Calculation of Neel temperature for $S=1/2$ Heisenberg quasi-one-dimensional antiferromagnets

V. Yu. Irkhin* and A. A. Katanin
Institute of Metal Physics, Ekaterinburg 620219, Russia

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Isotropic $S=1/2$ quasi-one-dimensional antiferromagnets are considered within the bosonization method. The $1/z_{\perp}$ corrections to the interchain mean-field theory (where $z_{\perp}$ is the number of nearest neighbors in transverse to chain directions) are obtained for the ground-state sublattice magnetization $\overline{S_0}$ and Neel temperature T_N. The corrections to T_N make up about 25% of mean-field value, while those to $\overline{S_0}$ are small enough (especially in the three-dimensional case). The fluctuation corrections obtained improve considerably the agreement with the experimental data for magnetic-chain compounds $KCuF_3$, Sr_2CuO_3, and Ca_2CuO_3.

I. INTRODUCTION

Systems containing chains of magnetic atoms are investigated for a long time from both theoretical and experimental point of view. There exist many real compounds which are ''almost'' one-dimensional (1D), i.e., have small interchain coupling. Here belong, e.g., $KCuF_3$, Sr_2CuO_3 (spin $S=1/2$), $CsNiCl_3$ ($S=1$), $CsVCl_3$ ($S=3/2$) etc. There are a number of approaches which give a possibility to perform calculations for purely 1D magnets (Bethe ansatz, exact numerical diagonalization, different versions of numerical renormalization group, quantum Monte-Carlo method etc.). At the same time, consideration of multichain problem with the use of these methods meets difficulties, so that theoretical approaches are of interest, which can adequately describe the situation in quasi-1D magnets in the presence of interlayer coupling and/or anisotropy.

As for purely 1D antiferromagnets, there is well-known theoretical result by Haldane[1] who mapped the spin-chain problem to nonlinear-sigma model (NLσM) and showed that the cases of integer and half-integer spins differ qualitatively (for a review see, e.g., Ref. 2). For half-integer spins, the so-called topological θ-term in the effective action occurs, which leads to unusual magnetic behavior of such chains. As follows from the Bethe ansatz solution for $S=1/2$ (the same situation holds for any half-integer spin value), ground state in this case already possesses quasi-long-range order. The excitation spectrum turns out to be gapless and spin correlators have a power-law behavior, but staggered magnetization is zero (the situation is reminiscent of the XY model below the Kosterlitz-Thouless point T_{KT}). It is natural to suppose that in such a state the true long-range order is induced by an arbitrarily small interchain coupling J' and/or magnetic anisotropy. For the isotropic Heisenberg model, this problem was investigated within different theoretical methods. The interchain mean-field theory[3–5] predicts for the ground-state staggered magnetization $\overline{S_0}$ and Neel temperature T_N the results

$$\overline{S_0}\propto\sqrt{|J'|/J},\quad T_N\propto|J'| \tag{1}$$

and therefore indeed yields occurrence of long-range order at arbitrarily small $|J'|$. The behavior (1) contradicts to the standard spin-wave theory, which does not distinguish between integer and half-integer spins and predicts in both the cases a finite critical value, $J'_c\sim Je^{-\pi S}$, so that at $|J'|<J'_c$ the quantity $\overline{S_0}$ vanishes and

$$\overline{S_0}\propto\ln|J'/J'_c|,\quad T_N\propto\overline{S_0}\sqrt{|J'|} \tag{2}$$

for $|J'|$ greater but not too close to J'_c.

This contradiction was resolved within the renormalization-group (RG) approach[2,6–8] which showed that for inverse-length scales $\mu\gg J'_c/J$ the standard two-dimensional NLσM scaling equations are applicable, and the spin-field scale factor Z_μ indeed satisfies $Z_\mu^{-1/2}\propto\ln\mu$. At the same time, for half-integer spins at $\mu\ll J'_c/J$ one has $Z_\mu^{-1/2}\propto\mu^{1/2}$. This means[6,7] that for both integer and half-integer spins and $|J'|\gg J'_c$ we have the spin-wave behavior (2), while for half-integer spins and $|J'|\ll J'_c$ Eq. (1) holds. (We suppose here that for half-integer spins the renormalized coupling constant satisfies $g_\mu<g_c$ where g_c is the critical 3D coupling constant. Apparently, this inequality holds in the absence of dimerization, see Refs. 6 and 7.)

In the extremely quantum case $S=1/2$ we have $J'_c\sim J$, so that $|J'|\ll J'_c$ in a broad region of $|J'|$. Therefore, one can conclude that interchain mean-field theory of Refs. 3–5 gives a qualitatively correct description of $S=1/2$ quasi-1D magnets. At the same time, this theory does not take into account interchain fluctuations. In particular, the calculated value of the Neel temperature is not sensitive to space dimensionality of the system, although in the $d=1+1$ case (both the dimensions are supposed to be spatial, but second one corresponds to the direction, transverse to the chain) we should have $T_N=0$; for the $d=1+2$ case the values of T_N turn out to be too high in comparison with experimental data.

To obtain the corrections to interchain mean-field theory, we use the $1/z_{\perp}$ expansion ($z_{\perp}$ is the number of nearest neighbors in directions transverse to the chain). This approach is similar to the expansion in $1/z$ (or inverse interaction radius $1/R$), which has been used to improve the standard mean-field theory of Heisenberg magnets many years ago in Refs. 9 and 10. This approach is also equivalent to the spin-fluctuation approach in the theory of itinerant magnets by Moriya.[11]

The plan of paper is as follows. In Sec. II we consider the bosonization of the system of interacting Heisenberg chains. In Sec. III we calculate fluctuation corrections to the inter-

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chain mean-field theory. In Sec. III we discuss the results and compare them with experimental data on magnetic chain compounds. In Appendix A, the perturbation theory in J' is considered and the first-order $1/z_\perp$ correction to the mean-field value of Neel temperature are calculated. In Appendix B, we demonstrate how the same results can be obtained more elegantly in spirit of the spin-fluctuation approach by Moriya. Finally, in Appendix C fluctuation corrections to the ground-state staggered magnetization are derived.

II. THE MODEL AND ITS BOSONIZATION

We consider the $S=1/2$ isotropic Heisenberg model of quasi-1D antiferromagnet

$$\mathcal{H}=J\sum_{n,i}\mathbf{S}_{n,i}\mathbf{S}_{n+1,i}+\frac{1}{2}J'\sum_{n,\langle ij\rangle}\mathbf{S}_{n,i}\mathbf{S}_{n,j}, \tag{3}$$

where n numerates sites along the chains and i,j are indices of the chains, $J>0$ and J' are intra- and interchain exchange parameters, respectively. We consider only the case $|J'|\ll J$.

Each chain can be ''bosonized'' with the use of the standard relations (see, e.g., Ref. 12)

$$\mathbf{S}_{n,i}=\mathbf{J}_i(x)+(-1)^n\mathbf{n}_i(x), \tag{4}$$

where

$$J_i^z(x)=\frac{\beta}{2\pi}\partial_x\varphi_i(x),$$
$$J_i^{\pm}(x)=\frac{\lambda}{\pi}\exp[\pm i\beta\theta_i(x)]\cos\beta\varphi_i(x) \tag{5}$$

are the cyclic vector current components and

$$n_i^z(x)=\frac{\lambda}{\pi}\cos\beta\varphi_i(x),$$
$$n_i^{\pm}(x)=\frac{\lambda}{\pi}\exp[\pm i\beta\theta_i(x)] \tag{6}$$

are their ''staggered'' analogs. Here, λ is the scale renormalization constant, $\varphi_i(x)$ is the boson operator, $\beta=\sqrt{2\pi}$.

Then we obtain the bosonized Hamiltonian in the form[13]

$$\begin{aligned}\mathcal{H}=&\frac{v}{2}\sum_i\int dx[\Pi_i^2+(\partial_x\varphi_i)^2]+g_u\sum_i\int dx\cos 2\beta\varphi_i\\&-\frac{J'\lambda^2}{2\pi^2}\sum_{i,\delta_\perp}\int dx[\cos(\beta\varphi_i)\cos(\beta\varphi_{i+\delta_\perp})\\&+\cos\beta(\theta_{i+\delta_\perp}-\theta_i)],\end{aligned} \tag{7}$$

where $v=\pi J/2$, Π_i is the momentum that is canonically conjugated to φ_i, and θ_i satisfies $\partial_x\theta_i=-\Pi_i$. The first line in Eq. (7) corresponds to a system of separate chains and has the form of a standard sine-Gordon Hamiltonian. First term in Eq. (7) describes a free-boson system, and the second one arises because of Umklapp scattering of original fermions (which arises after applying the Jordan-Wigner transformation); this term is marginal and produces logarithmic corrections to thermodynamic quantities.[4,14–16] Calculations (see Refs. 4 and 14) give $g_u/(2\pi)\simeq 0.25$. The second line of Eq. (7) describes the interaction between the chains. Note that only relevant terms are included in this summand since the marginal terms give smaller contribution (see Ref. 13).

III. MEAN-FIELD APPROXIMATION FOR BOSONIZED HAMILTONIAN AND $1/z_\perp$ CORRECTIONS

The simplest way of treating interchain exchange interactions is the mean-field approximation.[4] Decoupling the interaction term

$$\cos(\beta\varphi_i)\cos(\beta\varphi_{i+\delta_\perp})\rightarrow 2\langle\cos(\beta\varphi_{i+\delta_\perp})\rangle\cos(\beta\varphi_i) \tag{8}$$

we obtain

$$\begin{aligned}\mathcal{H}_{MF}=&\frac{v}{2}\sum_i\int dx[\Pi_i^2+(\partial_x\varphi_i)^2]+g_u\sum_i\int dx\cos 2\beta\varphi_i\\&-\frac{\lambda}{\pi}h_{MF}\sum_i\int dx\cos(\beta\varphi_i),\end{aligned} \tag{9}$$

where

$$h_{MF}=z_\perp J'\lambda\langle\cos(\beta\varphi_i)\rangle/\pi, \tag{10}$$

$z_\perp$ is the number of nearest neighbors in the transverse (to chain) directions ($z_\perp=4$ for simple cubic lattice). This approximation gives a possibility to reduce the multichain problem to a single-chain one in an effective staggered magnetic field. Introducing the function

$$B(h;T)=\frac{\lambda}{\pi}\langle\cos(\beta\varphi_i)\rangle_h, \tag{11}$$

which should be calculated in the presence of the last term in Eq. (9), we obtain the self-consistent equation for the sublattice magnetization $\overline{S}$ in the mean-field approximation in the form

$$\overline{S}_{MF}=B(z_\perp J'\overline{S}_{MF};T). \tag{12}$$

Despite the Hamiltonian, $\mathcal{H}_{MF}$, Eq. (9), has a one-chain form, calculation of the function $B(h;T)$ (which is an analog of the Brillouin function in the usual mean-field theory of Heisenberg magnets) at arbitrary T is a very complicated task. Scaling arguments suggest $B(h;T)=h^{1/3}f(h^{2/3}/T)$ with some scaling function $f(x)$. For $g_u=0$ (in this case, we have a standard sine Gordon, or, equivalently, massive Thirring model) $B(h;T)$ was calculated by Bethe ansatz in Ref. 17. However, in two following cases the calculation can be performed analytically: (i) $T=0$ where we have[4,5]

$$B(h;0)\simeq 0.677(h/v)^{1/3}[1+(g_u/2\pi)\ln(v/\Delta)]^{1/2}, \tag{13}$$

where

$$\Delta\simeq 2.085v^{1/3}h^{2/3}$$

and (ii) $h\rightarrow 0$ where

$$B(h,T)=h\chi_0(T). \tag{14}$$

Here, $\chi_0(T)$ is the staggered susceptibility of the system in the absence of h,[4,16]

$$\chi_0(T)=\frac{\tilde{\chi}_0}{T}L\left(\frac{\Lambda J}{T}\right),\quad \tilde{\chi}_0=\frac{\Gamma^2(1/4)}{4\Gamma^2(3/4)}\simeq 2.1884, \tag{15}$$

where we have picked out the factor $\tilde{\chi}_0$ for the sake of convenience and

$$L(\Lambda J/T)=C\left[\ln\frac{\Lambda J}{T}+\frac{1}{2}\ln\ln\frac{\Lambda J}{T}+\mathcal{O}(1)\right]^{1/2} \tag{16}$$

is the spin-field renormalization factor that arises because of the presence of the marginal operator; the single-chain numerical calculations[18] yield $C\simeq 0.15$, $\Lambda\simeq 5.8$. Thus, one can see that the above-mentioned scaling function $f(x)$ satisfies $f(x)\sim x$ at $x\to 0$ and $f(\infty)=\text{const}$. The result (14) gives a possibility to calculate the value of T_N in the mean-field theory since for $T\to T_N$ we just have $h_{MF}\to 0$. Thus, we obtain the equation[4]

$$T_N^{MF}=z_\perp J'\tilde{\chi}_0 L(\Lambda J/T_N^{MF}). \tag{17}$$

We have included in Eq. (16) a double-logarithmic term, which was not taken into account in Ref. 4 and modifies somewhat numerical results (see below). As discussed in the Introduction, the mean-field approximation (17) is not quite satisfactory to describe experimental data. In particular, the values of Neel temperatures are considerably overestimated.

The reason of this is that the mean-field approximation does not take into account the collective excitations, which substantially contribute to the thermodynamic properties. Such excitations can be considered within the random-phase approximation (RPA). The RPA spin susceptibilities are given by[4,5]

$$\chi^{+-}(\mathbf{q}_z,\omega)=\frac{\chi_0^{+-}(q_z,\omega)}{1-J'(q_x,q_y)\chi_0^{+-}(q_z,\omega)}, \tag{18a}$$

$$\chi^{zz}(\mathbf{q}_z,\omega)=\frac{\chi_0^{zz}(q_z,\omega)}{1-J'(q_x,q_y)\chi_0^{zz}(q_z,\omega)}, \tag{18b}$$

where, for the square lattice in the direction transverse to chains,

$$J'(q_x,q_y)=2J'(\cos q_x+\cos q_y), \tag{19}$$

$\chi_0(q,\omega)$ being the dynamical staggered susceptibility for the model (9) and we have taken into account only staggered components of the susceptibility. Again, $\chi_0(q,\omega)$ is given by simple analytical expressions only in two cases: $T=0$ (for the results see Ref. 5 and also Appendix C), and $h\to 0$ where we have[19,16] for both the susceptibilities

$$\chi_0(q_z,\omega)=\frac{1}{T}L\left(\frac{\Lambda}{T}\right)\tilde{\chi}_0(q_z/T,\omega/T), \tag{20}$$

$$\tilde{\chi}_0(k,\nu)=\frac{1}{4}\frac{\Gamma(1/4+ik_+)\Gamma(1/4+ik_-)}{\Gamma(3/4+ik_+)\Gamma(3/4+ik_-)},\ k_\pm=\frac{\nu\pm k}{4\pi}.$$

As it should be, $\chi_0(0,0)=\chi_0(T)$.

Now, we can calculate the spin-fluctuation corrections to interchain mean-field theory owing to collective modes. Similar to the case of the simplest mean-field approximation in the theory of Heisenberg magnets,[9,10] these corrections can be obtained within the $1/z$-expansion. Since we treat only transverse neighbors within the mean-field approach, one has to speak about the $1/z_\perp$ expansion. To construct this expansion, we consider the perturbation theory in $J'/\max(h_{MF},T)\sim 1/z_\perp$ (see Appendix A), which is an analog of expansion in $J/\max(h_{MF},T)\sim 1/z$ for three-dimensional Heisenberg magnets.[10] From this viewpoint, the above-discussed mean-field approximation is just the zeroth-order in $1/z_\perp$, so that the fluctuation corrections to this approximation can be obtained in a regular way. The leading (first order in $1/z_\perp$) corrections come from the diagrams which include one RPA-interaction line.

The details of calculations are discussed in Appendix A. For the Neel temperature we obtain to first order in $1/z_\perp$

$$T_N=kJ'z_\perp\tilde{\chi}_0 L(\Lambda/T_N), \tag{21}$$

where

$$k=\left\{1-\frac{\pi^2}{2\tilde{\chi}_0}\int_{-\infty}^{\infty}dr\int_0^1 d\tau\tilde{V}(r,\tau)\left[\frac{1}{8}F(r,\tau)+\frac{1}{2}G(r,\tau)\right]\right\}^{-1}, \tag{22}$$

$$\tilde{V}(r,\tau)=\int_{-\infty}^{\infty}\frac{dq_z}{2\pi}\times\sum_n\sum_{q_x,q_y}\frac{\cos q_x+\cos q_y}{2\tilde{\chi}_0-(\cos q_x+\cos q_y)\tilde{\chi}_0(q_z,2\pi in)}\times\exp(iq_zr-2\pi in\tau)$$

and $F(r,\tau)$, $G(r,\tau)$ are the four-point averages determined in Appendix A. The result (21) differs from the mean-field result (17) by a factor of k, which depends only on the lattice structure in the directions perpendicular to chains. Numerical calculation for $d=1+2$ case (simple cubic lattice) yields $k\simeq 0.70$. Thus, with account of the function $L(\Lambda/T_N)$, the lowering of T_N due to interchain fluctuation effects is about 25% of its mean-field value. For $d=1+2$ the integral in Eq. (22) is divergent and we have $T_N=0$.

The same result (21) can also be derived in a more elegant way within the spin-fluctuation approach by Moriya[11] (see Appendix B).

Corrections to the ground-state staggered magnetization are calculated in Appendix C. We have

$$\overline{S}_0=(0.677-0.311I)h_{MF}^{1/3}, \tag{23}$$

where the last term in the brackets represents the $1/z_\perp$ correction with

$$I=\begin{cases}0.038 & d=1+2\\ 0.193 & d=1+1.\end{cases} \tag{24}$$

Note that we do no take into account the logarithmic corrections owing to presence of the marginal operator, since there exists no simple ways of calculating dynamical staggered susceptibility at $T=0$ in the presence of such an operator. However, one can see that we have nearly 10% lowering of $\overline{S}_0$ for $d=1+1$ and only 2% lowering for $d=1+2$. Thus the fluctuation corrections to ground-state magnetization are much less important than those to the Neel temperature, and in the three-dimensional case they can be neglected.

IV. COMPARISON WITH THE EXPERIMENTAL DATA AND CONCLUSION

The results obtained enable one to perform quantitative comparison with experimental data on magnetic chain systems. Consider first the compound $KCuF_3$ with $S=1/2$. According to Ref. 20, we have $J=406$ K, $\overline{S}_0/S=0.25$. As discussed by Schulz,[4] this value of $\overline{S}_0$ corresponds to $J'/J=0.047$, so that $J'=19.1$ K. The simplest mean field approximation (17) yields $T_N=47$ K. From (21) we obtain $T_N=37.7$ K, which is somewhat lower in comparison with the experimental result of Ref. 20, $T_N=39$ K. Thus, our approximation slightly overestimates the effects of fluctuations, but improves reasonably the mean-field approximation. Contribution of the double-logarithmic term in Eq. (16) makes up about 5% and improves the agreement with the experimental data.

Another $S=1/2$ chain compound that is widely discussed in recent publications is Sr_2CuO_3, which has the following parameters:[21,22] $J=2600$ K, $T_N=5$ K. Direct experimental data for J' are absent, but using Eq. (21) and the experimental value of T_N we obtain $J'=1.85$ K. Then, we have from Eq. (23) $\overline{S}_0/S=0.042$, which is in agreement with the experimental data ($\overline{S}_0/S\leqslant 0.05$).

For Ca_2CuO_3 the experimental parameters have following values:[21,22] $S=1/2$, $J=2600$ K and $T_N=11$ K. From Eq. (21) we find $J'=4.3$ K and $\overline{S}_0/S=0.062$. Taking into account above results for Sr_2CuO_3 we find that the latter value is again in excellent agreement with the experimental data,[22] which give $\overline{S}_0(Ca_2CuO_3)/\overline{S}_0(Sr_2CuO_3)=1.5\pm 0.1$. Thus, the result (21) is sufficient to describe quantitatively real quasi-1D magnetic systems.

In the isotropic quasi-1D magnets under consideration, the fluctuation corrections modify only numerical factor in the expression for T_N. One can expect, however, that in the anisotropic case the form of functional dependence $T_N(J')$ will be also modified. The influence of anisotropy on the Neel temperature will be considered elsewhere. Another interesting question concerns quasi-1D magnets with half-integer spins $S>1/2$. As discussed in the Introduction, in this case there is a crossover from ''usual'' spin-wave behavior of staggered magnetization to non-spin-wave one. The expressions for T_N should be also changed because of this crossover.

Finally, despite the standard spin-wave theory yields a qualitatively correct description of integer-spin magnetic chains, the corresponding values of Neel temperatures are also overestimated in comparison with experimental data. Thus calculation of fluctuation corrections for these magnets is also of interest.

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APPENDIX A: PERTURBATION THEORY IN J' AND THE DIAGRAM TECHNIQUE FOR SPIN OPERATORS

In this appendix, we consider perturbation theory in J' for the field theory with the Lagrangian

$$\begin{aligned}\mathcal{L}=&\frac{v}{2}\sum_i\int d^2\mathrm{x}(\partial\varphi_i)^2+g_u\sum_i\int d^2\mathrm{x}\cos 2\beta\varphi_i\\&-\frac{\lambda}{\pi}h\sum_i\int d^2\mathrm{x}\cos(\beta\varphi_i)\\&-\frac{J'\lambda^2}{2\pi^2}\sum_{i,\delta_\perp}\int d^2\,\mathrm{x}[\cos(\beta\varphi_i)\cos(\beta\varphi_{i+\delta_\perp})\\&+\cos\beta(\theta_{i+\delta_\perp}-\theta_i)],\end{aligned}\tag{A1}$$

which corresponds to the Hamiltonian (7), the external staggered magnetic field h being introduced. In Eq. (7) we have used the complex coordinate $\mathrm{x}=x+iv\tau$. Further in this appendix we use the system of units where $v=1$. Consider the calculation of staggered magnetization

$$\overline{S}=\lambda\langle\cos(\beta\varphi_i)\rangle/\pi.$$

The perturbation theory in J' is constructed in a standard way (see, e.g., Ref. 23). To obtain the series in J' we write down the expression in the path integral formalism

$$\overline{S}=\frac{\lambda}{\pi}\frac{\int D\varphi\cos(\beta\varphi_i(0))\exp(-\mathcal{L}[\varphi])}{\int D\varphi\exp(-\mathcal{L}[\varphi])}.\tag{A2}$$

To zeroth order in J' (i.e., at $J'=0$) we have $\mathcal{L}=\mathcal{L}_0$ and

$$\overline{S}_0=B(h;T),\tag{A3}$$

where the function B was introduced in Eq. (11). Expanding Eq. (A2) in J' we obtain

$$\overline{S}=\frac{\lambda}{\pi}\frac{\int D\varphi\cos(\beta\varphi_i(0))\exp(-\mathcal{L}_0[\varphi])(1-\mathcal{L}_{int}+\mathcal{L}_{int}^2/2+\cdots)}{\int D\varphi\exp(-\mathcal{L}_0[\varphi])(1-\mathcal{L}_{int}+\mathcal{L}_{int}^2/2+\cdots)}$$
$$=\frac{\lambda}{\pi}\langle\cos(\beta\varphi_i(0))(1-\mathcal{L}_{int}+\mathcal{L}_{int}^2/2+\cdots)\rangle_{0,\mathrm{conn}}, \tag{A4}$$

where we have denoted $\langle\ldots\rangle_0=\int D\varphi\ldots\exp(-\mathcal{L}_0[\varphi])/\int D\varphi\exp(-\mathcal{L}_0[\varphi])$ and

$$\langle\cos(\beta\varphi_i(0))\mathcal{L}_{int}^n\rangle_{0,\mathrm{conn}}=\langle\cos(\beta\varphi_i(0))\mathcal{L}_{int}^n\rangle_0-\sum_{m=0}^{n-1}\frac{(n!)^2}{m!(n-m)!}\times\langle\cos(\beta\varphi_i(0))\mathcal{L}_{int}^m\rangle_0\langle\mathcal{L}_{int}^{n-m}\rangle_0. \tag{A5}$$

Each term in Eq. (A4) can be represented by its own diagram; the diagram technique is the same as that for spin operators[9,10] (some elements of the diagram technique are shown in Fig. 1). All diagrams are classified by powers of the parameter $J'/\max(h_{MF},T)\sim 1/z_\perp$. Diagrams of Fig. 2 have zeroth order in $1/z_\perp$. The summation of these diagrams leads to a shift of the external magnetic field by the mean field

$$h\rightarrow\tilde{h}=h+h_{MF},\quad h_{MF}=z_\perp J'\overline{S}. \tag{A6}$$

[The same result could be obtained by eliminating the mean-field term directly in Eq. (A1).] The diagrams of first order in $1/z_\perp$ [see Fig. 3(a)] have one RPA-interaction line [Fig. 3(b)]. These are directly connected to the RPA susceptibilities (18) by

$$V^{+-,zz}(\mathbf{q},\omega)=J'(q_x,q_y)+[J'(q_x,q_y)]^2\chi^{+-,zz}(q_z,\omega).$$

Thus, we obtain

$$V^{+-,zz}(\mathbf{q},\omega)=\frac{J'(q_x,q_y)}{1+\delta-J'(q_x,q_y)\chi_0^{+-,zz}(q_z,\omega)}, \tag{A7}$$

where

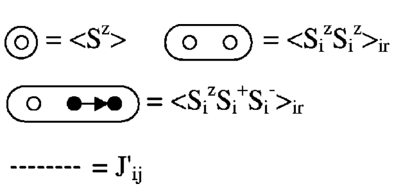

FIG. 1. Some elements of diagram technique for spin operators (for a detailed description see Ref. 10). The first three irreducible averages are determined by Eqs. (A9), (A12), and (A14).

$$\chi_0^{zz}(q_z,\omega)=\frac{\lambda^2}{\pi^2}\int d^2\mathrm{x}\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{x})\rangle_{0,ir}\times\exp(-iq_zx+i\omega_n\tau),$$
$$\chi_0^{+-}(q_z,\omega)=\frac{\lambda^2}{\pi^2}\int d^2\mathrm{x}\langle e^{i\beta[\theta_i(0)-\theta_i(\mathrm{x})]}\rangle_0\times\exp(-iq_zx+i\omega_n\tau), \tag{A8}$$

the two-operator irreducible average being given by

$$\langle AB\rangle_{ir}=\langle AB\rangle-\langle A\rangle\langle B\rangle \tag{A9}$$

and, following Ref. 11, we have introduced the correction δ in the denominator to satisfy the self-consistency requirement. In the case $T\leqslant T_N$ under consideration, this is determined by the condition $[\chi^{+-}(0,0)]^{-1}=0$, i.e. $\delta=z_\perp J'\chi_0^{+-}(0,0)-1$. Transforming Eq. (A7) back to the real space,

$$V^{+-,zz}(\mathrm{x})=T\sum_{i\omega_n}\int_{-\pi}^{\pi}\frac{dq_z}{2\pi}\sum_{q_x,q_y}V^{+-,zz}(\mathbf{q},i\omega_n)\times\exp(iq_zx-i\omega_n\tau), \tag{A10}$$

we obtain for the sublattice magnetization [see the diagrams of Fig. 3(a)]

$$\overline{S}=B(\tilde{h};T)+\frac{\lambda^3}{2\pi^3}\int d^2\mathrm{x}d^2\mathrm{y}[V^{zz}(\mathrm{x}-\mathrm{y})\times\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{x})\cos\beta\varphi_i(\mathrm{y})\rangle_{0,ir}+V^{+-}(\mathrm{x}-\mathrm{y})\times\langle\cos\beta\varphi_i(0)e^{i\beta\theta_i(\mathrm{x})}e^{-i\beta\theta_i(y)}\rangle_{0,ir}], \tag{A11}$$

where

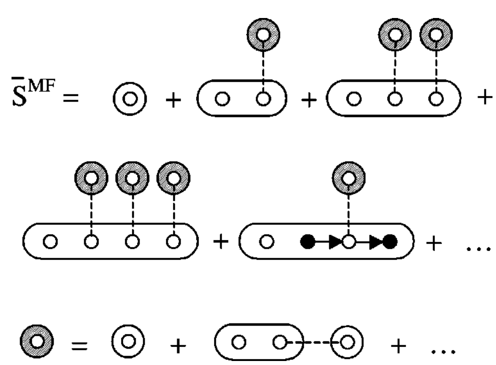

FIG. 2. Diagrams for staggered magnetization to zeroth order in $1/z_\perp$ (mean-field approximation).

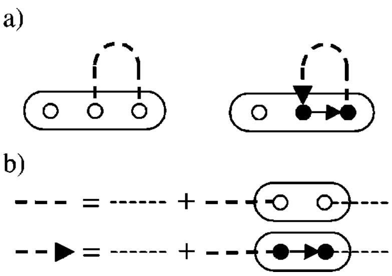

FIG. 3. (a) Diagrams of first order in $1/z_\perp$ for staggered magnetization. (b) Equations for RPA interaction lines.

$$\langle ABC\rangle_{ir}=\langle ABC\rangle-\langle A\rangle\langle BC\rangle_{ir}-\langle B\rangle\langle AC\rangle_{ir}-\langle AB\rangle_{ir}\langle C\rangle \tag{A12}$$

(all averages are calculated with $h\to\tilde{h}$). Up to this moment, we did not use a concrete form of $\mathcal{L}_0$. As already pointed in the main text, the only case where the averages in Eq. (A11) can be calculated analytically is the limit $\tilde{h}\to 0$. In this limit, we have

$$\begin{aligned}&\langle \cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{x})\cos\beta\varphi_i(\mathrm{y})\rangle_{0,ir}\\&=\frac{\lambda}{\pi}\tilde{h}\int d^2\mathrm{z}\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{z})\\&\quad\times\cos\beta\varphi_i(\mathrm{x})\cos\beta\varphi_i(\mathrm{y})\rangle_{0,ir},\end{aligned} \tag{A13}$$

where

$$\begin{aligned}\langle ABCD\rangle_{ir}=&\langle ABCD\rangle-\langle AD\rangle_{ir}\langle BC\rangle_{ir}-\langle BD\rangle_{ir}\langle AC\rangle_{ir}\\&-\langle AB\rangle_{ir}\langle CD\rangle_{ir}\end{aligned} \tag{A14}$$

and similar expression for transverse components; the averages in the right-hand side of Eq. (A13) are calculated at $\tilde{h}=0$. Thus we have at $h=0$, $h_{MF}\to 0$

$$\begin{aligned}\overline{S}=&\frac{\lambda^2}{\pi^2}h_{MF}\int d^2\mathrm{z}\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{z})\rangle\\&+\frac{\lambda^4}{2\pi^4}h_{MF}\int d^2\mathrm{x}\,d^2\mathrm{y}\,d^2\mathrm{z}[V^{zz}(\mathrm{x}-\mathrm{y})\\&\times\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{x})\cos\beta\varphi_i(\mathrm{y})\cos\beta\varphi_i(\mathrm{z})\rangle_{0,ir}\\&+V^{+-}(\mathrm{x}-\mathrm{y})\\&\times\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{z})e^{i\beta\theta_i(\mathrm{x})-i\beta\theta_i(\mathrm{y})}\rangle_{0,ir}].\end{aligned} \tag{A15}$$

Note that the SU(2) invariance guarantees at $\tilde{h}=0$

$$\begin{aligned}\int d^2\mathrm{x}\,d^2\mathrm{y}\,d^2\mathrm{z}[&\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{x})\cos\beta\varphi_i(\mathrm{y})\cos\beta\varphi_i(\mathrm{z})\rangle_{0,ir}\\&-3\langle\cos\beta\varphi_i(0)\cos\beta\varphi_i(\mathrm{x})e^{i\beta\theta_i(\mathrm{y})-i\beta\theta_i(\mathrm{z})}\rangle_{0,ir}]=0.\end{aligned} \tag{A16}$$

Calculating at $\beta^2=2\pi$ the averages in the right-hand side of Eq. (A15) in the presence of the marginal operator $g_u\cos 2\beta\varphi_i$ (which produces logarithmic corrections) we obtain

$$\begin{aligned}\overline{S}=&\frac{1}{2}h_{MF}L\left(\frac{\Lambda}{T}\right)\int d^2\mathrm{z}\frac{1}{|\varsigma(\mathrm{z})|}+\frac{1}{16}h_{MF}L^2\left(\frac{\Lambda}{T}\right)\int d^2\mathrm{x}\,d^2\mathrm{y}\,d^2\mathrm{z}V^{zz}(\mathrm{x}-\mathrm{y})\left[\frac{|\varsigma(\mathrm{z})\varsigma(\mathrm{x}-\mathrm{y})|}{|\varsigma(\mathrm{x})\varsigma(\mathrm{y})\varsigma(\mathrm{z}-\mathrm{x})\varsigma(\mathrm{z}-\mathrm{y})|}\right.\\&\left.+\frac{|\varsigma(\mathrm{z})\varsigma(\mathrm{z}-\mathrm{y})|}{|\varsigma(\mathrm{z})\varsigma(\mathrm{y})\varsigma(\mathrm{z}-\mathrm{x})\varsigma(\mathrm{x}-\mathrm{y})|}+\frac{|\varsigma(\mathrm{y})\varsigma(\mathrm{z}-\mathrm{x})|}{|\varsigma(\mathrm{z})\varsigma(\mathrm{x})\varsigma(\mathrm{z}-\mathrm{y})\varsigma(\mathrm{x}-\mathrm{y})|}-\frac{2}{|\varsigma(\mathrm{z})\varsigma(\mathrm{x}-\mathrm{y})|}-\frac{2}{|\varsigma(\mathrm{x})\varsigma(\mathrm{y}-\mathrm{z})|}-\frac{2}{|\varsigma(\mathrm{y})\varsigma(\mathrm{x}-\mathrm{z})|}\right]\\&+\frac{1}{4}h_{MF}L^2\left(\frac{\Lambda}{T}\right)\int d^2\mathrm{x}\,d^2\mathrm{y}\,d^2\mathrm{z}V^{+-}(\mathrm{x}-\mathrm{y})\frac{1}{|\varsigma(\mathrm{z})\varsigma(\mathrm{x}-\mathrm{y})|}\mathrm{Re}\left[\sqrt{\frac{\varsigma(\mathrm{x})\varsigma(\mathrm{z}-\mathrm{y})\overline{\varsigma(\mathrm{z}-\mathrm{x})}\,\overline{\varsigma(\mathrm{y})}}{\overline{\varsigma(\mathrm{x})}\,\overline{\varsigma(\mathrm{z}-\mathrm{y})}\varsigma(\mathrm{z}-\mathrm{x})\varsigma(\mathrm{y})}}-1\right],\end{aligned} \tag{A17}$$

where the bar states for the complex conjugate,

$$\varsigma(\mathrm{x})=\sinh(\pi T\mathrm{x})/(\pi T) \tag{A18}$$

and $L(\Lambda/T)$ is determined by Eq. (16). Introducing $\mathrm{r}=\mathrm{x}-\mathrm{y}$ instead of x and passing to the variables $\tilde{\mathrm{r}}=\mathrm{r}T$ etc. we obtain the result

$$\begin{aligned}\overline{S}=&\frac{1}{T}h_{MF}\tilde{\chi}_0L\left(\frac{\Lambda}{T}\right)\left\{1+\frac{\pi^2}{2T\tilde{\chi}_0}L\left(\frac{\Lambda}{T}\right)\right.\\&\left.\times\int d^2\mathrm{r}V(\mathrm{r})\left[\frac{1}{8}F(\mathrm{r})+\frac{1}{2}G(\mathrm{r})\right]\right\},\end{aligned} \tag{A19}$$

where

$$\tilde{\chi}_0=\frac{\pi}{2}\int d^2z\frac{1}{|\tilde{\varsigma}(z)|}\simeq 2.1184 \tag{A20}$$

and

$$F(\mathrm{r})=\int d^2\mathrm{y}\,d^2\mathrm{z}\Bigg[\frac{|\tilde{\mathrm{s}}(\mathrm{z})\tilde{\mathrm{s}}(\mathrm{r})|}{|\tilde{\mathrm{s}}(\mathrm{r+y})\tilde{\mathrm{s}}(\mathrm{y})\tilde{\mathrm{s}}(\mathrm{z-y-r})\tilde{\mathrm{s}}(\mathrm{z-y})|}+\frac{|\tilde{\mathrm{s}}(\mathrm{z})\tilde{\mathrm{s}}(\mathrm{z-y})|}{|\tilde{\mathrm{s}}(\mathrm{z})\tilde{\mathrm{s}}(\mathrm{y})\tilde{\mathrm{s}}(\mathrm{z-y-r})\tilde{\mathrm{s}}(\mathrm{r})|}+\frac{|\tilde{\mathrm{s}}(\mathrm{y})\tilde{\mathrm{s}}(\mathrm{z-y-r})|}{|\tilde{\mathrm{s}}(\mathrm{z})\tilde{\mathrm{s}}(\mathrm{r+y})\tilde{\mathrm{s}}(\mathrm{z-y})\tilde{\mathrm{s}}(\mathrm{r})|}-\frac{2}{|\tilde{\mathrm{s}}(\mathrm{z})\tilde{\mathrm{s}}(\mathrm{r})|}-\frac{2}{|\tilde{\mathrm{s}}(\mathrm{r+y})\tilde{\mathrm{s}}(\mathrm{y-z})|}-\frac{2}{|\tilde{\mathrm{s}}(\mathrm{y})\tilde{\mathrm{s}}(\mathrm{r+y-z})|}\Bigg] \tag{A21}$$

$$G(\mathrm{r})=\int d^2\mathrm{y}\,d^2\mathrm{z}\frac{1}{|\tilde{\mathrm{s}}(\mathrm{z})\tilde{\mathrm{s}}(\mathrm{r})|}\times\mathrm{Re}\left[\sqrt{\frac{\tilde{\mathrm{s}}(\mathrm{r+y})\tilde{\mathrm{s}}(\mathrm{z-y})\tilde{\mathrm{s}}(\overline{\mathrm{z}}-\overline{\mathrm{y}}-\overline{\mathrm{r}})\tilde{\mathrm{s}}(\overline{\mathrm{y}})}{\tilde{\mathrm{s}}(\overline{r}+\overline{y})\tilde{\mathrm{s}}(\overline{z}-\overline{y})\tilde{\mathrm{s}}(\mathrm{z-y-r})\tilde{\mathrm{s}}(\mathrm{y})}}-1\right]. \tag{A22}$$

In Eqs. (A20)–(A22) we have used

$$\tilde{\mathrm{s}}(\mathrm{x})=\sinh(\pi\mathrm{x}). \tag{A23}$$

Finally, using the connection (A6) between the mean field and the staggered magnetization and collecting all corrections to the denominator analogously to the usual three-dimensional Heisenberg magnets,[24] we obtain the result (21) of the main text.

APPENDIX B: SPIN-FLUCTUATION APPROACH TO THERMODYNAMICS OF QUASI-1D HEISENBERG MAGNETS

The results of previous appendix can be obtained in a much more simple way with the use of the spin-fluctuation approach proposed by Moriya[11] for description of thermodynamics of itinerant magnets where the Stoner theory (which is an analog of the mean-field theory in Heisenberg magnets) turns out to be quite not satisfactory. To apply the spin-fluctuation approach, we represent Hamiltonian (3) as

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{int},$$

$$\mathcal{H}_0=J\sum_{n,i}\mathbf{S}_{n,i}\mathbf{S}_{n+1,i}-h_{MF}\sum_{n,i}(-1)^{n+i}S^z_{i,n}, \tag{B1}$$

$$\mathcal{H}_{int}=\frac{1}{2}J'\sum_{\langle ij\rangle}(\mathbf{S}_{n,i}\mathbf{S}_{n,j})_{ir},$$

where $(AB)_{ir}=AB-\langle A\rangle\langle B\rangle$. With the use of the Hellmann-Feynman theorem, we obtain for the free energy

$$\mathcal{F}=\mathcal{F}_0(h_{MF})+\frac{1}{2}\sum_{\mathbf{q},i\omega_n}\int dJ'[\chi^{+-}(\mathbf{q},i\omega_n)+\chi^{zz}(\mathbf{q},i\omega_n)], \tag{B2}$$

where $\mathcal{F}_0(h_{MF})$ is the free energy corresponding to $\mathcal{H}_0$. Using the RPA results (18) one can find

$$\mathcal{F}=\mathcal{F}_0(h_{MF})+\frac{1}{2}\sum_{\mathbf{q},i\omega_n}\{\ln[1+J'(q_x,q_y)\chi_0^{+-}(q_z,i\omega_n)]+\ln[1+J'(q_x,q_y)\chi_0^{zz}(q_z,i\omega_n)]\}. \tag{B3}$$

Differentiating with respect to h_{MF} we readily obtain

$$\overline{S}=\overline{S}_{MF}+\frac{1}{2}\sum_{\mathbf{q},i\omega_n}\left[\frac{J'(q_x,q_y)}{1+J'(q_x,q_y)\chi_0^{+-}(q_z,i\omega_n)}\frac{\partial\chi_0^{+-}(q_z,i\omega_n)}{\partial h}+\frac{J'(q_x,q_y)}{1+J'(q_x,q_y)\chi_0^{zz}(q_z,i\omega_n)}\frac{\partial\chi_0^{zz}(q_z,i\omega_n)}{\partial h}\right]. \tag{B4}$$

This is just the result (A11) of Appendix A. Representing $\chi_0(q_z,i\omega_n)$ via boson variables, differentiating in h and calculating again the corresponding averages we return to Eq. (A19).

APPENDIX C: GROUND-STATE FLUCTUATION CORRECTIONS IN THE ABSENCE OF MARGINAL OPERATOR

In this appendix, we consider ground-state corrections to the mean-field value of sublattice magnetization. We use the expression (A11) [or, equivalently, (B4)], where at $T=0$ (Refs. 4 and 5),

$$\chi_0^{+-}=\frac{1}{4|J'|}\frac{\Delta^2}{\omega^2+v^2q^2+\Delta^2}, \tag{C1}$$

$$\chi_0^{zz}=\frac{Z'/Z}{4|J'|}\frac{\Delta^2}{\omega^2+v^2q^2+3\Delta^2} \tag{C2}$$

with

$$\Delta\simeq 6.175\,|J'|,\quad Z'/Z\simeq 0.49,\qquad \overline{S}_0\simeq 1.017|J'| \tag{C3}$$

and $h_{MF}=z_\perp J'\overline{S}_0$ (we neglect here the contribution of marginal operator). Differentiating Eq. (B4) in h_{MF} (with account of implicit dependence of J' on h_{MF}) we obtain after some algebraic manipulations

$$\overline{S}=\overline{S}_0-\frac{\Delta}{4\pi}\frac{\partial\Delta}{\partial h}I,\qquad I=\sum_q\left[(1-\Gamma'_q/2)\ln\frac{1}{1-\Gamma'_q}+(3-Z'\Gamma'_q/2Z)\ln\frac{1}{1-Z'\Gamma'_q/(3Z)}\right], \tag{C4}$$

where summation is performed over the transverse components, $\Gamma'_q=\cos q$ for $d=1+1$ and $\Gamma'_q=(\cos q_x+\cos q_y)/2$ for $d=1+2$. Calculating the integral I numerically we obtain the result (23) of the main text.

*Electronic address: Valentin.Irkhin@imp.uran.ru

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