

The $1/D$ Expansion for Low-Dimensional Classical Magnets

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The physical characteristics of two-dimensional classical ferro- and antiferromagnets have been calculated in the whole temperature range by an analytical approach based on the expansion in powers of $1/D$, where D is the number of spin components. This approach works rather well since it yields exact results for antiferromagnetic susceptibility and specific heat at $T=0$ already in the first order in $1/D$ and it is consistent with HTSE at high temperatures. For the quantities singular at $T=0$, such as ferromagnetic susceptibility and correlation length, the $1/D$ expansion supports their general- D functional form in the low-temperature range obtained by Fukugita and Oyanagi. The critical index η calculated in the first order in $1/D$ proves to be temperature dependent: $\eta = 2\theta/(\pi D)$ ($\theta = T/T_c^{(MFT)}$, $T_c^{(MFT)} = J_0/D$, J_0 is the zero Fourier component of the exchange interaction).

KEY WORDS: Low-dimensional magnets; spherical model; fluctuations; $1/D$ ($1/n$) expansion; correlation function.

1. INTRODUCTION

The physics of low-dimensional magnets has attracted the attention of researchers for several decades (see, e.g., ref. 1). Lately this interest has increased in connection with the high-temperature superconductivity.⁽²⁾ For layered magnetic systems accurate quantitative results on the high-temperature side can be obtained with the help of the high-temperature series expansion (HTSE).⁽³⁾ For classical models the longest series for internal energy and susceptibility were obtained in refs. 4 and 5. A comprehensive review on the application of the HTSE to different lattice models can be found in ref. 6.

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The HTSE approach works well for temperatures until below the antiferromagnetic susceptibility maximum. Complementary to this, some theories were developed primarily for the low-temperature range. In ref. 7 the renormalization group analysis was applied to the investigation of the long-wavelength, low-temperature behavior of the quantum antiferromagnet as described by the quantum nonlinear σ -model. A variational approach to the low-dimensional Heisenberg magnets without long-range order ("modified spin wave theory") was proposed by Takahashi.⁽⁸⁾ This approach proves to be rather successful at $T \ll J$ (J is the exchange integral), as is shown by the comparison with the exact solution for the one-dimensional classical Heisenberg model⁽⁴⁾ and with the data of Monte Carlo simulations and finite-size calculations for the square-lattice quantum Heisenberg models. However, this variational approach breaks down at $T \gtrsim J$ and, on the other hand, it is *not* a rigorous expansion in powers of T/J in the region $T \ll J$. Another drawback of the Takahashi theory is the impossibility of the generalization for the case of nonzero magnetic fields, since the condition of zero magnetization at $H = 0$ was enforced by hand and cannot be relaxed. One more approach to the low-dimensional Heisenberg magnets, the so-called "Schwinger boson mean field theory"⁽¹⁰⁾ based on functional methods, yields results almost equivalent to those of ref. 8, but with the proper factor 2/3 in the zero-temperature susceptibility of the Heisenberg antiferromagnet lacking.

In this article an analytical approach is proposed giving reasonable results for low-dimensional classical ferro- and antiferromagnets at arbitrary temperatures. The consideration sheds some light on quantum systems as well, since their physics in the undoped case is to a significant extent similar to that of classical ones.⁽²⁾ The idea of the method is the expansion in powers of $1/D$ for the model of D -component classical "spins" on a lattice introduced by Stanley⁽¹¹⁾ (see also ref. 27):

$$\mathcal{H} = -\mathbf{H} \sum_i \mathbf{m}_i - \frac{1}{2} \sum_{i,j} J_{ij} \mathbf{m}_i \mathbf{m}_j, \quad |\mathbf{m}| = 1 \quad (1.1)$$

In the limit $D \rightarrow \infty$ this model is equivalent to the spherical model⁽¹²⁾ and exactly soluble. In our earlier works⁽¹³⁾ a kind of diagram technique for classical spin systems was developed. This diagram technique proves to be very convenient, in particular, for the calculation of the high-temperature series. In ref. 13 the class of diagrams was located which survives in the limit $D \rightarrow \infty$ and recovers the exact solution for the spherical model. For three-dimensional classical Heisenberg and x - y models this class of diagrams (the $1/z$ or self-consistent Gaussian approximation, SCGA) results in an equation of state having an accuracy about 1% in the whole range of temperatures and magnetic fields, including the determination of

the phase transition temperature T_c . It was shown that all other contributions to the physical quantities of a magnetic system contain explicitly the powers of $1/D$ and can be classified by this parameter. This indicates a possibility of a regular $1/D$ expansion in the framework of the diagram technique for classical spin systems. Another version of this expansion was used earlier in refs. 14 and 15.

Actually, the model (1.1) is a particular case of the more general model⁽¹³⁾ of D -component "spins" with only $n \leq D$ components coupled by the interaction J . It is clear that just n can be considered as the number of the order parameter components determining the universality class of the system in the critical region. The critical indices for three-dimensional phase transitions obtained with the help of the $1/n$ expansion (see, e.g., ref. 16) are clearly independent of D . On the contrary, the nonuniversal quantities depend on both D and n . Here only the case $n = D$ will be considered; the model with $n \leq D$ is left for a subsequent consideration.

There are physical reasons by which the $1/D$ expansion for one- and two-dimensional classical Heisenberg model turns out to be much more efficient than one could expect considering the numerical value of $1/D$ for $D = 3$, and than it actually is for the calculation of the critical indices for three-dimensional systems. The point is that already the first-order approximation in $1/D$ gives the exact results for antiferromagnetic susceptibility, internal energy, and specific heat at $T \rightarrow 0$. Indeed, at $T \rightarrow 0$ there is a strong short-range order in the system, and each of the $(D - 1)$ susceptibilities of an antiferromagnet transverse with respect to the local spin configuration tends to the classical transverse value $1/(2J_0)$ ($J_0 = zJ$, z is the number of nearest neighbors), whereas the longitudinal one tends to zero.² Since there is no long-range order, the susceptibility of a sample is given by the average over local spin orientations, which yields $\chi(0) = 1/(2J_0) \cdot (1 - 1/D)$. For the Heisenberg model ($D = 3$) the D -dependent factor makes up exactly the famous number $2/3$. The internal energy of a magnet per spin takes on its saturated value $U(0) = -J_0/2$ at $T = 0$ —this result is independent of D and can be used for checking calculations in each order in $1/D$. Then, it can be argued that the specific heat at $T \rightarrow 0$ is given by $C(0) \equiv \partial U / \partial T |_{T=0} = (D - 1)/2$ (only $D - 1$ spin components transverse to the local molecular field contribute to the specific heat). On the other hand, on the high-temperature side the $1/D$ expansion recovers the leading order terms of the HTSE. Thus, it is plausible that this approximate solution, being well behaved on both sides of the temperature

² These arguments apply to bipartite lattices, such as the square lattice with the nearest-neighbor interaction, where the short-range order forms two "sublattices" with opposite magnetizations. This case is only considered throughout the paper.

interval, cannot deviate substantially from the exact one in the intermediate-temperature range as well.

Here the $1/D$ expansion for low-dimensional magnets is developed up to the first order in $1/D$. The remainder of the article is organized as follows. In Section 2 the applicability of the $1/D$ expansion is checked for a "toy" example of the classical linear chain magnet, for which the exact solution is available for arbitrary D .⁽¹⁷⁾ In Section 3 the diagram technique for classical spin systems is described. In Section 4 the self-consistent Gaussian approximation for systems without long-range order is formulated and the expansion of the SCGA results to the first order in $1/D$ is carried out. In Section 5 the D dependence of diagrams is analyzed and the additional diagrams of the leading order $1/D$ are found. In Section 6 the analytical expressions of the $1/D$ approximation are put into more convenient form and the low-temperature expansions for the internal energy and antiferromagnetic susceptibility of two-dimensional classical spin systems in the first order in $1/D$ are produced. In Section 7 we investigate the low-temperature behavior of ferromagnetic susceptibility and spin-spin correlation function.

2. ONE-DIMENSIONAL MAGNETS: A "TOY" EXAMPLE

The arguments in the Introduction apply equally well to one- and two-dimensional systems. It is convenient to check their applicability for a particular case of the linear chain magnet with the nearest neighbor interaction for which at $H=0$ the exact solution is available⁽¹⁷⁾ and the $1/D$ expansion can be obtained without any diagram technique. In particular, the normalized internal energy $\tilde{U} \equiv U/U(0)$ (which for systems with n.n. interactions coincides with the nearest neighbor correlation function $S_\delta = \langle \mathbf{m}_0 \mathbf{m}_\delta \rangle$) is given by

$$\tilde{U} = B(J/T); \quad B(\xi) = I_{D/2}(\xi)/I_{D/2-1}(\xi) \quad (2.1)$$

where B is the generalized Langevin function, and $I_\nu(\xi)$ is the modified Bessel function. The spin-spin correlation function S_r reads⁽¹⁷⁾

$$S_r = \langle \mathbf{m}_0 \mathbf{m}_r \rangle = [B(J/T)]^{1r} \quad (2.2)$$

where the interatomic spacing is set to unity: $a=1$. In the Fourier representation

$$S_{\mathbf{k}} = \sum_{\mathbf{r}} \exp(i\mathbf{k}\mathbf{r}) S_r = \frac{1 - B^2}{1 + B^2 - 2B\lambda_{\mathbf{k}}} \quad (2.3)$$

where $\lambda_{\mathbf{k}} \equiv J_{\mathbf{k}}/J_0 = \cos(k)$, $J_0 = zJ$ is the zero Fourier component of the exchange interaction, and $z = 2$ is the number of nearest neighbors. The wavevector-dependent susceptibility of a ferromagnet is given by

$$\chi_{\mathbf{k}} = \frac{1}{T} \sum_{\mathbf{r}} \exp(i\mathbf{k}\mathbf{r}) \langle m_0^x m_{\mathbf{r}}^x \rangle = \frac{1}{TD} S_{\mathbf{k}} \tag{2.4}$$

and the antiferromagnetic susceptibility $\chi_{\mathbf{k}}^{\text{AF}}$ can be expressed through that of a ferromagnet: $\chi_{\mathbf{k}}^{\text{AF}} = \chi_{\mathbf{b}-\mathbf{k}}$, where \mathbf{b} is the inverse lattice vector (for the linear chain $b = \pi$). Since $\lambda_0 = 1$ and $\lambda_{\mathbf{b}} = -1$, for the homogeneous susceptibilities with the use of (2.3) and (2.4) one gets

$$\chi_0 = \frac{1}{TD} \frac{1+B}{1-B}; \quad \chi_0^{\text{AF}} = \frac{1}{TD} \frac{1-B}{1+B} \tag{2.5}$$

The generalized Langevin function $B(\xi)$ in the above equations simplifies for small and large arguments, for D odd and in the case $D \gg 1$. In the region $x \equiv 2\xi/D \gg 1$

$$B(\xi) \cong 1 - \frac{D-1}{2\xi} + \frac{(D-1)(D-3)}{8\xi^2} + \frac{(D-1)(D-3)}{8\xi^3} + \dots \tag{2.6}$$

[for $D = 1$ or $D = 3$ the exponentially small corrections to (2.6) should be taken into account]. For $x \ll 1$

$$B(\xi) \cong \frac{\xi}{D} - \frac{\xi^3}{D^2(D+2)} + \frac{2\xi^5}{D^3(D+2)(D+4)} - \dots \tag{2.7}$$

In the case of large D in the first order in $1/D$

$$B(\xi) \cong f(x) + \frac{1}{D} \frac{x}{1+x^2} f^2(x) + \dots; \quad f(x) = \frac{x}{1+(1+x^2)^{1/2}} \tag{2.8}$$

Finally, for $D = 1, 3$ the function B takes on the well-known forms

$$B(\xi) = \begin{cases} \tanh(\xi), & D = 1 \\ \coth(\xi) - 1/\xi, & D = 3 \end{cases} \tag{2.9}$$

Dealing with the D -component vector model described by the Hamiltonian (1.1), it is convenient to choose the mean-field phase transition temperature $T_c^{(\text{MFT})} = J_0/D$ as the energy scale. In terms of the dimensionless temperature variable $\theta \equiv T/T_c^{(\text{MFT})}$ [$\xi = D/(2\theta)$] the low-temperature expansions of internal energy (2.1) and dimensionless anti-

ferromagnetic susceptibility $\tilde{\chi}_0^{\text{AF}} \equiv J_0 \chi_0^{\text{AF}}$ of the linear chain model are as follows:

$$\tilde{\chi}_0 \cong 1 - \left(1 - \frac{1}{D}\right)\theta + \frac{1}{2}\left(1 - \frac{1}{D}\right)\left(1 - \frac{3}{D}\right)\theta^2 + \frac{1}{D}\left(1 - \frac{1}{D}\right)\left(1 - \frac{3}{D}\right)\theta^3 + \dots \quad (2.10)$$

and

$$\tilde{\chi}_0^{\text{AF}} \cong \frac{1}{2}\left(1 - \frac{1}{D}\right) + \frac{1}{2D}\left(1 - \frac{1}{D}\right)\theta - \frac{1}{8}\left(1 - \frac{1}{D}\right)\left(1 - \frac{2}{D} - \frac{7}{D^2}\right)\theta^2 + \dots \quad (2.11)$$

It can be seen from (2.10) and (2.11) that, indeed, in the one-dimensional case specific heat and antiferromagnetic susceptibility at $T \rightarrow 0$ are exact in the first order in $1/D$, and, generally, their n th temperature derivatives at $T \rightarrow 0$ are exact in the $(n+1)$ th order in $1/D$. At high temperatures ($\theta \gg 1$) with the help of (2.7) and (2.5) one gets for energy

$$\tilde{U} \cong \frac{1}{2\theta} - \frac{D}{D+2} \frac{1}{8\theta^3} + \frac{D^2}{(D+2)(D+4)} \frac{1}{16\theta^5} + \dots \quad (2.12)$$

and for the spin-spin correlation function $S_0 = \theta \tilde{\chi}_0$

$$S_0 \cong 1 + \frac{1}{\theta} + \frac{1}{2\theta^2} + \frac{1}{D+2} \frac{1}{2\theta^3} - \frac{D-2}{D+2} \frac{1}{8\theta^4} - \frac{3D-4}{(D+2)(D+4)} \frac{1}{8\theta^5} + \dots \quad (2.13)$$

[in the antiferromagnetic case the signs at the odd powers of θ in (2.13) are reversed]. It is seen from (2.12) and (2.13) that at high temperatures the $1/D$ expansion correctly reproduces the leading term of the energy and the three leading terms of the susceptibility. The general recurrence relations for the coefficients in the formulas (2.12) and (2.13) can be found in ref. 17.

The temperature dependences of internal energy (2.1) and antiferromagnetic susceptibility (2.5) for the classical Heisenberg model ($D=3$) together with the first-order approximation in $1/D$ obtained with the help of (2.8) are represented below in Figs. 4 and 5. It is seen that, as was argued above, the accuracy of the $1/D$ expansion is good enough, and that the latter is a substantial improvement over the zeroth order in $1/D$ (spherical) approximation. As could be expected, for internal energy the accuracy is higher, and the two curves are almost indistinguishable. As we will see below, the situation is qualitatively the same for the square-lattice

ferro- and antiferromagnets, where the exact solution is unknown and the diagram technique developed in ref. 13 is to be applied. This diagram technique is described in detail in the next section.

3. THE DIAGRAM TECHNIQUE FOR CLASSICAL SPIN SYSTEMS

The diagrammatic representation of the thermal average of any quantity \mathcal{A} characterizing a classical spin system (say, $\mathcal{A} = m_i^\alpha$, $\alpha = 1, 2, \dots, D$) can be obtained by expanding the expression

$$\langle \mathcal{A} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{j=1}^N d\mathbf{m}_j \mathcal{A} \exp(-\beta \mathcal{H}); \quad |\mathbf{m}_j| = 1 \quad (3.1)$$

($\beta = 1/T$ and N is the number of spins in the lattice) in powers of the interaction part V_{int} of the Hamiltonian (1). The one-site averages of the spin components with the “bare” hamiltonian \mathcal{H}_0 are determined by the derivatives of the “bare” partition function \mathcal{Z}_0 ,

$$\mathcal{Z}_0(\xi) = \text{const} \cdot \xi^{-(D/2-1)} I_{D/2-1}(\xi) \quad (3.2)$$

($\xi = |\xi|$, $\xi = \beta \mathbf{H}$) with respect to the appropriate components ξ_α . In the diagram technique the main role is played by the cumulant averages, the “bare” values of which are given by

$$\langle m^{\alpha_1} m^{\alpha_2} \dots m^{\alpha_p} \rangle_0^{\text{cum}} \equiv A_{\alpha_1 \alpha_2 \dots \alpha_p}(\xi) = \frac{\partial^p A(\xi)}{\partial \xi_{\alpha_1} \partial \xi_{\alpha_2} \dots \partial \xi_{\alpha_p}} \quad (3.3)$$

where $A(\xi) = \ln \mathcal{Z}_0(\xi)$. In particular,

$$\begin{aligned} A_\alpha(\xi) &= B_0(\xi) \xi_\alpha \equiv B(\xi) \xi_\alpha / \xi \\ A_{\alpha\beta}(\xi) &= B_0(\xi) \delta_{\alpha\beta} + B_1(\xi) \xi_\alpha \xi_\beta \\ A_{\alpha\beta\gamma}(\xi) &= B_1(\xi) (\xi_\alpha \delta_{\beta\gamma} + \xi_\beta \delta_{\gamma\alpha} + \xi_\gamma \delta_{\alpha\beta}) + B_2(\xi) \xi_\alpha \xi_\beta \xi_\gamma \\ A_{\alpha\beta\gamma\delta}(\xi) &= B_1 \cdot 3\mathcal{P}(\delta_{\alpha\beta} \delta_{\gamma\delta}) + B_2 \cdot 6\mathcal{P}(\xi_\alpha \xi_\beta \delta_{\gamma\delta}) + B_3 \xi_\alpha \xi_\beta \xi_\gamma \xi_\delta \end{aligned} \quad (3.4)$$

where

$$B_n(\xi) = \left(\frac{1}{\xi} \frac{\partial}{\partial \xi} \right)^n \frac{B}{\xi} \quad (3.5)$$

$B(\xi)$ is given by (2.1), $\delta_{\alpha\beta}$ is the component Kronecker symbol, and \mathcal{P} is the symmetrization operator. In the limit $\xi \rightarrow 0$ the quantities B_n tend to

the constants determined by the expansion (2.7), so in (3.4) only the first terms of even-component cumulants survive.

The usual (noncumulant) averages, including the different-site ones, are expressed through the cumulants

$$\begin{aligned} \langle m_i^\alpha m_j^\beta \rangle_0 &= A_{\alpha\beta} \delta_{ij} + A_\alpha A_\beta \\ \langle m_i^\alpha m_j^\beta m_k^\gamma \rangle_0 &= A_{\alpha\beta\gamma} \delta_{ijk} + A_{\alpha\beta} A_\gamma \delta_{ij} + A_{\beta\gamma} A_\alpha \delta_{jk} + A_{\gamma\alpha} A_\beta \delta_{ki} + A_\alpha A_\beta A_\gamma \end{aligned} \quad (3.6)$$

etc., where δ_{ij} and δ_{ijk} are the site Kronecker symbols. In the graphical language the decomposition (3.6) corresponds to all possible groupings of small circles (spin components) into oval blocks (cumulant averages). The circles coming from V_{int} (the "inner" circles) are connected pairwise by the wavy interaction lines, and the summation over their coordinates and component indices is carried out in diagram expressions. One should not take into account disconnected diagrams [those containing disconnected parts with no "outer" circles coming from \mathcal{A} in (3.1)], since these diagrams are compensated for by the expansion of the partition function \mathcal{Z} in (3.1). The consideration of numerical factors shows that each diagram contains the factor $1/n_s$, where n_s is the number of the symmetry group elements of a diagram (the symmetry operations do not concern outer circles). For practical calculations it is more convenient to use the Fourier representation and calculate integrals over the Brillouin zone rather than lattice sums. As the lattice sums are subject to the constraint that the coordinates of the circles belonging to the same block coincide with each other [see (3.6)], in the Fourier representation the sum of wavevectors coming to any block along interaction lines is zero.

The diagram technique for classical spins is a generalization of the "longitudinal part" of the spin operator diagram technique^(18,19) and reduces to it for the Ising model without transverse field. In this case $A_z = B$, $A_{zz} = B'$, $A_{zzz} = B''$, etc. For the classical Heisenberg model the present diagram technique proves to be much more efficient than the spin operator diagram technique, since it takes advantage of classical properties of spin vectors in the explicit form. An earlier approach close to the present one is the linked cluster expansion.⁽²⁰⁾

To illustrate the rules of the diagram technique for classical spin systems, let us calculate a few leading order terms of the HTSE for the energy of a ferromagnet. The energy due to one spin U is given by the average of the Hamiltonian (1), in which the summation over one of two indices is "frozen." The contributions to U up to the order $1/T^3$ are given by the diagrams represented in Fig. 1, where the interaction line coming from the Hamiltonian (1) (the outer interaction line) not participating in

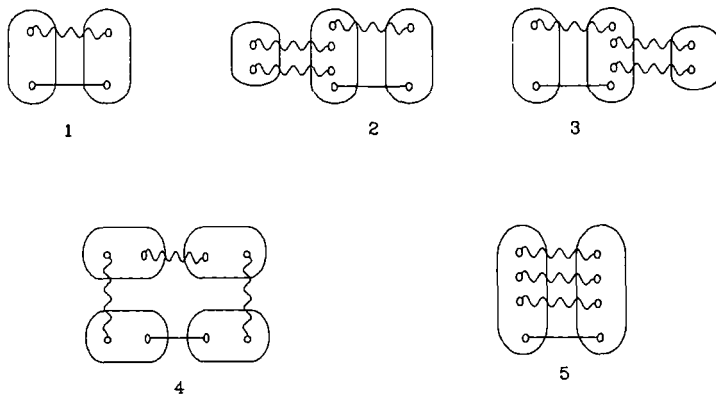


Fig. 1. The diagrams for internal energy of a classical spin system at high temperatures.

symmetry operations is designated by the straight line. The first diagram yields

$$U^{(1)} = -v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \beta J_{\mathbf{q}}(J_{\mathbf{q}}/2) \sum_{\alpha=1}^D A_{\alpha\alpha}^2 \quad (3.7)$$

where $\beta J_{\mathbf{q}}$ and $J_{\mathbf{q}}/2$ correspond to inner and outer lines, the integral is carried out over d -dimensional Brillouin zone, and v_0 is the unit cell volume. For hypercubic lattices $v_0 = a^d$, i.e., $v_0 = 1$ for $a = 1$. Then, dividing (3.7) by $U(0) = -J_0/2$ and adopting $\beta J_{\mathbf{q}} = (D/\theta) \lambda_{\mathbf{q}}$ in (3.7), one gets the corresponding contribution to the normalized energy \tilde{U} ,

$$\tilde{U}^{(1)} = \frac{D}{\theta} P_2 \sum_{\alpha} A_{\alpha\alpha}^2; \quad P_n = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \lambda_{\mathbf{q}}^n \quad (3.8)$$

For the linear chain $\lambda_q = \cos(q)$ and $P_2 = 1/2$; for the square lattice $\lambda_q = \frac{1}{2}[\cos(q_x) + \cos(q_y)]$ and $P_2 = 1/4$. Generally, for the n.n. interaction $P_2 = 1/z$ —this result is obvious if one calculates P_2 as a lattice sum. The cumulant $A_{\alpha\alpha}$ in (3.8) is calculated with the use of (3.4), (3.5), and (2.7) for $\xi = 0$; the obvious result is $A_{\alpha\alpha} = 1/D$. Thus, $\tilde{U}^{(1)} = 1/(z\theta)$. The higher-order contributions to \tilde{U} are calculated similarly. The sum of two equivalent diagrams 2 and 3 is given by

$$\tilde{U}^{(2+3)} = \frac{2}{2!} \left(\frac{D}{\theta}\right)^3 P_2^2 \sum_{\alpha\beta} A_{\alpha\alpha} A_{\beta\beta} A_{\alpha\alpha\beta\beta} = -\frac{2}{z^2\theta^3} \quad (3.9)$$

In (3.9) the sum over α, β is calculated with the use of (3.4) [for $\xi = 0$ the four-spin cumulant $A_{\alpha\alpha\beta\beta} = B_1(0)(1 + 2\delta_{\alpha\beta})$]; the factor $2!$ in the

denominator is the number of the symmetry group elements n_s of the diagrams connected with the equivalence of the interaction lines of the lateral "double-legged" fragments. The fourth diagram in Fig. 1 gives

$$\tilde{U}^{(4)} = \left(\frac{D}{\theta}\right)^3 P_4 \sum_x A_{xx}^4 = \frac{P_4}{\theta^3} \quad (3.10)$$

where $P_4 = 3/8$ for the linear chain and $P_4 = 9/64$ for the square lattice. Finally, the contribution of the fifth diagram in Fig. 1 reads

$$\tilde{U}^{(5)} = \left(\frac{D}{\theta}\right)^3 P^{(4)} \sum_{\alpha\beta} A_{\alpha\beta}^2 \left[\frac{1}{3!} \delta_{\alpha\beta} + \frac{1}{2!} (1 - \delta_{\alpha\beta}) \right] = \frac{2}{D+2} \frac{1}{z^3 \theta^3} \quad (3.11)$$

where $P^{(4)}$ is the three-loop integral:

$$P^{(4)} = v_0^3 \int \frac{d\mathbf{q}_1 d\mathbf{q}_2 d\mathbf{q}_3}{(2\pi)^{3d}} \lambda_{\mathbf{q}_1} \lambda_{\mathbf{q}_2} \lambda_{\mathbf{q}_3} \lambda_{\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3} = \frac{1}{z^3} \quad (3.12)$$

(the value of this integral is evident in the coordinate representation). The combination in the square brackets in (3.11) is due to the fact that for $\alpha = \beta$ there are three identical inner interaction lines, and for $\alpha \neq \beta$ there are two of them. The resulting high-temperature series for \tilde{U} (up to the fifth order in $1/\theta^5$) for the square lattice model is

$$\tilde{U} = \frac{1}{4\theta} + \frac{1}{64} \frac{D+4}{D+2} \frac{1}{\theta^3} - \frac{1}{256} \frac{D^2+3D-12}{(D+2)(D+4)} \frac{1}{\theta^5} + \dots \quad (3.13)$$

[cf. (2.12)]. For the zero Fourier component of the spin-spin correlation function $S_0 = \theta \tilde{\chi}_0$ of the square lattice ferromagnet similar calculations yield

$$S_0 = 1 + \frac{1}{\theta} + \frac{3}{4\theta^2} + \frac{4D+9}{8(D+2)} \frac{1}{\theta^3} + \frac{19D+50}{64(D+2)} \frac{1}{\theta^4} + \frac{20D^2+147D+284}{128(D+2)(D+4)} \frac{1}{\theta^5} + \dots \quad (3.14)$$

[cf. (2.13)]. It should be noted that one need not, however, consider the diagrammatic representations for both U and S . It is more convenient to calculate the diagrams for the wavevector-dependent correlator $S_{\mathbf{q}}$ and then to obtain energy with the help of the formula

$$U = -\frac{1}{2} v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} S_{\mathbf{q}} J_{\mathbf{q}} \quad (3.15)$$

In addition to the properties described above, the diagram technique for classical spin systems possesses such a feature as the possibility of the renormalization of interaction lines and blocks, which allows one to perform extensive diagram summations. This will be demonstrated in the next two sections.

4. THE SELF-CONSISTENT GAUSSIAN APPROXIMATION

The simplest infinite series of diagrams that can be summed up in the spin diagram technique is the "tree" series comprising all diagrams with no closed loops with integration over wavevectors.⁽¹⁹⁾ Taking into account only tree diagrams results in the mean-field approximation. For one- and two-dimensional magnets having no long-range order these diagrams, being proportional to powers of magnetization $\langle m^x \rangle$, are equal to zero. The next class of diagrams (which was summed up for the Ising model in ref. 19) takes into account only *pair* correlations of the molecular field acting on a given spin from its neighbors, which results in the Gaussian statistics of the molecular field fluctuations. In ref. 13 the self-consistent approximation for classical Heisenberg models based on a Gaussian set of diagrams was proposed, which proved to be very efficient in three dimensions. For the Ising model such an approximation was exploited earlier in refs. 21–23.

The reduced version of the SCGA for systems without long-range order is represented in Fig. 2. The analytical form of these diagram equations reads

$$\begin{aligned} \tilde{\lambda}_{xx} &= \exp \left[\sum_{x=1}^D \frac{1}{n_x!} \left(l \frac{\partial^2}{\partial \xi_x^2} \right)^{n_x} \right] A(\xi) \\ &= \frac{1}{\pi^{D/2}} \int d^D r \exp(-r^2) A_{xx}(2l^{1/2} \mathbf{r}) \end{aligned} \quad (4.1)$$

and

$$l = \frac{1}{2!} v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{\beta J_{\mathbf{q}}}{1 - \tilde{\lambda}_{xx} \beta J_{\mathbf{q}}} \quad (4.2)$$

These are the system of nonlinear equations for the cumulant spin average $\tilde{\lambda}_{xx}$ renormalized by Gaussian fluctuations and the dispersion of these fluctuations (normalized by temperature) l . With the use of the explicit form of A_{xx} from (3.4) and taking advantage of the symmetry, one can simplify the D -dimensional integral (4.1) to

$$\tilde{\lambda}_{xx} = \frac{2}{Dl^{1/2} \Gamma(D/2)} \int_0^\infty dr r^D \exp(-r^2) B(2l^{1/2} r) \quad (4.3)$$

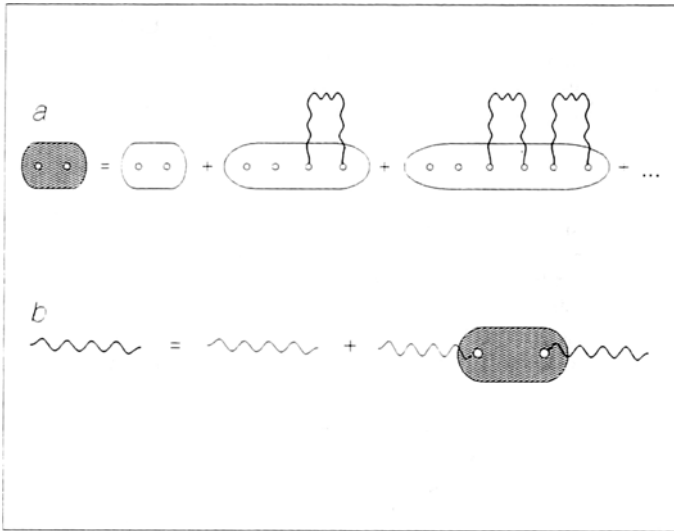


Fig. 2. The self-consistent Gaussian approximation (SCGA) for classical magnets: (a) the block summation for the cumulant one-site two-spin average $\tilde{\lambda}_{xx}$; (b) the Dyson equation for the renormalized interaction.

It is convenient to introduce a dimensionless quantity $G = (D/\theta) \tilde{\lambda}_{xx}$ [see (2.10) for θ] and to rewrite (4.2) as

$$l = \frac{D}{2\theta G} [P(G) - 1]; \quad P(G) = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{1 - G\lambda_{\mathbf{q}}} \quad (4.4)$$

For the square lattice with the n.n. interaction $P(G) = (2/\pi) \mathbf{K}(k)$, $k = G$, $\mathbf{K}(k)$ is the elliptic integral of the first kind, and for the linear chain $P(G) = 1/(1 - G^2)^{1/2}$.

Generally, the quantities of interest, the normalized internal energy \tilde{U} and the wavevector-dependent susceptibility of a ferromagnet $\tilde{\chi}_{\mathbf{k}}$, can be expressed as functions of the compact (irreducible) part of the two-spin correlation function $\hat{\lambda}_{xx}(\mathbf{q})$ comprising the diagrams that cannot be cut by one interaction line:

$$\tilde{U} = \theta \left(v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{1 - \hat{G}_{\mathbf{q}} \lambda_{\mathbf{q}}} - 1 \right); \quad \hat{G}_{\mathbf{q}} = \frac{D}{\theta} \hat{\lambda}_{xx}(\mathbf{q}) \quad (4.5)$$

and

$$\tilde{\chi}_{\mathbf{k}} = \frac{\hat{G}_{\mathbf{k}}}{1 - \hat{G}_{\mathbf{k}} \lambda_{\mathbf{k}}} \quad (4.6)$$

The susceptibility of an antiferromagnet is given by $\tilde{\chi}_{\mathbf{k}}^{AF} = \tilde{\chi}_{\mathbf{b}-\mathbf{k}}$, where \mathbf{b} is the inverse lattice vector [for the square lattice $\mathbf{b} = (\pi, \pi)$]. It is seen that the quantity $\tilde{\Lambda}_{xx}(\mathbf{q})$ is analogous to the self-energy part in other diagram techniques. In the SCGA the quantity G is independent of wavevector, and $G \rightarrow 1$ at $T \rightarrow 0$, ensuring the divergence of ferromagnetic susceptibility $\tilde{\chi}_0$. Since $\lambda_{\mathbf{b}} = -1$, in the SCGA the antiferromagnetic susceptibility $\tilde{\chi}_{\mathbf{b}}$ tends to the classical transverse value $1/2$ at $T \rightarrow 0$ instead of the proper value $(1/2)(1 - 1/D)$. To obtain the latter, one should take into account some additional diagrams of the order of $1/D$ giving rise to the wavevector dependence of $\hat{\Lambda}_{xx}$.

Before going beyond the SCGA, let us consider its properties in the case $D \gg 1$. For large D the product $r^D \exp(-r^2)$ in the integrand of (4.3) becomes sharply peaked at $r = r_0 = (D/2)^{1/2}$ and the integral can be evaluated by the pass method. In the first order in $1/D$ the result reads

$$G \equiv \frac{D}{\theta} \tilde{\Lambda}_{xx} \cong \frac{2}{\theta x_0} f(x_0) + \frac{1}{D} \Delta(x_0) + \dots \tag{4.7}$$

where $x_0 \equiv 2(2l_0)^{1/2}$, $l_0 \equiv l/D$, $f(x)$ is given by (2.8), and

$$\Delta(x_0) = \frac{1}{2\theta x_0} \left[-f(x_0) + x_0 f'(x_0) + x_0^2 f''(x_0) + \frac{4x_0}{1+x_0^2} f^2(x_0) \right] \tag{4.8}$$

In the limit $D \rightarrow \infty$ the Δ term in (4.7) can be dropped, and the system of equations (4.7) and (4.4) after the elimination of l reduces to the equation for the quantity G in the spherical limit

$$\theta GP(G) = 1 \tag{4.9}$$

It is seen that $G(\theta)$ monotonously decreases; $G(0) = 1$. For the linear chain (4.9) can be solved analytically to yield $G = 1/(1 + \theta^2)^{1/2}$.

The $1/D$ correction to the quantity G due to the Δ term in (4.7) can be calculated perturbatively. For δG determined by $G^{(SCGA)} = G + \delta G/D$ [henceforth G means the solution of (4.9)] one gets

$$\delta G = \frac{2P-1}{GP'+P} \Delta = -\frac{2}{\theta} \frac{(P-1)^3}{P(2P-1)^2 (GP'+P)} \tag{4.10}$$

where $P = P(G)$ and $P' = dP/dG$.

To end this section we consider the high- and low-temperature behavior of the quantities G , δG , P , and P' , which will be needed subsequently. At high temperatures ($\theta \gg 1$) the solution of (4.9) gives [see (3.8) for P_n]

$$G \cong \theta^{-1} - P_2 \theta^{-3} + (3P_2^2 - P_4) \theta^{-5} + O(\theta^{-7}) \tag{4.11}$$

which is sufficient for the determination of P to the order θ^{-6} :

$$P = 1 + P_2\theta^{-2} + (P_4 - 2P_2^2)\theta^{-4} + (P_6 - 6P_2P_4 + 7P_2^3)\theta^{-6} + O(\theta^{-8}) \quad (4.12)$$

Now one can calculate energy $\tilde{U} = \theta(P - 1)$ to the order θ^{-5} . In particular, for the square lattice with n.n. interaction $P_2 = 1/4$, $P_4 = 9/64$, and $P_6 = 25/256$, hence $P_4 - 2P_2^2 = 1/64$, $P_6 - 6P_2P_4 + 7P_2^3 = -1/256$, and the $D \rightarrow \infty$ limit of the expansion (3.13) is recovered. As $P' \cong 2P_2\theta^{-1} + O(\theta^{-3})$, the quantity δG of (4.10) is very small at high temperatures: $\delta G \cong -2P_2^3\theta^{-7} + O(\theta^{-8})$.

In the low-temperature region we focus our attention on the two-dimensional case, where the quantity G is exponentially close to unity. For the n.n. square lattice [see (4.4)]

$$P(G) \cong \frac{1}{\pi} \ln \left(\frac{8}{1-G} \right); \quad 1 - G \ll 1 \quad (4.13)$$

and G itself found from (4.9) reads

$$G \cong 1 - 8 \cdot \exp(-\pi/\theta) \quad (4.14)$$

Now the quantities P and P' are given by

$$P \cong \frac{1}{\theta} + O \left(\exp \left(\frac{-\pi}{\theta} \right) \right); \quad P' \cong \frac{1}{\pi} \frac{1}{1-G} \cong \frac{1}{8\pi} \exp \left(\frac{\pi}{\theta} \right) \quad (4.15)$$

and the $1/D$ correction δG , (4.10), reads

$$\delta G \cong -\frac{1}{2\theta P'} \frac{(1-\theta)^3}{(1-\theta/2)^2} \cong \frac{1}{P'} \left[-\frac{1}{2\theta} + 1 + O(\theta) \right] \quad (4.16)$$

5. THE $1/D$ EXPANSION

As we have seen in the preceding section, the self-consistent Gaussian approximation yields the exact results for the spherical model in the limit $D \rightarrow \infty$. This means that all other diagrams except those taken into account in Fig. 2 are small for $D \gg 1$. Our task in this section is to choose among them the diagrams whose leading terms are of the order of $1/D$. For the estimation of diagrams in the case $D \gg 1$ it is convenient to use the scaled variables $x = 2\xi/D$ [see (2.6)–(2.8)] and $\theta = T/T_c^{(MFT)} = TD/J_0$ [see (2.10)], whose characteristic values are of order unity. Now it is seen that each inner interaction line gives the factor $D: \beta J_q = (D/\theta) \lambda_q$, and the cumulant spin averages determined by (3.3) are proportional to

$$A_{\alpha_1 \alpha_2 \dots \alpha_n} \propto D^{1-n} \quad (5.1)$$

The estimate (5.1) shows that for $D \gg 1$ the unification of two smaller blocks into one larger one gives an additional factor $1/D$. Indeed,

$$A_{\alpha_1 \alpha_2 \dots \alpha_n} \cdot A_{\alpha_{n+1} \dots \alpha_{n+m}} \propto D^{2-m-n}$$

whereas

$$A_{\alpha_1 \alpha_2 \dots \alpha_{m+n}} \propto D^{1-m-n}$$

The third source of D dependence of diagrams is the summation over spin vector components. For $D \gg 1$ each summation yields the factor D in the leading order, which corresponds to the combinations of component indices maximally different from each other. In particular, in the summation over α, β in (3.9) the contribution of the terms with $A_{\alpha\alpha\alpha}(0) = 3B_1(0)$ is of order D , whereas that of the terms $A_{\alpha\alpha\beta\beta}(0) = B_1(0)$ is of order D^2 .

For an illustration, consider the D dependences of the HTSE contributions to energy calculated in the preceding section. These are $\tilde{U}^{(1)} \propto D \cdot (1/D)^2 \cdot D \propto 1$ (one inner interaction line, two blocks $A_{\alpha\alpha}$, and one summation over α), $\tilde{U}^{(2+3)} \propto D^3 \cdot (1/D)^2 \cdot (1/D^3) \cdot D^2 \propto 1$ (three inner interaction lines, two blocks $A_{\alpha\alpha}$, one block $A_{\alpha\alpha\beta\beta}$, and two summations), $\tilde{U}^{(4)} \propto D^3 \cdot (1/D)^4 \cdot D \propto 1$ (three inner interaction lines, four blocks $A_{\alpha\alpha}$, and one summation), and $\tilde{U}^{(5)} \propto D^3 \cdot (1/D^3)^2 \cdot D^2 \propto 1/D$ (three inner interaction lines, two blocks $A_{\alpha\alpha\beta\beta}$, and two summations). Note that the diagram 5 in Fig. 1 having larger spin blocks is of a combined smallness bearing two additional small factors, $1/D$ and $1/z$, in comparison with other diagrams in Fig. 1. This is a general feature making the $1/D$ expansion developed here and the “ $1/z$ approximation” (SCGA) developed earlier⁽¹³⁾ strongly connected with each other.

Now, the additional set of diagrams for the compact part $\hat{A}_{\alpha\alpha}$ of the leading order $1/D$ chosen with the help of the estimation method given above is represented in Fig. 3. Keeping only the lowest order terms in $1/D$, one can write down the analytical expressions for the four contributions to $\hat{A}_{\alpha\alpha}$:

$$\begin{aligned} \hat{A}_{\alpha\alpha}^{(1)} &= \frac{1}{2} V_0 \tilde{\Lambda}_{\alpha\alpha\beta\beta}^2 \tilde{\Lambda}_{\alpha\alpha\beta\beta\gamma\gamma} v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} V_{\mathbf{q}} \tilde{V}_{\mathbf{q}} \\ \hat{A}_{\alpha\alpha}^{(2)} &= \frac{1}{2} L_0 \tilde{\Lambda}_{\alpha\alpha\beta\beta}^3 v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} A_{\mathbf{q}} \tilde{V}_{\mathbf{q}} \\ \hat{A}_{\alpha\alpha}^{(3)} &= \frac{1}{2} \tilde{\Lambda}_{\alpha\alpha\beta\beta} \tilde{\Lambda}_{\alpha\alpha\beta\beta\gamma\gamma} v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} V_{\mathbf{q}} \tilde{V}_{\mathbf{q}} \\ \hat{A}_{\alpha\alpha}^{(4)}(\mathbf{k}) &= \tilde{\Lambda}_{\alpha\alpha\beta\beta}^2 v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{\beta J_{\mathbf{k}-\mathbf{q}}}{1 - \tilde{\Lambda}_{\alpha\alpha} \beta J_{\mathbf{k}-\mathbf{q}}} \tilde{V}_{\mathbf{q}} \end{aligned} \tag{5.2}$$

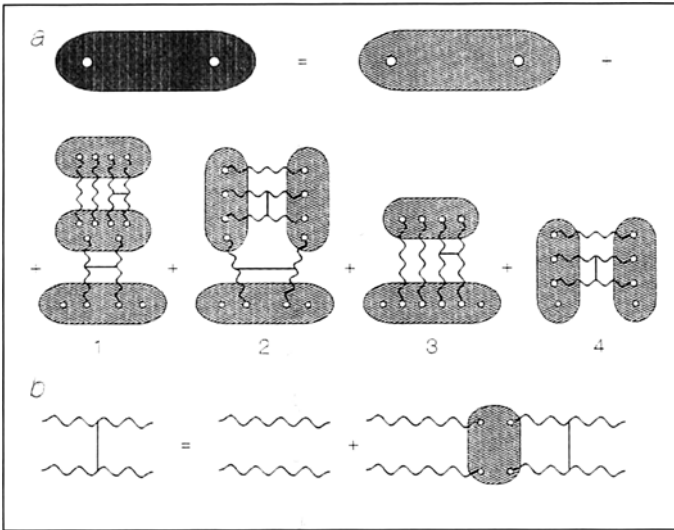


Fig. 3. (a) The additional diagrams of the order of $1/D$ for the compact part $\tilde{\lambda}_{xx}$ of the spin correlation function $\langle m^2 m^2 \rangle$; (b) the ladder equation for the four-spin correlation line.

In (5.2) $\tilde{\lambda}_{xx} = \theta G/D$, the quantity G is given by the solution of (4.9),

$$\begin{aligned}
 V_{\mathbf{q}} &= \frac{D}{2!} v_0 \int \frac{d\mathbf{p}}{(2\pi)^d} \frac{\beta J_{\mathbf{p}}}{1 - \tilde{\lambda}_{xx} \beta J_{\mathbf{p}}} \frac{\beta J_{\mathbf{q} - \mathbf{p}}}{1 - \tilde{\lambda}_{xx} \beta J_{\mathbf{q} - \mathbf{p}}} \\
 A_{\mathbf{q}} &= D v_0 \int \frac{d\mathbf{p}}{(2\pi)^d} \left(\frac{\beta J_{\mathbf{p}}}{1 - \tilde{\lambda}_{xx} \beta J_{\mathbf{p}}} \right)^2 \frac{\beta J_{\mathbf{q} - \mathbf{p}}}{1 - \tilde{\lambda}_{xx} \beta J_{\mathbf{q} - \mathbf{p}}}
 \end{aligned}
 \tag{5.3}$$

and $\tilde{V}_{\mathbf{q}} = V_{\mathbf{q}} L_{\mathbf{q}} = V_{\mathbf{q}} / (1 - \tilde{\lambda}_{\alpha\alpha\beta\beta} V_{\mathbf{q}})$. The factors D in (5.3) are the results of summation over spin vector components. The four- and six-spin cumulants $\tilde{\lambda}_{\alpha\alpha\beta\beta}$ and $\tilde{\lambda}_{\alpha\alpha\beta\beta\gamma\gamma}$ ($\alpha \neq \beta \neq \gamma$) are given by formulas analogous to (4.1). In the leading order in $1/D$ only the first terms of the expressions (3.4) should be taken into account. Calculating the Gaussian integrals by the pass method in the lowest order in $1/D$, one gets

$$\begin{aligned}
 \tilde{\lambda}_{\alpha\alpha\beta\beta} &\cong \left(\frac{2}{D} \right)^3 \left(\frac{1}{x} \frac{d}{dx} \right) \frac{f(x)}{x} \Big|_{x=v_0} \\
 \tilde{\lambda}_{\alpha\alpha\beta\beta\gamma\gamma} &\cong \left(\frac{2}{D} \right)^5 \left(\frac{1}{x} \frac{d}{dx} \right)^2 \frac{f(x)}{x} \Big|_{x=v_0}
 \end{aligned}
 \tag{5.4}$$

where $f(x)$ and x_0 are given by (2.8) and (4.7). With the use of the explicit form $x_0 = 2\{P(G)[P(G) - 1]\}^{1/2}$ the quantities $\tilde{\Lambda}_{\alpha\alpha\beta\beta}$ and $\tilde{\Lambda}_{\alpha\alpha\beta\beta\gamma\gamma}$ can be expressed as functions of G :

$$\tilde{\Lambda}_{\alpha\alpha\beta\beta} \cong -\left(\frac{2}{D}\right)^3 \frac{1}{(2P)^2(2P-1)}; \quad \tilde{\Lambda}_{\alpha\alpha\beta\beta\gamma\gamma} \cong \left(\frac{2}{D}\right)^5 \frac{3P-1}{(2P)^3(2P-1)^3} \quad (5.5)$$

To get the expressions for energy \tilde{U} and susceptibility $\tilde{\chi}_k$ in the first order in $1/D$, one should represent the quantity \hat{G}_k in (4.5) and (4.6) as

$$\hat{G}_k = G + \frac{1}{D} \Delta G_k; \quad \Delta G_k = \delta G + \frac{D^2}{\theta} \sum_{i=1}^4 \hat{\Lambda}_{\alpha\alpha}^{(i)}(\mathbf{k}) \quad (5.6)$$

[δG is given by (4.10)] and expand the expressions (4.5) and (4.6) in the first order in ΔG . For energy one thus gets

$$\tilde{U} = \tilde{U}_0 + \frac{1}{D} \Delta \tilde{U} \quad (5.7)$$

where $\tilde{U}_0 = \theta(P-1) = 1/G - \theta$ is the normalized energy in the spherical limit and

$$\Delta \tilde{U} = \theta v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{\lambda_q \Delta G_q}{(1 - G\lambda_q)^2} \quad (5.8)$$

The result for the susceptibility reads

$$\tilde{\chi}_k = \frac{G}{1 - G\lambda_k} + \frac{1}{D} \frac{\Delta G_k}{(1 - G\lambda_k)^2} \quad (5.9)$$

Further, collecting all terms of (5.2) into ΔG_k , (5.6), and making some rearrangements, one gets

$$\Delta G_k = \Delta G_0 + M_k \quad (5.10)$$

where

$$\begin{aligned} \Delta G_0 &= \frac{2G}{GP' + P} - v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{2G}{r_q(1 - G\lambda_q)} \\ &+ \frac{G^2}{GP' + P} v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{r_q} \frac{\partial r_q}{\partial G} \end{aligned} \quad (5.11)$$

$P' = \partial P / \partial G$, $P(G)$ is given by (4.4),

$$r_q = v_0 \int \frac{d\mathbf{p}}{(2\pi)^d} \frac{1}{(1 - G\lambda_p)} \frac{1}{(1 - G\lambda_{q-p})} \quad (5.12)$$

and

$$M_{\mathbf{k}} = 2G^2 v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{r_{\mathbf{q}}} \frac{\lambda_{\mathbf{q}} - \lambda_{\mathbf{q}-\mathbf{k}}}{(1 - G\lambda_{\mathbf{q}})(1 - G\lambda_{\mathbf{q}-\mathbf{k}})} \quad (5.13)$$

At zero wavevector ($\mathbf{k} = 0$) the quantity $M_{\mathbf{k}}$ vanishes, and in (5.10) $\Delta G_{\mathbf{k}} = \Delta G_0$. The results analogous to (5.9)–(5.13) were obtained by a different method in refs. 14 and 15. With the concrete form of $\Delta G_{\mathbf{k}}$ the expression (5.8) for $\Delta \tilde{U}$ simplifies to

$$\tilde{U} = \frac{2P'}{P(GP' + P)} - \frac{1}{GP' + P} v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{r_{\mathbf{q}}} \frac{\partial r_{\mathbf{q}}}{\partial G} \quad (5.14)$$

Before further processing of the formulas obtained, note that the analytical structure of the $1/D$ approximation for two-dimensional classical magnets, characterized by the repeated integrations over the Brillouin zone, is much more complicated than that of the one-loop theories,^(8,10) and it requires some work to produce low-temperature expansions of physical quantities and to rearrange the formulas obtained to the form convenient for numerical analysis. The details of calculation will be given in the next sections. Now we make some comments on the general analytical structure of the $1/D$ approximation. As is known, in one- and two-dimensional magnets with continuous symmetry long-range order is “washed out” by long-wavelength magnons, which reveals itself in the divergence of the one-loop integral of the type (4.2) at $T < T_c$, if one starts from the mean-field approximation. In three-dimensional systems⁽¹³⁾ this integral determines the spin-wave correction to magnetization. In low-dimensional case this divergence is removed at any $T \neq 0$ by the gap in the magnon spectrum. At $T \rightarrow 0$ this gap goes to zero with the quantity $1 - G$, and the integral l of (4.2) goes to infinity. The question is how to reconcile this divergence with the finiteness of most thermodynamic quantities of low-dimensional magnets at $T \rightarrow 0$, which must hold in each order in $1/D$. This question is solved differently in Takahashi’s modified spin wave theory⁽⁸⁾ and in the self-consistent Gaussian approximation. In Takahashi’s theory the constraint is imposed by hand that the total magnetization, i.e., the ground-state value minus the spin-wave correction, be zero. In the SCGA all powers of the divergent one-loop integral l are summed up, which ensures finiteness of energy and antiferromagnetic susceptibility at $T \rightarrow 0$ and yields exact results in the spherical limit $D \rightarrow \infty$. In the $1/D$ approximation there is no analog of the Gaussian diagram series (the further terms of such series would be of higher orders in $1/D$), and two-loop integrals diverge even stronger than the one-loop integral l at $T \rightarrow 0$. This divergence is restrained by the ladder diagram sequence for the four-spin correlation line (see Fig. 3b).

6. INTERNAL ENERGY AND ANTIFERROMAGNETIC SUSCEPTIBILITY

In this section the expressions for physical quantities of two-dimensional magnets more convenient for numerical calculations and low-temperature expansion will be worked out. First, the function $r_{\mathbf{q}}$ of (5.14), which plays a major role in the theory, is divergent at low temperatures ($G \rightarrow 1$) and $\mathbf{q} \rightarrow 0$. In the long-wavelength region ($x \equiv q^2/4 \ll 1$) $r_{\mathbf{q}}$ is given by

$$r_{\mathbf{q}} \cong \begin{cases} \frac{1}{\pi c}; & x \ll c; \quad c \equiv 1 - G \ll 1 \\ \frac{2}{\pi x} \ln\left(\frac{x}{c}\right); & x \gg c; \quad \ln\left(\frac{8}{c}\right) \cong \frac{\pi}{\theta} \end{cases} \quad (6.1)$$

(the expression for $r_{\mathbf{q}}$ in the general case $x \sim c$ is given in Appendix C). For convenience of the evaluation of the integrals in (5.11) and (5.14) we introduce a less singular function $\psi_{\mathbf{q}}$ determined by

$$\psi_{\mathbf{q}} = \frac{1}{G} v_0 \int \frac{d\mathbf{p}}{(2\pi)^d} \frac{\lambda_{\mathbf{q}} - G\lambda_{\mathbf{p}}\lambda_{\mathbf{q}-\mathbf{p}}}{(1 - G\lambda_{\mathbf{p}})(1 - G\lambda_{\mathbf{q}-\mathbf{p}})} = \frac{1}{G^2} [2P - 1 - (1 - G\lambda_{\mathbf{q}})r_{\mathbf{q}}] \quad (6.2)$$

In the region $x \ll 1$

$$\psi_{\mathbf{q}} \cong \begin{cases} \frac{2}{\pi} \ln\left(\frac{8}{c}\right) - 1 - \frac{1}{\pi}; & x \ll c \\ \frac{2}{\pi} \ln\left(\frac{8}{x}\right) - 1; & x \gg c \end{cases} \quad (6.3)$$

i.e., $\psi_{\mathbf{q}}$ is only logarithmically divergent at small x and is not large at $x \sim 1$ [cf. (6.1)]. At low temperatures the "staggered" value of $\psi_{\mathbf{q}}$ is given by $\psi_{\mathbf{b}} = -1 + O(c)$. Now with the use of (6.2) one gets

$$r_{\mathbf{q}} = (2P - 1) \frac{1 - a\psi_{\mathbf{q}}}{1 - G\lambda_{\mathbf{q}}} \quad (6.4)$$

and

$$\frac{1}{r_{\mathbf{q}}} \frac{\partial r_{\mathbf{q}}}{\partial G} = \frac{2}{G} + \frac{\lambda_{\mathbf{q}}}{1 - G\lambda_{\mathbf{q}}} + \frac{2(GP' - 2P + 1)}{G(2P - 1)} \frac{1}{1 - a\psi_{\mathbf{q}}} - \frac{a}{1 - a\psi_{\mathbf{q}}} \frac{\partial \psi_{\mathbf{q}}}{\partial G} \quad (6.5)$$

where

$$a = \frac{G^2}{2P - 1} \quad (6.6)$$

In (6.5) the term with P' , which is exponentially large at small temperatures [see (4.15)], contains the main contributions to the integral (5.12) coming from the regions $\mathbf{p} \cong 0$ and $\mathbf{p} \cong \mathbf{q}$. In the long-wavelength region (see Appendix C)

$$\frac{\partial \psi_{\mathbf{q}}}{\partial G} = \begin{cases} \frac{2}{\pi c}; & x \ll c \\ -\frac{2}{\pi x} \ln\left(\frac{x}{c}\right) + \frac{6}{\pi x}; & x \gg c \end{cases} \quad (6.7)$$

i.e., the derivative $\partial \psi_{\mathbf{q}} / \partial G$ behaves similarly to $r_{\mathbf{q}}$, (6.1). With the use of (6.4) and (6.5) the expression for ΔG_0 , (5.11), can be put into the form

$$\Delta G_0 = \frac{G(P+3)}{GP'+P} - \frac{2G}{GP'+P} \frac{3P-1}{2P-1} I_1 - \frac{G^2}{GP'+P} I_2 \quad (6.8)$$

where

$$I_1 = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{1 - a\psi_{\mathbf{q}}}; \quad I_2 = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{a}{1 - a\psi_{\mathbf{q}}} \frac{\partial \psi_{\mathbf{q}}}{\partial G} \quad (6.9)$$

Now it is explicitly seen that ΔG_0 is exponentially small at low temperatures, as it should be. For the $1/D$ correction to energy (5.14) one gets

$$\Delta \bar{U} = \frac{2GP' - P(P+1)}{GP'(GP'+P)} - \frac{2a}{G^3} \frac{GP' - 2P + 1}{GP' + P} I_1 + \frac{1}{GP' + P} I_2 \quad (6.10)$$

For the calculation of antiferromagnetic susceptibility $\chi_0^{\text{AF}} = \chi_{\mathbf{b}}$ the quantity $M_{\mathbf{b}}$, (5.13), is needed. Taking into account the identity $\lambda_{\mathbf{b}-\mathbf{q}} = -\lambda_{\mathbf{q}}$, one can transform $M_{\mathbf{b}}$ to

$$M_{\mathbf{b}} = 4av_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{1 - a\psi_{\mathbf{q}}} \frac{\lambda_{\mathbf{q}}}{1 + G\lambda_{\mathbf{q}}} \quad (6.11)$$

Here at low temperature ($G \rightarrow 1$) the integrand diverges at $\mathbf{q} \rightarrow \mathbf{b}$. Since $\psi_{\mathbf{b}} = -1 + O(1-G)$, it is convenient to break up (6.11) into two parts: $M_{\mathbf{b}} = M_{\mathbf{b}}^{(0)} + M_{\mathbf{b}}^{(1)}$, where [see (6.6)]

$$M_{\mathbf{b}}^{(0)} = \frac{4a}{1+a} v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{\lambda_{\mathbf{q}}}{1 + G\lambda_{\mathbf{q}}} = -\frac{4G(P-1)}{2P-1+G^2} \quad (6.12)$$

and

$$M_{\mathbf{b}}^{(1)} = \frac{4aG^2}{2P-1+G^2} I_3; \quad I_3 = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{1 + \psi_{\mathbf{q}}}{1 - a\psi_{\mathbf{q}}} \frac{\lambda_{\mathbf{q}}}{1 + G\lambda_{\mathbf{q}}} \quad (6.13)$$

The expressions (6.10)–(6.13) are convenient for both numerical calculation and low-temperature expansion of the internal energy and antiferromagnetic susceptibility of two-dimensional magnets. For the internal energy (6.10) at low temperatures, omitting exponentially small terms, with the help of (4.15), one gets

$$\Delta \tilde{U} = 2\theta - 2aI_1 \tag{6.14}$$

Since at $\theta \ll 1$ the quantity $a \cong (\theta/2)/(1-\theta/2) \ll 1$ and $\psi_{\mathbf{q}}^n$ are integrable functions [see (6.3)], one can expand (6.14) in powers of $a\psi_{\mathbf{q}}$ and then of θ . As a result one gets [see (5.7)]

$$\tilde{U} \cong 1 - \left(1 - \frac{1}{D}\right)\theta - \frac{1}{2D}(1 + W_1)\theta^2 - \frac{1}{4D}(1 + 2W_1 + W_2)\theta^3 + \dots \tag{6.15}$$

where ($G \rightarrow 1$)

$$W_1 = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \psi_{\mathbf{q}} = v_0^2 \int \frac{d\mathbf{p} d\mathbf{q}}{(2\pi)^{2d}} \frac{\lambda_{\mathbf{p}+\mathbf{q}} - \lambda_{\mathbf{p}}\lambda_{\mathbf{q}}}{(1-\lambda_{\mathbf{p}})(1-\lambda_{\mathbf{q}})} \tag{6.16}$$

$$W_2 = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \psi_{\mathbf{q}}^2$$

The integrals W_n depend on the lattice structure alone and are in some sense analogs of the Watson integral for three-dimensional lattices. Note that in the low-dimensional case two integrations are needed to ensure convergence of lattice integrals. For the square lattice with n.n. interaction $W_1 = 0$ and $W_2 = 0.534$. The formula (6.15) should be compared with (2.10).

The low-temperature behavior of the antiferromagnetic susceptibility in the 1/D approximation [see (5.9)] is determined by the term $M_{\mathbf{b}}$ alone, since all other contributions are exponentially small. For $M_{\mathbf{b}}$ one gets

$$M_{\mathbf{b}} = -2(1-\theta) + \frac{\theta^2}{1-\theta/2} I_3 \tag{6.17}$$

which results in the low-temperature expansion

$$\tilde{\chi}_0^{\text{AF}} = \frac{1}{2} \left(1 - \frac{1}{D}\right) + \frac{1}{2D}\theta + \frac{\tilde{W}_1}{4D}\theta^2 + \frac{\tilde{W}_2}{8D}\theta^3 + \dots \tag{6.18}$$

where ($G \Rightarrow 1$)

$$\tilde{W}_n = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{\lambda_{\mathbf{q}}}{1 + \lambda_{\mathbf{q}}} (1 + \psi_{\mathbf{q}})^n \tag{6.19}$$

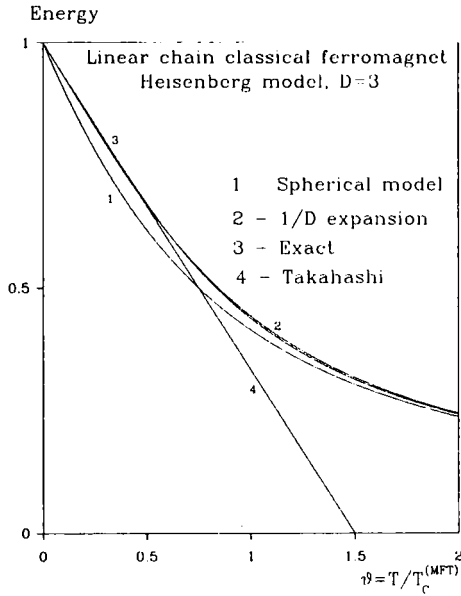


Fig. 4. The temperature dependence of the normalized internal energy of the linear chain classical Heisenberg model; $\theta = T/T_c^{(MFT)}$.

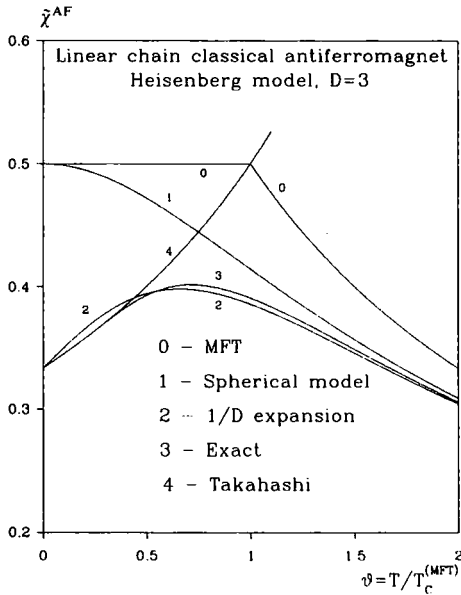


Fig. 5. The temperature dependence of the normalized antiferromagnetic susceptibility $\tilde{\chi}^{AF} = J_0 \chi^{AF}$ of the linear chain classical Heisenberg model.

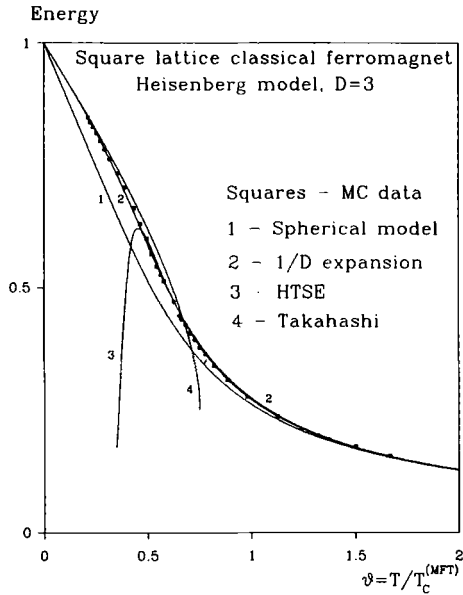


Fig. 6. The temperature dependence of normalized internal energy of the square lattice classical Heisenberg model.

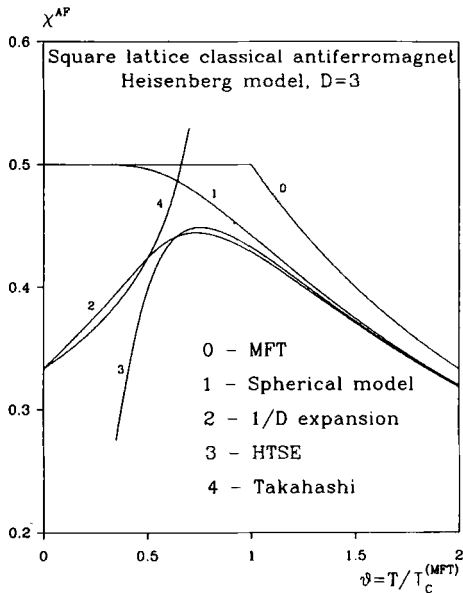


Fig. 7. The temperature dependence of antiferromagnetic susceptibility of the square lattice classical Heisenberg model. The HTSE curve was obtained by the summation of the series for $1/\bar{\chi}^{AF}$ calculated with the use of the series for $\bar{\chi}^{AF}$.⁽⁵⁾

are the other analogs of the Watson integral. For the square lattice with n.n. interaction, $\tilde{W}_1 = 0.0935$ and $\tilde{W}_2 = 0.470$. The formula (6.18) should be compared with (2.11).

The numerical results for internal energy (5.9) of the square lattice classical Heisenberg model ($D=3$) obtained with the use of the formulas of this section and the numerical solution of Eq. (4.9) for the quantity G are represented in Figs. 6 and 7. The comparison with the results of the other methods (HTSE,^(4,5) MC simulations⁽²⁴⁾) shows that the $1/D$ approximation is fairly reasonable in the whole temperature range. The accuracy of the $1/D$ approximation in two dimensions is comparable with that in one dimension (cf. Figs. 4 and 5). Useful formulas for numerical calculation of $\psi_{\mathbf{q}}$ are developed in Appendices A and B.

A propos of the results obtained at low temperatures for energy \tilde{U} and antiferromagnetic susceptibility $\tilde{\chi}_0^{\text{AF}}$, it should be noted that both quantities are determined by the short-range order. Correspondingly, the formulas (6.18) and (6.21) contain integrals determined by the whole Brillouin zone. For the long-wavelength quantities such as ferromagnetic susceptibility $\tilde{\chi}_0$ and spin-spin correlation function $S_{\mathbf{k}}$ the situation is more subtle, and nontrivial long-wavelength integrals appear in the calculations. This is the subject of the next section.

7. FERROMAGNETIC SUSCEPTIBILITY AND SPIN-SPIN CORRELATION FUNCTION

For the calculation of the ferromagnetic susceptibility $\tilde{\chi}_0$ of two-dimensional classical magnets at low temperatures one has to consider the exponentially small $1/D$ corrections to the quantity G in (5.6). It is seen already from (4.16) that the $1/D$ expansion for the ferromagnetic susceptibility is not homogeneous and fails in the vicinity of the singularity point $\theta=0$, where $1/(D\theta) \gtrsim 1$. Nevertheless, as we will see below, the inhomogeneity of the $1/D$ expansion does not impede the determination of the true form of singular quantities at $\theta \ll 1$.

Taking into account that in (6.8) $P \cong 1/\theta$ and $I_1 = 1 + O(\theta)$, one gets

$$\Delta G_0 \cong \frac{1}{P'} \left[\frac{1}{\theta} - I_2 + O(\theta) \right] \quad (7.1)$$

The integral I_2 can be represented as $I_2 = I_{20} + I_{21}$, where

$$I_{20} = av_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{\partial \psi_{\mathbf{q}}}{\partial G}; \quad I_{21} = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{a^2}{1 - a\psi_{\mathbf{q}}} \frac{\partial \psi_{\mathbf{q}}}{\partial G} \quad (7.2)$$

The integral I_{20} can be calculated with the use of (6.2). In the low-temperature range, neglecting exponentially small terms, one gets

$$I_{20} \cong a \frac{\partial}{\partial G} [(1-G)(P-1)^2] \cong -\frac{1}{2\theta} + \frac{3}{4} + \frac{1}{\pi} + O(\theta) \quad (7.3)$$

[see (4.15)]. The integral I_{31} is more complicated and it is calculated in Appendix C. Here we note that because of the factor $a^2 \propto \theta^2$ in (7.2) the contribution to I_{21} from the main part of the Brillouin zone ($q \sim 1$), where $\partial\psi_q/\partial G \sim 1/\theta$, is $O(\theta)$ and may be neglected. Thus, for the calculation of I_{21} the long-wavelength form of ψ_q can be used. The result of the calculation reads

$$I_{21} \cong -\frac{1}{2\theta} + \frac{3}{\pi} \ln\left(\frac{\pi}{\theta}\right) + \frac{1}{4} - \frac{3}{\pi} + \frac{4}{\pi} \ln(2) + \frac{\gamma_0}{\pi} + O(\theta) \quad (7.4)$$

where $\gamma_0 = 0.273$. Now, adopting (7.3) and (7.4) in (7.1) and inserting ΔG_0 of (7.1) into (5.6), one gets

$$1 - \hat{G}_0 \cong 8 \exp\left(-\frac{\pi}{\theta}\right) \left(1 - \frac{2\pi}{D\theta} + \frac{3}{D} \ln\frac{1}{\theta} + \frac{c_0}{D}\right) \quad (7.5)$$

where $c_0 = \pi - 2 + \ln(16\pi^3) + \gamma_0 = 7.62$. The expression for $1 - \hat{G}_0$ should be adopted in (4.6). The $1/D$ corrections become high at small θ . This means that the actual form of the quantity $1 - \hat{G}_0$ in our approximation is

$$1 - \hat{G}_0 \cong 8 \left(1 + \frac{c_0}{D}\right) \theta^{-3/D} \exp\left[-\frac{\pi}{\theta} \left(1 + \frac{2}{D}\right)\right] \quad (7.6)$$

The latter is consistent with the functional form of the result obtained by the Monte Carlo renormalization group analysis for arbitrary D ,⁽²⁵⁾

$$\begin{aligned} \tilde{\chi}_0 &= c'_D \theta^{3/(D-2)} \exp\left(\frac{\pi}{\theta} \frac{D}{D-2}\right) \\ c'_3 &= (1.62-2.68) \cdot 10^{-5} \\ c'_4 &= (1.41-2.12) \cdot 10^{-3} \\ c'_5 &= (7.30-9.08) \cdot 10^{-3} \end{aligned} \quad (7.7)$$

It is seen that it is difficult to determine the prefactor c'_D in (7.7) by the $1/D$ expansion, which is reflected in the large value of the constant c_0 in (7.6). In the case $D=2$ the expression (7.7) goes to infinity, which corresponds to the diverging of susceptibility in the temperature range below the Berezinsky-Kosterlitz-Thouless transition.

The correlation length ξ and the \mathbf{k} -dependent spin-spin correlation function $S_{\mathbf{k}}$ are determined by the small- \mathbf{k} ($k \ll 1$) behavior of the denominator of (4.6):

$$1 - \hat{G}_{\mathbf{k}} \lambda_{\mathbf{k}} \cong 1 - \hat{G}_0 + k^2/4 - M_{\mathbf{k}}/D \quad (7.8)$$

where $1 - \hat{G}_0$ is given by (7.5) and the expansion $\lambda_{\mathbf{k}} \cong 1 - k^2/z$ ($z=4$) was used. It can be shown that at $k \ll 1$ and $\theta \ll 1$ the relevant contribution to $M_{\mathbf{k}}$, (5.20), is due to the long-wavelength region $q \ll 1$. The details of calculation are given in Appendix D. The correlation length is determined by $\xi = \kappa^{-1}$, where $k = i\kappa$ is the zero of (7.8). In the spherical approximation ($D \rightarrow \infty$) $\kappa = \kappa_0$, $\kappa_0^2 = 32 \exp(-\pi/\theta)$. In the first order in $1/D$ it is sufficient to calculate $M_{\mathbf{k}}$ for $k = k_0 = i\kappa_0$. As a result one gets

$$\kappa^2 \equiv \xi^{-2} = 32 \exp\left(-\frac{\pi}{\theta}\right) \left(1 - \frac{2\pi}{D\theta} + \frac{2}{D} \ln \frac{1}{\theta} + \frac{c_1}{D}\right) \quad (7.9)$$

where $c_1 = c_0 - \ln(\pi) + \gamma_1 = 7.36$, $\gamma_1 = 0.8811$. This is also consistent with the functional form of the result of ref. 25,

$$\xi^{-1} = c_D \theta^{-1/(D-2)} \exp\left(-\frac{\pi}{2\theta} \frac{D}{D-2}\right) \quad (7.10)$$

$$c_3 = 451; \quad c_4 = 39.2; \quad c_5 = 19.0$$

but again the prefactor c_D here cannot be compared with the result of the $1/D$ expansion. Thus, one can conclude that the $1/D$ expansion works well for calculation of the physical quantities of two-dimensional ferro- and antiferromagnets nonsingular at $T=0$, such as internal energy and antiferromagnetic susceptibility, and that it is less efficient in comparison with other methods for the analysis of the singular ones.

The spin-spin correlation function $S_{\mathbf{k}}$ in the $1/D$ approximation proves to be of a non-Ornstein-Zernike form. The calculation of $M_{\mathbf{k}}$ at $\kappa \ll k \ll 1$ (the details are given in Appendix D) shows that in the region $\ln(k/\kappa) \gg 1$, i.e., $(\theta/\pi) \ln(1/k) \ll 1$ (this condition requires larger values of k than just $k \gg \kappa$) the wavevector-dependent susceptibility $\tilde{\chi}_{\mathbf{k}} = S_{\mathbf{k}}/\theta$ is given by

$$\frac{1}{4} k^2 \tilde{\chi}_{\mathbf{k}} \cong 1 - \frac{1}{D} \left[1 + \frac{2\theta}{\pi} \ln\left(\frac{1}{k}\right)\right] \cong \left(1 - \frac{1}{D}\right) k^{2\theta/\pi D} \quad (7.11)$$

which implies $S_{\mathbf{k}} \propto 1/k^{2-\eta}$, $\eta = 2\theta/(\pi D)$. The dependences of $-\ln(k^2 \tilde{\chi}_{\mathbf{k}}/4)$ versus $\ln(1/k)$ for different values of θ are represented in Fig. 8. It can

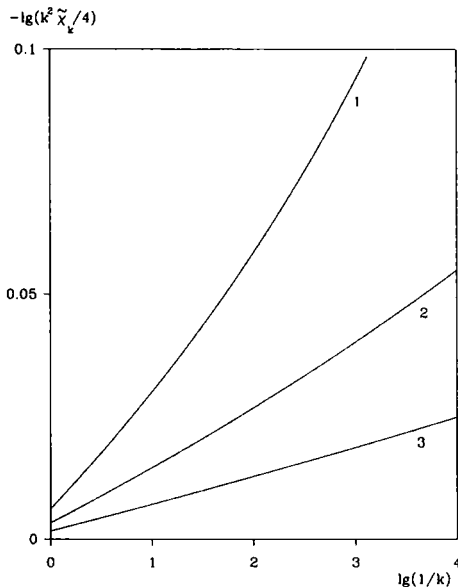


Fig. 8. The non-Ornstein-Zernike behavior of the spin-spin correlation function $S_k = \theta \tilde{\chi}_k$ of the square-lattice classical Heisenberg model in the $1/D$ approximation; (1) $\theta = 0.1$; (2) $\theta = 0.05$; (3) $\theta = 0.025$.

be seen that the linear dependence is realized only at sufficiently small temperatures and large wavevectors. Note that in the one-dimensional case [see (2.3)] the correlation function has the Ornstein-Zernike form.

8. DISCUSSION

In this article the $1/D$ expansion for classical spin systems on a lattice has been developed and applied to two-dimensional Heisenberg ferro- and antiferromagnets. It proves that for the quantities nonsingular at $T=0$, such as internal energy and antiferromagnetic susceptibility, the $1/D$ expansion is uniform for all temperatures and works rather well for $D=3$. The reason is that the exact results for thermodynamic quantities at $T=0$ are recovered already in the first order in $1/D$ and the $1/D$ expansion is consistent with HTSE at high temperatures. For singular quantities, such as ferromagnetic susceptibility and correlation length, the $1/D$ expansion is inhomogeneous at low temperatures, but, nevertheless, it yields the asymptotic forms of the singular quantities at $\theta \ll 1$ [see, e.g., (7.5) and (7.6)].

An important feature of the approach proposed here is the correspondence between the order of the $1/D$ expansion and the number of loops (i.e., the number of independent integrations over the Brillouin zone) in the diagrams taken into account. That is, in the zeroth order in $1/D$ (spherical or self-consistent Gaussian approximations) all one-loop diagrams are taken into account (see Fig. 2) and the approximation of the first order in $1/D$ is given by two-loop diagrams (see Fig. 3). It is expected that the three-loop approximation of the order $1/D^2$ would be a substantial improvement at low temperatures, since it yields, in particular, the exact values of both $\chi^{\text{AF}}(0)$ and $\partial\chi^{\text{AF}}/\partial T|_{T=0}$.

It is interesting to note that using the conjecture that the coefficients in the low-temperature expansions of energy and antiferromagnetic susceptibility are polynomials in $1/D$ allows one to determine *exactly* one additional coefficient in each order in $1/D$. For example, the coefficients in the terms of orders θ^2 in (6.15) and θ in (6.18) for the two-dimensional classical model become exact only in the second order in $1/D$ [cf. (2.10) and (2.11)]. Nevertheless, these coefficients can be determined exactly with the use of the present $O(1/D)$ results and the additional condition that for $D=1$ ($S=1/2$ Ising model) they vanish (there are no powers of temperature in the low-temperature expansions, only exponentials). As a result, these coefficients acquire additional factors $(1 - 1/D)$:

$$\tilde{U} \cong 1 - \left(1 - \frac{1}{D}\right)\theta - \frac{1}{2D} \left(1 - \frac{1}{D}\right) (1 + W_1)\theta^2 + \dots \quad (8.1)$$

$$\tilde{\chi}_0^{\text{AF}} = \frac{1}{2} \left(1 - \frac{1}{D}\right) + \frac{1}{2D} \left(1 - \frac{1}{D}\right)\theta + \dots \quad (8.2)$$

[recall that for the square lattice $W_1 = 0$; see (6.16)].

The fact that at low temperatures the $1/D$ expansion yields exact results for specific heat and antiferromagnetic susceptibility up to the n th order in temperature in the $(n+1)$ th order in $1/D$ can be used for the development of the low-temperature expansions of the physical quantities of spin systems. However, this way seems to be too indirect and heavy. It would be better to obtain the low-temperature expansions directly using the small parameter $\theta \ll 1$. But for systems without long-range order the situation at $\theta \ll 1$ is not so simple as for three-dimensional ones, and this problem requires a special investigation.

Comparing the present results with those of the other lattice theories for low-dimensional magnets, we note that the latter do not go beyond a one-loop approach. The most successful of them proposed by Takahashi⁽⁸⁾ for the Heisenberg model proves to be rather good at low temperature.

For the one-dimensional classical Heisenberg model, neglecting small exponentials, Takahashi's theory yields

$$\tilde{U} \cong 1 - \frac{2}{3}\theta; \quad \tilde{\chi}_0^{\text{AF}} \cong \frac{1}{3} \frac{1}{1 - \theta/3}; \quad \theta \ll 1 \quad (8.3)$$

[cf. (2.10) and (2.11)], which reproduces the exact results (2.1) and (2.2) with the accuracy of the order of $\exp(-3/\theta)$. Comparing this with the $1/D$ expansion [see (2.10) and (2.11)], we conclude that (8.3) actually contains all powers of $1/D$ and, accordingly, all relevant many-loop diagrams. It does not necessarily contradict the one-loop nature of the Takahashi theory, since the latter is based on variational, rather than on a perturbative approach, and in the one-dimensional case all many-loop integrals can be calculated analytically giving simple results. In the two-dimensional case the situation is different, because already two-loop integrals over the Brillouin zone cannot be calculated analytically. For the square-lattice classical Heisenberg model, neglecting exponentially small terms, the results of the Takahashi approach can be expressed in the form³

$$\tilde{U} \cong \frac{1}{2} \left[1 + \left(1 - \frac{4}{3}\theta \right)^{1/2} \right] - \frac{1}{3}\theta \cong 1 - \frac{2}{3}\theta - \frac{1}{9}\theta^2 - \frac{2}{27}\theta^3 - \dots \quad (8.4)$$

$$\tilde{\chi}_0^{\text{AF}} \cong \frac{2}{3} \frac{1}{1 + [1 - (4/3)\theta]^{1/2}} \cong \frac{1}{3} + \frac{1}{9}\theta + \frac{2}{27}\theta^2 + \frac{5}{81}\theta^3 + \dots \quad (8.5)$$

These results should be compared with (6.15) and (6.18) for $D = 3$ [cf. also (8.1) and (8.2)]. Whereas the factors $1/9 = (1/2D)(1 - 1/D)$ in (8.4) and (8.5) seem to be correct, in contrast to the factors $1/(2D) = 1/6$ in (6.16) and (6.18), it seems unlikely that all many-loop integrals over the Brillouin zone in all orders in $1/D$ could fold into simple numbers like $2/27$ and $5/81$. Comparison with the MC simulation results for energy⁽²⁴⁾ (see Fig. 6) shows that actually the $1/D$ expansion is not worse than (8.4) and (8.5) at low temperatures and is remarkably good in the whole temperature range. It would be very desirable to make such a comparison for antiferromagnetic susceptibility. Another interesting task is to generalize the Takahashi theory for arbitrary D and to compare it with the $1/D$ expansion.

As for ferromagnetic susceptibility χ_0 and correlation length ξ in two dimensions, the $1/D$ expansion supports the arbitrary- D RG results (7.7) and (7.10) obtained by Fukugita and Oyanagi,⁽²⁵⁾ which for $D = 3$ take on the form

$$S_0 \cong \theta \tilde{\chi}_0 \propto \theta^4 \exp\left(\frac{3\pi}{\theta}\right); \quad \xi \propto \theta \exp\left(\frac{3\pi}{2\theta}\right) \quad (8.6)$$

³ The low-temperature expansion of the antiferromagnetic susceptibility of the square-lattice classical model produced by Takahashi himself seems to be incorrect.

as well as similar results by Shenker and Tobochnik⁽²⁴⁾ obtained earlier for the classical Heisenberg model. On the contrary, the preexponents proportional to θ^2 and *const* for S_0 and ξ obtained by Takahashi and some other researchers seem to be incorrect.

An interesting problem, the investigation of which is planned for the nearest future, is the calculation of the physical quantities of low-dimensional magnets in the presence of a magnetic field. This problem is significant for both one- and two-dimensional systems and it cannot be handled with such theories as that of ref. 8. The underlying physics is non-trivial here, as is reflected by the impermutability of limits $T \rightarrow 0$ and $H \rightarrow 0$. In particular, for the antiferromagnetic susceptibility of bipartite lattice systems we have $\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} \chi(H, T) = 1/(2J_0) \cdot (1 - 1/D)$ and $\lim_{H \rightarrow 0} \lim_{T \rightarrow 0} \chi(H, T) = 1/(2J_0)$. The general functional form of $\chi(H, T)$ in the $1/D$ approximation containing these features can be determined regularly in the framework of the method proposed.

APPENDIX A. THE FUNCTION $\psi_{\mathbf{q}}$ FOR A GENERAL LATTICE

The function $\psi_{\mathbf{q}}$, (6.2), is not divergent in the low-temperature limit ($G \rightarrow 1$) at $\mathbf{q} \neq 0$, because the numerator of (6.2) compensates for the small value of the denominator at $\mathbf{p} = 0$ and $\mathbf{p} = \mathbf{q}$. However, the integral (6.2) is still inconvenient for the direct numerical calculation since the integrand has singularities at $\mathbf{p} = 0$ and $\mathbf{p} = \mathbf{q}$. In particular, for $p \ll 1$, $\lambda_{\mathbf{p}} \cong 1 - O(p^2)$ and $\lambda_{\mathbf{p}-\mathbf{q}} \cong \lambda_{\mathbf{q}} - \mu_{\mathbf{q}}\mathbf{p} - O(p^2)$, where $\mu_{\mathbf{q}} = \partial\lambda_{\mathbf{q}}/\partial\mathbf{q}$; thus the integrand behaves as $\mu_{\mathbf{q}}\mathbf{p}/p^2$. This singularity gives zero contribution to the integral, but it can spoil numerical results. To remedy this drawback, we make some identical transformations of (6.2) to get a nonsingular integrand. First, (6.2) can be written as

$$\psi_{\mathbf{q}} = \frac{1}{G} v_0 \int \frac{d\mathbf{p}}{(2\pi)^d} \frac{\lambda_{\mathbf{q}} - G\lambda_{\mathbf{p}}\lambda_{\mathbf{q}-\mathbf{p}}}{2 - G(\lambda_{\mathbf{p}} + \lambda_{\mathbf{q}-\mathbf{p}})} \left(\frac{1}{1 - G\lambda_{\mathbf{p}}} + \frac{1}{1 - G\lambda_{\mathbf{q}-\mathbf{p}}} \right) \quad (\text{A.1})$$

Since the two parts of (A.1) give the same contribution to $\psi_{\mathbf{q}}$, one can drop the second term in the square brackets and multiply the first one by 2. Then the integrand can be symmetrized with respect to the change of the sign of \mathbf{p} :

$$\psi_{\mathbf{q}} = \frac{1}{G} v_0 \int \frac{d\mathbf{p}}{(2\pi)^d} \frac{1}{1 - G\lambda_{\mathbf{p}}} \left[\frac{\lambda_{\mathbf{q}} - G\lambda_{\mathbf{p}}\lambda_{\mathbf{q}-\mathbf{p}}}{2 - G(\lambda_{\mathbf{p}} + \lambda_{\mathbf{q}-\mathbf{p}})} + \frac{\lambda_{\mathbf{q}} - G\lambda_{\mathbf{p}}\lambda_{\mathbf{q}+\mathbf{p}}}{2 - G(\lambda_{\mathbf{p}} + \lambda_{\mathbf{q}+\mathbf{p}})} \right] \quad (\text{A.2})$$

Here the integrand is well behaved at $\mathbf{p} = 0$, and (A.2) is convenient for computations.

APPENDIX B. THE FUNCTION $\psi_{\mathbf{q}}$ FOR THE SQUARE LATTICE

For the square lattice with the nearest neighbor interaction $\lambda_{\mathbf{k}} = \frac{1}{2}(\cos k_x + \cos k_y)$, and in the expression for the function $\psi_{\mathbf{q}}$, (6.2), one can perform one of the integrations over p_x, p_y analytically. In fact, it is more convenient to calculate the function $r_{\mathbf{q}}$, (5.12), first, and then to determine $\psi_{\mathbf{q}}$ from (6.2). For $r_{\mathbf{q}}$ with the use of formula (1.5.9.32) of ref. 26 one gets

$$r_{\mathbf{q}} = \int_{-\pi}^{\pi} \frac{dp_y}{2\pi} Q(p_y, \mathbf{q})$$

$$Q = \frac{1}{\mathcal{D}} \left[\frac{a_+ - a_- \cos(q_x)}{(a_-^2 - g^2)^{1/2}} + \frac{a_- - a_+ \cos(q_x)}{(a_+^2 - g^2)^{1/2}} \right] \quad (\text{B.1})$$

$$\mathcal{D} = (a_+ - a_-)^2 + (1 - \cos q_x)[2a_+ a_- - g^2(1 + \cos q_x)]$$

$$a_{\pm} = 1 - g \cdot \cos(p_y \pm q_y/2); \quad g = G/2$$

It can be seen that in the low-temperature limit ($G \rightarrow 1, g \rightarrow 1/2$) both terms of Q , (B.1), are divergent at $\mathbf{q} \rightarrow 0$, whereas Q itself remains finite for $p_y \neq 0$. To put it into explicit form, we transform the expression for Q to

$$Q = \frac{1 - \cos(q_x)}{\mathcal{D}} \left(\frac{a_+}{S_+} + \frac{a_-}{S_-} \right) + \frac{1}{\mathcal{D}} \frac{(a_+ - a_-)^2 (a_+ + a_-)}{S_+ S_- (S_+ + S_-)} \quad (\text{B.2})$$

where $S_{\pm} = (a_{\pm}^2 - g^2)^{1/2}$. At low temperature the function Q is singular at $p_y = \pm q_y/2$, which hampers the numerical integration over p_y . Thus, it is more convenient to write down the quadrature for $\psi_{\mathbf{q}}$ directly, which with the use of the identity

$$\int_{-\pi}^{\pi} \frac{dp_y}{2\pi} \frac{1}{S_{\pm}} = P(G)$$

can be transformed to the final form

$$\psi_{\mathbf{q}} = \frac{1}{G^2} \int_0^{\pi} \frac{dp_y}{\pi} \left[\frac{1}{S_+} + \frac{1}{S_-} - 1 - (1 - G\lambda_{\mathbf{q}}) Q(p_y, \mathbf{q}) \right] \quad (\text{B.3})$$

In the limit $T \rightarrow 0$ the integrand of (B.3) becomes discontinuous (but not divergent) at $p_y = q_y/2$. This must be taken into account in the computation of $\psi_{\mathbf{q}}$.

APPENDIX C. LONG-WAVELENGTH INTEGRALS FOR FERROMAGNETIC SUSCEPTIBILITY

The function r_q , (5.12), in the long-wavelength ($x \equiv q^2/4 \ll 1$), low-temperature ($1 - G \ll 1$) region can be calculated analytically in a straightforward manner. For the square lattice the result reads

$$r_q \cong \frac{2}{c\pi} \tilde{r}(y); \quad y = x/c; \quad c \equiv 1 - G \ll 1 \quad (\text{C.1})$$

$$\tilde{r}(y) = \frac{1}{2} \frac{1}{[y(y+4)]^{1/2}} \ln \left[1 + \frac{[y(y+4)]^{1/2} \{y+2 + [y(y+4)]^{1/2}\}}{2} \right]$$

It is seen that $\tilde{r}(0) = 1/2$ and $\tilde{r}(y) \cong \ln(y)/y$ for $y \gg 1$ [cf. (6.1)]. Then, with the same assumptions, the derivative $\partial\psi_q/\partial G$ can be calculated with the help of (6.2) and (C.1) to yield

$$\frac{\partial\psi}{\partial G} \cong \frac{2}{c\pi} \left[v(y) - \frac{y-2}{y+4} \tilde{r}(y) \right] \quad (\text{C.2})$$

$$v(y) = 3 \frac{[y(y+4)]^{1/2} (2y^2 + 7y + 4) + 2y^3 + 11y^2 + 14y + 2}{\left((y+4) \{ [y(y+4)]^{1/2} + y + 1 \} \times \{ [y(y+4)]^{1/2} (y+2) + y^2 + 4y + 2 \} \right)}$$

The limiting forms of $v(y)$ are $v(0) = 3/4$ and $v(y) \cong 3/y$ for $y \gg 1$ [cf. (6.7)].

Now we proceed to the calculation of the integral I_{21} , (7.2). The relevant terms of I_{21} , i.e., those $O(1/\theta)$ and $O(1)$, are determined by the long-wavelength region. However, one cannot simply extend the integration in (7.2) to infinity, since in this case the integral will diverge at the upper bound. Thus, we express in (7.2) ψ_q through r_q with the use of (6.2) and write

$$I_{21} = v_0 \int \frac{d\mathbf{q}}{(2\pi)^d} \left[\frac{G^2}{r_q(1 - G\lambda_q)} - a \right] \frac{\partial\psi_q}{\partial G}$$

$$\cong \frac{1}{\pi} \int_0^{A/c} dy \left[\frac{1}{(y+1)\tilde{r}(y)} - \frac{2a}{\pi} \right] \left[v(y) - \frac{y-2}{y+4} \tilde{r}(y) \right] \quad (\text{C.3})$$

where the upper bound corresponds to $q^2 \sim x = A \sim 1$. Then we break up I_{21} into two parts: $I_{21} = I_{210} + I_{211}$, where

$$I_{210} = \frac{1}{\pi} \int_0^{A/c} dy f_0(y); \quad I_{211} = \frac{1}{\pi} \int_0^{A/c} dy [f(y) - f_0(y)] \quad (\text{C.4})$$

$f(y)$ is the integrand of (C.3) and $f_0(y)$ is its asymptotic form in the range $y \gg 1$. We use [see (C.1) and (C.4)]

$$f_0(y) = \frac{1}{y + \rho} \left[\frac{1}{\ln(y + \rho)} - \frac{2a}{\pi} \right] \left[3 - \ln(y + \rho) \right] \quad (C.5)$$

where the parameter $\rho > 1$ is adopted to ensure the convergence of I_{210} at the lower bound $y = 0$. Evaluation of I_{210} with the use of $a \cong (\theta/2)/(1 - \theta/2)$ [see (6.6)] and $\ln(8/c) \cong \pi/\theta$ [see (4.13) and (4.15)] yields

$$I_{210} = -\frac{1}{2\theta} + \frac{3}{\pi} \ln\left(\frac{\pi}{\theta}\right) - \frac{3}{\pi} + \frac{1}{4} - \frac{3}{\pi} \ln \ln(\rho) + \frac{1}{\pi} \ln(\rho) + O(\theta) \quad (C.6)$$

Now, since the difference $f(y) - f_0(y)$ in I_{211} , (C.4), rapidly diminishes with the increasing of y , the integral I_{211} is determined by the region $y \sim 1$ ($x \sim c$), and the upper bound in I_{211} may be set to infinity. Neglecting the terms with a which are $O(\theta)$, one gets

$$I_{211} = \frac{4}{\pi} \ln(2) - \frac{1}{\pi} \ln(\rho) + \frac{3}{\pi} \ln \ln(\rho) + \frac{\gamma_0}{\pi} + O(\theta) \quad (C.7)$$

where

$$\gamma_0 = -3 \ln \ln(\rho) + \int_0^\infty dy \left[\frac{v(y)}{(y+1)\tilde{r}(y)} - \frac{3}{(y+\rho)\ln(y+\rho)} \right] = 0.273 \quad (C.8)$$

It is obvious that γ_0 is independent of ρ . The resultant expression for I_{21} is given by (7.4).

APPENDIX D. LONG-WAVELENGTH INTEGRALS FOR THE SPIN-SPIN CORRELATION FUNCTION

In this Appendix the long-wavelength form of the quantity $M_{\mathbf{k}}$ ($x_k \equiv k^2/4 \ll 1$) in the low-temperature region will be developed. Since $r_{\mathbf{q}} \sim 1/\theta$ for $q \sim 1$ [see (6.1)], the main part of the Brillouin zone yields a small contribution to $M_{\mathbf{k}}$, (5.13), being of the order of $a \sim \theta \ll 1$. Thus, in the calculation of $M_{\mathbf{k}}$ one can use the long-wavelength approximation:

$$M_{\mathbf{k}} \cong -\frac{2}{\pi} \int_0^A dx \frac{I(x, x_k)}{r_{\mathbf{q}}(x+c)} = -\frac{k^2}{4} \int_0^{A/c} dy \frac{\tilde{I}(y, y_k)}{(y+1)\tilde{r}(y)} \quad (D.1)$$

where $A \sim 1$, $\tilde{r}(y)$ is given by (C.1), $y_k = x_k/c = k^2/(4c)$, and I is the average with respect to the angle of the vector \mathbf{q} :

$$I(x, x_k) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi_q \frac{\lambda_q - \lambda_{q-k}}{1 - G\lambda_{q-k}} = y_k \tilde{I}(y, y_k) \quad (\text{D.2})$$

$$\tilde{I}(y, y_k) = \frac{1}{y_k} \left[-1 + \frac{1+y}{[(1+y+y_k)^2 - 4yy_k]^{1/2}} \right]$$

For small k ($y_k \ll 1$, i.e., $k \ll 1/\xi$)

$$\tilde{I}(y, y_k) = \frac{y-1}{(y+1)^2} + \frac{y^2-4y+1}{(y+1)^4} y_k + O(y_k^2) \quad (\text{D.3})$$

The integral (D.1) can be treated with the same method that was applied to I_{21} in Appendix C. Using the asymptotic form $\tilde{I} \cong 1/(y+\rho)$, one gets

$$M_k \cong -\frac{k^2}{4} \left[\ln\left(\frac{\pi}{\theta}\right) - f(y_k) + O(\theta) \right] \quad (\text{D.4})$$

where

$$f(y_k) = \ln \ln(\rho) + \int_0^\infty dy \left[\frac{1}{(y+\rho) \ln(y+\rho)} - \frac{\tilde{I}(y, y_k)}{(y+1) \tilde{r}(y)} \right] \quad (\text{D.5})$$

and $\rho > 1$. For the calculation of the correlation length $\xi = \kappa^{-1}$ in the first order in $1/D$ it is sufficient to calculate M_k for $k = k_0 = i\kappa_0$ ($\kappa_0 = 4c$), i.e., for $y_k = -1$. This should be done carefully, since $\tilde{I}(y, -1)$ is divergent at $y = 0$. So, we write $f(-1) = f_0 + f_1$, where

$$f_0 = 2 \int_0^\infty dy \left[\frac{1}{y+\rho} - \tilde{I}(y, -1) \right] = 2[2 - \ln(\rho)] \quad (\text{D.6})$$

and

$$f_1 = \ln \ln(\rho) + \int_0^\infty dy \left\{ \frac{1}{y+\rho} \left[\frac{1}{\ln(y+\rho)} - 2 \right] - \tilde{I}(y, -1) \left[\frac{1}{(y+1) \tilde{r}(y)} - 2 \right] \right\} \quad (\text{D.7})$$

has a well-behaved integrand [$\tilde{r}(0) = 1/2$]. As a result of computations one gets $f(-1) = 0.8811$. For a comparison, the small- k expansion of f calculated with the use of (D.3) yields $f(y_k) \cong f(0)(1 + \alpha y_k)$ with $f(0) = 0.8875$ and $\alpha = 0.006983$, which gives 0.8813 for $y_k = -1$. Now, adopting M for $k = i\kappa_0$ in (7.8), one obtains the formula (7.9) for correlation length in the $1/D$ approximation.

For the calculation of spin-spin correlation function S_k for $k \gg \kappa$, we should investigate the behavior of the function $f(y_k)$, (D.5), for $y_k \gg 1$. It turns out that after eliminating small terms of orders $1/y_k$ and $1/\sqrt{y_k}$ from (D.5), f becomes a function of "slow" variable $\ln(y_k) = 2 \ln(k/\kappa_0)$. In the limit $y_k \gg 1$ the function $\tilde{I}(y, y_k)$ simplifies to $\tilde{I} \cong \tilde{I}_0 + \tilde{I}_1$, where \tilde{I}_0 is peaked at $y = y_k$:

$$\tilde{I}_0 = \frac{1}{[(y_k - y)^2 + 4y_k]^{1/2}} \tag{D.8}$$

and \tilde{I}_1 is a steplike function:

$$\tilde{I}_1 = \frac{1}{y_k} \left[-1 + \frac{y - y_k}{[(y_k - y)^2 + 4y_k]^{1/2}} \right] \cong -\frac{2}{y_k} \theta(y_k - y) \tag{D.9}$$

[here $\theta(x)$ is the step function]. The corrections to (D.8) and (D.9) are of the order $1/y_k^2$. It is convenient to integrate out the peak part of the integral (D.5) analytically. Since near $y = y_k \gg 1$ the function $\tilde{r}(y)$ takes on its asymptotic form [see (C.1)], one can break up (D.5) into two parts: $f = f_0 + f_1$, where

$$f_0 = \frac{1}{\ln(y_k + \rho)} \int_0^\infty dy \left[\frac{1}{y + \rho} - \tilde{I}(y, y_k) \right] = \frac{2 - \ln(\rho)}{\ln(y_k + \rho)} \tag{D.10}$$

and

$$f_1 = \ln \ln(\rho) + \int_0^\infty dy \left\{ \frac{1}{y + \rho} \left[\frac{1}{\ln(y + \rho)} - \frac{1}{\ln(y_k + \rho)} \right] - \tilde{I}(y, y_k) \left[\frac{1}{(y + 1) \tilde{r}(y)} - \frac{1}{\ln(y_k + \rho)} \right] \right\} \tag{D.11}$$

In (D.11) the peak of \tilde{I} at $y = y_k$ is compensated for by the difference in square brackets. Thus, the representation (D.10), (D.11) is convenient for the numerical calculation of $f(y_k)$ for arbitrary y_k . Note that (D.10), (D.11) recovers (D.6), (D.7) if we choose $\ln(1 - \rho) = 1/2$, i.e., $\rho = e^{1/2} + 1 = 2.6487$. Such a choice of ρ guarantees good behavior of the integrand of (D.11) for both $y_k = -1$ and $y_k \gg 1$.

For the analytical calculation of the function $f(y_k)$, (D.5), in the limit $y_k \gg 1$ it is convenient to represent it in the ρ -independent form. Replacing the upper bound of the integration by $A \rightarrow \infty$, one gets

$$f(y_k) = \ln \ln(A) + \frac{2 - \ln(A)}{\ln(y_k)} + \int_0^A dy \tilde{I}(y, y_k) \left[\frac{1}{\ln(y_k)} - \frac{1}{(y + 1) \tilde{r}(y)} \right] \tag{D.12}$$

Using the asymptote $(y + 1) \tilde{r}(y) \cong \ln(y)$ in the relevant region $y \sim y_k \gg 1$ and the representation of \tilde{I} (D.8), (D.9), we can transform expression (D.12) to

$$\begin{aligned} f(y_k) &\cong \ln \ln(A) + \frac{2 - \ln(A)}{\ln(y_k)} \\ &+ \int_0^{y_k} dy \left(\frac{1}{y_k - y} - \frac{2}{y_k} \right) \frac{\ln(y/y_k)}{\ln(y) \ln(y_k)} \\ &+ \int_{y_k}^A \frac{dy}{y - y_k} \frac{\ln(y/y_k)}{\ln(y) \ln(y_k)} \end{aligned} \quad (\text{D.13})$$

In (D.13) the quantity $4y_k$ entering \tilde{I}_0 , (D.8), is omitted, since it introduces an error of the order $1/\sqrt{y_k}$ to $f(y_k)$. Then after some transformations, the function $f(y_k)$ takes on the final form

$$\begin{aligned} f(y_k) &\cong \ln \ln(y_k) - 1 + \frac{2}{\ln(y_k)} - \frac{2}{\ln^2(y_k)} \int_0^1 dz \frac{\ln(z)}{1 + \ln(z)/\ln(y_k)} \\ &- \frac{2}{\ln^3(y_k)} \int_0^1 \frac{dz}{1 - z} \frac{\ln^2(z)}{1 - \ln^2(z)/\ln^2(y_k)} \end{aligned} \quad (\text{D.14})$$

which can be easily expanded in powers of $1/\ln(y_k)$. Now, with the help of (4.6), (7.8), and (D.4) for $k \gg x$ we write

$$\frac{\tilde{\chi}_k k^2}{4} \cong 1 - \frac{1}{D} \left\{ \ln \left(\frac{\pi}{\theta} \right) - f \right\} \quad (\text{D.15})$$

In the case $\ln(y_k) \gg 1$, using the first two terms of (D.14) and the formula $\ln(y_k) \cong \pi/\theta - 2 \ln(1/k)$, one arrives at the formula (7.11).

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