HIGH TEMPERATURE SERIES EXPANSION FOR THE SPIN $\frac{1}{2}$ XY-MODEL IN A MAGNETIC FIELD

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Series expansions for the partition function and the fluctuation in the long range order parameter are presented for the spin $1/2$ XY-model on the f.c.c. lattice with an external magnetic field in the z-direction.

The high temperature series expansions for the spin $\frac{1}{2}$ XY-model in zero magnetic field have been studied extensively by Betts et al. [1-4]. With a magnetic field the full Hamiltonian is the sum of two commuting parts H_1 and H_2 :

$$H_1 = -H \sum_i \sigma_i^z, \quad H_2 = -2J \sum_{\langle ij \rangle} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) = -J \sum_{\langle ij \rangle} (a_i^+ a_j + a_i a_j^+)$$

and the partition function can, with $K = \beta J$, be written as

$$Z = (2 \cosh \frac{1}{2} \beta H)^N \sum_{n=0}^{\infty} \frac{K^n}{n!} \text{Tr} \left\{ \prod_i [\exp(\beta H \sigma_i^z) (2 \cosh \frac{1}{2} \beta H)^{-1}] \left(\sum_{\langle ij \rangle} (a_i^+ a_j + a_i a_j^+) \right)^n \right\}.$$

The different terms in this sum give rise to the ordered directed graphs of ref. [3], and the graphs and their ordering of arrows have to satisfy the conditions mentioned there in order to give a non-zero contribution. The contribution to the trace of a given ordered graph can be seen to be given by

$$\exp(\beta H r) [1 + \exp(\beta H)]^{-s}$$

where s is the number of vertices of the graph and r is the number of vertices that in the ordered product of creation and annihilation operators appear first with a creation operator. Adding up the contributions of the different graphs, we obtain for the f.c.c. lattice the following result:

$$\begin{aligned} \frac{1}{N} \ln Z = & \ln(2 \cosh \frac{1}{2} \beta H) + 6x^2y K^2 + 8x^3(y+y^2) K^3 + \{x^2y + 22x^3(y+y^2) + 22x^4(y+y^3) - 50x^4y^2\} K^4/2 \\ & + \{2x^3(y+y^2) + 20x^4(y+y^3) + 120x^4y^2 + 14x^5(y+y^4) - 110(y^2+y^3)\} K^5 \\ & + \{x^2y + 82x^3(y+y^2) + 811x^4(y+y^3) + 6034x^4y^2 + 1656x^5(y+y^4) \\ & + 9264x^5(y^2+y^3) + 970x^6(y+y^5) - 17740x^6(y^2+y^4) - 1020x^6y^3\} K^6/60 \\ & + \{3x^3(y+y^2) + 72x^4(y+y^3) + 648x^4y^2 + 380x^5(y+y^4) + 10394x^5(y^2+y^3) + 488x^6(y+y^5) \\ & + 364x^6(y^2+y^4) - 30264x^6y^3 + 257x^7(y+y^6) - 9261x^7(y^2+y^5) + 21244x^7(y^3+y^4)\} K^7/15 \\ & + \{x^2y + 266x^3(y+y^2) + 6678x^4(y+y^3) + 78878x^4y^2 + 45648x^5(y+y^4) + 1745544x^5(y^2+y^3) \\ & + 113712x^6(y+y^5) - 5624696x^6(y^2+y^4) + 12090784x^6y^3 + 114128x^7(y+y^6) - 1500464x^7(y^2+y^5) \\ & - 27250944x^7(y^3+y^4) + 56092x^8(y+y^7) - 3589984x^8(y^2+y^6) + 26250148x^8(y^3+y^5) \\ & + 28650448x^8y^4\} K^8/3360 \end{aligned}$$

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$$\begin{aligned}
& + \{85x^3(y+y^2) + 3876x^4(y+y^3) + 54072x^4y^2 + 41868x^5(y+y^4) + 2287548x^5(y^2+y^3) + 168162x^6(y+y^5) \\
& + 19276728x^6(y^2+y^4) + 64999788x^6y^3 + 281979x^7(y+y^6) + 21944151x^7(y^2+y^5) - 32060178x^7(y^3+y^4) \\
& + 244314x^8(y+y^7) - 10423692x^8(y^2+y^6) - 126618426x^8(y^3+y^5) + 141144408x^8y^4 + 113016x^9(y+y^8) \\
& - 12141456x^9(y^2+y^7) + 204414912x^9(y^3+y^6) + 131383128x^9(y^4+y^5)\} K^9/7560 \\
& + \dots
\end{aligned}$$

where we abbreviated $y = \exp(\beta H)$ and $x = (1+y)^{-1}$. The square of the long range order fluctuation may also be expressed in the same way:

$$\begin{aligned}
Y \equiv \frac{1}{N} \sum_{i,j=1}^N \langle a_i^+ a_j + a_i a_j^+ \rangle &= 1 + 24x^2yK + 132x^3(y+y^2)K^2 + \{4x^2y + 88x^3(y+y^2) + 468x^4(y+y^3) + 1320x^4y^2\} K^3 \\
&+ \{34x^3(y+y^2) + 424x^4(y+y^3) + 2544x^4y^2 + 1225x^5(y+y^4) + 7979x^5(y^2+y^3)\} K^4 \\
&+ \{x^2y + 82x^3(y+y^2) + 1264x^4(y+y^3) + 9210x^4y^2 + 6318x^5(y+y^4) \\
&+ 97842x^5(y^2+y^3) + 12711x^6(y+y^5) + 176266x^6(y^2+y^4) + 382606x^6y^3\} K^5/5 \\
&+ (112x^3(y+y^2) + 3246x^4(y+y^3) + 29368x^4y^2 + 26267x^5(y+y^4) + 711205x^5(y^2+y^3) + 84544x^6(y+y^5) \\
&+ 2921136x^6(y^2+y^4) + 6904480x^6y^3 + 131143x^7(y+y^6) + 3800031x^7(y^2+y^5) + 15160346x^7(y^3+y^4)) K^6/30 \\
&+ (x^2y + 266x^3(y+y^2) + 8814x^4(y+y^3) + 102978x^4y^2 \\
&+ 92058x^5(y+y^4) + 3490714x^5(y^2+y^3) + 438372x^6(y+y^5) + 30444042x^6(y^2+y^4) \\
&+ 89755128x^6y^3 + 1065194x^7(y+y^6) + 76977434x^7(y^2+y^5) + 362450012x^7(y^3+y^4) \\
&+ 1347679x^8(y+y^7) + 81842422x^8(y^2+y^6) + 548159021x^8(y^3+y^5) + 968025916x^8y^4) K^7/210 \\
&+ \dots
\end{aligned}$$

In computing these contributions, extensive use was made of the tables of lattice constants of Baker et al. [5].

The same expansions, with different expressions for x and y , also apply to the model proposed by Takagi [6] for liquid ^3He – ^4He mixtures, at least to the superfluid driven stratification part of his Hamiltonian. If e.g. we resume our formula for the partition function of the XY -model by

$$\frac{1}{N} \ln Z - \ln(2 \cosh \frac{1}{2} \beta H) = F(x, y, K),$$

then the partition function Z for the Takagi-Hamiltonian is given by

$$\frac{1}{N} \ln Z + \ln x' = F(x', y', 2K)$$

where

$$y' = \exp(\beta(H_1 + H_2)), \quad x' = [1 + y'(1 + \exp(-2\beta H_1))]^{-1};$$

H_1 and H_2 are essentially the difference and the sum of the chemical potentials of ^4He and ^3He . For more details, we refer to [6]. A numerical analysis of this model will be presented in a forthcoming publication.

A preliminary analysis has been done for the Y -series of the XY -model, by ratio method and Padé approximants [7]. The results are given in fig. 1, where they are compared with the molecular field results. For higher magnetic fields, the uncertainty on the critical temperature becomes too large to give decisive results, and more sophisticated methods will have to be applied. The critical exponent γ does not show a significant variation with H .

Fig. 1. The critical temperature for the spin $1/2$ XY-model on a f.c.c. lattice as a function of the magnetic field in the z-direction. The dotted line gives the molecular field result and the solid line the result of our series expansions.

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