

Non-Abelian Random Polygons: A New Model in Statistical Physics

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A model in statistical physics is presented based on assigning non-Abelian phase factors to the turning points of polygons in three dimensions. This model allows for an exact solution and exhibits an unexpectedly rich phase structure. The model as well as the solution are obtained by a generalization of the methods of Kac and Ward and by mapping the problem to a Markov process as was done by Feynman for the two-dimensional Ising model.

KEY WORDS: Random; polygons; three-dimensional; Ising.

1. INTRODUCTION

One of the most fascinating models in statistical physics is the Ising model. Originally it was designed to understand the critical behavior of ferromagnetic materials. However, it turned out soon that despite its simple appearance, the construction of the solution would be extremely complicated if the dimension of the lattice is more than one and so far it has not been possible to obtain the free energy in closed form for a three dimensional lattice. A major achievement was reached by Onsager and Kaufmann, who solved the Ising model in two dimensions.^(1,2) The solution was constructed using transfer-matrix methods. An alternative solution strategy was initiated by Kac and Ward,⁽³⁾ who considered combinatorial methods. This solution strategy leads to the requirement of finding a huge determinant. The method of Kac and Ward has been simplified considerably by Feynman, who translated the finding of the determinant into the evaluation of weighted sum of paths, and conjectured an unproved identity concerning the canceling of unwanted paths in the sum. In practice, the sum can be performed by interpreting the problem as a Markov

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random walk process. The unsolved identity was proven by Sherman,⁽⁵⁾ whereas Feynman's contribution is very neatly explained in ref. 5.

With the advent of lattice gauge theories there was a revival of interest in the Ising model because it served as a playground for studying these theories using a Z_2 local symmetry. Moreover, it was demonstrated by Kavalov and Sedrakyán, that there is also an intimate connection with models of surfaces with fermionic structure.⁽⁶⁾ In particular, in this work, a generalization of the Kac-Ward factor for the three-dimensional Ising model is proposed in which elements of the group $SU(2)$ are considered. The authors refer to unpublished work of Polyakov and Dotsenko. Fermionic models in three dimensions have also been considered by Bazhanonov and Stroganov.⁽⁷⁾

A closed-form approximation for the three dimensional Ising model has been proposed by He, Xu and Hao in ref. 8. These authors generalize the phase factors which are associated with the turning points of the polygons in a three dimensional lattice to elements of the group $SU(2)$. In this way they arrive at a closed-form approximation for the free energy.

In this paper, a new model in statistical physics is presented. The model is obtained by combining the approach of Kac, Ward and Feynman with the approach of Kavalov, Sedrakyán, Polyakov and Dotsenko. The model is *not* equivalent to the three-dimensional Ising model, however it resembles some similarity with the 3D Ising model. For example, the value of the critical coupling is, $K^* = 0.2402186\dots$, whereas for the 3D Ising model, $K^* = 0.2216595\dots$ ⁽⁹⁾ In fact, the model *is* equivalent to the approximate solution that was obtained by He, Xu and Hao. In fact, their model, being defined as an approximation of the three-dimensional Ising model, can be viewed as a statistical system without reference to the Ising model and be interpreted also as a definition of a model for random polygons with non-abelian phase factors.²

The new model essentially generalizes the Kac-Ward phase factor, associated to each turn on a 2D lattice, to non-abelian unitary group elements on a 3D lattice. Therefore, we name the new model NARP (non-abelian random polygons). The model can be solved exactly and an expression for the free energy will be derived. It turns out the phase structure exhibits unexpected features. Therefore, we believe that our model and solution method is interesting enough to be presented since it may be generalized to higher dimensions and larger groups. In particular, our solution method which is based on the application of modern software technologies, allows for such generalizations.

² After submission of the manuscript the authors became aware of the work in ref. 8, which contains many ideas similar to ours.

This paper is organized as follows. Since the Ising model has played a major role in setting up the model, we give a brief summary of the Ising model and the solution method relevant for this work in Section 2. The NARP model is defined in Section 3. We set up the conditions for the (non-abelian) phase factors which are associated to the moves along the polygons in a lattice. In this paper we will consider simple cubic lattices but this restriction is not essential. In Section 4, the closed-form solution is obtained. In Section 5, the free energy of the solution is analyzed and in Section 6, a comparison with related work of He, Xu and Hao is discussed.

2. DEFINITION OF THE ISING MODEL

The Ising model consists of a D -dimensional lattice with sites, i . In each site is defined a spin s_i , which can interact with its nearest neighbors. The value of the spin variable can be $+1$ or -1 . The energy corresponding to a definite spin configuration is

$$H(s_1, s_2, \dots, s_N) = -J \cdot \sum_{\langle ij \rangle} s_i s_j \quad (1)$$

where $\langle ij \rangle$ runs over all distinct pairs of neighboring sites of the lattice. The number of sites is N and J is the strength of the interaction. The partition function at inverse temperature β is given by

$$Z = \sum_{s_1} \sum_{s_2} \dots \sum_{s_N} \exp -\beta H(s_1, s_2 \dots s_N) \quad (2)$$

The Helmholtz free energy per spin is

$$f = -\frac{1}{\beta} \lim_{N \rightarrow \infty} \left(\frac{1}{N} \log Z \right) \quad (3)$$

In all solution methods, the Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ play an important role.

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (4)$$

2.1. The Two-Dimensional Ising Model

In this section the solution of the square two-dimensional Ising model based on the method of Kac is briefly summarized, since it serves as a good

starting point for our three-dimensional case. Let us restart with the partition function

$$Z = \sum_{\text{all states}} \exp(-K \Sigma^* s_i s_j) \quad (5)$$

with $K = \beta J$. In this formula the star corresponds to all neighbouring pairs in the lattice and Z can be rewritten as

$$Z = \sum_{\text{all states}} \Pi^* \exp(-K s_i s_j) \quad (6)$$

Since $\exp(-K s_i s_j) = \exp(-K)$ if $s_i s_j = 1$ and $\exp(-K s_i s_j) = \exp(K)$ if $s_i s_j = -1$, we find that

$$Z = \sum_{\text{all states}} \Pi^* C_0 (1 + s_i s_j T) \quad (7)$$

where $C_0 = \cosh(K)$ and $T = \tanh(K)$. We can extract the factor C_0 from the sum, by noting that there are ND bonds in a D dimensional lattice of N sites.

The partition function can then be viewed as a sum over all closed graphs in a D -dimensional lattice, such that in every graph each bond can contribute only once. The partition function becomes

$$Z = 2^N C_0^{ND} \sum_L d(L) T^L \quad (8)$$

where the sum is over all closed graphs on the lattice and $d(L)$ is the number of closed graphs of length L that can be put on the lattice. The summation over self-avoiding loops is a very difficult task to perform. An alternative approach is applied, whereby all loops are allowed but a weight factor is assigned to each loop, such that effectively the self-avoidance is realized by canceling weights. For the two-dimensional Ising problem a correct set of weight factors is provided by the following rules:

For each closed loop one should assign

- a factor $\phi = e^{\pi i/4} T$ for a turn to the left,
- a factor $\phi = e^{-\pi i/4} T$ for a turn to the right,
- a factor $\phi = T$ for going straight-on,
- a factor $\phi = 0$ for a U-turn.

Note that the factors $e^{\pi i/4}$ and $e^{-\pi i/4}$ are elements of the group $U(1)$ which is isomorphic to $SO(2)$, i.e. the group of rotations in a plane. The choice of the angle, $\pi/4$, is such that a full rotation over 2π results into a weight factor -1 .

The basic idea is to replace the summing over all self-avoiding loops, by summing over all loops where the phase factors assigned to the loops cancel out unwanted graphs. The sum over all loops can be performed by solving a recurrent random-walk problem.^(12, 13) A closed graph may consist of several polygons. The composition is such that no bond is used twice. In order to perform the sum, a specific point (the origin) on the lattice is chosen. From now on we will consider the factor

$$Z_1 = \sum_L d(L) T^L \tag{9}$$

The corresponding part of the free energy is related to Z_1 by $Z_1 = \exp(-\beta N f_1)$, i.e. the total free energy reads

$$f = f_1 - \frac{1}{\beta} \log(2C_0^D) \tag{10}$$

Since the free energy is proportional to the number of lattice sites, we may consider f as the free energy per lattice site. Each polygon occurs L times in the summing over all sites. Since only different polygons are counted, we obtain

$$-\beta f_1 = \sum_L \frac{h(L)}{L} T^L \tag{11}$$

where $h(L)$ is the number of ways that one can return to the starting point in L steps without traversing the same bond twice.

It is evident that

$$-\beta T \frac{df_1}{dT} = \sum_L h(L) T^L \tag{12}$$

This sum expresses the number of polygons that exist and pass through the origin.

The role of the phase factors is to provide the cancelation while the restriction to self-avoidance is omitted, i.e. bonds may be traversed several times.

In Feynman's approach the following identification is made:

$$\sum_L d(L) T^L = \left(-\frac{1}{2}\right) \sum_L \Gamma(L) T^L \quad (13)$$

The sum on the right is the sum over all paths weighted with the loop-phase factor, $\Gamma(L) = \prod_{i=1}^L \phi_i$. Here, the factor $(-\frac{1}{2})$ compensates for the minus sign in the phase factor and the fact that each loop can be traversed in two directions.

3. DEFINITION OF THE NARP MODEL

As has been mentioned in the foregoing section, it was possible to obtain correct loop-counting for the two-dimensional Ising model by including appropriate weightfactors to the loops. The weight factors for each loop were constructed by including an element of $U(1)$ to each point along the path where a turn is made. Since a simple graph with four turns of 90 degrees generates a phase factor -1 , we keep in mind that in a two-dimensional plane a loop corresponds to a full rotation, i.e. there is a mapping of the phase factors into $O(2)$. In order to define the NARP model, we will use similar methods. In particular, for the generation of loops in three dimensions, we use the fact that the group of rotations in R^3 is locally isomorphic to the group $SU(2)$. Therefore, for a loop in R^3 we will define a phase factor at each turn selected from $SU(2)$.

Our starting point is the selection of a coordinate system in R^3 . We choose a right-handed frame as is illustrated in Fig.1. A rotation of 90

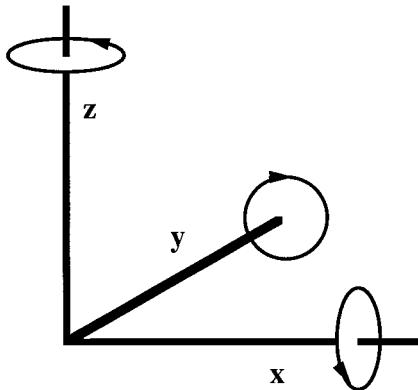


Fig. 1. Right-handed coordinate system for the 3D lattice.

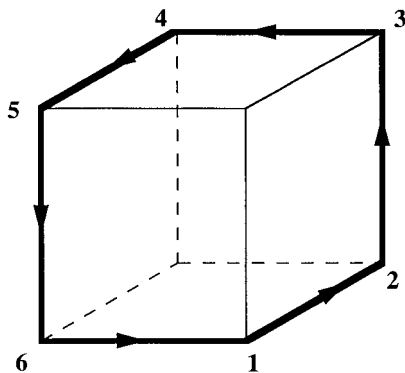


Fig. 2. Simplest path in the Ising model which is essentially three dimensional.

degrees is defined to be positive if the corresponding cross product projected on the axis of rotation is positive. In particular $\hat{x} \times \hat{y} = \hat{z}$ corresponds to a rotation of \hat{x} of 90 degrees around the z-axis, etc. The positive rotations around the principal axes are illustrated in Fig.1. Let us consider a loop in R^3 , which is essentially three-dimensional and which contains rotations around all three axes. In Fig. 2 such a loop along the sides of a cube is shown.

In each corner a phase factor is defined, which is taken from the group SU(2) as follows:

- corner-1: positive rotation $r_z^+(\theta_z) = \exp(i(\theta_z/2) \sigma_z)$
- corner-2: positive rotation $r_x^+(\theta_x) = \exp(i(\theta_x/2) \sigma_x)$
- corner-3: negative rotation $r_y^-(\theta_y) = \exp(-i(\theta_y/2) \sigma_y)$
- corner-4: positive rotation $r_z^+(\theta_z) = \exp(i(\theta_z/2) \sigma_z)$
- corner-5: positive rotation $r_x^+(\theta_x) = \exp(i(\theta_x/2) \sigma_x)$
- corner-6: negative rotation $r_y^-(\theta_y) = \exp(-i(\theta_y/2) \sigma_y)$

For reasons of symmetry we assume that $\theta_x = \theta_y = \theta_z = \theta$.

The phase factor for the loop of Fig. 2 is

$$\Gamma = r_z^+ r_x^+ r_y^- r_z^+ r_x^+ r_y^- \tag{14}$$

The construction of the phase factors for the two-dimensional Ising model satisfied the condition that a simple square generates a total phase factor equal to -1 . Since the planar loops form a subset of the total collection of loops in the three dimensional lattice, we select $\theta = \pi/2$ for the simple cubic lattice.

The NARP model is defined as follows:

Rule 1. For each turning point of a polygon in the simple cubic lattice, a phase factor is provided according to the following assignments:

- a counter clock wise rotation around the z-axis of 90 degrees in the (xy)-plane: r_z^+
- a clock wise rotation around the z-axis of 90 degrees in the (xy)-plane: r_z^-
- a counterclock wise rotation around the x-axis of 90 degrees in the (yz)-plane: r_x^+
- a clock wise rotation around the x-axis of 90 degrees in the (yz)-plane: r_x^-
- a counterclock wise rotation around the y-axis of 90 degrees in the (zx)-plane: r_y^+
- a clock wise rotation around the y-axis of 90 degrees in the (zx)-plane: r_y^-

Rule 2. After evaluation of the product of all phase factors, the trace is taken divided by two, i.e. $\phi = \frac{1}{2} Tr(\prod_{i=1}^N r_i)$.

Rule 3. A phase factor $\omega \hat{1}$ is assigned to a step straight-on with ω a real positive constant.

Rule 4. A phase factor $\hat{0}$ is assigned to a U-turn.

Rule 5. For each link a factor $T = \tanh(K)$ is inserted.

In order to evaluate an arbitrary chain of phase factors, it is interesting to generate some tables for performing the calculations. Let us consider the phase factor of Fig. 2. After application of rule no. 1, and the fact that $\sigma_i \sigma_j = i \sigma_k$ where $(i, j, k) = (x, y, z)$: cyclic permutations, we obtain

$$\Gamma = \left(\frac{1}{2}(1 + i\sigma_x - i\sigma_y + i\sigma_z)\right)^3 \quad (15)$$

Introducing the specific SU(2) elements:

$$U = \frac{1}{2}(1 + i\sigma_x + i\sigma_y + i\sigma_z)$$

$$X = \frac{1}{2}(1 - i\sigma_x + i\sigma_y + i\sigma_z)$$

$$Y = \frac{1}{2}(1 + i\sigma_x - i\sigma_y + i\sigma_z)$$

$$Z = \frac{1}{2}(1 + i\sigma_x + i\sigma_y - i\sigma_z)$$

we may use the Pauli matrices to write these elements as

$$U = \frac{1}{2} \begin{bmatrix} 1+i & 1+i \\ -1+i & 1-i \end{bmatrix} \tag{16}$$

$$X = \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ -1-i & 1-i \end{bmatrix} \tag{17}$$

$$Y = \frac{1}{2} \begin{bmatrix} 1+i & -1+i \\ 1+i & 1-i \end{bmatrix} \tag{18}$$

$$Z = \frac{1}{2} \begin{bmatrix} 1-i & 1+i \\ -1+i & 1+i \end{bmatrix} \tag{19}$$

These matrices have the following properties:

$$U^2 = -U^\dagger, \quad X^2 = -X^\dagger, \quad Y^2 = -Y^\dagger, \quad Z^2 = -Z^\dagger \tag{20}$$

Since $\Gamma = Y^3$ we obtain $\Gamma = -1$. So we managed to get the phase factor -1 for a simple closed loop in three dimensions, analogously to the phase factors that were used by Kac in two dimensions.

The multiplication table of the elementary phase factors r_i^\pm , is found in Table 1. Here we defined three matrices

$$\Sigma_x = i\sigma_x, \quad \Sigma_y = i\sigma_y, \quad \Sigma_z = i\sigma_z$$

which have the property that $\Sigma_x^2 = \Sigma_y^2 = \Sigma_z^2 = -\hat{1}$.

In order to evaluate an arbitrary phase factor, Table 2 gives the multiplication rules for $(U, X, Y, Z, U^\dagger, X^\dagger, Z^\dagger, \Sigma_x, \Sigma_y, \Sigma_z)$.

The finite subgroup of $SU(2)$ that we are considering here, consists of 24 elements, being

$$\left[\begin{array}{c} 1, -1, U, -U, X, -X, Y, -Y, Z, -Z, U^\dagger, -U^\dagger, \\ X^\dagger, -X^\dagger, Y^\dagger, -Y^\dagger, Z^\dagger, -Z^\dagger, \Sigma_x, -\Sigma_x, \Sigma_y, -\Sigma_y, \Sigma_z, -\Sigma_z \end{array} \right] \tag{21}$$

Table 1. Multiplication Table of the Elementary Phase Factors

Factor	r_x^+	r_y^+	r_z^+	r_x^-	r_y^-	r_z^-
r_x^+	Σ_x	Z	U	1	Y	X^\dagger
r_y^+	U	Σ_y	X	Y^\dagger	1	Z
r_z^+	Y	U	Σ_z	X	Z^\dagger	1
r_x^-	1	X	Z^\dagger	$-\Sigma_x$	U^\dagger	Y^\dagger
r_y^-	X^\dagger	1	Y	Z^\dagger	$-\Sigma_y$	U^\dagger
r_z^-	Z	Y^\dagger	1	U^\dagger	X^\dagger	$-\Sigma_z$

Table 2. Multiplication Rules for $(U, X, Y, Z, U^\dagger, X^\dagger, Z^\dagger, \Sigma_x, \Sigma_y, \Sigma_z)$

Factor	U	X	Y	Z	U^\dagger	X^\dagger	Y^\dagger	Z^\dagger	Σ_x	Σ_y	Σ_z
U	$-U^\dagger$	Σ_y	Σ_z	Σ_x	1	Y	Z	X	$-Y^\dagger$	$-Z^\dagger$	$-X^\dagger$
X	Σ_z	$-X^\dagger$	Z^\dagger	U	Y^\dagger	1	Σ_y	$-\Sigma_x$	Y	$-U^\dagger$	$-Z$
Y	Σ_x	U	$-Y^\dagger$	X^\dagger	Z^\dagger	$-\Sigma_y$	1	Σ_z	$-X$	Z	$-U^\dagger$
Z	Σ_y	Y^\dagger	U	$-Z^\dagger$	X^\dagger	Σ_x	$-\Sigma_z$	1	$-U^\dagger$	$-Y$	X
U^\dagger	1	Z^\dagger	X^\dagger	Y^\dagger	$-U$	$-\Sigma_z$	$-\Sigma_x$	$-\Sigma_y$	Z	X	Y
X^\dagger	Z	1	Σ_x	$-\Sigma_z$	$-\Sigma_y$	$-X$	U^\dagger	Y	$-Z^\dagger$	Y^\dagger	U
Y^\dagger	X	$-\Sigma_x$	1	Σ_y	$-\Sigma_z$	Z	$-Y$	U^\dagger	U	$-X^\dagger$	Z^\dagger
Z^\dagger	Y	Σ_z	$-\Sigma_y$	1	$-\Sigma_x$	U^\dagger	X	$-Z$	X^\dagger	U	$-Y^\dagger$
Σ_x	$-Z^\dagger$	Z	$-U^\dagger$	$-X$	Y	$-Y^\dagger$	X^\dagger	U	-1	$-\Sigma_z$	Σ_y
Σ_y	$-X^\dagger$	$-Y$	X	$-U^\dagger$	Z	U	$-Z^\dagger$	Y^\dagger	Σ_z	-1	$-\Sigma_x$
Σ_z	$-Y^\dagger$	$-U^\dagger$	$-Z$	Y	X	Z^\dagger	U	$-X^\dagger$	$-\Sigma_y$	Σ_x	-1

This subgroup can be obtained from the 3 generators $[r_x^+, r_y^+, r_z^+]$. Note that $r_i^- = (r_i^+)^7$, and therefore does not correspond to an independent generator.

We will now discuss the rule no. 2 and no. 3. In order to set up phase factors for the solution of the two-dimensional Ising model, the phase factors for going straight-on was chosen to be simply one. However, we may adapt this rule for setting up a new model. A few choices of ω are now considered. Consider the loop, which is depicted in Fig. 3. The corresponding phase factor Γ for the loop is:

$$\Gamma = r_y^- r_y^+ r_z^+ r_z^- r_{unknown} r_z^+ r_x^+ r_y^- = \Sigma_z r_{unknown} r_z^+ Y \quad (22)$$

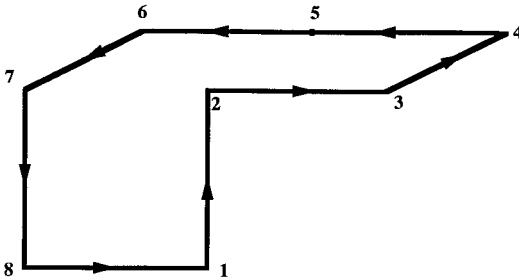


Fig. 3. Example of a path in the Ising model which contains a site where the path goes straight on.

If we choose $r_{unknown} = 1$, then $\Gamma \neq -1$. Alternatively, if we choose $r_{unknown} = r_x^+$, then

$$\Gamma = \Sigma_z UY = \Sigma_z \Sigma_z = -1 \tag{23}$$

The choice $r_{unknown} = r_x^-$ gives

$$\Gamma = \Sigma_z Z^\dagger Y = \Sigma_z (-\Sigma_y) = -\Sigma_x \tag{24}$$

If we had selected $r_{unknown} = r_x^+$ for all straight-ons in the positive and negative x-directions, we would not obtain a phase factor equal to -1 , if traversing the loop in the opposite direction. For the opposite traversal we obtain -1 if we set $r_{unknown} = r_x^-$. Since $Tr\Sigma_{x,y,z} = 0$, we adapt the following additional rules

- a step straight-on in the x-direction: $r_x^+ + r_x^- = \sqrt{2} \hat{1}$
- a step straight-on in the y-direction: $r_y^+ + r_y^- = \sqrt{2} \hat{1}$
- a step straight-on in the z-direction: $r_z^+ + r_z^- = \sqrt{2} \hat{1}$

This corresponds to the choice $\omega = \sqrt{2}$ in rule no. 3. In order to construct the complete phase factor we can take the trace after multiplication of all matrix insertions and multiply by $(-\frac{1}{2})$. In ref. 8, the Ising model is approximated with the parameter $\omega = 1$ for the straight-on rule.

Setting up phase factors for closed loops by applying the trace of SU(2) elements was suggested by Polyakov and Dotsenko and further exploited by Kavalov and Sedrakyan.⁽⁶⁾ However, these authors consider contours in three dimensional space, which have no torsion. Consequently, their directions of research proceed according to the U(1) subgroup structure contained in SU(2), albeit in a three-fold replication.

It is also interesting to compare our proposition to the generalization that was advocated by Kac and Ward. These authors generalized the two-dimensional situation by stating that the next step of the walk on the lattice can be one of five different cases, being (1) straight on, (2) turn to the left, (3) turn to the right, (4) turn upwards and (5) turn downwards. The meaning of the five cases is defined relatively to the bond on which one is approaching the lattice site. Of course, such a local observer's point of view differs considerably from the absolute frame view which we have proposed here. Indeed Kac and Ward showed that their generalization ran into conflictuous values of phase factors for non-planar loops.

4. THE RANDOM WALK APPROACH IN THREE DIMENSIONS

In this section we will mimic the calculation that Feynman performed for the two-dimensional Ising model and extend it to three dimensions. The

sum over all loops can be performed by solving a recurrent random-walk problem.

Restarting from Eq. (8), the partition function becomes

$$Z = 2^N C_0^{3N} \sum_L d(L) T^L \quad (25)$$

Herein, $d(L)$ is the number of closed loops of length L that can exist on the cubic lattice. In order to perform the sum a specific point on the lattice is chosen, the origin, and again from now on we will consider

$$Z_1 = \sum_L d(L) T^L \quad (26)$$

The corresponding part of the free energy is related to Z_1 by $Z_1 = \exp(-\beta N f_1)$, i.e. the total free energy reads

$$f = f_1 - \frac{1}{\beta} \log(2C_0^3) \quad (27)$$

Since the free energy is proportional to the number of lattice sites. we may consider f as the free energy per lattice site.

$$-\beta f_1 = \sum_L \frac{h(L)}{L} T^L \quad -\beta T \frac{df_1}{dT} = \sum_L h(L) T^L \quad (28)$$

where $h(L)$ is the number of ways that one can return to the starting point in L steps.

This last sum expresses the number of polygons that exist and pass through the origin. The key ingredient in Feynman's approach is the following identification:

$$\sum_L d(L) T^L = \left(-\frac{1}{2}\right) \sum_L \frac{1}{2} \text{Tr}[\Gamma(L)] T^L \quad (29)$$

The sum on the right is the sum over all paths weighted with the loop amplitude. Here, the factor $(-\frac{1}{2})$ compensates for the minus sign in the phase factor and the fact that each loop can be traversed in two directions. The other factor $\frac{1}{2}$ compensates the $\text{Tr} 1 = 2$ evaluation. Summarizing, we have generalized the Feynman conjecture as follows:

$$Z = 2^N C_0^{3N} Z_1 \quad (30)$$

$$Z_1 = \exp(-\beta N f_1) \quad (31)$$

$$-\beta f_1(T) = \int_0^T dt \left(-\frac{1}{4t}\right) \left\{ \sum_L \text{Tr} \Gamma(L) t^L \right\} \quad (32)$$

Let us now evaluate the 2×2 matrix $A(t)$

$$A(t) = \sum_L \Gamma(L) t^L \tag{33}$$

Following the method of Feynman we need to introduce the directional transition amplitudes for arriving in a lattice site $\vec{r} = (x, y, z)$ after n steps:

$$\psi_n(\vec{r}) = \begin{pmatrix} U_n(x, y, z) \\ D_n(x, y, z) \\ R_n(x, y, z) \\ L_n(x, y, z) \\ B_n(x, y, z) \\ F_n(x, y, z) \end{pmatrix} \tag{34}$$

The amplitudes are defined as follows:

- U : moving upwards, i.e. along the $z+$ direction
- D : moving downwards, i.e. along the $z-$ direction
- R : moving to the right, i.e. along the $x+$ direction
- L : moving to the left, i.e. along the $x-$ direction
- B : moving to the back, i.e. along the $y+$ direction
- F : moving to the front, i.e. along the $y-$ direction

This gives rise to the following recursion relations:

$$\begin{aligned} U_{(n+1)}(x, y, z) &= \omega \hat{1} T U_n(x, y, z-1) + r_y^- T R_n(x, y, z-1) \\ &\quad + r_y^+ T L_n(x, y, z-1) + r_x^+ T B_n(x, y, z-1) \\ &\quad + r_x^- T F_n(x, y, z-1) \end{aligned}$$

$$\begin{aligned} D_{(n+1)}(x, y, z) &= \omega \hat{1} T D_n(x, y, z+1) + r_y^+ T R_n(x, y, z+1) \\ &\quad + r_y^- T L_n(x, y, z+1) + r_x^- T B_n(x, y, z+1) \\ &\quad + r_x^+ T F_n(x, y, z+1) \end{aligned}$$

$$\begin{aligned} R_{(n+1)}(x, y, z) &= r_y^+ T U_n(x-1, y, z) + r_y^- T D_n(x-1, y, z) \\ &\quad + \omega \hat{1} T R_n(x-1, y, z) + r_z^- T B_n(x-1, y, z) \\ &\quad + r_z^+ T F_n(x-1, y, z) \end{aligned}$$

$$L_{(n+1)}(x, y, z) = r_y^- TU_n(x+1, y, z) + r_y^+ TD_n(x+1, y, z) \\ + \omega \hat{1} TL_n(x+1, y, z) + r_z^+ TB_n(x+1, y, z) \\ + r_z^- TF_n(x+1, y, z)$$

$$B_{(n+1)}(x, y, z) = r_x^- TU_n(x, y-1, z) + r_x^+ TD_n(x, y-1, z) \\ + r_z^+ TR_n(x, y-1, z) + r_z^- TL_n(x, y-1, z) \\ + \omega \hat{1} TB_n(x, y-1, z)$$

$$F_{(n+1)}(x, y, z) = r_x^+ TU_n(x, y+1, z) + r_x^- TD_n(x, y+1, z) \\ + r_z^- TR_n(x, y+1, z) + r_z^+ TL_n(x, y+1, z) \\ + \omega \hat{1} TF_n(x, y+1, z)$$

Using Fourier transforms of the amplitudes according to

$$U_n(x, y, z) = \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\xi d\eta dv U_n(\xi, \eta, v) \exp(i\xi x + i\eta y + ivz) \quad (35)$$

and

$$U_n(\xi, \eta, v) = \sum_{x=-\infty}^{\infty} \sum_{y=-\infty}^{\infty} \sum_{z=-\infty}^{\infty} U_n(x, y, z) \exp(-i\xi x - i\eta y - ivz) \quad (36)$$

and similar transforms for the other directional amplitudes, we obtain

$$\psi_{(n+1)}(\xi, \eta, v) = T \star M \psi_n(\xi, \eta, v) \quad (37)$$

The matrix M is given by

$$M = \begin{bmatrix} \omega \hat{1} e^{-iv} & 0 & r_y^- e^{-iv} & r_y^+ e^{-iv} & r_x^+ e^{-iv} & r_x^- e^{-iv} \\ 0 & \omega \hat{1} e^{iv} & r_y^+ e^{iv} & r_y^- e^{iv} & r_x^- e^{iv} & r_x^+ e^{iv} \\ r_y^+ e^{-i\xi} & r_y^- e^{-i\xi} & \omega \hat{1} e^{-i\xi} & 0 & r_z^- e^{-i\xi} & r_z^+ e^{-i\xi} \\ r_y^- e^{i\xi} & r_y^+ e^{i\xi} & 0 & \omega \hat{1} e^{i\xi} & r_z^+ e^{i\xi} & r_z^- e^{i\xi} \\ r_x^- e^{-i\eta} & r_x^+ e^{-i\eta} & r_z^+ e^{-i\eta} & r_z^- e^{-i\eta} & \omega \hat{1} e^{-i\eta} & 0 \\ r_x^+ e^{i\eta} & r_x^- e^{i\eta} & r_z^- e^{i\eta} & r_z^+ e^{i\eta} & 0 & \omega \hat{1} e^{i\eta} \end{bmatrix} \quad (38)$$

The solution for ψ becomes

$$\psi_n(\xi, \eta, v) = (T \star M)^n \psi_0(\xi, \eta, v) \quad (39)$$

With the use of this result into $A(t)$ we obtain

$$\begin{aligned}
 A(t) &= \sum_L \Gamma(L) t^L \\
 &= \text{Tr} \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\xi d\eta dv \text{tr} \left(\sum_{n=1}^{\infty} (tM)^n \right) \\
 &= \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\xi d\eta dv \text{Trtr} \left(\frac{1}{1-tM} - 1 \right) \tag{40}
 \end{aligned}$$

After substitution we obtain

$$\begin{aligned}
 -\beta f_1(T) &= \frac{1}{2^5 \pi^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\xi d\eta dv \text{Trtr} \log(1 - T \star M) \\
 &= \frac{1}{2^5 \pi^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\xi d\eta dv \log \det(1 - T \star M) \tag{41}
 \end{aligned}$$

We can now substitute the rotation matrices for the evaluation of the determinant. The generic matrix, Q , of which the determinant needs to be evaluated is

$$Q = \begin{bmatrix}
 \alpha & 0 & 0 & 0 & 1 & -1 & 1 & 1 & 1 & i & 1 & -i \\
 0 & \alpha & 0 & 0 & 1 & 1 & -1 & 1 & i & 1 & -i & 1 \\
 0 & 0 & \alpha^* & 0 & 1 & 1 & 1 & -1 & 1 & -i & 1 & i \\
 0 & 0 & 0 & \alpha^* & -1 & 1 & 1 & 1 & -i & 1 & i & 1 \\
 1 & 1 & 1 & -1 & \beta & 0 & 0 & 0 & (1-i) & 0 & (1+i) & 0 \\
 -1 & 1 & 1 & 1 & 0 & \beta & 0 & 0 & 0 & (1+i) & 0 & (1-i) \\
 1 & -1 & 1 & 1 & 0 & 0 & \beta^* & 0 & (1+i) & 0 & (1-i) & 0 \\
 1 & 1 & -1 & 1 & 0 & 0 & 0 & \beta^* & 0 & (1-i) & 0 & (1+i) \\
 1 & -i & 1 & i & (1+i) & 0 & (1-i) & 0 & \gamma & 0 & 0 & 0 \\
 -i & 1 & i & 1 & 0 & (1-i) & 0 & (1+i) & 0 & \gamma & 0 & 0 \\
 1 & i & 1 & -i & (1-i) & 0 & (1+i) & 0 & 0 & 0 & \gamma^* & 0 \\
 i & 1 & -i & 1 & 0 & (1+i) & 0 & (1-i) & 0 & 0 & 0 & \gamma^*
 \end{bmatrix} \tag{42}$$

In this matrix, α, β, γ are complex numbers and $\alpha^*, \beta^*, \gamma^*$ their complex conjugates. At first sight this matrix looks deterrent for calculating the determinant. However, by setting

$$\alpha = a + ib, \quad \beta = c + id, \quad \gamma = e + if$$

and using computer algebraic software, e.g. "Mathematica,"⁽¹⁴⁾ the determinant can be easily computed. The result is

$$\begin{aligned} \det(Q) = & \{-256 + 16 \cdot (a^2 + b^2 + c^2 + d^2 + e^2 + f^2) \\ & + 32 \cdot (ac + ae + ce) \\ & - 8 \cdot [(a^2 + b^2) \cdot ce + (c^2 + d^2) \cdot ae + (e^2 + f^2) \cdot ac] \\ & + (a^2 + b^2) \cdot (c^2 + d^2) \cdot (c^2 + f^2)\}^2 \end{aligned} \quad (43)$$

After substitution of the actual values for α, β, γ , i.e.

$$\alpha = \sqrt{2} \left(\omega - \frac{e^{iv}}{T} \right) \quad \beta = \sqrt{2} \left(\omega - \frac{e^{i\xi}}{T} \right) \quad \gamma = \sqrt{2} \left(\omega - \frac{e^{i\eta}}{T} \right) \quad (44)$$

we arrive at the main result of this paper, being that the Helmholtz free energy per spin, $f(T)$, for the NARP model is

$$-\beta f(T) = \log(2C_0^3) + \frac{1}{2^4 \pi^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\xi d\eta dv \log\{T^6 |G(\xi, v, \eta)|\} \quad (45)$$

with $u = 1/\omega T$

$$\begin{aligned} G(\xi, v, \eta) = & -32 + 36\omega^2 - 12\omega^4 + \omega^6 \\ & + (-24\omega^2 + 16\omega^4 - 2\omega^6) Au \\ & + (12\omega^2 - 12\omega^4 + 3\omega^6 + (8\omega^2 - 20\omega^4 + 4\omega^6) B) u^2 \\ & + ((8\omega^4 - 4\omega^6) A + (24\omega^4 - 8\omega^6) C) u^3 \\ & + (3\omega^6 - (4\omega^4 - 4\omega^6) B) u^4 - 2\omega^6 Au^5 + \omega^6 u^6 \end{aligned} \quad (46)$$

and setting $\cos \xi = x, \cos v = y, \cos \eta = z$ and

$$\begin{aligned} A(x, y, z) &= x + y + z \\ B(x, y, z) &= xy + yz + zx \\ C(x, y, z) &= xyz. \end{aligned} \quad (47)$$

5. FURTHER ANALYSIS OF THE HELMHOLTZ FREE ENERGY

In order to study the critical points it is required to sort out for which values of K the function G vanishes. These points correspond to non-analytic behaviour of the Helmholtz free energy, and consequently we may expect phase transitions to occur for these values. In this section, we will study the case $\omega = \sqrt{2}$. This value corresponds to a unit normalization of the loop phases.

Let us rewrite the integral as a multiple integral from $-1 \rightarrow 1$. After rearranging various terms, we may separate f into its analytic and non-analytic parts:

$$-\beta f_A(T) = \frac{5}{2} \log 2 + 3 \log \sinh K \tag{48}$$

$$-\beta f_{NA}(T) = \frac{1}{2\pi^3} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \frac{dx}{\sqrt{1-x^2}} \frac{dy}{\sqrt{1-y^2}} \frac{dz}{\sqrt{1-z^2}} \log |G(x, y, z; u)| \tag{49}$$

whereas here $G(x, y, z; u)$ is a polynomial in x, y, z and u .

$$G(x, y, z; u) = u^2(u^4 - 2Au^3 + (3 + 2B)u^2 + 4Cu - 4B) \tag{50}$$

The structure of the surface $G(x, y, z; u) = 0$ can be visualized by scanning the cube $-1 \leq x, y, z \leq 1$ for each value of u . Such a graphical analysis can be done by solving explicitly for one of the variables. For instance, an explicit solution for z is given by

$$z(x, y; u) = \frac{u^4 + 3u^2 - 2u^3(x + y) + (2u^2 - 4)xy}{2u^3 - 2(u^2 - 2)(x + y) - 4uxy} \tag{51}$$

The following results are obtained:

- $u > 3$: There are no points in the cube such that $G = 0$. For these values of u there is no critical behaviour.
- $u = 3$: Merely the point $(x, y, z) = (1, 1, 1)$ corresponds to $G = 0$.
- $2 < u < 3$: There is surface in the upper tip of the cube for which $G = 0$. In Fig. 4 the surface for $u = 2.5$ is shown.
- $u = 2$: The edges $(x = 1, y = 1)$, $(y = 1, z = 1)$ and $(x = 1, z = 1)$ correspond to $G = 0$.
- $1 < u < 2$: In Fig. 5 the surface for $u = 1.2$ is shown.

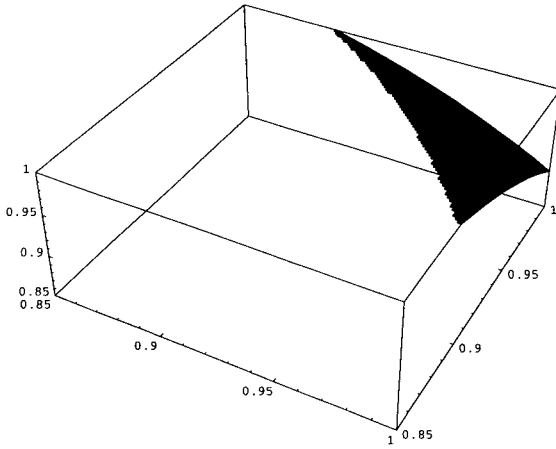


Fig. 4. Upper corner of the cube showing the surface on which $G=0$. This figure corresponds to $u=2.5$.

- $u=1$: The point $(x, y, z) = (-1, -1, -1)$ also gives $G=0$, The surface and the isolated point $(x, y, z) = (-1, -1, -1)$ are shown in Fig. 6.
- $1/\sqrt{2} < u < 1$: The surface $G=0$ is shown in Fig. 7 for $u=0.85$.
- $u \leq 1/\sqrt{2}$: This case is not relevant since it corresponds to $T \geq 1$.

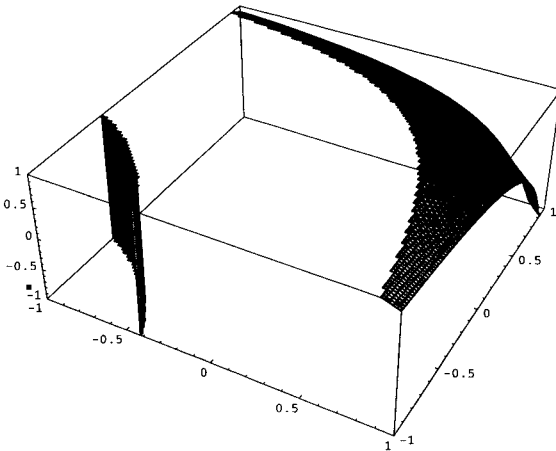


Fig. 5. Upper corner of the cube showing the surface on which $G=0$. This figure corresponds to $u=1.2$. The steep rim corresponds to (x, y) -values for which z is indefinite.

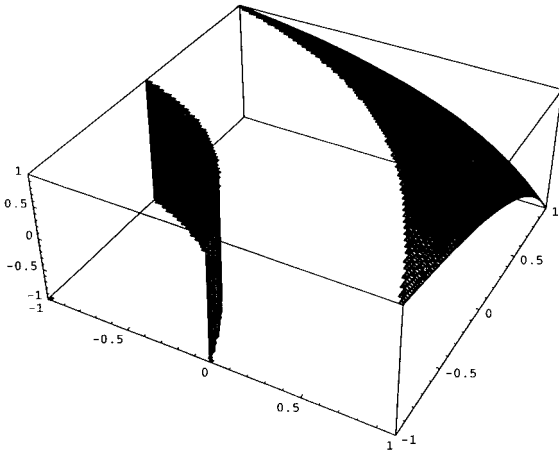


Fig. 6. Upper corner of the cube showing the surface on which $G=0$. This figure corresponds to $u = 1.0$. The steep rim corresponds to $y = x + 1/2x - 1$ for which z is indefinite.

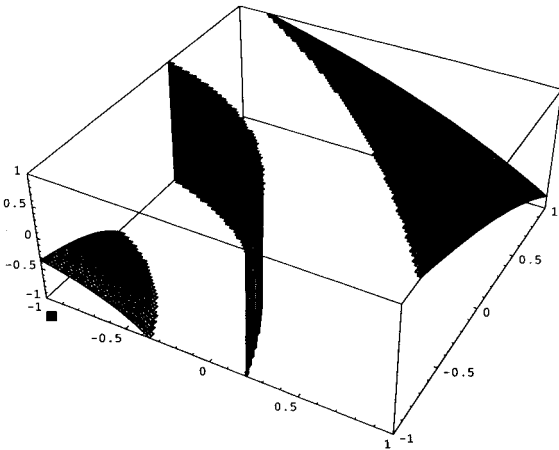


Fig. 7. Upper corner of the cube showing the surface on which $G=0$. This figure corresponds to $u = 0.85$. The steep rim corresponds to (x, y) -values for which z is indefinite.

The transition point from non-critical behaviour to critical behaviour is found at $u=3$. This value corresponds to $T=1/3\sqrt{2}=0.235702$. Since $T=\tanh(K)$ the critical value for K is³

$$K^*=0.2402186.. \quad (52)$$

It is worthwhile to compare the structure of the function $G(x, y, z; u)$ with the function that one encounters for the two-dimensional Ising model. For the latter case one obtains with $u=\sinh(2K)$ ⁽⁵⁾

$$G(x, y, u) = u + \frac{1}{u} - (x + y) \quad -1 \leq x, y \leq 1 \quad (63)$$

The *only* point in the (x, y) -plane for which $G=0$, is $(x, y)=(1, 1)$. In our result, K^* is not an isolated zero point of G in the integration domain but the onset of an interval $[K^*, \infty)$, i.e. for these values of K , there are always points, lines or surfaces for which the function G vanishes. Naively one might expect that the NARP model remains in a critical state from zero temperature up to $T_c=K^*/k_B$, but this is not the case. A formal argument for understanding the regular behaviour of the Helmholtz free energy, despite the appearance of zeros in the integrand is given by extending an observation of Green and Hurst for the 2D Ising model.^(10,11) The free energy is written as a triple contour integral

$$-\beta f \simeq \frac{1}{i^3} \oint_{C_1} \oint_{C_2} \oint_{C_3} \frac{dz_1}{z_1} \frac{dz_2}{z_2} \frac{dz_3}{z_3} G(z_1 + z_1^{-1}, z_2 + z_2^{-1}, z_3 + z_3^{-1}; u) \quad (53)$$

A singularity can in general be easily avoided by changing the integration path, unless a pinching of the contours occurs from opposite sides.

In Fig. 8, the free energy of the NARP model is plotted. The result is obtained by numerical integration. and in Fig. 9, the first derivative is plotted. The derivative is obtained by numerical differentiation of the free energy, using a five-point interpolation scheme.

Since the free energy is explicitly known, it should be possible to obtain the behaviour of some observables around the transition temperature. Though being inspired by the Ising model, the NARP model is

³ This value can be compared with numerical results obtained from numerical renormalization group methods,⁽¹⁵⁾ which give values around 0.25. A method based on numerically estimating the partition function⁽¹⁶⁾ gives a value around 0.24. Therefore, the older calculations suggest that we may actually have a solution to the 3D Ising model. However, more recent calculations contradict with this conclusion⁽⁹⁾ therefore the NARP model is not equivalent to the 3D Ising model.

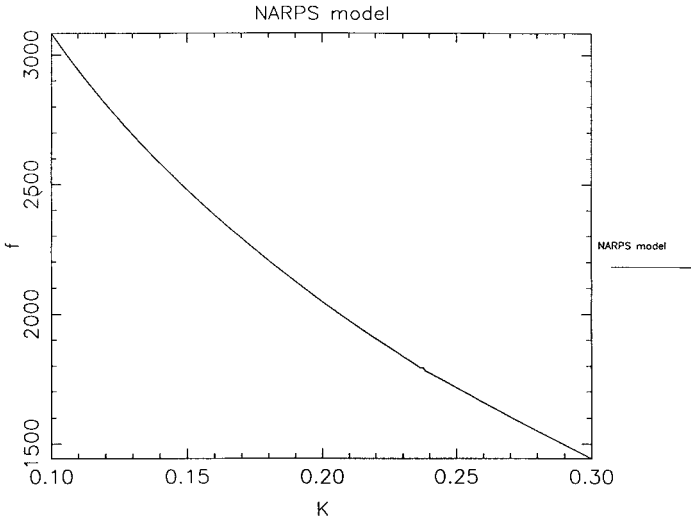


Fig. 8. Free energy of the NARP model.

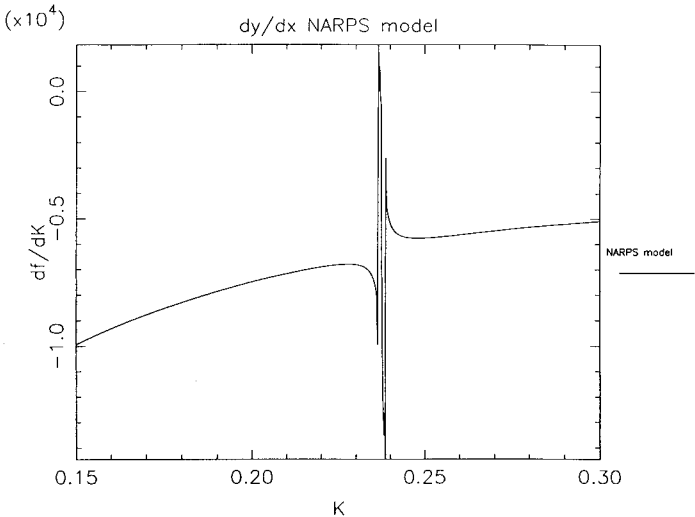


Fig. 9. First derivative of the free energy of the NARP model.

not defined in terms of spins but in terms of random polygons. Therefore, we will not deal with observables which correspond to magnetization. The specific heat is a candidate for further studying the singular behaviour. The internal energy per site, w , is

$$w = \frac{\partial}{\partial \beta} (\beta f) \quad (54)$$

and the heat capacity per site is

$$c = k_B \beta^2 \frac{\partial^2}{\partial \beta^2} (-\beta f) \quad (55)$$

After substitution of the results we obtain the following expression for the specific heat per site

$$\frac{c}{k_B} = K^2 (1 - \omega^2 u^2) \left(-2u \frac{\partial \tilde{f}}{\partial u} + \left(\frac{1}{\omega^2} - u^2 \right) \frac{\partial^2 \tilde{f}}{\partial u^2} \right) \quad (56)$$

and $\tilde{f}(u) = -\beta f(u(T))$ is given in Eq. (45). The three-fold integration in the expression for the Helmholtz free energy complicates the isolation of the asymptotic behaviour considerably. In particular, the familiar arguments from the 2D Ising model, which exploit properties of the elliptic integrals or hypergeometric functions cannot be transposed to our situation. Therefore, we will be using somewhat more heuristic arguments. The non-analytic behaviour of the Helmholtz free energy is determined by the behaviour around $(x, y, z) \simeq (1, 1, 1)$ for u above u_c .

We will analyze the case $\omega = \sqrt{2}$, but this is not essential. Furthermore we consider the upper right corner of the integration domain and return back to the variables ξ , v and η . By using a Taylor expansion of the functions A , B and C , we obtain that

$$\begin{aligned} r^2 &= \xi^2 + v^2 + \eta^2 \\ A &= 3 - \frac{1}{2}r^2 \\ B &= 3 - r^2 \\ C &= 1 - \frac{1}{2}r^2 \end{aligned} \quad (57)$$

and with $r_0 \simeq O(2\pi)$ some upper bound for the integration domain,

$$\tilde{f}_{NA} \simeq \int_0^{r_0} r^2 dr \log |G(r^2, u)| \quad (58)$$

with

$$G(r^2, u) = u^2(u^4 - (6 - r^2)u^3 + (9 - 2r^2)u^2 + (4 - 2r^2)u + 4r^2 - 12) \quad (59)$$

We can rewrite G as

$$\begin{aligned} G(r^2; u) &= a(u)r^2 + b(u) \\ a(u) &= u^2(u^3 - 2u^2 - 2u + 4) \\ b(u) &= u^2(u - 3)(u^3 - 3u^2 + 4) \end{aligned}$$

The nature of the singularity around $u_c = 3$, can be derived from the following integral result

$$\begin{aligned} \tilde{f}_{NA} &\simeq \int_0^{r_0} r^2 dr \log |G(r^2, u)| \\ &= \frac{1}{3} r_0^3 \log(ar_0^2 + b) - \frac{2}{9} r_0^3 + \frac{2}{3} \frac{b}{a} r_0 \\ &\quad + \begin{cases} \frac{1}{3} \left(\frac{|b|}{a}\right)^{3/2} \log\left(\frac{r_0 + \sqrt{|b|/a}}{r_0 - \sqrt{|b|/a}}\right) & \text{if } b < 0 \\ -\frac{2}{3} \left(\frac{b}{a}\right)^{3/2} \arctan\left(\frac{r_0}{\sqrt{b/a}}\right) & \text{if } b > 0 \end{cases} \end{aligned}$$

Although the zero of G is in the integration domain for $u < 3$, the result is regular. In particular, we obtain the following nature of the singularity for the specific heat c around the critical point K^*

$$c \simeq \begin{cases} \text{constant} & \text{if } K > K^* \\ \frac{1}{\sqrt{K^* - K}} & \text{if } K < K^* \end{cases} \quad (60)$$

6. COMPARISON WITH RELATED WORK

The hunt for a polynomial expression in the integrand of the free energy of the simple cubic Ising model, the so-called *critical polynomial*, has been ongoing, since the discovery of the Onsager solution for the two dimensional Ising model. A recent status has been presented by Fisher.⁽¹⁷⁾ In that work a warning is placed that such a polynomial may not even exist, since a mere matching of the value of K^* is not sufficient for having obtained a solution of the 3D Ising model.

A polynomial of the type in the foregoing section has been proposed by He, Xu and Hao. Their approximation of the 3D-Ising model corresponds to $\omega = 1$ in our work. In this case, we obtain

$$G(x, y, z; u) = u^6 - 2Au^5 + 3u^4 + (4A + 16C)u^3 + (3 - 8B)u^2 - 10Au - 7 \quad (61)$$

The onset of critical behaviour takes place for $x = y = z = 1$. This results into the following equation for u .

$$G(1, 1, 1; u) = ((u - 1)^2 - 2)^2 ((u - 1)^2 - 8) = 0 \quad (62)$$

The positive roots of this equation are $u_1^* = 1/T_1^* = 1 + \sqrt{2}$ and $u_2^* = 1/T_2^* = 1 + 2\sqrt{2}$, and correspond to $T_c = 0.4142$ and $T_c = 0.2612$. The values have also been reported in ref. 8.

Noting that if ω becomes larger, then T^* becomes smaller, we have obtained a closed-form relation of $T^*(\omega)$ from the root-equation, which is obtained from Eq. (46)

$$(\omega^2 u^2 - 2\omega^2 u + \omega^2 - 8)(\omega^2 u^2 - 2\omega^2 u + \omega^2 - 2)^2 = 0 \quad (63)$$

The result is

$$T^* = \frac{1}{\omega \pm 2\sqrt{2}} \quad T^* = \frac{1}{\omega \pm \sqrt{2}} \quad (64)$$

In particular, the choice $\omega = \sqrt{3}$, gives $T^* = 0.2192753$, whereas the Ferrenberg–Landau (FL) value is $T^* = 0.2180992 \pm 0.0000025$. An overview of some “special” values for ω is given in Table 3. Of course, so far, any deeper motivation for choosing one of these values is lacking. Moreover, although numbers like $\sqrt{3}$ or $\sqrt{\pi}$ are close to ω_{FL} , they fall outside the error bars.

Table 3

ω	K^*	T^*	Model
$\sqrt{\pi} \simeq 1.77$	0.2208726	0.2173497	
1.75664259	0.2216595(26)	0.2180992(25)	FL
$\sqrt{3} \simeq 1.73$	0.2228946	0.2192753	
$\sqrt{2}$	0.2402186	0.2357023	this work
1	0.2674000	0.2612039	He, Xu, Hao

7. CONCLUSIONS

We have followed Feynman's method to construct a model in statistical physics using non-abelian phase factors for turning points in random polygons. The model is exactly solvable, and the free energy is analysed in detail. The essential part in the calculation consists of identifying the sum over all graphs corresponding to an unconstrained random walk problem with complex weights. The model exhibits an asymmetric phase transition point.

Our result may contribute to a better understanding of random-walk problems in three dimensions with non-abelian transition amplitudes, since an explicit solution for such a model has been constructed.

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