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Density of Yang–Lee zeros and Yang–Lee edge singularity for the antiferromagnetic Ising model

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Abstract

The microcanonical transfer matrix is used to evaluate the exact partition function of the antiferromagnetic (AF) Ising model on $L \times L$ square lattices in an arbitrary nonzero external magnetic field at arbitrary temperature. The precise distribution of the Yang–Lee zeros in the complex $x = e^{-2\beta H}$ plane for the AF Ising model is determined as a function of temperature. Some of the Yang–Lee zeros for the AF Ising model lie on the negative real x axis, and the number of the zeros on the negative real axis is increased as temperature increases. The zeros on the negative real axis accumulate at their right end x_e. In the thermodynamic limit ($L \to \infty$), the density of the zeros $g(x)$ on the negative real axis of the AF Ising model diverges at x_e for *all* temperatures. Therefore, the AF Ising model has the Yang–Lee edge singularity x_e whose existence has been known in the ferromagnetic models only for $T > T_c$. For the AF Ising model the density of zeros near x_e is given by $g(x) \sim (x - x_e)^{-1/6}$, in the same way for the ferromagnetic models.

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1. Introduction

The two-dimensional Ising model is the simplest model showing phase transitions at finite temperatures, and consequently it has played a central role in our understanding of phase transitions and critical phenomena. Yang and Lee [1] proposed a mechanism for the occurrence of phase transitions in the thermodynamic limit and yielded an insight into the problem of the ferromagnetic (FM) Ising model in an arbitrary nonzero external magnetic field at arbitrary temperature by introducing the concept of the zeros of the partition function in the *complex* magnetic field plane (Yang–Lee zeros). They [2] also formulated the celebrated circle theorem which states that the Yang–Lee zeros of the FM Ising model lie on the unit circle in the complex $x = e^{-2\beta H}$ plane. However, the properties of the Yang–Lee zeros of the antiferromagnetic (AF) Ising model [3–7] are much less well understood than those of the FM model. Fisher [8] found that the partition function zeros in the complex temperature plane (Fisher zeros) are also important in understanding phase transitions, and showed that for the square lattice Ising model in the absence of magnetic field the Fisher zeros in the complex $a = e^{2\beta J}$ plane lie on two circles (the FM circle $a_{\rm FM} = 1 + \sqrt{2}e^{i\theta}$ and the AF circle $a_{\rm AF} = -1 + \sqrt{2}e^{i\theta}$) in the thermodynamic limit.

If the density of zeros [2,5,9–28] is found, the free energy, the equation of state, and all other thermodynamic functions can be obtained. However, very little is known about the actual form of the density of zeros.

In this paper, by enumerating the exact number of states for the Ising model on $L \times L$ square lattices in an arbitrary nonzero external magnetic field at arbitrary temperature, we investigate the density of the Yang–Lee zeros for the AF Ising model whose properties are not known. In Section 2 we briefly discuss the number of states for the Ising model. In Section 3 the known properties of the density of the Yang–Lee zeros for the FM Ising model are briefly reviewed. In Section 4 we discuss the density of the Yang–Lee zeros for the AF Ising model.

2. Number of states

The Ising model in an external magnetic field H on a lattice with N_s sites and N_b bonds is defined by the Hamiltonian

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

where J is the coupling constant, $\langle i, j\rangle$ indicates a sum over all nearest-neighbor pairs of lattice sites, and $\sigma_i = \pm 1$. The partition function of the Ising model is

$$Z = \sum_{\{\sigma_n\}} e^{-\beta\mathcal{H}},$$

where $\{\sigma_n\}$ denotes a sum over 2^{N_s} possible spin configurations and $\beta = (k_B T)^{-1}$. If we define the number of states, $\Omega(E, M)$, with a given energy

$$E = \frac{1}{2} \sum_{\langle i,j\rangle} (1 + \sigma_i \sigma_j) \tag{2}$$