Modern Physics Letters B, Vol. 8, No. 2 (1994) 127–130

ISING TRANSITION TEMPERATURES FOR QUASICRYSTALS: DOES THE TOPOLOGY MATTER?

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Received 30 October 1993

We study by Monte Carlo simulation the variation of the Ising critical temperature on pentagonal two-dimensional quasicrystals with the change of the continuous parameter that controls the local isomorphism of the quasicrystals.

The Ising model on any lattice is defined by the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} s_i s_j \,, \tag{1}$$

where the spins $s_i = \pm 1$ are located at the sites i, and the summation is over nearest neighbours only. The universal critical behavior of this model is well understood, though several unanswered questions remain.[1] The situation is not so transparent for nonuniversal quantities, the most important one of which is the transition temperature T_c. There are various ways of putting bounds on T_c, but what of the lattice actually determines remains obscure.[2] One of the reasons may be the unavailability of simple, tunable translationally invariant (Bravais) lattices. With the advent of quasicrystals, it is now possible to have nonisomorphic classes of lattices that can be parametrized by a number $\gamma \in [0, 1)$.[3] Since the lattice structure, both global and local, can be tuned continuously, the transition temperature is expected to change continuously. Such a variation might lead to new insights. Our purpose is to determine the T_c vs γ curve.

We consider two-dimensional quasicrystals which are dual to the periodic pentagonal grid, $\mathbf{e}_n = (\cos 2\pi n/5,\ \sin 2\pi n/5)$, $n = 1, 2, \ldots, 5$. The grid consists of lines $\mathbf{x}_n$ in each direction such that

$$\mathbf{x}_n \cdot \mathbf{e}_n = p + \gamma_n \,, \tag{2}$$

where p is an integer. Note that each γ_n determines the relative shift of the set of lines (for different p) from the origin. The important quantity for us is

$$\gamma = \sum \gamma_n \,. \tag{3}$$

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It is known that the lattices with γ differing by an integer are locally isomorphic.[3] It therefore suffices to consider γ in the range $[0, 1)$ with $\gamma = 0$ and $\gamma = 1$ as the well-known Penrose lattice.[3] By construction, the grid lattice is always four-coordinated, but the quasicrystals have coordination numbers in the range 3 to 9. Since the quasicrystals are obtained from periodic pentagrids, the ratio of the fat to skinny rhombi is $\tau : 1$, where $\tau = (\sqrt{5} + 1)/2$ is the golden mean.[3]

It is now well-accepted that the critical exponents on such lattices do not depend on their structure or the lack of translational invariance.[4,5] But T_c is expected to change. We performed Monte Carlo (MC) simulation of the Ising models on such quasicrystals for various values of γ.

The standard important sampling MC procedure is adopted. For a given lattice, new spin configurations are generated by flipping the spins one at a time. Whether a spin is to be flipped or not is determined by comparing the Boltzmann factor associated with the change in energy to a random number between 0 and 1.[6]

To extract the relevant information at different temperatures, we follow the histogram approach.[7,8] We determine, at a given temperature T, the histogram $P_T(E, S)$, where E is the total energy and $S = \sum s_i$ is the total magnetization. The probability distribution at any other temperature T' is then obtained from the formula

$$P_{T'}(E, S) = P_T(E, S) \exp[-E(K' - K)]/Z(T'), \tag{4}$$

where

$$Z(T') = \sum_{E,S} P_T(E, S) \exp[-E(K' - K)], \tag{5}$$

$K = J/kT$, and $K' = J/kT'$. Once we know the probability distribution, the averages can be calculated easily.

The transition temperature is determined by using the fourth cumulant

$$U_N = 1 - \langle S^4 \rangle / (3\langle S^2 \rangle^2) \tag{6}$$

for a lattice with N points.[9] It is known that $U_N \to 2/3$ as $T \to 0$, and it goes to zero as $T \to \infty$. Right at T_c, U_N has a size-independent (i.e. fixed-point) value. Therefore,

$$R_{NN'}(T) = 1 - \frac{U_N(T)}{U_{N'}(T)} \tag{7}$$

goes to zero at $T = T_c$. Hence, T_c can be determined by locating the root of $R_{NN'}(T)$ without any adjustable parameter.

For each γ, we choose lattices of various sizes, typically in the range 300 to 800. MC simulation is done at $kT/J = 2.4$ for 10^5 steps and the first 10^4 steps are excluded for thermalization. We choose the smallest size as N' in Eq. (7). For all the cases studied, $R_{NN'}(T)$ can be fitted very well by a cubic equation of the type $R_{NN'}(T) = a_0 + a_1 T + a_2 T^2 + a_3 T^3$ (T is in units of k/J; see Fig. 1). The solution

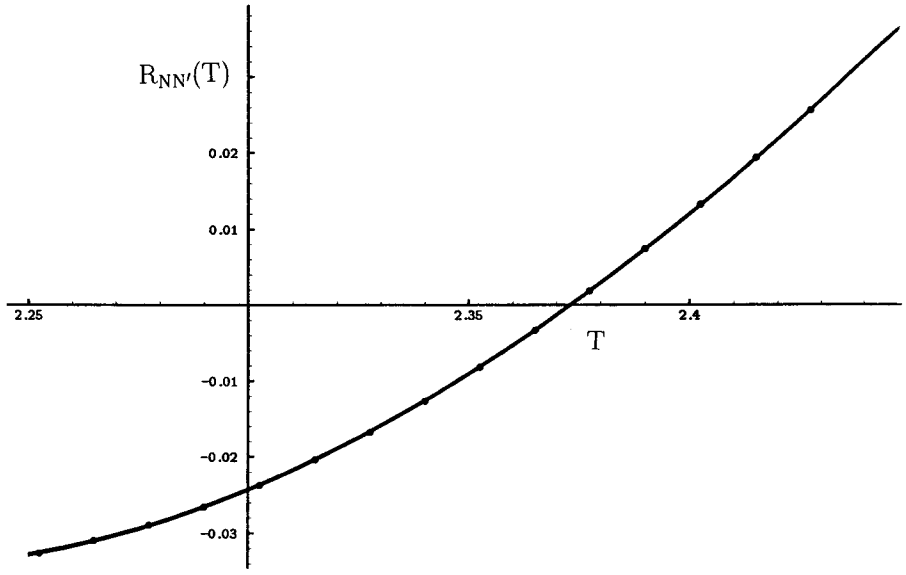

Fig. 1. A representative plot of $R_{NN'}(T)$ vs T for $N = 421$ and $N' = 291$. Note that T is in units of kT/J. The solid line is a cubic fit to the data and only a few points are shown for clarity.

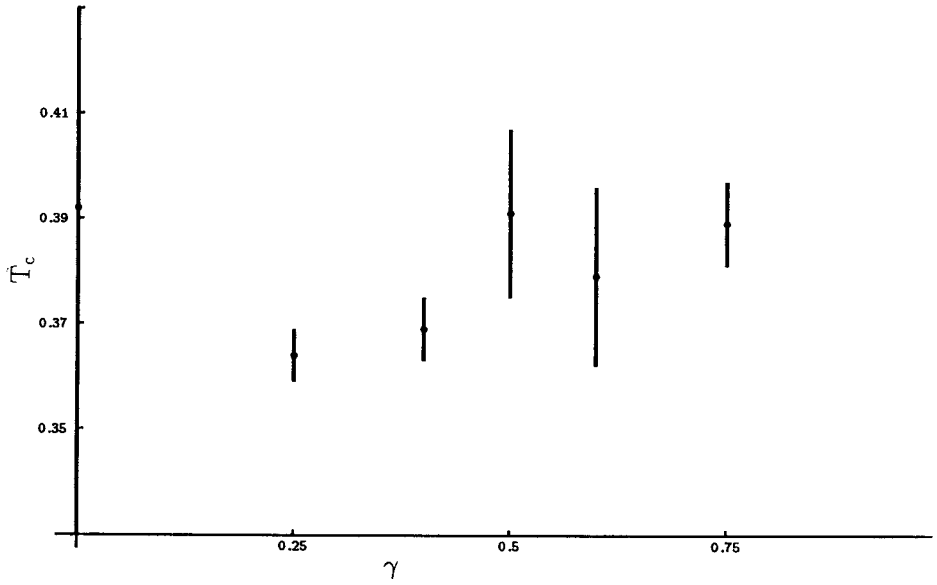

Fig. 2. T_c vs γ curve. T_c is in units of k/J. The accurate value (see Ref. 5) for the Penrose lattice ($\gamma = 0$) is shown in the plot. The error bars indicate the spread in the value.

of the cubic equation then gives T_c. The results for various γ are shown in Fig. 2. The figure includes the accurate estimate of T_c for the Penrose lattice from Ref. 5.

By construction, all of these lattices have a four-coordinated dual lattice. Therefore, the mean field transition temperature on the dual lattice will be independent of γ. If we use duality transformation at this stage, all of the quasicrystals would have the same mean field transition temperature. The actual variation we find is very small, but still there is an interesting pattern. However, our accuracy is limited because of the small sizes. A study of this problem on bigger lattices might reveal more interesting features.

Acknowledgements

It is a pleasure to thank Suprava Mishra for many helpful discussions, especially regarding the histogram method. Support for this work from DST through grant no. SP/YS/P12/89 is gratefully acknowledged.

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