Yang-Lee Edge in the High-Temperature Limit

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For Ising ferromagnets on two 4-coordinated lattices in 2 and 3 dimensions we use an exact transformation of the partition function to show that the length of the arc segment of the unit circle containing Yang-Lee zeros behaves as $A/\sqrt{T}$ at high temperatures $T$. Our consideration leads to a new lower bound on the amplitude $A$.

Yang and Lee\cite{1,2} pointed out that zeros of the partition function of an Ising ferromagnet lie on the unit circle

$$z = e^{i\theta}, \quad -\pi < \theta \ll \pi$$

in the complex $z = e^{-2H}$ plane, where $H$ is the reduced external magnetic field. At infinite temperature ($T = \infty$) the spins are noninteracting and the partition function reduces to $(z^{1/2} + z^{-1/2})^N$, where $N$ is the total number of spins. The zeros are therefore $N$-fold degenerate at $\theta = \pi$. As the temperature is lowered, the zeros spread into an arc segment of the unit circle centered about $\theta = \pi$ and extending between two Yang-Lee edges at $\theta(T) = \pm[\pi - \frac{1}{2}\Delta(T)]$. The length $A(T)$ of the arc segment grows as the temperature is lowered, eventually reaching $A(T_c) = 2\pi$ (zeros distributed over the whole unit circle) at the critical temperature $T_c$. While the precise expression of $A(T)$ remains unknown,\cite{4} Kurtze and Fishers have argued from a consideration of the high-temperature series expansion that at high temperatures the gap width behaves as

$$\Delta(T) = A/\sqrt{T}, \quad T \to \infty$$

In addition, upper and lower bounds on $A(T)$ have also been obtained.\cite{6}

In this note we use an exact transformation of Ising partition functions to explicitly establish the high-temperature behavior (1) for two 4-coordinated lattices in 2 and 3 dimensions. We also obtain a new lower bound on the amplitude $A$, which is better than that obtained previously.\cite{6}

In two dimensions we establish Eq. (1) for the Kagomé lattice. But we consider first a
related honeycomb lattice with reduced nearest-neighbor interactions $K$ and an external magnetic field $H = -i\theta \theta^2$ where $\theta = \text{real}$. It is convenient to introduce the real variables

$$ x = e^{2K} \cos(\theta/3) \quad y = e^{2K} \sin(\theta/3), $$

or, equivalently, $e^{4K} = x^2 + y^2$, $\theta/3 = \tan^{-1}(y/x)$, and consider the regime in the $xy$-plane (see Fig. 1) in which zeros of the Ising partition function lie. In these variables the azimuth angle of a point in the $xy$-plane is precisely $\theta/3$.

We now consider a Kagomé Ising model of $N$ sites related to the honeycomb lattice by a decoration and star-triangle transformation. Since this relation is standard, we quote only the final resulting expression:

$$ Z_{\text{Kag}}(h, R) = (2e^R \cosh L)^{-2N^3}(2e^K \cosh H)^N Z_{\text{HC}}(H, K) $$

Here, $R$ and $h$ are, respectively, the reduced nearest-neighbor interaction and the magnetic field of the Kagomé Ising model, and $Z_{\text{Kag}}$ and $Z_{\text{HC}}$ are the respective partition functions. The Ising parameters in Eq. (3) are related by

$$ e^{4K} = 1 + (\sinh 2L/\cosh h)^2 $$

$$ e^{4H/3} = \cosh(h + 2L)/\cosh(h - 2L) $$

FIG. 1. Regime of Yang-Lee zeros. All zeros are distributed continuously in the shaded region.

As indicated by Eq. (2), the constant temperature $K$ loci for the honeycomb lattice are concentric circles in the $xy$-plane centered about the origin. At infinite temperature ($K = 0$) the locus is the circle $r = e^{2K} = 1$, and the zeros are all located at $\theta = \pi$, or $\theta/3 = 60^\circ$, the point A in Fig. 1. The loci for fixed but finite $K$ are circles of radii $r > 1$, on which zeros are distributed in a segment extending from the line $\theta/3 = 60^\circ$ to a Yang-Lee edge. The size of the segment grows as the temperature is lowered, eventually reaching the $x$-axis at the critical temperature $e^{2K_c} = 2 + \sqrt{3}$, the point B in Fig. 1. Thus, the Yang-Lee edge traces out a continuous Yang-Lee boundary connecting A and B, with zeros distributed continuously above it in the shaded region in Fig. 1.

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with
\[ \cosh 2L = \frac{e^{4R} + 1}{2} \]  
(5)

Using Eq. (4), Eq. (2) can be rewritten as
\[ x = \cosh 2L, \quad y = i \sinh 2L \tanh h. \]  
(6)

While the transformation Eq. (3) holds quite generally for real and complex \( h \) and \( R \), for \( x \), \( y \) real as dictated by Eq. (2), Eqs. (5) and (6) imply either \( R < 0, 0 < x < 1, L = \text{imaginary}, h = \text{real} \), or \( R > 0, x > 1, L = \text{real}, h = \text{imaginary} \). Furthermore, the transformation Eq. (3) maps every zero of \( Z_{HC} \) onto a zero of \( Z_{Kg} \) and vice versa (albeit not necessarily one-one). It follows that zeros of the two partition functions coincide and are confined by the same Yang-Lee boundary. We can then apply the boundary in Fig. 1 to the Kagomé lattice.

For \( R < 0 \) it is known that the Kagomé partition function is free of zeros for real \( h \), a fact consistent with the regime of the zero distribution shown in Fig. 1. For fixed ferromagnetic \( R > 0 \), zeros of the partition function are distributed on lines \( x = \text{constant} \). Particularly, the locus \( R = 0 \) corresponds to \( x = 1 \), and the Yang-Lee edge of the Kagomé Ising lattice approaches the point \( C \) in the infinite temperature \( (R = 0) \) limit. Writing the magnetic field of the Kagomé lattice as
\[ h = -i\phi/2, \]  
(7)

where \( \phi = \text{real} \), we obtain from Eq. (6)
\[ \lim_{T \to \infty} [\sinh 2L \tan(\phi/2)] = y_0, \]  
(8)

where \( y_0 \) is the coordinate of the point \( C \). Substituting \( \phi = \pi - \frac{1}{2} \Delta(T) \) and expanding for small \( \Delta(T) \), we obtain from Eq. (8) the expression
\[ \Delta(T) = \frac{8}{y_0} \frac{\sqrt{T}}{kT}, \quad T \to \infty \]  
(9)

where \( J \) is the Kagomé Ising interaction. Now, \( \phi \) is monotonically decreasing in \( L \). This implies that \( y_0 \) is monotonically decreasing in \( x \), and thus, from Fig. 1, \( y_0 < \sqrt{3}/2 \). Using this last inequality and comparing Eq. (9) with Eq. (1), we are led to
\[ A > 16 \sqrt{\frac{1}{3k}}. \]  
(10)

This is a lower bound of the amplitude \( A \), which is better than the bound \( A > \frac{8\sqrt{J}}{J/k} \) derived previously for 4-coordinated lattices.\(^6\)

In 3 dimensions we consider a 3-coordinated hydrogen-peroxide lattice.\(^9,10\) The same sequence of decoration and star-triangle transformations transform the hydrogen-peroxide
lattice into a hyper-Kagomé lattice which is 4-coordinated.” Then, the same analysis can be carried through and, as a result, we establish the high-temperature behavior Eq. (1) and the bound Eq. (10) for the hyper-Kagomé lattice.

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