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LETTER TO THE EDITOR

GROUND STATE PROPERTIES OF AN ANISOTROPIC HEISENBERG MODEL*

DARKO V. KAPOR[a], KATARINA R. SURLA[b], DUŠAN I. SURLA[b], JOVAN P. ŠETRAJČIĆ[a] and MARIO J. ŠKRINJAR[a]

a) *Institute of Physics, Faculty of Sciences, Dr I. Đuričića 4,* 21000 *Novi Sad, Yugoslavia*

b) *Institute of Mathematics, Faculty of Sciences, Dr I. Đuričića 4,* 21000 *Novi Sad, Yugoslavia*

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Energy gap and spin deviation in the ground state of an anisotropic Heisenberg model are expanded in terms of small anisotropy parameter up to the fourth power of the anisotropy parameter. It is shown that the fourth-order terms in Bose-operators give much more significant contribution than it was previously estimated.

We have discussed a particular version of anisotropic Heisenberg ferromagnetic model on the simple cubic lattice, for spin 1/2, first introduced by Buyers et al.[1] and discussed in detail by Belorizky et al.[2,3,4]. The Hamiltonian is given by

$$H = -\frac{1}{2} \sum_{\substack{\vec{n},\vec{m} \\ (n.n.)}} J_{\vec{n}\vec{m}} \vec{S}_{\vec{n}} \vec{S}_{\vec{m}} + J' \sum_{\vec{n}} \sum_{r=x,y,z} S^{r}_{\vec{n}} S^{r}_{\vec{n}+\vec{\varepsilon}_r} - g \mu_B \mathscr{H} \sum_{\vec{n}} S^{z}_{\vec{n}}.$$

*Preliminary results were reported at the 8th Yugoslav Conference on the Physics of Condensed Matter, Poreč, 21—24 September 1982.

The anisotropy is introduced through the additional coupling along three axes ($\vec{\varepsilon}_r$ is the vector connecting given site with its neighbour along r-axis) characterized by the anisotropy parameter $\delta = J'/J$.

In our previous paper[5] we have presented the general formulae for the dispersion law and average magnetization obtained in the Dyson-Maleev representation[6,7] by the Green's function method. We have also discussed[8] the behaviour of the energy gap $\lim_{\vec{k}\to 0} E(\vec{k}) = E(0)$ in the ground state ($T = 0$ K) in the leading approximation (of order δ^2).

We have continued with this calculation in order to examine in more detail two important consequences of the anisotropy: energy gap and spin deviation in the ground state.

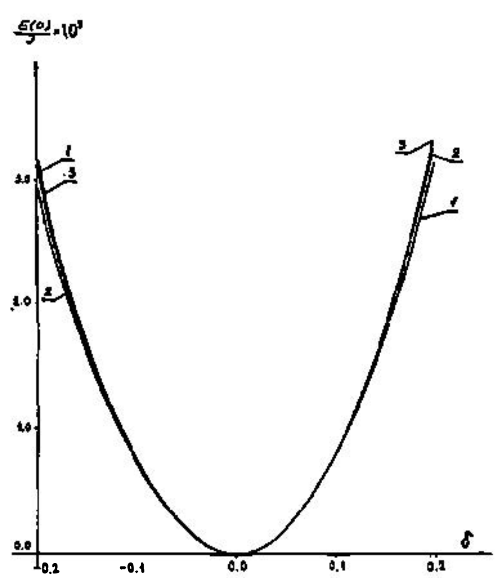

Fig. 1: Energy gap $\frac{E(0)}{J}$ for small anisotropy

1 — $0.078143\,\delta^2$

2 — $0.078143\,\delta^2 + 0.016902\,\delta^3$

3 — $0.078143\,\delta^2 + 0.016902\,\delta^3 + 0.022489\,\delta^4$.

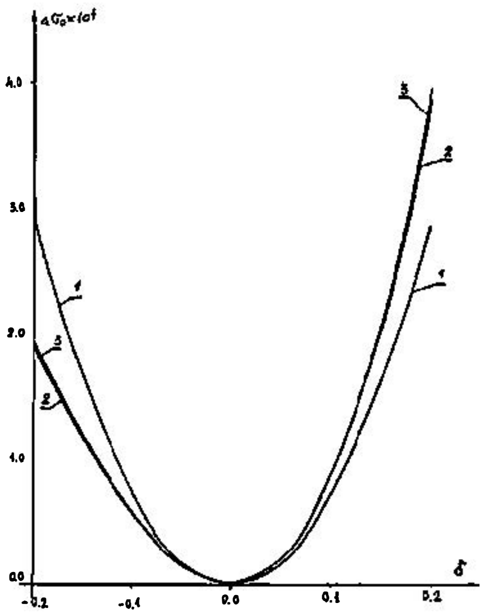

Fig 2: Spin deviation for small anisotropy

1 — $0.007172\,\delta^2$

2 — $0.007172\,\delta^2 + 0.012831\,\delta^3$

3 — $0.007172\,\delta^2 + 0.012831\,\delta^3 + 0.002518\,\delta^4$.

Expanding all relevant quantities up to δ^4 (for $0 < \delta \ll 1$), we have obtained the expressions for these two quantities, which are rather long, so we shall not quote them here. (The complete expressions were presented on the 8th Yugoslav Symposium on Condensed Matter Physics, 21—24 IX 1982, Poster Session).

The lattice sums figuring in these expressions were calculated numerically using the Gaussian quadrature formulae on the *Varian* 73 *computer* of the Institute of Mathematics, University of Novi Sad, with the accuracy of 10^{-9} giving the results:

$$\frac{E(0)}{J} = 0.078143\,\delta^2 + 0.016902\,\delta^3 + 0.022489\,\delta^4$$

$$\Delta\sigma_0 \equiv 1 - \frac{\langle S^z \rangle}{S} = 0.007172\,\delta^2 + 0.012831\,\delta^3 + 0.002518\,\delta^4.$$

It can be seen that the energy gap is much more sensitive to the corrections of order δ^3 and δ^4, than the spin deviation.

It is also interesting to compare the leading terms in δ^2 with the results of previous papers. The energy gap with the coefficient 0.078 agrees in order of magnitude with the results 0.092[4] and 0.095[8]. On the other hand, the spin deviation was overestimated in our previous paper[5] by an order of magnitude, due to overseeing the factors 8 in front of the lattice sum.

The final conclusion that was put forward by this work is that fourth-order terms in boson operators have significant contribution in the ground state. A similar calculation for finite temperatures is now in progress.

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OSOBINE OSNOVNOG STANJA JEDNOG ANIZOTROPNOG HAJZENBERGOVOG MODELA

DARKO V. KAPOR[a], KATARINA R. SURLA[b], DUŠAN I. SURLA[b], JOVAN P. ŠETRAJČIĆ[a] i MARIO J. ŠKRINJAR[a]

a) *Institut za fiziku, Prirodno-matematički fakultet, Dr I. Đuričića* 4, 21000 *Novi Sad*

b) *Institut za matematiku, Prirodno-matematički fakultet, Dr I. Đuričića* 4, 21000 *Novi Sad*

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Energetski procep i devijacija spina u osnovnom stanju jednog modela anizotropnog Hajzenbergovog feromagnetika su razvijani po stepenima malog parametra anizotropije do četvrtog stepena parametra anizotropije. Pokazano je da je doprinos članova IV reda po Boze-operatorima mnogo značajniji nego što se to do sada smatralo.