THE XY-MODEL AND THE SELF-AVOIDING WALK APPROXIMATION[‡]

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The SAW-approximation is calculated for the quantum-mechanical XY-model for spin $\frac{1}{2}$ in a parallel magnetic field. For this purpose we derive an exact expression for the internal weight factors of the polygon graphs.

In this approximation we obtain an analytic expression for the phase-separation line in the (H, T) -phase. The critical exponents are the same as for classical models.

1. Introduction

The usual procedure to derive series expansions for lattice models is to establish a correspondence between the different terms in an expansion of some thermodynamic functions and the different graphs that can be drawn on a lattice, according to some specific rules¹⁾. The contribution of each graph factorizes in two parts, the first being a numerical constant (lattice constant) derived from the number of embeddings of the graph in the underlying lattice, the second being an internal weight factor of the graph, determined by the hamiltonian.

In the self-avoiding walk (SAW) approximation²⁾ one rejects in every order of the expansion all graphs except the one with the largest lattice constant. In this way one obtains the closed polygons as SAW-graphs for the free energy and the open chains for susceptibility-type functions. This SAW-approximation has been applied quite successfully⁴⁾ to several classical models, like the Ising model^{3,4)} and the classical Heisenberg model⁴⁾, which have the advantage that the internal weight factors of the graphs can be determined rather easily. The asymptotic expressions for the lattice constants of the SAW-graphs with a large number of bonds are given in standard notation by

$$n^{-1}u_n \sim \mu^n n^{-h-1} \quad (1a)$$

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and

$$c_n \sim \mu^n n^g \quad (1b)$$

for closed polygons and open chains respectively. μ is the connective constant of the lattice (e.g. $\mu \simeq 10.035$ for the f.c.c. lattice) and in three dimensions $h = \frac{7}{4}$, $g = \frac{1}{6}$. As a result one obtains a critical point at μ^{-1} and critical exponents which are somewhere between the mean-field exponents, and the exact exponents.

This partial success allows us to expect that an analogous approximation to the thermodynamic functions of the XY-model will also give non-trivial results, which should contain an improvement over the mean-field approximation. Betts *et al.*^{1,5}) have derived a graphical representation of the high-temperature series expansions for this model, and this method has been extended by Dekeyser and Rogiers⁶) to the case where an external parallel magnetic field is present. The main difficulty in applying the SAW-approximation to this quantum-mechanical model is to obtain an asymptotic expression for the internal weight factors of the SAW-graphs.

2. The self-avoiding walk approximation for the partition function

In ref. 6 it has been shown that the partition function Z for the spin $\frac{1}{2}$ XY hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} (a_i^+ a_j + a_j^+ a_i) - H \sum_i S_i^z, \quad (2)$$

where $\langle ij \rangle$ indicates a summation over all nearest-neighbour pairs, may be expanded (with $\beta = 1/kT$) as

$$\begin{aligned} \frac{1}{N} \log Z = \log \left(2 \cosh \frac{\beta H}{2} \right) + \sum_{n=2}^{\infty} \sum_{s=2}^n \sum_{m=1}^{s-1} A(n, s, m) \frac{(\beta J)^n}{(n-1)!} \\ \times (1+y)^{-s} y^m, \end{aligned} \quad (3)$$

where

$$y = \exp(\beta H). \quad (4)$$

This expansion is a result of a summation over the contributions of all ordered graphs of arrows between the lattice points (vertices), where an arrow pointing from j to i comes from the operator $(a_i^+ a_j)$. When we read the operators in a given contributing ordering from right to left, some vertices will first appear with an annihilation operator (an arrow tail), others with a creation operator (an arrow

head); we call them of type I or II, respectively. In the following example, vertex 1 is of type II, vertices 2 and 3 are of type I:

$$(a_2^+ a_1 a_3^+ a_2 a_1^+ a_3).$$

In considering the $n!$ orderings of a given graph g_{ns} with n arrows and s vertices, let us call $X(g_{ns}, m)$ the number of these orderings with exactly m vertices of type I, the remaining $(s - m)$ ones then being of type II. The contribution of the graph g_{ns} to (3) is then shown⁶) to be given by

$$\frac{(\beta J)^n}{n!} N(g_{ns}) S(g_{ns}) (1 + y)^{-s} \sum_{m=0}^s X(g_{ns}, m) y^m, \quad (5)$$

where N and S are the lattice constant and the symmetry factor of the graph. The functions $X(g, m)$ obey the rules

$$X(g_{ns}, 0) = 0 = X(g_{ns}, s) \quad (6)$$

and

$$X(g_{ns}, m) = X(g_{ns}, s - m). \quad (7)$$

In the self-avoiding walk approximation, we only retain the closed-polygon graphs P_n , for which $s = n$. Except for their large lattice constants, we can find here an extra justification for this SAW-approximation in the fact that these are the only graphs for which all $n!$ orderings give a non-zero (positive) contribution.

The lattice constants $N(P_n)$ are given asymptotically by (1a), and $S(P_n) = 2$, since there are two ways to walk around a polygon.

Since the number of vertices of type I does not change in a cyclic permutation of the arrow ordering as was shown in ref. 6, all $X(g_{ns}, m)$ are entire multiples of n , and we therefore prefer to work with the reduced weights:

$$T(n, m) = n^{-1} X(P_n, m). \quad (8)$$

In the SAW-approximation, we thus obtain the free energy of the XY-model from

$$F = \frac{1}{N} \log Z \simeq \log (2 \cosh \tfrac{1}{2} \beta H) + 2 \sum_{n=2}^{\infty} \frac{(\beta J / (1 + y))^n}{(n - 1)!} N(P_n) \sum_{m=0}^n y^m T(n, m). \quad (9)$$

We may remark at this point that the Takagi model, treated in ref. 6 in analogy with the XY-model, will not exhibit a tricritical point in the SAW-approximation. In the partition function for this model, we have to replace in (3) the factor

$(1 + y)^{-s}$ by x^s , where x is an independent variable, arising from the presence of a second field variable. The only effect of this factor in the approximation (9) is to rescale the temperature from βJ into βJx , and this can never lead to a tricritical point.

3. Properties of the $T(n, m)$

On a closed polygon P_n all orderings of the arrows give a non-vanishing contribution for the spin $\frac{1}{2}$ XY model, since only the presence of two creation (or annihilation) operators on the same vertex can cause the vanishing of the contribution. Therefore

$$\sum_m T(n, m) = (n - 1)!. \quad (10)$$

Furthermore, no ordering gives $m = 0$ or $m = n$, and only the n orderings in which one walks along the polygon in an uninterrupted way give $m = 1$, since only at the starting vertex do we find an arrow tail before a head. Thus

$$T(n, 0) = T(n, n) = 0, \quad T(n, 1) = T(n, n - 1) = 1. \quad (11)$$

We now derive a recursion relation for the reduced weights. Let us therefore consider all $(n - 1)!$ orderings of an $(n - 1)$ -polygon with vertices labeled $1, 2, \dots, n - 1$. We want to put an extra vertex with label n between the $(n - 1)$ - and the 1-vertex, by replacing $(a_1^+ a_{n-1})$ by $(a_n^+ a_{n-1})$ and adding a new factor $(a_1^+ a_n)$. If we put this new factor in front of the other factors, then all the cyclic permutations of these $(n - 1)!$ orderings give all $n!$ new orderings.

$T(n, m)$ is then by its definition equal to the number of the new orderings with $(a_1^+ a_n)$ in front, and with exactly m vertices of type I.

In the original ordering we may encounter two different situations:

a) Vertex 1 was of type I; this means that the operators were ordered like

$$\dots (a_1^+ a_{n-1}) \dots (a_2^+ a_1) \dots$$

The addition of a new vertex transforms this into

$$(a_1^+ a_n) \dots (a_n^+ a_{n-1}) \dots (a_2^+ a_1) \dots,$$

which has the same m -value as before, since vertex 1 is still of type I and the new vertex n is of type II.

b) Vertex 1 was of type II, the operators were ordered as

$$\dots (a_2^+ a_1) \dots (a_1^+ a_{n-1}) \dots$$

With the n th vertex this gives

$$(a_1^+ a_n) \cdots (a_2^+ a_1) \cdots (a_n^+ a_{n-1}) \cdots$$

Here vertex 1 changes its type from II to I, and if we want to arrive at m vertices of type I, we must start from an original ordering with $(m - 1)$ vertices of type I.

In order to obtain the $T(n, m)$ desired orderings, we must thus start from those orderings out of the $X(P_{n-1}, m)$ ones which are in situation a) and from those of the $X(P_{n-1}, m - 1)$ ones which are in situation b). Due to the rotational symmetry of the polygon the number of permutations in which a given vertex is of type I is the same for all vertices, and it must be equal to $X(P_n, m) m/n$. The number of permutations for which a given vertex is of type II is then $X(P_n, m) (n - m)/n$. This means that we finally obtain

$$T(n, m) = \frac{m}{n-1} X(P_{n-1}, m) + \frac{(n-1) - (m-1)}{n-1} X(P_{n-1}, m-1)$$

or

$$T(n, m) = mT(n-1, m) + (n-m)T(n-1, m-1). \quad (12)$$

To the existence of such a recursion relation was already hinted by Lee⁷). The solution of this relation with the boundary conditions (11) is given by

$$T(n, m) = \sum_{k=0}^m (-1)^k \binom{n}{k} (m-k)^{n-1}. \quad (13)$$

For a given n these functions have a sharp maximum at $m = n/2$, in the neighbourhood of which they behave almost like a gaussian exponential.

4. The thermodynamic functions

By substituting (13) in (9) one now obtains for the summation over m

$$\begin{aligned} \sum_{m=0}^n y^m T(n, m) &= \sum_{m=0}^n \exp(\beta H m) \sum_{k=0}^m (-1)^k \binom{n}{k} (m-k)^{n-1} \\ &= \sum_{k=0}^n (-1)^k \binom{n}{k} \exp(\beta H k) \sum_{p=0}^{n-k} \exp(\beta H p) p^{n-1} \\ &\simeq (-1/\beta H)^n (n-1)! \exp(\beta H n) \sum_{k=0}^n (-1)^k \binom{n}{k} \\ &\quad \times \sum_{j=n}^{\infty} (-\beta H)^j (n-k)^j / j!. \end{aligned} \quad (14)$$

We approximated the sum over $p = m - k$ by an integral, which approximation we expect to be valid in the asymptotic limit for large n . The sum over k may now be recognized to produce the Stirling numbers of the second kind^{8,9)}:

$$\sum_{k=0}^n (-1)^k \binom{n}{k} (n-k)^j = n! \mathcal{S}_j^{(n)} \quad (15)$$

and since⁸⁾

$$n! \sum_{j=n}^{\infty} \mathcal{S}_j^{(n)} \frac{(-\beta H)^j}{j!} = (\exp(-\beta H) - 1)^n, \quad (16)$$

we finally obtain for the singular part of the free energy (9), also using (1a):

$$F_s \sim 2 \sum_n \left[\frac{J\mu}{H} \operatorname{tgh} \frac{\beta H}{2} \right]^n n^{-h-1} \sim 2\Gamma(-h) \left[-\log \left(\frac{J\mu}{H} \operatorname{tgh} \frac{\beta H}{2} \right) \right]^h. \quad (17)$$

This expression is only valid in the high-temperature domain, *i.e.* for $\beta < \beta_c$ where the critical temperature is determined by the singularity of the logarithm appearing in (17):

$$\beta_c = \frac{2}{H} \operatorname{tgh}^{-1} \left(\frac{H}{J\mu} \right). \quad (18)$$

This expression for the boundary in the (H, T) -phase between the ferro- and paramagnetic phases is the same expression as derived by mean-field theory, except for the appearance of μ instead of the coordination number q of the lattice. As a consequence we obtain

$$kT_c(H=0)/J = \mu/2 \quad (19)$$

which is 5.017 for the f.c.c. lattice, compared to 6 in mean-field theory and 4.524 from series expansion analysis. The ground state critical field predicted by (18) is

$$H_c(T=0) = J\mu \quad (20)$$

compared to Jq in mean-field theory. Austen and Plischke¹⁰⁾ argued that $H_c(0)$ should be exactly equal to Jq ; series expansion analysis is inconclusive.

For $\beta \gtrsim \beta_c$, the free energy (17) behaves like

$$F_s \sim 2\Gamma(-h) \left[\frac{\mu^2 - (H/J)^2}{2\mu} J(\beta_c - \beta) \right]^h \quad (21)$$

which gives as specific heat critical exponent $\alpha = 2 - h$. This is the same exponent as derived by the SAW-approximation for the Ising and classical Heisenberg model, which seems to indicate that the argument by de Gennes¹¹), namely that all SAW-approximations belong to the universality class $n = 0$, may also be applied to the quantum models. (21) gives also a prediction on the amplitudes of the specific heat singularity.

In an analogous way one can derive the fluctuation series^{5,6}) from the open chain graphs. Its singular part, which gives also the singular part of the transverse susceptibility, has the same form as (21), but with h replaced by $(-g - 1)$. The critical exponent γ is $(g + 1)$, i.e. $\gamma = \frac{7}{6}$ for $d = 3$ instead of $\gamma = 1.33$ from series expansions. The amplitude predicted for the susceptibility singularity does not agree with series analysis results⁶); an increase of the amplitudes is predicted with increasing H , whereas series analysis indicates a decrease.

5. The classical XY-model

For the classical XY-model, or plane rotator, one has to calculate instead of (5) the contribution of the n -sided polygons in the following way, by integrating over the angles Ω_i of the vectors S_i with fixed length $S = \frac{1}{2}$:

$$(\beta J)^n N(P_n) C^{-n} \left(\prod_{i=1}^n \int d\Omega_i \right) \exp \left(\beta H \sum_{j=1}^n S_j^z \right) (S_1^x S_2^x + S_1^y S_2^y) \cdots (S_n^x S_1^x + S_n^y S_1^y) \quad (22)$$

where C is the normalization

$$C = \int d\Omega \exp(\beta H S^z) = \frac{8\pi}{\beta H} \sinh \frac{\beta H}{2}. \quad (23)$$

This gives for the singular part of the free energy

$$F_s \sim \sum_n \left[\frac{2J\mu}{H} \left(\coth \frac{\beta H}{2} - \frac{2}{\beta H} \right) \right]^n n^{-h-1}; \quad (24)$$

and the classical phase diagram is determined by

$$\coth \frac{\beta_c H}{2} - \frac{2}{\beta_c H} = \frac{H}{2J\mu}. \quad (25)$$

6. Conclusion

We have derived the SAW-approximation for the thermodynamic functions of the quantum-mechanical XY -model for spin $\frac{1}{2}$. The critical exponents are the same as the SAW-exponents for the Ising model, confirming an argument by de Gennes¹¹). The phase diagram in the (H, T) -plane is determined analytically and we obtain the mean-field phase boundary scaled by a factor μ/q . The predictions on the critical amplitude are contradicted by series analysis.

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