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BUDAPEST

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ON THE SPECTRUM OF SINGLET EXCITATIONS OF THE S=1/2 LINEAR HEISENBERG ANTIFERROMAGNET

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ABSTRACT

We examined the spectrum of singlet excitations of the nearest neighbour Heisenberg antiferromagnet by extrapolation from numerical results for small rings. The inferred shape of the lower edge of the spectrum is radically different from that predicted by Ovchinnikov and seems to be better approximated by the result valid for triplet excitations.

РЕЗЮМЕ

Рассматривается спектр синглетных возбуждений гамильтониана Гейзенберга при антиферромагнитном взаимодействии ближайших соседей методом экстраполяции из результатов для маленьких колец. Найденная форма нижней грани спектра существенно отличается от формы, предсказанной Овчинниковым, и, по-видимому, является более близкой к результату для грани спектра триплетных возбуждений.

KIVONAT

Az elsőszomszéd Heisenberg antiferromágnes szinglet spektrumát vizsgáltuk a kis gyürükre kapott numerikus eredményekből való extrapoláció segitségével. A spektrum alsó élére vonatkozó sejtésünk lényegesen különbözik az Ovcsinnyikov által megjósolttól és láthatóan jobb közelitést ad a tripletspektrumra érvényes eredmény.

The large number of quasi-one-dimensional magnetic systems available for experimental investigation has inspired a great deal of work on one-dimensional models of magnetism. Of particular theoretical interest is the Heisenberg antiferromagnetic chain described by the Hamiltonian $H=J\sum_i \vec{S}_i \cdot \vec{S}_{i+1}$ with $J>0$ for spin $S=1/2$. The reason for this is twofold: first, it has proved to be the first quantum-mechanical many-body system yielding to exact treatment, at least in certain aspects [1], [2] and second, because the $S=1/2$ case is suspect of showing anomalous behaviour even for higher dimensions. Such doubts about the general validity of the conventional picture of antiferromagnetism have recently been expressed by Anderson [3] and were further corroborated by Fazekas and Anderson [4]. Thus, by examining the $S=1/2$ linear chain one may hope to gain insight into the nature of non-Néel-type behaviour of other $S=1/2$ antiferromagnets. In a subsequent publication we intend to draw a parallel between certain features of the linear chain and triangular antiferromagnets [5].

Theoretical efforts to unravel the properties of the excitation spectrum have mainly been concentrated on the triplet spectrum. We mention here the numerical investigations by Orbach [6], Mattheiss [7], and by des Cloizeaux and Pearson [8], and the exact solution given by the latter authors in the same paper. In this work the form

$$\varepsilon_{tr}(q) = \frac{1}{2} J\pi |\sin q| \qquad /1/$$

was established for the lower edge of the triplet spectrum. Less attention has been paid to the singlet excitations though it should have been apparent from the results of Orbach [6], and Mattheiss [7] that there are low-lying singlet excitations and they are bound to show up in the low temperature thermal properties. Making use of Bethe's Ansatz Ovchinnikov [9] proposed a formula for the lower edge of the singlet spectrum

$$\varepsilon_s(q) = J\pi |\sin \frac{q}{2}| \qquad /2/$$

where $-\frac{\pi}{2} \leq q \leq \frac{\pi}{2}$, i.e. this branch of excitations is supposed to terminate halfway to the zone boundary. Though it has an initial slope identical to that of /1/, at $q=\pi/2$ it will attain the value $J\pi/\sqrt{2}\sim 2.3$ J, significantly higher than the corresponding triplet value.

As a part of extensive numerical investigation of low-dimensional S=1/2 Heisenberg antiferromagnets we have calculated the singlet spectra of closed chains for the lattice site numbers N=2,4,6,8 and 10 making use of Hulthén's [2] method. Numerical results will not be tabulated here for they are obviously the same as those obtained, though not fully published, by Orbach [6]. Figures 1. and 2. give the graphic representation of the spectra for N=8, and 10 respectively. On the vertical axes excitation energies in units of J, and on the horizontal axes the wave vector $q=Q-Q_o$, where always Q_o the wave vector of the ground state is chosen as the origo, is plotted. Fig.1. actually could have been extracted from Fig. 7. of Ref. [7]; we give it together with Fig. 2. to make the trend with increasing N easier to see. We emphasize that the same numerical data have been obtained by a number of authors before; it is the extrapolation to large N's and the juxtaposition of the results with those of Ovchinnikov [9] that we believe is new.

As it is apparent from Figs. 1. and 2., the distribution of singlet levels is roughly symmetrical about $q=\pi/2$ and the lower edge of the spectrum seems to tend to a well-defined smooth curve. The only exception in this latter respect is at the point next to the ground state $q=2\pi/N$ where the lowest energy fails to fit the otherwise fairly sinelike curve. Perhaps we could describe the situation by saying that the corresponding excitation is "missing". Whether such a statement remains valid for any N we are not able to guess.

Fig. 3. gives extrapolations for a few characteristic points of the lower edge by plotting their energies vs 1/N. Circles represent the zone-edge $q=\pi$ excitations; their energy clearly tends to zero. To determine what is the lowest excitation energy belonging to $q=\pi/2$ we plotted what seemed to be the largest energies belonging to the lower edge for N=6,8 and 10. These are denoted by crosses and belong to $q=\pi/3, \pi/2, 3\pi/5$ for N=6,8,10 respectively. The seemingly remarkably accurate extrapolation gives the value $\varepsilon_s(\frac{\pi}{2}) = 1.56J$, a very good approximation to $\pi J/2$, the same as formula /1/ would give.

In view of the above results and considering how numerical results for the triplet spectra converge /see Figs. 1-3. of Ref [8]/ to the well-established form /1/, we feel justified in drawing the conclusion that <u>the lower edge of the singlet spectrum is nearly, and probably exactly, identical to that of the triplet spectrum as given by /1/</u>. The "missing point" indicates that such a statement needs corrections but in our opinion the formula /2/ given by Ovchinnikov [9] certainly does <u>not</u> belong to the lowest-lying singlet excitations: the extrapolations for $q=\pi/2$, and particularly for $q=\pi$ look pretty reliable.

Finally we would like to point out that probably there are low-lying singlet excitations other than those belonging to the lower edge near the points $q=0$ and $q=\pi$. In Fig. 3. we represented by diamonds the lowest excitations having the same wave number as the ground state. The extrapolation here is not too accurate, admitting a range of values between zero and, say, 0.6J. But at least the absence of a singlet gap for $q=0$ is not excluded. This is a reasonable expectation: there is a continuum of excitations for each q and we see no reason why the lower edge should be disjoint from it.

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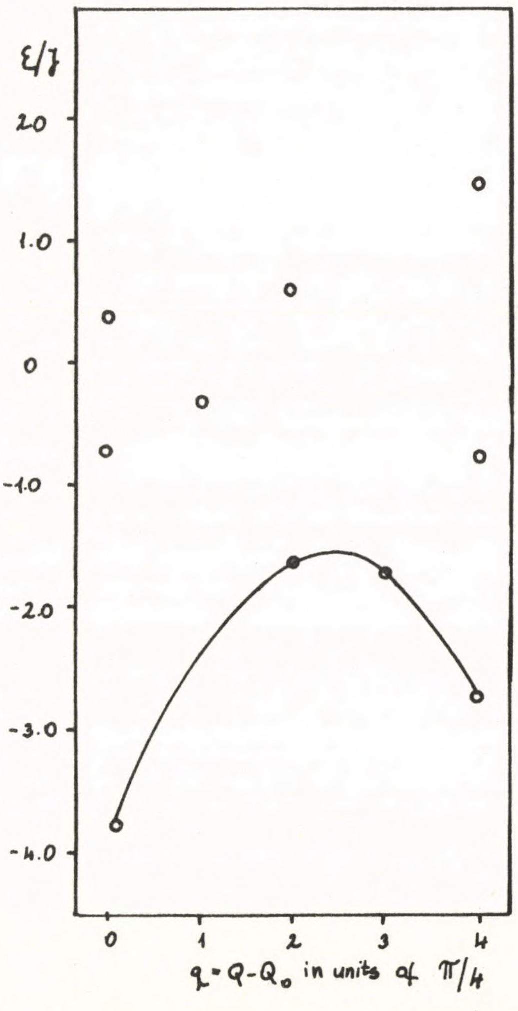

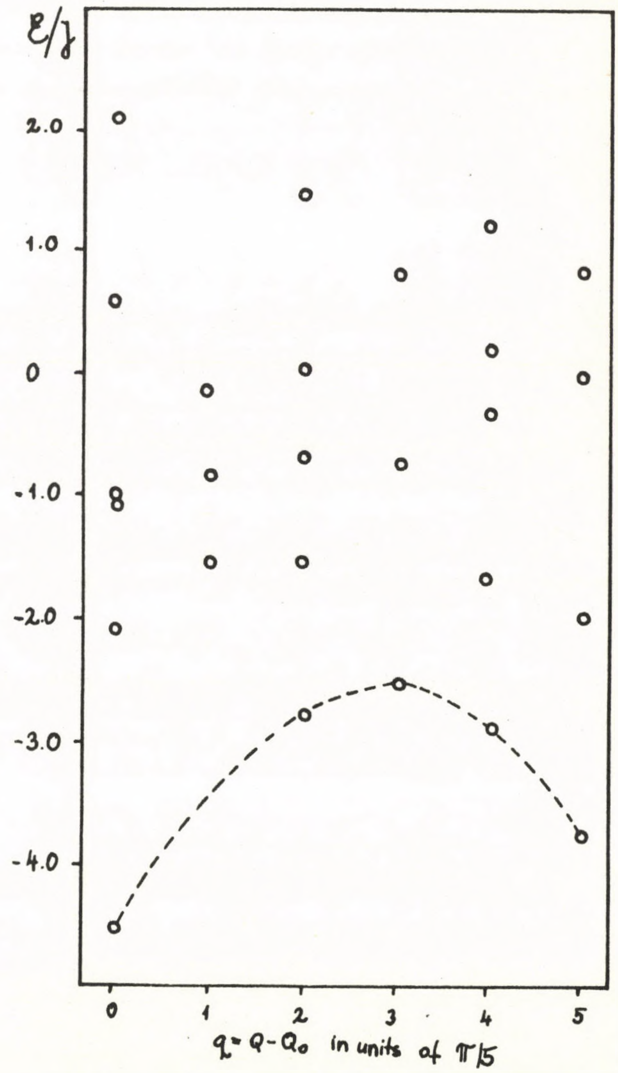

Fig.1. *The singlet spectrum of the antiferromagnetic Heisenberg Hamiltonian for a ring of N=8 spins. Energies are given in units of J, and wave numbers in units of π/4. Only half of the zone is shown. The dashed curve, just as in Fig. 2., is a smooth interpolation for the lower edge.*

Fig.2. *The singlet spectrum for the ring of N=10 spins. Energies are in units of J, while wave numbers in units of π/5. Note that the wave vector is measured from that of the ground state, i.e. from $Q_0=\pi$. The smooth interpolation for the lower edge considers the point belonging to q= =π/5 as "missing".*

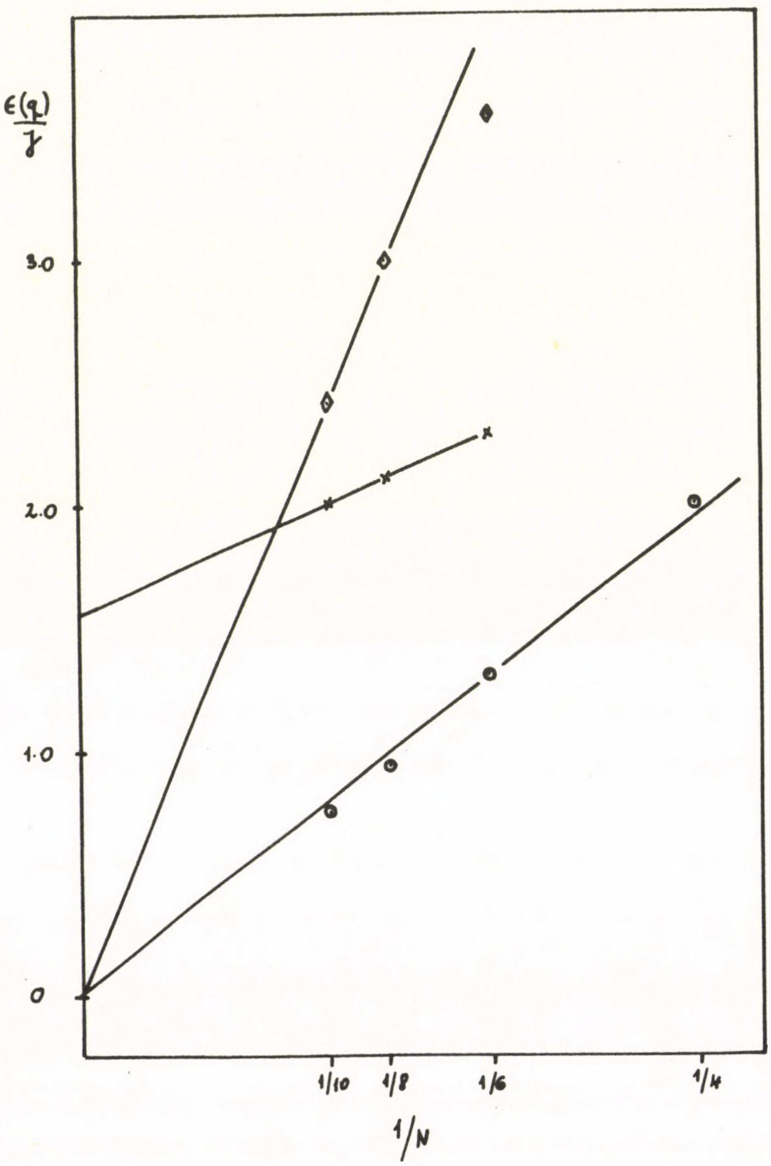

Fig.3. The extrapolation of certain singlet excitation energies for large N's. Circles represent excitation energies /in units of J/ of the zone-edge $q=\pi$ mode; crosses belong to the largest excitation energies on the lower edge; diamonds represent the lowest excitation energies for $q=0$. The fit to these latter ones is one of the extremal ones admitted by the data: the large uncertainty is obvious.

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