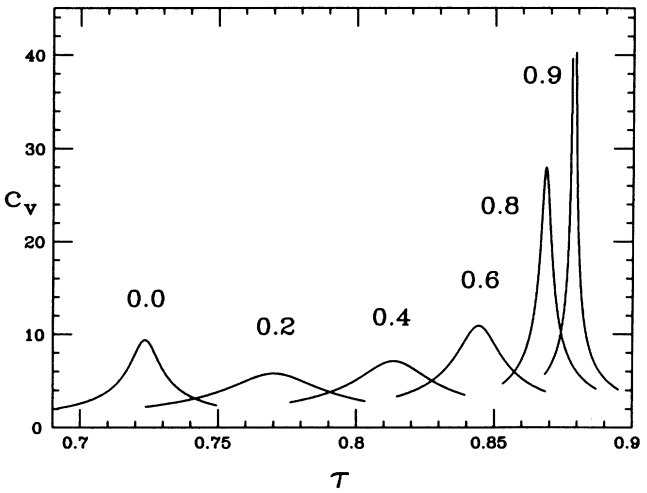

FIG. 3. Shown here are the reduced specific heats plotted vs reduced temperature for $p_7 < p_{7c}$ determined by differentiating the fits to Eq. (4) in the text for the $N=2585$ lattice. The maximum is seen to decrease as p_7 is lowered from p_{7c}, indicating the disappearance of the phase transition. The curve for $p_7=0.9$ is nondivergent, with a maximum of $c_v \simeq 95$.

In terms of the universal behavior of the critical point, the values of the specific-heat exponent α obtained in the fit to (3) were 0.642(4), 0.655(2), and 0.625(2) for the $N=376$, 984, and 2576 lattice sizes, respectively. The uncertainties in these values were determined by the standard method of fixing all other parameters while adjusting α to increase χ^2 by one. Although this is a standard definition, we feel the quoted uncertainties to be, perhaps, a factor of 5–10 too small. The value for α obtained here is suspiciously close to the den Nijs conjectured value $\alpha=\frac{2}{3}$ (Ref. 17) for the undiluted $q=4$ Potts model in two dimensions, shown to be the same for both the square and Penrose lattices.[6] We have no reason to believe the quenched anisotropically diluted system is in the same universality class, thus we conjecture that the critical point obtained here is in a new universality class.

Figures 4(a) and 4(b) show the coexisting energies ε_1 and ε_2, and transition temperatures τ^*, respectively, of the first-order phase transitions for $p_7 > p_{7c}$. The uncertainties in both figures are approximately the size of the plotting symbols and have been excluded. It is apparent from these figures that the anisotropic dilution of the 7NN sites behaves as a "symmetry-breaking field." This is because the low-temperature phase can be reached from the high-temperature phase via a path around the critical point, while never undergoing a phase transition.

Finally, it must be emphasized that the systems simulated are finite and we can only infer the results in the $N\to\infty$ limit. Finite-size scaling is, unfortunately, not applicable to the lattice sizes presented here for two reasons. First, the latent heats (coexisting energy differences) shown for $p_7=1.0$ in Fig. 4(a), for example, do not show a trend that might reveal the latent heat in the $N\to\infty$ limit. A $q=5$ Potts model simulation on the undiluted square lattice[6] displayed a similar behavior in the latent heats, with a 50^2 lattice system's latent heat being approximately four times larger than the infinite lattice's known exact value. If the situation is similar for the Penrose lattice system's latent heat, we cannot expect the results presented here to be *quantitatively* accurate predictions of the $N\to\infty$ values. Secondly, we are unable to perform a useful finite-size scaling of the critical point because p_{7c} cannot be determined with arbitrary accuracy for each value of N. This is apparent from Figs. 4, where the successive removal of just one lattice site produces large changes in the transition energies and temperature. Only bounds can be placed above and below the critical point, which do not provide adequate information for finite-size scaling. In spite of these considerations, we expect the qualitative picture that has emerged from the simulation will remain unchanged as the lattice size is increased.

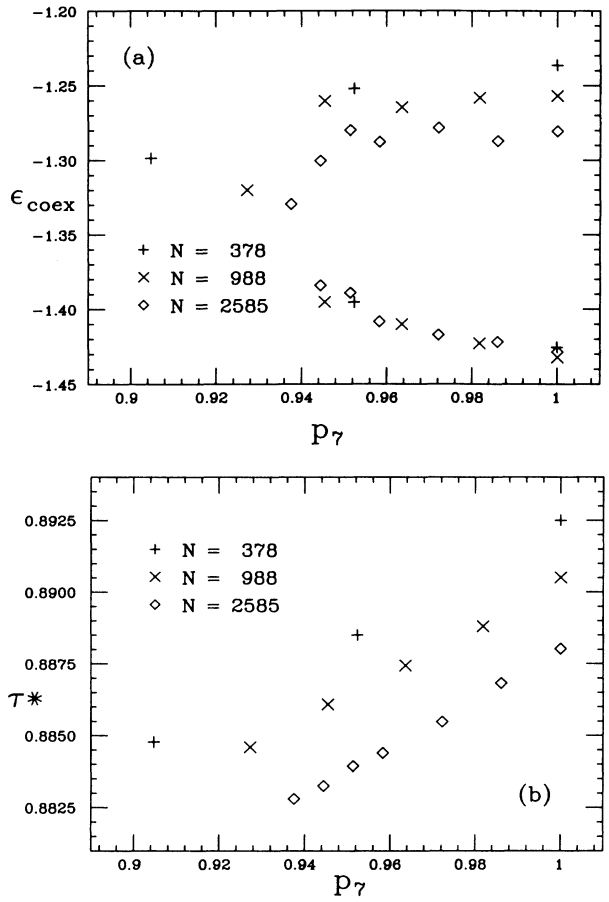

FIG. 4. The (a) coexisting energies ε_1 and ε_2, and (b) transition temperatures τ^* are shown vs the anisotropic dilution variable p_7. The critical point is at $p_{7c}=0.941(3)$ for the $N=2585$ lattice. Uncertainties are approximately the size of the plotting symbol and have been excluded.

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