SOME CRITICAL PROPERTIES OF A THREE-DIMENSIONAL SYSTEM OF RANDOMLY MIXED HEISENBERG AND ISING BONDS*

By A. Pękalski

Institute of Theoretical Physics, University of Wrocław**

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Using the high temperature series expansion method, the three-dimensional system of randomly mixed Heisenberg and Ising bonds is considered. The dependence of critical temperature and susceptibility critical exponent γ on concentration of Heisenberg-type bonds is found to be continuous. The crossover exponent is estimated.

In the previous papers [1, 2] we have investigated some critical properties of a random mixture of two kinds of bonds: isotropic Heisenberg-like and anisotropic Ising-like. Using the high temperature series expansion method we have calculated five terms in the susceptibility series for the square lattice. From those series we have been able to estimate the dependence of the critical temperature and the susceptibility index γ on the concentration of one kind of bonds. In this note we present a continuation of the previous investigations for the case of two three dimensional lattices, the b.c.c. and s.c. Since the physical mechanism responsible for the considered system is the same as before, and the method used here is the same as that employed in [1, 2], we refer the reader to [1, 2] and references cited therein for all the details.

The coefficients of the susceptibility series for the b.c.c. lattice and arbitrary spin are

$$a_1 = 16/3X\Lambda_1,$$

$$a_2 = 1/45\{X^2[1120\Lambda_1^2+64\mu_2]-X[120\lambda_2+48\mu_2]\},$$

$$a_3 = 1/675\{X^3[78400\Lambda_1^3-2400\Lambda_1\lambda_2+8160\Lambda_1\mu_2+1440\lambda_3+864\mu_3]$$
$$-X^2[16800\Lambda_1\lambda_2+6720\Lambda_1\mu_2+960\lambda_3+576\mu_3]$$
$$+X[960\lambda_3+96\mu_3]\},$$

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** Address: Instytut Fizyki Teoretycznej, Uniwersytet Wrocławski, Cybulskiego 36, 50-205 Wrocław, Poland.

$$
\begin{aligned}
a_4 = 1/14175\{&X^4[7521920\Lambda_1^4 - 470400\Lambda_1^2\lambda_2 + 1097600\Lambda_1^2\mu_2 + 282240\Lambda_1\lambda_3 \\
&+ 169344\Lambda_1\mu_3 - 107520\lambda_1^4 + 24192\lambda_2\mu_2 + 29568\mu_2^2 + 3456\mu_4] \\
&- X^3[80640\Lambda_1^4 + 2391200\Lambda_1^2\lambda_2 + 940800\Lambda_1^2\mu_2 + 171360\Lambda_1\lambda_3 \\
&+ 112896\Lambda_1\mu_3 - 25200\lambda_2^2 + 132048\lambda_2\mu_2 + 74592\mu_2^2 + 53760\lambda_1^4 + 25200\lambda_4 + 6624\mu_4] \\
&+ X^2[188160\Lambda_1\lambda_3 + 18816\Lambda_1\mu_3 + 176400\lambda_2^2 + 150528\lambda_2\mu_2 \\
&+ 39312\mu_2^2 + 25200\lambda_4 + 3984\mu_4] \\
&- X[12600\lambda_4 + 720\mu_4]\},
\end{aligned}
$$

$$
\begin{aligned}
a_5 = 1/297675\{&X^5[718332160\Lambda_1^5 - 74793600\Lambda_1^3\lambda_2 + 137965184\Lambda_1^3\mu_2 \\
&+ 705600\Lambda_1\lambda_2^2 - 1373568\Lambda_1\lambda_2\mu_2 + 6325312\Lambda_1\mu_2^2 \\
&+ 41489280\Lambda_1^2\lambda_3 + 24893568\Lambda_1^2\mu_3 - 423360\lambda_2\lambda_3 - 846720\mu_2\lambda_3 \\
&- 2032128\lambda_2\mu_3 + 907200\mu_2\mu_3 - 211680\Lambda_1\lambda_4 + 635040\Lambda_1\mu_4 \\
&+ 22353408\Lambda_1\lambda_1\lambda_2\mu_1 - 25589760\Lambda_1\lambda_1^4 + 10160640\lambda_1^3\lambda_2 \\
&+ 7451136\mu_1^3\lambda_2 + 90720\lambda_5 + 38880\mu_5] \\
&- X^4[13547520\Lambda_1^5 + 196000000\Lambda_1^3\lambda_2 + 9031680\Lambda_1\lambda_1^4 + 121664256\Lambda_1^3\mu_2 \\
&+ 24366720\Lambda_1^2\lambda_3 + 16595712\Lambda_1^2\mu_3 - 13171200\Lambda_1\lambda_2^2 \\
&+ 18527488\Lambda_1\lambda_2\mu_2 + 15861888\Lambda_1\mu_2^2 + 330822912\Lambda_1\lambda_1\lambda_2\mu_1 \\
&+ 4798080\Lambda_1\lambda_4 + 1270080\Lambda_1\mu_4 + 4656960\lambda_2\lambda_3 + 2540160\mu_2\mu_3 \\
&+ 423360\lambda_2\mu_3 + 451584\mu_2\lambda_3 + 110575360\lambda_2\lambda_1^3 + 110274304\lambda_2\mu_1^3 \\
&+ 181440\lambda_5 + 77760\mu_5] \\
&+ X^3[40748400\Lambda_1\lambda_2^2 + 52454304\Lambda_1\lambda_2\mu_2 + 8382528\Lambda_1\mu_2^2 + 26836320\Lambda_1^2\lambda_3 \\
&+ 2765952\Lambda_1^2\mu_3 + 4798080\Lambda_1\lambda_4 + 776160\Lambda_1\mu_4 + 7281792\Lambda_1\lambda_1\lambda_2\mu_1 \\
&+ 677376\Lambda_1^3\mu_2 + 4480560\lambda_2\lambda_3 + 1552320\mu_2\mu_3 + 2328480\mu_2\lambda_3 \\
&+ 1255968\lambda_2\mu_3 + 3951360\lambda_2\lambda_1^3 + 2427264\lambda_2\mu_1^3 + 532224\lambda_5 \\
&+ 64800\mu_5] \\
&- X^2[2469600\Lambda_1\lambda_4 + 141120\Lambda_1\mu_4 + 4939200\lambda_2\lambda_3 + 282240\mu_2\mu_3 \\
&+ 1968624\mu_2\lambda_3 + 296352\lambda_2\mu_3 + 526176\lambda_5 + 25920\mu_5] \\
&+ X[193536\lambda_5 + 4320\mu_5]\},
\end{aligned}
$$

where

$$
X := S(S+1), \quad \lambda_n := p(J^{\mathrm{H}})^n, \quad \mu_n := (1-p)(J^{\mathrm{I}})^n,
$$

and

$$\Lambda_1 := \lambda_1 + \mu_1.$$

For the s.c. lattice the coefficients are

$$a_1 = 4X\Lambda_1,$$

$$a_2 = 1/15\{X^2[200\Lambda_1^2 + 16\mu_2] - X[30\lambda_2 + 12\mu_2]\},$$

$$\begin{aligned} a_3 = {} & 1/225\{X^3[10000\Lambda_1^3 - 600\Lambda_1\lambda_2 + 1400\Lambda_1\mu_2 + 360\lambda_3 + 216\mu_3] \\ & - X^2[3000\Lambda_1\lambda_2 + 1200\Lambda_1\mu_2 + 240\lambda_3 + 144\mu_3] \\ & + X[240\lambda_3 + 24\mu_3]\}, \end{aligned}$$

$$\begin{aligned} a_4 = {} & 1/4725\{X^4[686560\Lambda_1^4 - 84000\Lambda_1^2\lambda_2 + 50400\Lambda_1\lambda_3 + 128800\Lambda_1^2\mu_2 \\ & + 30240\Lambda_1\mu_3 - 8960\lambda_1^4 + 3360\lambda_2\mu_2 + 4960\mu_2^2 + 864\mu_4] \\ & - X^3[6720\Lambda_1^4 + 301000\Lambda_1^2\lambda_2 + 29400\Lambda_1\lambda_3 + 117600\Lambda_1^2\mu_2 \\ & + 20160\Lambda_1\mu_3 + 4480\lambda_1^4 + 22260\lambda_2\mu_2 + 13080\mu_2^2 + 1656\mu_4 \\ & - 6300\lambda_2^2 + 6300\lambda_4] \\ & + X^2[33600\Lambda_1\lambda_3 + 3360\Lambda_1\mu_3 + 26880\lambda_2\mu_2 + 31500\lambda_2^2 + 6300\lambda_4 \\ & + 7020\mu_2^2 + 996\mu_4] \\ & - X[3150\lambda_4 + 180\mu_4]\}, \end{aligned}$$

$$\begin{aligned} a_5 = {} & 1/99225\{X^5[46867520\Lambda_1^5 - 9290400\Lambda_1^3\lambda_2 + 11272352\Lambda_1^3\mu_2 + 176400\Lambda_1\lambda_2^2 \\ & + 3998400\Lambda_1\lambda_2\mu_2 + 669200\Lambda_1\mu_2^2 + 5292000\Lambda_1^2\lambda_3 + 3175200\Lambda_1^2\mu_3 \\ & + 110376\Lambda_1\mu_4 - 52920\Lambda_1\lambda_4 - 1630720\Lambda_1\lambda_1^4 - 105840\lambda_2\lambda_3 \\ & + 1199520\mu_2\lambda_3 - 381024\lambda_2\mu_3 + 220752\mu_2\mu_3 + 611226\lambda_2\mu_1^3 \\ & + 846720\lambda_2\lambda_1^3 + 1833678\Lambda_1\lambda_1\lambda_2\mu_1 + 22680\lambda_5 + 9720\mu_5] \\ & - X^4[752640\Lambda_1^5 + 501760\Lambda_1\lambda_1^4 + 17326400\Lambda_1^3\lambda_2 + 10734528\Lambda_1^3\mu_2 \\ & - 2352000\Lambda_1\lambda_2^2 + 1864800\Lambda_1\mu_2^2 - 2665600\Lambda_1\lambda_2\mu_2 + 2940000\Lambda_1^2\lambda_3 \\ & + 2116800\Lambda_1^2\mu_3 + 846720\Lambda_1\lambda_4 + 224784\Lambda_1\mu_4 + 30077376\Lambda_1\lambda_1\lambda_2\mu_1 \\ & + 10050880\lambda_1^3\lambda_2 + 9768640\mu_1^3\lambda_2 + 811440\lambda_2\lambda_3 + 449568\mu_2\mu_3 \\ & + 169344\lambda_2\mu_3 + 34860\mu_2\lambda_3 + 45360\lambda_5 + 19440\mu_5] \\ & + X^3[5071500\Lambda_1\lambda_2^2 + 1033200\Lambda_1\mu_2^2 + 4733400\Lambda_1\lambda_2\mu_2 + 3381000\Lambda_1^2\lambda_3 \\ & + 352800\Lambda_1^2\mu_3 + 846720\Lambda_1\lambda_4 + 138264\Lambda_1\mu_4 + 606816\Lambda_1\lambda_1\lambda_2\mu_1 \\ & + 767340\lambda_2\lambda_3 + 310464\lambda_2\mu_3 + 404040\mu_2\lambda_3 + 276528\mu_2\mu_3 \end{aligned}$$

$$+329280\lambda_1^3\lambda_2+94080\mu_1^3\lambda_2+56448\Lambda_1^3\mu_2+133056\lambda_5+16200\mu_5]$$
$$-X^2[441000\Lambda_1\lambda_4+25200\Lambda_1\mu_4+882000\lambda_2\lambda_3+70560\lambda_2\mu_3$$
$$+351540\mu_2\lambda_3+50400\mu_2\mu_3+131544\lambda_5+6480\mu_5]$$
$$+X[48384\lambda_5+1080\mu_5]\}.$$

Using the ratio method (see e.g. [3]) we can estimate the dependence of the critical temperature on the concentration p of Heisenberg-type bonds, and then from the formula [4]

$$\gamma_n = nr_n y^{-1} - n + 1$$

TABLE I

kT_c/J as a function of concentration p of Heisenberg-type bonds for the b.c.c. lattice, $S = 1$ and different values of constant couplings

p	$J^H = J^I = 1$	$J^H = 1,\ J^I = 2$	$J^H = 2,\ J^I = 1$	$J^H = 5,\ J^I = 1$	$J^H = 1,\ J^I = 5$
0	9.032	18.064	9.032	9.032	45.161
0.1	8.946	17.136	9.673	11.932	41.652
0.2	8.856	16.204	10.326	14.830	38.140
0.3	8.762	15.266	10.984	17.711	34.624
0.4	8.662	14.320	11.640	20.582	31.104
0.5	8.552	13.362	12.287	23.461	27.575
0.6	8.428	12.385	12.920	26.359	24.034
0.7	8.284	11.373	13.537	29.280	20.467
0.8	8.111	10.300	14.134	32.223	16.836
0.9	7.899	9.103	14.711	35.188	12.983
1.0	7.634	7.634	15.268	38.171	7.634

TABLE II

kT_c/J_{eff} as a function of concentration p of Heisenberg-type bonds for the b.c.c. lattice, $S = 1$ and different values of constant couplings. $J_{eff} := J[p(J^H/J)+(1-p)(J^I/J)]$

p	$J^H = 1,\ J^I = 2$	$J^H = 2,\ J^I = 1$	$J^H = 1,\ J^I = 5$	$J^H = 5,\ J^I = 1$
0	9.032	9.032	9.032	9.032
0.1	9.019	8.794	9.055	8.523
0.2	9.000	8.605	9.081	8.239
0.3	8.900	8.449	9.112	8.050
0.4	8.950	8.314	9.148	7.916
0.5	8.908	8.191	9.192	7.820
0.6	8.846	8.075	9.244	7.753
0.7	8.748	7.963	9.303	7.705
0.8	8.583	7.852	9.353	7.672
0.9	8.275	7.743	9.274	7.650
1.0	7.634	7.634	7.634	7.634

where $r_n = a_n/a_{n-1}$, and y is the limit of the sequence $\{r_n\}$, the same dependence for the susceptibility exponent γ can be obtained. The results are presented in Tables I and II and Fig. 1 for b.c.c. lattice and spin $S = 1$. Qualitative behaviour for other spin values and the s.c. lattice is similar. In Table I the dependence of critical temperature (reduced by J) on the concentration p of Heisenberg-type bonds in shown. In Table II we have the same dependence but the critical temperature is divided by $J_{\text{eff}} := J[pJ^{\text{H}}/J+(1-p)J^{\text{I}}/J]$. Figure 1 gives the change of the susceptibility index γ

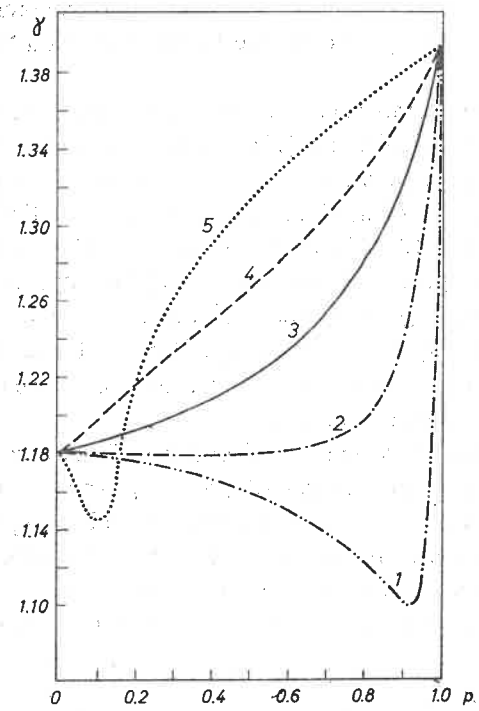

Fig. 1. Critical index γ vs concentration p of Heisenberg-type bonds for the b.c.c. lattice and $S = 1$. $1 - J^{\text{H}}/J = 5$, $J^{\text{I}}/J = 1$; $2 - J^{\text{H}}/J = 2$, $J^{\text{I}}/J = 1$; $3 - J^{\text{H}}/J = J^{\text{I}}/J = 1$; $4 - J^{\text{H}}/J = 1$, $J^{\text{I}}/J = 2$; $5 - J^{\text{H}}/J = 1$, $J^{\text{I}}/J = 5$

with p. As can be seen from these data, the change from Ising-like values of T_c and γ ($p = 0$) to the Heisenberg-like ones ($p = 1$) depends strongly on the coupling constants ratio. This change is nearly uniform over the whole range of p for $J^{\text{I}} = J^{\text{H}}$, and is more rapid in the small p region for $J^{\text{H}} > J^{\text{I}}$, and in the large p region for $J^{\text{I}} < J^{\text{H}}$. The local minimum in the γ vs p curve around $p = 0.1$ (for $J^{\text{H}} = 5J^{\text{I}}$) seems to be an artifact connected with the shortness of the series, as for shorter series (4 terms) this minimum is deeper. On the other hand the minimum of γ for $J^{\text{I}} = 5J^{\text{H}}$ changes but slightly when one term in the series is added. Therefore, the random mixture of Heisenberg and Ising bonds (which for $0 < p < 1$ corresponds to neither Heisenberg nor Ising systems) differs from the mixed Heisenberg-Ising models [5, 6] where the transition from one system to another was sharp, i.e. as long as there was anisotropy the value of critical

exponent γ remained practically fixed at its Ising (anisotropic) value, and changed discontinuously when the system became isotropic. General behaviour of the random system, i.e. its smooth transition from an anisotropic ($p = 0$) to isotropic ($p = 1$) cases is the same in two and three dimensions. Let us stress that the differences in critical properties of mixed and random system are not surprising. Apart from pure Heisenberg and Ising models, which are of course the same in both systems, in the mixed one all bonds are always anisotropic with only degree of anisotropy varying, whereas the random system is composed of isotropic and anisotropic bonds and it is impossible to predict at what concentration of, say, anisotropic bonds the system will show overall anisotropic behaviour.

For the two extreme homogeneous systems the series obtained here are identical with those given by Van Dyke and Camp [7] and Rushbrooke et al. [8] for Ising and Heisenberg models, respectively. Numerical values of the critical temperature and critical exponent γ for the two pure models obtained in this paper for the b.c.c. lattice and $S = 1$ are equal $kT_c/J = 7.634$, $\gamma = 1.396$ for the Heisenberg model and $kT_c/J = 9.032$, $\gamma = 1.181$ for the Ising model. This agrees well with the value given by Rushbrooke and Wood [9] for the Heisenberg model, $kT_c/J = 7.6020$. For the exponent γ usually a value between 1.405 and 1.375 is adopted [6]. The critical temperature for the b.c.c. lattice and spin $S = 1$ for the Ising model has, to the best of our knowledge, never been published. The critical exponent γ is believed to be equal 1.23 [6].

For the two dimensional system the divergence of the susceptibility at $p = 1$ was identified with the Stanley-Kaplan singularity, which gives spin-dependent T_{SK}. In three diemensions there is no Stanley-Kaplan singularity, hence both T_c and γ for $p = 1$ should be independent on the value of the spin. This indeeed is the case. The existing difference of the order of 0.05 for γ can be attributed to short series.

Additionally, we calculated the values of the crossover exponent ϕ from the formula [10]

$$\phi_k = (k-1+\delta)\left[\frac{h_k}{h_{k-1}} - 1\right], \qquad h_k = \left(\frac{d \ln a_k}{d(1-p)}\right)_{(1-p)=0}$$

where δ is a fitting parameter. To obtain ϕ from ϕ_k again the ratio method has been used. We found that ϕ depends rather weakly on the coupling constants ratio, for we have (for the b.c.c. lattice)

$$\phi = 1.180 \pm 0.055 \quad (\delta = 0.1) \quad \text{for } J^{\mathrm{I}} = J^{\mathrm{H}}$$

$$\phi = 1.210 \pm 0.025 \quad (\delta = 0.1) \quad \text{for } J^{\mathrm{I}} = 2J^{\mathrm{H}}$$

$$\phi = 1.175 \pm 0.06 \quad (\delta = 0.1) \quad \text{for } 2J^{\mathrm{I}} = J^{\mathrm{H}}.$$

Since to determine ϕ we have only five terms in the susceptibility series, the above values are only rough estimates. They differ, however, significantly from the value obtained for the square lattice in the same approximation $\phi = 2.15$ [2]. This agrees with a common belief that ϕ should be of the order of γ, and in two dimensions greater value of ϕ could be connected with the large value of γ_{SK} for the Stanley-Kaplan singularity.

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