Self-consistent Gaussian approximation for classical spin systems: Thermodynamics

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The self-consistent Gaussian approximation (SCGA) for classical spin systems described by a completely anisotropic D-component vector model is proposed, which takes into account fluctuations of the molecular field and thus is a next step beyond the molecular field approximation. The SCGA is sensitive to the lattice dimension and structure and to the form of spin interactions and yields rather accurate values of the field-dependent magnetization $m(H,T)$ and other thermodynamic functions in the whole plane (H,T) excluding the vicinity of the critical point $(0,T_c)$, where the SCGA breaks down, showing a first-order phase transition. The values of T_c themselves can be determined in the SCGA with an accuracy better than 1% for actual three-dimensional structures. At low and high temperatures the SCGA recovers the leading terms of the spin-wave theory, the low- and high-temperature series expansions, respectively. The accuracy of the SCGA increases with the increase of the spin dimension D, and in the limit $D\to\infty$ the exact solution for the spherical model is recovered.

I. INTRODUCTION

The models considering spin as a classical vector variable of a fixed length are the most studied ones in the theory of temperature-induced phase transitions on a lattice. The reason for this is that quantum effects that are always present in real magnetic systems and can make calculations more intricate play, however, a secondary role at (and above) T_c and do not change the critical behavior. Classical models are also a good approximation to magnetics with large spin values S, such as, e.g., the Heisenberg systems EuO and EuS having $S=7/2$. Generally, for systems described by the Heisenberg model $H(S)$ with $S\gg 1$ quantum effects become irrelevant in the temperature range $T\gtrsim T_c/S$, where the whole Brillouin zone is populated by spin waves and their occupation numbers become large. Additionally, the arbitrary-S Ising model $I(S)$ without a transverse field can be treated with the same methods as classical ones, because no spin commutators appear and quantum effects are trivial. An advantage of classical vector models is that they can be formulated for an arbitrary number of spin components, as was done by Stanley.[1–3] Such a generalization is important since some magnetics with a complicated structure possess an order parameter with $n>3$ symmetric components (see Refs. 4, 5, and references therein).

In the absence of an analytical solution to the phase transition problem in three dimensions such numerical methods as low-temperature series expansions (LTSE's) for the $I(1/2)$ model[6] and high-temperature series expansions (HTSE's) for the $I(1/2)$,[7–10] $I(S)$,[11,12] $H(S)$,[13,14] $H(\infty)$,[15,16] and classical plane rotator and x-y models,[17] as well as for the general n-component vector model O(n),[1,3,19–21] were successfully applied for an accurate calculation of thermodynamic quantities in a wide temperature range including the vicinity of T_c. It gave the results for the critical indices of magnetic systems and favored the creation of scaling and universality concepts. With the development of computational facilities and algorithms the series methods were permanently improved. As the latest benchmark the recent calculation[21] of the HTSE series for the reduced susceptibility $T\chi(T)$ of the O(n) models up to $(J/T)^{19}$ can be considered. Another very efficient numerical method competing with series expansions is based on Monte Carlo (MC) simulations (see, e.g., Refs. 22,10). An extraction of accurate results for infinite systems from the simulation data for the lattices with a finite linear dimension L is based usually on finite-size scaling.[23] An alternative approach also using simulations is the chiral perturbation theory in powers of $1/L$ (see, e.g., Ref. 24 and references therein).

Lately the ideas of the statistical theory of magnetism together with the methods of calculation have penetrated into the field theory. In particular, the lattice-regularized scalar Higgs model in the chiral limit, which can be identified with the four-component classical Heisenberg model O(4) in four dimensions,[18] was studied with the HTSE (Refs. 19,20) and MC simulation[25,26] methods. Recently Rajagopal and Wilczek[27,28] have related the two-flavor quantum chromodynamics (QCD) to the O(4) vector model in three dimensions, the gauge coupling constant g^2 determining the temperature and the quark mass m_q being proportional to the applied magnetic field. This has initiated an extensive numerical work (see Refs. 29–31 and references therein).

Although HTSE's produce the series coefficients usually with the help of such diagram methods as the linked cluster expansion (LCE),[32,33] the results are represented as a sum of ''bare'' (unrenormalized) diagrams, each proportional to some power of J/T. Alternatively, there were attempts starting from the early years to sum up some ''important'' infinite diagrams series to obtain a closed-form equation for a magnetic system in terms of renormalized diagrams, which should be a good analytical approximation in the whole temperature range. It was shown, in particular, how the mean field approximation (MFA) can be obtained diagrammatically (see, e.g., Refs. 34,35). A further renormalization of diagrams for the Ising model by Horwitz and Callen[35] led to an improvement of the MFA taking into account self-consistently Gaussian fluctuations of the molecular field. This important work remained seemingly unappreciated,

since the resulting equations were not numerically investigated in a satisfactory way and the real accuracy of the approximation was not recognized. Only much later was this self-consistent Gaussian approximation (SCGA) for the Ising systems independently rediscovered and numerically analyzed in Ref. 36.

The methods developed by Horwitz and Callen[35] for the Ising model were generalized for the quantum Heisenberg model in the subsequent paper, Ref. 37. This first version of the spin diagram technique (SDT) had not, however, succeeded in formulating a Gaussian approximation for the Heisenberg systems, since due to quantum effects transverse spin cumulants acquire a time dependence and cannot be renormalized in a desirable way.

Later a similar diagram technique was formulated independently in Refs. 38,39 and further developed in Refs. 40,41. Although the SDT allows one to write down diagrammatic perturbation series for all temperatures in a regular way and recovers the known spin-wave and LTSE results in the ordered state, as well as the HTSE ones above T_c, summation of nontrivial diagram sequences in all orders of a perturbation theory (apart from the usual cases of Dyson and vertex equations) seems to be impossible. Due to the use of the Wick theorem for the calculation of averages of transverse spin components the number and complexity of diagrams increase dramatically with each order and most of diagrams are divergent at $T>T_c$ and compensate each other only in final expressions. The latter is not the case only for Ising systems, where there are no problems with the noncommutativity of different spin components and quantum effects are trivial. In the classical limit $S\to\infty$, which is of a primary importance in the theory of temperature-induced phase transitions, the quantum SDT does not essentially simplify.

In Ref. 42 an alternative diagram technique for classical spin systems was proposed, which explicitly takes advantage of their classical properties and is much simpler than the quantum SDT. It allows, in particular, calculation of thermodynamic quantities of a system without dealing with its dynamics. In the static case all spin components can be treated similarly, and the consideration can be carried out for a generalized completely anisotropic model of D component classical spin vectors ($|\mathbf{m}|=1$) on a lattice:

$$\mathscr{H}=-\mathbf{H}\sum_i \mathbf{m}_i-\frac{1}{2}\sum_{ij} J_{ij}\sum_{\alpha=1}^{D} \eta_\alpha m_{\alpha i} m_{\alpha j}. \qquad (1.1)$$

If the exchange interaction $\eta_\alpha J_{ij}$ is isotropic, i.e., all anisotropy factors $\eta_\alpha=1$, this model reduces to the one pioneered by Stanley,[1–3] who proved[2] that it is in the limit $D\to\infty$ equivalent to the exactly soluble spherical model.[43] An important particular case of the general model (1.1) is the so-called n-D model,[42] where $n\leqslant D$ spin components are coupled by the exchange interaction with an equal strength and the rest $D-n$ ones are ''free'' (i.e., $\eta_\alpha=1$ for $\alpha\leqslant n$ and $\eta_\alpha=0$ for $\alpha>n$). The n-D model contains as particular cases the $S=1/2$ Ising model $I(1/2)$, for $n=D=1$, the classical Ising model $I(\infty)$ for $n=1$, $D=3$, the plane rotator model for $n=D=2$, the classical x-y model for $n=2$, $D=3$, and the classical Heisenberg model $H(\infty)$ for $n=D=3$. The variable n is the number of the order parameter components and determines the universality class of a system. The total number of spin components, D, enters only such nonuniversal quantities as T_c. It is clear that the expansion of the critical indices for the large number of components can be only the $1/n$ expansion. To the contrary, we shall see below that the absolute values of thermodynamic quantities are naturally developed in powers of $1/D$ for $D\gg 1$, which is not automatically the same as $1/n$ for $n\neq D$.

In Ref. 42 the self-consistent Gaussian approximation by Horwitz and Callen was generalized for systems with continuous spin symmetry and it was shown that in the limit $D\to\infty$ the SCGA becomes exact and yields the solution of the spherical model, whereas all other diagrams die out as at least $1/D$. Accordingly, the SCGA becomes more accurate for high spin dimensions D and works better for the $H(\infty)$ model ($n=D=3$) than for the $I(1/2)$ one ($n=D=1$). Numerical calculations for $I(S)$ (Ref. 36) and $H(\infty)$ (Ref. 44) models have shown that for different three-dimensional lattice structures the SCGA yields the magnetization m and other thermodynamic quantities in the whole temperature range excluding the close vicinity of T_c with an overall accuracy about 1%, including the determination of T_c itself.

In Refs. 36,42,44 the SCGA was only briefly described, and its analytical properties need to be explained in more detail. Principally important is to test the SCGA on models with lattice dimensionality $d\geqslant 4$ (hypecubic lattices) and to compare its results with those of the $1/d$ expansion[45,46] and MC calculations.[10] In this case the SCGA should be more accurate, since nontrivial effects of the fluctuation interaction (i.e., non-Gaussian effects) die out.[47] In view of applications in the field theory mentioned above it is important to extend calculations to O(n) models ($n=D$) with $n\geqslant 4$ and to make a comparison with the $1/n$ expansion.[48–50] Some other tasks are to perform a numerical solution of the SCGA equations in the case of a nonzero magnetic field, to make a comparison with the experimental data on Eu chalcogenides, and to consider the lattices with the next nearest neighbor (nnn) interactions. The solution of the problems mentioned above, as well as a detailed statement of the SCGA, is the aim of the present article.

In Sec. II a simple derivation and analysis of the SCGA for the Ising systems without using diagrams is given. In Sec. III the classical spin diagram technique and construction of the SCGA for a general Hamiltonian (1.1) are described in more detail. In Sec. IV the analytic properties of the SCGA in different limiting cases are investigated, including the spherical limit, where the known results are generalized for the anisotropic Hamiltonian (1.1). In Sec. V the results of the numerical solution of the SCGA equations for different classical spin models on different lattices are presented and compared with the available HTSE, LTSE, MC-simulation, and $1/D$ expansion results, as well as with the experimental data on EuO and EuS. In Sec. VI some further applications of the SCGA and the possibilities of its generalization are discussed.

II. IDEA OF SCGA

If in (1.1) the magnetic field $\mathbf{H}$ is directed along the ordering axis z ($\eta_z=1$), then the z component of the molecu-

lar field $\mathbf{H}_i$ acting on the spin on a site i is given by

$$H_{zi}=H+\sum_j J_{ij}m_{zj}. \tag{2.1}$$

The MFA consists in neglecting fluctuations of $\mathbf{H}_i$, which in the spatially homogeneous case leads to the Curie-Weiss equation for the magnetization $m\equiv\langle m_z\rangle$:

$$m=B(\beta\langle H_z\rangle),\quad \langle H_z\rangle=H+mJ_0, \tag{2.2}$$

where $B(\xi)$ is the Langevin function, $\beta\equiv 1/T$, and J_0 is the zero Fourier component of the exchange interaction. The second moment of fluctuations of the α component of the molecular field $\mathbf{H}_i$, which were neglected in the MFA, can be expressed as

$$\sigma_{2\alpha}=\sum_{jj'} J_{ij}J_{ij'}\eta_\alpha^2\langle\Delta m_{\alpha j}\Delta m_{\alpha j'}\rangle$$
$$=v_0\int\frac{d\mathbf{q}}{(2\pi)^d}(\eta_\alpha J_{\mathbf{q}})^2 S_{\alpha\alpha}(\mathbf{q}), \tag{2.3}$$

where $\Delta\mathbf{m}\equiv\mathbf{m}-\langle m_z\rangle\mathbf{e}_z$, $S_{\alpha\alpha}(\mathbf{q})$ is the spin-spin correlation function, v_0 is the unit cell volume, and d is the lattice dimensionality. If correlations of spins on different lattice sites j,j' are neglected, then for systems with nearest neighbor (equivalent neighbor) interactions the integral over the Brillouin zone in (2.3) is proportional to $1/z$ and small for a large number of equivalent neighbors z. This is justified in the temperature range $T\gg T_c$, but for $T\sim T_c$ the correlations in (2.3) should be taken into account. For low-dimensional systems ($d=1,2$) the lattice integral in (2.3) diverges with lowering the temperature at $\mathbf{q}=0$, which invalidates the MFA. For three-dimensional systems the magnitude of the molecular field fluctuations σ_2 remains finite and not very large, which is reflected by the shift of the actual values of T_c in about 30% downwards from T_c^{MFA} depending on the lattice structure and the details of spin interactions in (1.1). The latter makes feasible an improvement of the MFA in $d\geqslant 3$ dimensions, which consists in taking into account molecular field fluctuations described *only* by the set of their second moments $\sigma_{2\alpha}$. This means that the averages of an arbitrary number of molecular field components decay pairwise, which is equivalent to the use of the *Gaussian* distribution function for the molecular field fluctuations. For the Ising model ($\eta_\alpha=0$ for $\alpha\neq z$) this leads, in particular, to the expression for magnetization m being given by a Langevin function with a spreaded argument:

$$m=\frac{1}{(2\pi\sigma_{2z})^{1/2}}\int_{-\infty}^{\infty}dH_{z,\mathrm{fl}}\exp\left(-\frac{H_{z,\mathrm{fl}}^2}{2\sigma_{2z}}\right)$$
$$\times B[\beta(\langle H_z\rangle+H_{z,\mathrm{fl}})] \tag{2.4}$$

or

$$m=\widetilde{B}(\xi_z,l_z)=\frac{1}{\pi^{1/2}}\int_{-\infty}^{\infty}dz\ e^{-z^2}B(\xi_z+2l_z^{1/2}z), \tag{2.5}$$

where $\xi_z\equiv\beta(H+mJ_0)$ and $l_z\equiv\beta^2\sigma_{2z}/2$. To obtain a closed system of equations, one can calculate the spin-spin correlation function $S_{zz}(\mathbf{q})$ in (2.3) in the simplest Ornstein-Zernike approximation:

$$S_{zz}(\mathbf{q})=\frac{\widetilde{B}'(\xi_z,l_z)}{1-\widetilde{B}'(\xi_z,l_z)\beta J_{\mathbf{q}}}, \tag{2.6}$$

where the derivative of the Langevin function, $B'\equiv dB/d\xi$, is also renormalized by Gaussian fluctuations analogously to (2.5). This system of nonlinear equations for m and l_z given by (2.5), (2.6), and (2.3) with $\alpha=z$ was obtained in a very technical manner by Horwitz and Callen[35] and was solved numerically in Ref. 36. Note that the integral over the Brillouin zone σ_{2z}, Eq. (2.3), is taken into account in (2.5) in all orders of a perturbation theory. Such a self-consistent Gaussian approximation is, like all closed-form approximations in the theory of phase transitions, not a rigorous expansion in some small parameter. It is an approach taking into account some physically significant diagram structures self-consistently in all orders of a perturbation theory and reproducing the leading orders in the perturbatively treatable regions $T\ll T_c$ and $T\gg T_c$. In the next section the SCGA will be derived for a general form of the spin-vector Hamiltonian (1.1) with the use of the classical spin diagram technique.

III. CLASSICAL SPIN DIAGRAM TECHNIQUE AND THE SCGA

This diagram technique can be considered as a simplified form of the quantum linked cluster expansion[37] or of the quantum SDT,[38,39] making use of the classical properties of spin vectors. A perturbative expansion of the thermal average of any quantity $\mathscr{A}$ characterizing a classical spin system (e.g., $\mathscr{A}=m_z$) can be obtained by rewriting (1.1) as $\mathscr{H}=\mathscr{H}_0+\mathscr{H}_{\mathrm{int}}$, where $\mathscr{H}_0$ is the MFA Hamiltonian with the molecular field $\langle H_z\rangle$ determined by (2.2), and expanding the expression

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

in powers of $\mathscr{H}_{\mathrm{int}}$. The integration in (3.1) is carried out with respect to the orientations of the D-dimensional unit vectors $\mathbf{m}_j$ on each of the total N lattice sites. Averages of various spin vector components on various lattice sites with the Hamiltonian $\mathscr{H}_0$ can be expressed through spin cumulants, or semi-invariants, which will be considered below, in the following way:

$$\langle m_{\alpha i}\rangle_0=\Lambda_\alpha,$$
$$\langle m_{\alpha i}m_{\beta j}\rangle_0=\Lambda_{\alpha\beta}\delta_{ij}+\Lambda_\alpha\Lambda_\beta,$$
$$\langle m_{\alpha i}m_{\beta j}m_{\gamma k}\rangle_0=\Lambda_{\alpha\beta\gamma}\delta_{ijk}+\Lambda_{\alpha\beta}\Lambda_\gamma\delta_{ij}+\Lambda_{\beta\gamma}\Lambda_\alpha\delta_{jk}$$
$$+\Lambda_{\gamma\alpha}\Lambda_\beta\delta_{ki}+\Lambda_\alpha\Lambda_\beta\Lambda_\gamma, \tag{3.2}$$

etc., where δ_{ij}, δ_{ijk}, etc., are the site Kronecker symbols equal to 1 for all site indices coinciding with each other and to zero in all other cases. For the one-site averages ($i=j=k=\cdots$) (3.2) reduces to the well-known representation of moments through semi-invariants, generalized for a

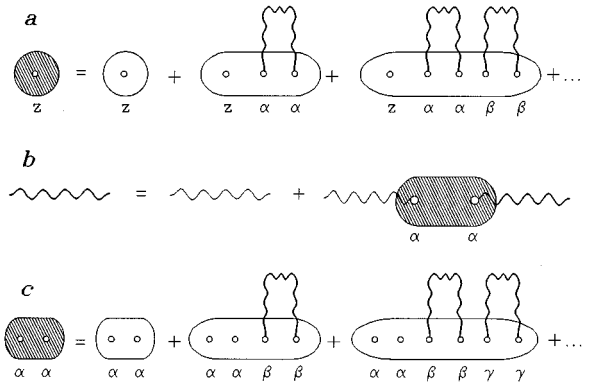

FIG. 1. Self-consistent Gaussian approximation (SCGA) for classical spin systems. (a) and (c) Block summations for the renormalized magnetization and pair spin cumulant averages; (b) Dyson equation for the renormalized interaction line.

multiple-component case. In the graphical language (see Fig. 1) the decomposition (3.2) corresponds to all possible groupings of small circles (spin components) into oval blocks (cumulant averages). The circles coming from $\mathscr{H}_{\rm int}$ (the ''inner'' circles) are connected pairwise by the wavy interaction lines representing the quantity $\eta_\alpha \beta J_{ij}$ in (1.1). In diagram expressions summations over site indices i and component indices α of inner circles are carried out. One should not take into account disconnected (unlinked) diagrams [i.e., those containing disconnected parts with no ''outer'' circles belonging to $\mathscr{A}$ in (3.1)], since these diagrams are compensated for by the expansion of the partition function $\mathscr{Z}$ in the denominator of (3.1). Consideration of combinatorial numbers shows that each diagram contains the factor $1/n_s$, where n_s is the number of symmetry group elements of a diagram. The symmetry operations do not concern outer circles, which serve as a distinguishable ''root'' to build up more complicated or renormalized diagrams. Such combinatorial factors are present, in particular, in the formulas (3.15) and (3.16). For practical calculations it is usually more convenient to use the Fourier representation and to calculate integrals over the Brillouin zone rather than lattice sums. As due to the Kronecker symbols in (3.2) lattice sums are subject to the constraint that the coordinates of the circles belonging to the same block coincide with each other, in the Fourier representation the sum of wave vectors coming to or going out of any block along interaction lines is zero. The cumulant spin averages in (3.2) can be obtained by differentiating the generating function $\Lambda(\xi)$ over appropriate components of the dimensionless field $\boldsymbol{\xi} \equiv \beta \mathbf{H}$:[42]

$$\Lambda_{\alpha_1 \alpha_2 \cdots \alpha_p}(\boldsymbol{\xi}) = \frac{\partial^p \Lambda(\xi)}{\partial \xi_{\alpha_1} \partial \xi_{\alpha_2} \cdots \partial \xi_{\alpha_p}}, \quad \Lambda(\xi) = \ln \mathscr{Z}_0(\xi), \tag{3.3}$$

where $\xi \equiv |\boldsymbol{\xi}|$,

$$\mathscr{Z}_0(\xi) = \text{const} \times \xi^{-(D/2-1)} I_{D/2-1}(\xi) \tag{3.4}$$

is the partition function of a D-component classical spin, and $I_\nu(\xi)$ is the modified Bessel function. A similar technique was applied by Lüsher and Weisz[20] to generate HTSE's for a more general n-component ϕ^4 model. For several lowest-order cumulants differentiation in (3.3) leads to the following expressions:

$$\begin{aligned}
\Lambda_\alpha(\boldsymbol{\xi}) &= B_0(\xi)\xi_\alpha = B(\xi)\xi_\alpha/\xi, \\
\Lambda_{\alpha\beta}(\boldsymbol{\xi}) &= B_0(\xi)\delta_{\alpha\beta} + B_1(\xi)\xi_\alpha\xi_\beta, \\
\Lambda_{\alpha\beta\gamma}(\boldsymbol{\xi}) &= B_1(\xi)(\xi_\alpha\delta_{\beta\gamma} + \xi_\beta\delta_{\gamma\alpha} + \xi_\gamma\delta_{\alpha\beta}) + B_2(\xi)\xi_\alpha\xi_\beta\xi_\gamma, \\
\Lambda_{\alpha\beta\gamma\delta}(\boldsymbol{\xi}) &= B_1 3\mathscr{P}(\delta_{\alpha\beta}\delta_{\gamma\delta}) + B_2 6\mathscr{P}(\xi_\alpha\xi_\beta\delta_{\gamma\delta}) \\
&\quad + B_3\xi_\alpha\xi_\beta\xi_\gamma\xi_\delta,
\end{aligned} \tag{3.5}$$

where $\delta_{\alpha\beta}$ is the spin component Kronecker symbol, $\mathscr{P}$ is the symmetrization operator,

$$B_n(\xi) \equiv \left(\frac{1}{\xi}\frac{\partial}{\partial \xi}\right)^n \frac{B(\xi)}{\xi}, \tag{3.6}$$

and

$$B(\xi) = d\Lambda(\xi)/d\xi = I_{D/2}(\xi)/I_{D/2-1}(\xi) \tag{3.7}$$

is the Langevin function of D-component classical spins, which can be expressed through elementary functions for odd values of D:

$$B(\xi) = \begin{cases} \tanh(\xi) & D=1, \\ \coth(\xi) - 1/\xi & D=3, \\ 1/[\coth(\xi) - 1/\xi] - 3/\xi, & D=5, \end{cases} \tag{3.8}$$

etc. The small- and large-argument expansions of the Langevin function $B(\xi)$ have the form

$$\begin{aligned}
B(\xi) \cong \frac{\xi}{D} - \frac{\xi^3}{D^2(D+2)} + \frac{2\xi^5}{D^3(D+2)(D+4)} \\
- \frac{5\xi^7}{D^4(D+2)(D+4)(D+6)}\left(1 + \frac{2}{5(D+2)}\right) + \cdots
\end{aligned} \tag{3.9}$$

and

$$B(\xi) \cong 1 - \frac{D-1}{2\xi} + \frac{(D-1)(D-3)}{8\xi^2} + \cdots, \tag{3.10}$$

respectively. One can see from (3.9) that the functions $B_n(\xi)$, Eq. (3.6), are all finite at $\xi=0$: $B_0(0)=1/D$, $B_1(0) = -2/[D^2(D+2)]$, $B_2 = 16/[D^3(D+2)(D+4)]$, etc. Accordingly, the spin cumulants $\Lambda_{\ldots}$ in (3.5) with an even number of coinsiding indices are given in this case by their first terms:

$$\Lambda_{\alpha\alpha} = B_0(0), \quad \Lambda_{\alpha\alpha\beta\beta} = B_1(0)(1 + 2\delta_{\alpha\beta}), \tag{3.11}$$

etc., whereas all other cumulants turn to zero. At large arguments from (3.6) and (3.10) follows $B_n(\xi) \propto \xi^{-(1+2n)}$. In this limit all terms of (3.5) yield comparable contributions into $\Lambda_{\ldots}$, and a k-spin cumulant decays generally as $\Lambda_{\alpha_1\alpha_2..\alpha_k} \propto \xi^{-(k-1)}$. If, however, the field $\boldsymbol{\xi}$ is directed along some axis z, then in the cumulant averages containing z components of spins the leading terms can cancel each other. In

particular, the two-spin cumulant $\Lambda_{\alpha\beta}$ in (3.5), which plays a big role in the following, can be rewritten explicitly as

$$\Lambda_{\alpha\beta}(\boldsymbol{\xi})=\frac{B(\xi)}{\xi}\left(\delta_{\alpha\beta}-\frac{\xi_\alpha\xi_\beta}{\xi^2}\right)+B'(\xi)\frac{\xi_\alpha\xi_\beta}{\xi^2}. \quad (3.12)$$

For $\boldsymbol{\xi}=\xi\mathbf{e}_z$ this expression simplifies to $\Lambda_{zz}=B'(\xi)$ and $\Lambda_{\alpha\alpha}=B(\xi)/\xi$ $(\alpha\neq z)$. Now from (3.10) one can see that, for $\xi\gg 1$, $\Lambda_{zz}\propto\xi^{-2}$, whereas $\Lambda_{\alpha\alpha}\propto\xi^{-1}$.

The simplification of spin cumulants for $\boldsymbol{\xi}=\xi\mathbf{e}_z$ mentioned above takes place in the unrenormalized diagrams generated initially by the expansion of (3.1) in powers of $\mathscr{H}_{\rm int}$ since there is only one nonzero component of the molecular field: $\xi_z=\xi=\beta(H+mJ_0)$. The complete form of spin cumulants (3.5), (3.12) is needed, however, for the construction of the SCGA, which allows for both longitudinal and *transverse* fluctuations of the molecular field. The latter is the essense of the diagram technique for the multiple-component classical spin systems presented here. In the Ising case the classical spin diagram technique coincides with the ''Ising part'' of the standard quantum SDT (Refs. 38,39,51) and can be used with Brillouin functions B_S of a general spin S. In the Refs. 39,51 the reader can find more technical details concerning the construction of the SDT for Ising systems, which play the same role in the present classical SDT.

Before proceeding to the construction of the SCGA we should make a remark about the numerical calculation of the generalized Langevin function $B(\xi)$ (3.7) for arbitrary D. One can see from (3.8) that for $D>1$ the function $B(\xi)$ contains terms divergent at $\xi\to 0$, although $B(\xi)$ itself is well behaved. This hampers numerical calculations, and the situation is aggravated for the derivative $B'(\xi)$ and for the functions $B_n(\xi)$ (3.6) entering the spin cumulants (3.5), as well as for higher spin dimensionalities D. The best way of calculating $B(\xi)$ is based on using the *backward* recursion relation with respect to D:

$$B(D,\xi)=\frac{\xi}{D+\xi B(D+2,\xi)}, \quad (3.13)$$

which can be derived from (3.7) and the three-term recursion relation for the modified Bessel functions $I_\nu(\xi)$. This formula yields the proper small-argument behavior of $B(D,\xi)$, Eq. (3.9), to leading order even for an inaccurate $B(D+2,\xi)$, and the proper behavior at $\xi\gg 1$ to leading order described by (3.10) can be guaranteed, if we choose the first two terms of the large-D expansion[52]

$$B(\xi)\cong f(x)+\frac{1}{D}\frac{x}{1+x^2}f^2(x)+O\left(\frac{1}{D^2}\right),$$

$$x\equiv 2\xi/D, \quad f(x)\equiv\frac{x}{1+(1+x^2)^{1/2}} \quad (3.14)$$

as an initial condition for the recurrence formula (3.13). This procedure proves to be extremely good: Already one application of (3.13) yields $B(\xi)$ with an accuracy not worse than 0.6% for $D=1$, 0.35% for $D=2$, and 0.25% for $D=3$ in the whole range of ξ, and the process converges fast with the increase of the iterations number.

The self-consistent Gaussian approximation consists in taking into account *pair* correlations of the molecular field acting on a given spin from its neighbors, which implies the Gaussian statistics of molecular field fluctuations. The corresponding diagram sequence is represented in Fig. 1 and is equivalent to the following closed system of nonlinear equations for magnetization $m\equiv\langle m_z\rangle$ and the normalized second moments $l_\alpha\equiv\beta^2\sigma_{2\alpha}/2!$ [cf. (2.3) and (2.5)] of the molecular field fluctuations:

$$m=\widetilde{\Lambda}_z,$$

$$l_\alpha=\frac{1}{2!}v_0\int\frac{d\mathbf{q}}{(2\pi)^d}\frac{\eta_\alpha\beta J_{\mathbf{q}}}{1-\widetilde{\Lambda}_{\alpha\alpha}\eta_\alpha\beta J_{\mathbf{q}}}, \quad \alpha=1,2,\ldots,D. \quad (3.15)$$

Here the spin cumulants $\widetilde{\Lambda}_{\ldots}$ renormalized by Gaussian fluctuations of the molecular field are given according to Figs. 1(a), 1(c) by the series

$$\widetilde{\Lambda}_{\ldots}=\Lambda_{\ldots}+\sum_{\alpha=1}^{D}\Lambda_{\ldots\alpha\alpha}l_\alpha+\sum_{\alpha,\beta=1}^{D}\left(1-\delta_{\alpha\beta}+\frac{1}{2!}\delta_{\alpha\beta}\right)\Lambda_{\ldots\alpha\alpha\beta\beta}l_\alpha l_\beta+\cdots, \quad (3.16)$$

where the ''bare'' spin cumulants $\Lambda_{\ldots}$ are given by (3.3) or (3.5). This series describing the influence of pair-correlated fluctuations of different components of the molecular field can be rewritten as

$$\widetilde{\Lambda}_{\ldots}=\prod_{\alpha=1}^{D}\sum_{n_\alpha=0}^{\infty}\frac{1}{n_\alpha!}\left(l_\alpha\frac{\partial^2}{\partial\xi_\alpha^2}\right)^{n_\alpha}\Lambda_{\ldots}(\boldsymbol{\xi})=\exp\left[\sum_{\alpha=1}^{D}l_\alpha\frac{\partial^2}{\partial\xi_\alpha^2}\right]\Lambda_{\ldots}(\boldsymbol{\xi}). \quad (3.17)$$

Such exponential differential operators were considered by Horwitz and Callen[35] for the Ising model. A generalization of their results for the multiple-component case yields the closed formula

$$\widetilde{\Lambda}_{\ldots}=\frac{1}{\pi^{D/2}}\int d^Dr e^{-r^2}\Lambda_{\ldots}(\boldsymbol{\zeta}), \quad (3.18)$$

where $\boldsymbol{\zeta}$ is the spreaded molecular field given by

$$\boldsymbol{\zeta}\equiv\beta(H+mJ_0)\mathbf{e}_z+2\sum_{\alpha=1}^{D}l_\alpha^{1/2}r_\alpha\mathbf{e}_\alpha, \quad (3.19)$$

$\mathbf{e}_\alpha$ is the unit vector in the direction α, and the integration in (3.18) is performed with respect to the D-component vector variable $\mathbf{r}\equiv\{r_\alpha\}$. It can be seen that the renormalized spin cumulants $\widetilde{\Lambda}_{\ldots}$ are functions of m and all l_α. In the Ising case the SCGA system of equations (3.15) reduces to the one obtained by Horwitz and Callen,[35] which was described in the preceding section, since here only l_z in (3.15) is nonzero and $\widetilde{\Lambda}_{zz}=\widetilde{B}'(m,l_z)$. The expression for l_α in (3.15) differs from (2.3) in that a zero term of the type $\int d\mathbf{q}J_{\mathbf{q}}\sim J_{ii}=0$ was added for convenience, which allows one to formulate the diagram technique in terms of renormalized interactions.

The number of unknown variables in the nonlinear system of SCGA equations (3.15) is for a general form of the Hamiltonian (1.1) equal to $D+1$. Thus, for example, for a com-

pletely anisotropic Heisenberg model there are four unknown variables m, l_x, l_y, and l_z. In a more complicated case with the magnetic field transverse to the ordering axis z, which is not considered here, one should take into account different magnetization components and nondiagonal moments of molecular field fluctuations, $l_{\alpha\beta}$ with $\alpha\neq\beta$, and the number of unknowns increases considerably. Similar takes place for antiferromagnets in magnetic field and for multiple-sublattice structures. Of a practical interest is the case when in the Hamiltonian (1.1) there are groups of equivalent transverse ($\alpha\neq z$) spin components having anisotropy factors η_α, and hence the moments l_α, equal to each other. In this case the number of unknowns in (3.15) diminishes; denoting such a group with the index x and introducing $r_x^2\equiv\Sigma_{\alpha\in x}r_\alpha^2$ and n_x as the number of equivalent components in the group, one can simplify the D-dimensional integral in (3.18) with the help of the identity

$$\frac{1}{\pi^{n_x/2}}\int d^{n_x}r_{\alpha\in x}e^{-r_x^2}\cdots=\frac{2}{\Gamma(n_x/2)}\int dr_x r_x^{n_x-1}e^{-r_x^2}\cdots \tag{3.20}$$

and make a replacement $\xi_\alpha^2\Rightarrow\xi_x^2/n_x$, where $\xi_x\equiv 2l_x^{1/2}r_x$ and $l_x\equiv l_{\alpha\in x}$, in the pair spin cumulants $\Lambda_{\alpha\alpha}$, Eq. (3.12), entering (3.18). Thus, in particular, for the O(n) model all components with $\alpha\neq z$ are equivalent, and there are three independent variables in the SCGA equations (3.15): m, l_z, and $l_x=l_\alpha$. The Gaussian integrals (3.18) reduce in this case to two-dimensional ones over r_z and r_x, and in (3.20) $n_x=n-1$. Above T_c in the absence of a magnetic field $m=0$ and all spin components are equivalent; there is only one unknown variable $l_z=l_\alpha$ in (3.15), and the intergal $\widetilde{\Lambda}_{\alpha\alpha}$, Eq. (3.18), becomes one dimensional.

The SCGA system of equations (3.15) determines the equation of state of a magnetic system, i.e., the magnetization as a function of temperature and magnetic field, $m(T,H)$. The caloric properties of a magnetic system in the SCGA can also be determined. In particular, the energy of a spin system $U\equiv\langle\mathscr{H}\rangle$ can be obtained by averaging the Hamiltonian (1.1) and using the expression for the renormalized spin correlation function $S_{\alpha\alpha}(\mathbf{q})$ determined by (2.3) in the form

$$S_{\alpha\alpha}(\mathbf{q})=\frac{\widetilde{\Lambda}_{\alpha\alpha}}{1-\widetilde{\Lambda}_{\alpha\alpha}\eta_\alpha\beta J_{\mathbf{q}}} \tag{3.21}$$

[cf. (2.6)]. Using the definition of l_α in (3.15) one gets

$$\begin{aligned}U&=-Hm-\frac{1}{2}J_0m^2-\frac{1}{2}v_0\int\frac{d\mathbf{q}}{(2\pi)^d}J_{\mathbf{q}}\sum_{\alpha=1}^{D}\eta_\alpha S_{\alpha\alpha}(\mathbf{q})\\&=-Hm-\frac{1}{2}J_0m^2-T\sum_{\alpha=1}^{D}l_\alpha\widetilde{\Lambda}_{\alpha\alpha};\end{aligned} \tag{3.22}$$

i.e., the energy can be obtained as a by-product of the numerical solution of the SCGA equations (3.15). Now the heat capacity $C_H=\partial U(T,H)/\partial T$ can be obtained by the differention of (3.22). The most strong result is, however, that for the free energy $F=-T\ln\mathscr{Z}$ of a system. Its diagrammatic derivation, which was accomplished by Horwitz and Callen[35] for the Ising model, is a rather complicated combinatorial problem, since the free-energy diagrams have no distinguishable outer circles, which could be used as a root for building renormalized diagrams. But the generalization of the corresponding results for the multiple-component case is straightforward and yields

$$\beta F=\frac{\beta}{2}J_0m^2-\widetilde{\Lambda}-\sum_{\alpha=1}^{D}L_\alpha+\sum_{\alpha=1}^{D}l_\alpha\widetilde{\Lambda}_{\alpha\alpha}, \tag{3.23}$$

where $\widetilde{\Lambda}$ is the generating function of spin cumulants (3.3) renormalized by Gaussian fluctuations [see (3.18)] and

$$L_\alpha=-\frac{1}{2!}v_0\int\frac{d\mathbf{q}}{(2\pi)^d}\ln(1-\widetilde{\Lambda}_{\alpha\alpha}\eta_\alpha\beta J_{\mathbf{q}}). \tag{3.24}$$

Considering in (3.23) m and l_α as free parameters, i.e., $F=F(T,H,m,\{l_\alpha\})$, and using the identities $\partial\widetilde{\Lambda}_{\dots}/\partial\xi_\alpha=\widetilde{\Lambda}_{\dots\alpha}$ and $\partial\widetilde{\Lambda}_{\dots}/\partial l_\alpha=\widetilde{\Lambda}_{\dots\alpha\alpha}$, one can obtain the SCGA system of equations (3.15) from the requirement that F be stationary with respect to m and l_α: $\partial F/\partial m=0$ and $\partial F/\partial l_\alpha=0$. The expression for the energy U, Eq. (3.22), can be also obtained from (3.23): $U=\partial(\beta F)/\partial\beta$.

IV. ANALYTICAL PROPERTIES OF THE SCGA AND THE SPHERICAL LIMIT

In this section the behavior of the SCGA solution for classical spin systems is analyzed in the regions of high and low temperatures, in the spherical limit ($D\to\infty$), and in the vicinity of the critical point. It is convenient to choose the dimensionless temperature variable $\theta\equiv T/T_c^{\mathrm{MFA}}$, where $T_c^{\mathrm{MFA}}=J_0/D$, and the dimensionless magnetic field $h\equiv H/J_0$, and susceptibility $\widetilde{\chi}\equiv J_0\chi$. Then the (unspreaded) molecular field in (3.19) is written as $\xi_z=\beta(H+mJ_0)=(D/\theta)(h+m)$, and the quantities l_α, Eq. (3.15), transform to

$$\begin{aligned}&l_\alpha=\frac{D}{2\theta\widetilde{G}_\alpha}[P(\eta_\alpha\widetilde{G}_\alpha)-1],\quad \widetilde{G}_\alpha\equiv\frac{D}{\theta}\widetilde{\Lambda}_{\alpha\alpha},\\&P(X)\equiv v_0\int\frac{d\mathbf{q}}{(2\pi)^d}\frac{1}{1-X\lambda_{\mathbf{q}}},\end{aligned} \tag{4.1}$$

where $\lambda_{\mathbf{q}}\equiv J_{\mathbf{q}}/J_0$ satisfies $1-\lambda_{\mathbf{q}}\propto k^2$ for $a_0k\ll 1$; a_0 is the lattice spacing. The lattice integral $P(X)$ has the following properties:

$$P(X)\cong\begin{cases}1+X^2/z, & X\ll 1,\\ W-c(\delta X)^{1/2}, & \delta X\ll 1,\quad d=3,\\ W-c\,\delta X\ln(c'/\delta X), & \delta X\ll 1,\quad d=4,\end{cases} \tag{4.2}$$

where $\delta X\equiv 1-X$, z is the number of equivalent neighbors, and W (the Watson integral) and c,c' are lattice-dependent constants. For low-dimensional systems ($d=1,2$) the function $P(X)$ diverges for $X\to 1$; for $d\geqslant 5$ the leading term of the expansion of $P(X)$ about $X=1$ is nonsingular. The values of the Watson integral W are 1.344 66 for the fcc lattice ($z=12$), 1.393 20 for the bcc lattice ($z=8$), 1.516 39 for the simple cubic (sc) lattice ($z=6$), 1.792 88 for the diamond lattice ($z=4$), 1.239 65 for the $d=4$ hypercubic (hpc) lattice ($z=8$), and 1.156 31 for the $d=5$ hpc one ($z=10$). For

hypecubic lattices with $d \gg 1$ one has $W \cong 1+1/z$ with $z=2d$. The difference $W-1$ measures in the SCGA deviations from the molecular field behavior and tends to zero if $z \to \infty$.

In the high-temperature region ($\theta \gg 1$) the second moments of the molecular field fluctuations, $\sigma_{2\alpha}$, Eq. (2.3), should be temperature independent and, correspondingly, $l_\alpha \equiv \beta^2 \sigma_{2\alpha}/2! \propto \theta^{-2}$. In this case the renormalized spin cumulants $\tilde{\Lambda}_{\ldots}$, Eq. (3.18), are given for $l_\alpha \ll 1$ by the expansion (3.16), where the first order terms written out correspond to diagrams with one integration loop in Figs. 1(a), 1(c). Now using (3.11) one can calculate the quantity $\tilde{G}_\alpha$ in (4.1) in the lowest order: $\tilde{G}_\alpha \cong \theta^{-1} \ll 1$. Then from (4.1) and (4.2) follows $l_\alpha \cong \eta_\alpha^2 D/(2\theta^2 z) \ll 1$, which justifies the initial assumption. The latter can be used to find a more accurate value of $\tilde{G}_\alpha$ up to θ^{-3} from the first two terms of (3.16) and (3.11). This allows one to determine the reduced susceptibilities $\theta \tilde{\chi}_\alpha(\mathbf{q}) = D S_{\alpha\alpha}(\mathbf{q})$ [see (3.21)] in the SCGA up to θ^{-3}. For a particular case of the n-D model ($\eta_\alpha = 1$ for $\alpha \leqslant n$ and $\eta_\alpha = 0$ for $\alpha > n$) we write down the *complete* expression for the longitudinal ($\alpha \leqslant n$) reduced susceptibility up to θ^{-3}, which can be obtained with the help of the classical SDT without using the SCGA and has the form

$$\theta \tilde{\chi}_\parallel \cong 1 + \frac{1}{\theta} + \left(1 - \frac{1}{z}\frac{n+2}{D+2}\right)\frac{1}{\theta^2} + \left(1 - \frac{2}{z}\frac{n+2}{D+2} + \frac{2}{z^2}\frac{n+2}{(D+2)^2}\right)\frac{1}{\theta^3} + \cdots . \quad (4.3)$$

Here all terms except the last one are contained in the SCGA, the latter being relatively small as $1/[z(D+2)]$. Such a situation takes place in the high-temperature range for other thermodynamic functions [e.g., the energy (3.22)], too, as well as in higher orders of a perturbation theory — corrections to the SCGA are determined by two small parameters $1/z$ and $1/(D+2)$. It can be seen from (4.3) that for the models with $n=D$ the dependence of $\chi_\parallel$ on D comes practically only from these correction terms and remains weak not too close to T_c. In the SCGA the D dependence of the reduced susceptibility of a spin system, as well as of its energy, appears only in the order θ^{-7} due to the last $1/(D+2)$-correction term in (3.9) and is very weak. For this reason also the values of T_c determined in the SCGA from the divergence of susceptibility are for the models with $n=D$ very close to each other and to the one of the spherical model. From the expression (4.3) it can be seen that in the case of a large number of spin components the susceptibility developes in a natural way in powers of $1/D$ and not of $1/n$, as was mentioned in the Introduction. The same is valid for other thermodynamic quantities as well.

In the low-temperature region ($\theta \ll 1$) the expansion of thermodynamic quantities in powers of θ is more complicated, because the longitudinal and transverse spin components are nonequivalent and all expressions depend on magnetization, which should be calculated self-consistently in each order. The small-fluctuation expansion (3.16) is valid in the range $\theta \ll 1$, too, since the high-order spin cumulants diminish as appropriate powers of $1/\xi \propto \theta$ [see the discussion after (3.11)]. In the zero-field case, starting from $\xi = (D/\theta)m \cong D/\theta$, one can estimate different terms of the low-temperature expansion (3.16) for the magnetization $m = \tilde{\Lambda}_z$. One gets ($\alpha \neq z$)

$$\Lambda_z = B \cong 1 - (D-1)/(2\xi) \cong 1 - \theta(D-1)/(2D),$$
$$\Lambda_{\alpha\alpha} = B/\xi \cong \theta/D, \quad (4.4)$$
$$\Lambda_{zz} = B' \cong (D-1)/(2\xi^2) \cong \theta^2(D-1)/(2D^2),$$
$$\Lambda_{z\alpha\alpha} = (\partial/\partial\xi)(B/\xi) \cong -\theta^2/D^2, \quad \Lambda_{zzz} \cong \theta^3(D-1)/D^3,$$

etc., the first of these formulas being the MFA expression for magnetization m up to first order in θ. Now it can be seen that in the low-temperature range $\tilde{G}_z \cong (D/\theta)\Lambda_{zz} \propto \theta$, (4.1) yields $l_z \sim$ const, and the contribution of longitudinal fluctuations into m given by $\Lambda_{zzz} l_z$ in (3.16) is small as θ^3. The leading contribution to m comes from transverse fluctuations (spin waves), since $\tilde{G}_\alpha \cong 1$ and $l_\alpha \cong [P(\eta_\alpha)-1]D/(2\theta) \gg 1$. For the absolute value of the second moment of the molecular field fluctuations, $\sigma_{2\alpha} = 2T^2 l_\alpha$, Eq. (2.3), the latter means $\sigma_{2\alpha} \propto \theta \ll 1$. Now the magnetization m is given for $\theta \ll 1$ by the formula

$$m \cong 1 - \frac{\theta}{2D}\sum_{\alpha=2}^{D} P(\eta_\alpha) \quad (4.5)$$

of the lowest-order spin-wave theory, where the sum includes only transverse components. For the n-D model (4.5) simplifies to[42]

$$m \cong 1 - \frac{\theta}{2D}[(n-1)W + D - n] \quad (4.6)$$

[see (4.2)]. Such a linear dependence replaces for classical ferromagnets the quantum Bloch law $m \cong 1 - a\theta^{3/2}$.

In the next order of a perturbation theory in $\theta \ll 1$ with the help of (3.16) and (4.5) one gets

$$\tilde{G}_\alpha \cong 1 - (\theta/D)[P(\eta_\alpha) - 1], \quad (4.7)$$

which in the case $\eta_\alpha = 1$ leads for three-dimensional systems due to (4.2) to the singular negative contribution to l_α, Eq. (4.1), and, as a consequence, to a *positive* contribution to magnetization $\propto \theta^{3/2}$ in addition to the leading negative linear term in (4.5). The latter is an artifact of the SCGA related to the unbalanced renormalization of spin-spin correlation functions. This is, however, an effect of the next order of magnitude, which is suppressed by the magnetic field or in the anisotropic case $\eta_\alpha < 1$.

In the spherical limit $D \to \infty$, the SCGA becomes exact, since all other more complicated diagrams die out[42,52] as at least $1/D$. The Langevin function (3.7) simplifies in this limit to the first term of the formula (3.14). The expression for the square of the *spreaded* value of the scaled argument $x = 2\zeta/D$ in (3.18) reads

$$x^2 = \left[\frac{2}{\theta}(h+m) + \frac{4}{D} l_z^{1/2} r_z\right]^2 + \frac{16}{D^2}\sum_{\alpha=2}^{D} l_\alpha r_\alpha^2 . \quad (4.8)$$

Since, according to (4.1), $l_{\alpha,z} \propto D$, the spreading of the z component of the molecular field in (4.8) can be neglected, whereas the transverse contributions to (4.8), each of them is

small as $1/D$, are essential due to their number of the order D. The renormalized cumulants $\tilde{\Lambda}_{\alpha\alpha}$ ($\alpha \neq z$) entering the SCGA equations (3.15) are in the limit $D \to \infty$ all equal to each other and given according to (3.5) by $\tilde{\Lambda}_{\alpha\alpha} \cong \tilde{B}_0$, so that we can introduce $G = (D/\theta)\tilde{B}_0$. The Gaussian integrals (3.18) are for $D \gg 1$ easily calculated by applying the identity

$$\frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} dx e^{-x^2} f(ax^2) \cong f(a/2), \quad a \ll 1, \tag{4.9}$$

for an arbitrary function f successively $D-1$ times. Thus, the integration leads simply to the replacement $r_\alpha^2 \Rightarrow 1/2$ in (4.8), and SCGA equations (3.15) reduce after some transformations to

$$\frac{m}{h} = \frac{G}{1-G} \tag{4.10}$$

and

$$1 - m^2 = G \frac{\theta}{D} \sum_{\alpha=2}^{D} P(\eta_\alpha G). \tag{4.11}$$

Comparing these results with (4.5) one can identify the spherical model as a model which is described in the whole temperature range by an effective lowest-order spin-wave theory. In a zero magnetic field ($h=0$) the magnetization m disappears above T_c, and the quantity G, which can be determined from (4.11), increases from 0 to 1 with lowering temperature from ∞ to T_c. Below T_c for $h=0$ from (4.10) follows $G=1$, and m^2 determined from (4.11) is a linear function of temperature. It turns to zero at the critical point

$$\theta_c^{(\infty)} = \left[\frac{1}{D} \sum_{\alpha=2}^{D} P(\eta_\alpha) \right]^{-1}, \tag{4.12}$$

which reduces to the well-known result[43] $\theta_c^{(\infty)} = 1/W$ in the isotropic case $\eta_\alpha = 1$ considered by Stanley.[2] The corresponding result for the n-D model ($n/D = \text{const} \leqslant 1$) was obtained in Ref. 42. The general formula (4.12), as well as the whole equation of state (4.10), (4.11), shows a crossover to MFA behavior in the case $\eta_\alpha \to 0$, $\eta_z = 1$, i.e., for the ''spherical Ising model''; see (1.1). In the anisotropic case, i.e., for any $\eta_\alpha < 1$, the singularity of the function $P(X)$ at $X=1$ [see (4.2)] is suppressed, and the critical indices of the spherical model coincide with those of the MFA.

Now we proceed to the investigation of the behavior of the SCGA solution for classical spin systems in the critical region. The first step is to search for T_c as a point at which the longitudinal correlation function given by (3.21) with $\alpha = z$ diverges at $\mathbf{q}=0$ for $h=0$. This leads to the condition $\tilde{G}_z \equiv (D/\theta)\tilde{\Lambda}_{zz} = 1$, which in the isotropic case ($\eta_\alpha = 1$) with the use of the symmetrization (3.20) can be transformed to the following nonlinear equation for θ_c:[42]

$$\theta_c = \frac{2D}{\Gamma(D/2)} \int_0^\infty dr\, r^{D-1} e^{-r^2} F(2 l_c^{1/2} r),$$

$$l_c = D(W-1)/(2\theta_c), \tag{4.13}$$

where [cf. (3.12)]

$$F(\xi) = \left(1 - \frac{1}{D}\right) \frac{B(\xi)}{\xi} + \frac{B'(\xi)}{D}. \tag{4.14}$$

In the particular case $D=1$ this equation reduces to the one obtained by Horwitz and Callen[35] for the Ising model. As was stressed above by the analysis of the susceptibility HTSE, Eq. (4.3), this θ_c should be very close to that of the spherical model, the latter underestimating T_c in (5–8)% for three-dimensional systems. Equation (4.13) can be solved analytically in two limiting cases: (i) for $D \gg 1$ using the $1/D$ expansion results of Ref. 52 and (ii) for $W-1 \ll 1$, when the spreading of molecular field fluctuations in (4.13) is small and the deviation from the spherical result is due to the last correction term in (3.9). In these limiting cases θ_c is given by

$$\theta_c \cong \frac{1}{W} \times \begin{cases} 1 - \dfrac{2}{D} \dfrac{(W-1)^3}{W(2W-1)^2}, & D \gg 1, \\ 1 - \dfrac{2}{D+2}(W-1)^3, & W-1 \ll 1. \end{cases} \tag{4.15}$$

Considering the values of the Watson integrals W listed after (4.2), one can see that, indeed, the correction terms in (4.15) are typically small.

An attempt to simplify the SCGA equations (3.15) about such a defined transition temperature θ_c and to calculate the spontaneous magnetization m just below θ_c shows that θ_c is actually the lower spinodal boundary of a fictitious first order phase transition occurring in the SCGA due to its inaccuracy in a close critical region; i.e., the magnetization jumps to a finite value by crossing θ_c from above. This instability is due to the singular behavior of the function $P(X)$ near $X=1$ [see (4.2)]. The decrease of $\tilde{G}_z$ from 1 below θ_c related to the increase of magnetization leads to a sharp decrease of molecular field fluctuations and hence to a further increase of magnetization and so on. Analytically the absence of a continuous solution $m(\theta)$ below θ_c can be shown the most easily for the Ising model, where in the vicinity of θ_c the SCGA simplifies to a system of equations

$$\delta\tilde{G}_z + (2D/\theta)\tilde{B}'''\delta l_z = 2[(D/\theta)\tilde{B}' - 1],$$

$$\delta\tilde{G}_z + [1/(D+2)](D/\theta)^3 \tilde{B}''' m^2 = 0. \tag{4.16}$$

Here the spread derivatives $\tilde{B}^{[n]}$ are calculated with $l_{zc} = D(W-1)/(2\theta_c)$ and δl_z is determined as $\delta l_z = l_{zc} - D[P(1-\delta\tilde{G}_z) - 1]/[2\theta(1-\delta\tilde{G}_z)] > 0$. Below θ_c the right part of the first of Eqs. (4.16) is positive, and this equation has no solution since the negative singular term with δl_z ($\tilde{B}''' < 0$) dominates over the positive one with $\delta\tilde{G}_z$. This is the case for lattice dimensions $d=3,4$; for $d \geqslant 5$ the situation depends on the numerical factors in (4.16),

and if (4.16) has a solution, then the MFA behavior of the spontaneous magnetization with the critical index $\beta=1/2$ is reproduced. The latter is consistent with the renormalization group analysis of Larkin and Khmelnitski.[47]

The breakdown of the SCGA in the close critical region shows that this approximation is more sensitive to critical effects than other closed-form approximations always reproducing the MFA behavior. In the next section it will be shown that the *upper* spinodal boundary of the phase transition determined from the temperature dependence of magnetization yields a much better approximation for T_c than the lower one. It is so because the inverse susceptibility turns to zero at T_c with zero derivative, and even small inaccuracies in determination of the susceptibility can exert a great effect on determination of T_c. On the contrary, inaccuracies in magnetization produce a smaller effect on T_c due to the infinite slope of m at T_c.

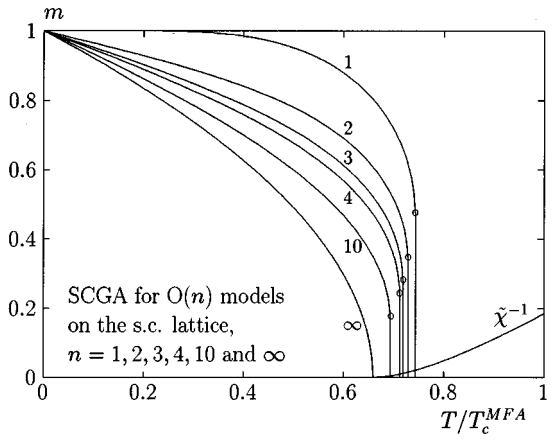

FIG. 2. Temperature dependences of spontaneous magnetization and zero-field susceptibility of the O(n) models on the sc lattice in the SCGA.

V. NUMERICAL RESULTS AND COMPARISONS

The SCGA system of nonlinear equations (3.15) was solved for different lattices and different types of the spin Hamiltonan (1.1) by the Newton-Raphson iterative method. For the fcc, bcc, sc, and diamond lattices the analytic expressions for the lattice integrals $P(X)$, Eq. (4.1), given by Joyce[53] were used. For hypercubic lattices $P(X)$ was reduced to one-dimensional integrals with the modified Bessel function $I_0(x)$ and calculated numerically. In other cases $P(X)$ was calculated by a direct integration over the Brillouin zone ($k_{x,y,z}\in[0,\pi]$) with the use of three-dimensional product quadratures composed of five- or ten-point one-dimensional Gaussian quadratures. The accuracy of these quadratures is so high that one does not need to analytically separate the divergence of the integrand in (4.1) at $q\to 0$ for $X=1$. The Gaussian integrals (3.18) were calculated for the Ising model with the use of five-, six-, or eight-point Gauss-Hermite quadratures, for the x-y, plane rotator, and completely anisotropic Heisenberg models, with the use of the corresponding product quadratures. For the models with equivalent spin components, such as O(n) with $n\geqslant 3$, the symmetrized integrals of the type (3.20) were approximated by five-, six- or eight-point generalized Gauss-Hermite quadratures corresponding to the weight function $|x|^{\alpha}\exp(-x^2)$ with $\alpha=1,2,3$ (Ref. 54) and $\alpha=2,4,6,8$ (Ref. 55). The latter was sufficient to calculate O(n) models up to $n=10$. The relative accuracy of calculations is not worse than 0.1%, which exceeds the intrinsic accuracy of the SCGA.

The results represented in Table I, Fig. 2, and Fig. 3 show that the deviations from the MFA due to molecular field fluctuations increase with the inverse of the number of interacting neighbors, z, or, rather, with the difference $W-1$ [see (4.2)] depending on the lattice structure. Among the three-dimensional lattices considered here the extreme cases are the diamond lattice ($z=4$) and the equivalent neighbor fcc-sc lattice ($z=18$) with 12 face-centered-cubic nearest neighbors and 6 simple cubic next nearest ones. For the O(n) models ($n=D$) the deviations of the magnetization m from the MFA solutions increase with the increase of n (see Fig. 2): $I(1/2)\Rightarrow$ plane rotator $\Rightarrow H(\infty)\Rightarrow$ spherical model, whereas the susceptibilities $\tilde{\chi}$ are practically the same for all models. The latter could be expected from the analysis of the susceptibility HTSE, Eq. (4.3), and of the lower spinodal boundary of the SCGA equations (4.13). For the n-D models with increasing n and $D=\text{const}$ [$I(\infty)\Rightarrow$ classical x-$y\Rightarrow H(\infty)$] the deviations from the MFA are increasing stronger than for O(n) ones. This feature is in accordance with the functional form of the susceptibility HTSE Eq. (4.3).

The temperature dependences of magnetization and other thermodynamic quantities calculated with increasing temperature are smooth functions of T up to some ''upper spinodal boundary'' after which in a zero magnetic field the magnetization jumps to zero. This feature results from the inaccuracy of the SCGA in a close critical region and was discussed in more detail at the end of Sec. IV. The discontinuities of thermodynamic functions in the SCGA diminish with the increase of the number of interacting neighbors, z, and the number of spin components, D, as well as with the decrease of the number of interacting spin components, n. For the quantities which are less singular at the critical point (e.g., the energy; see Ref. 44) these discontinuities are essen-

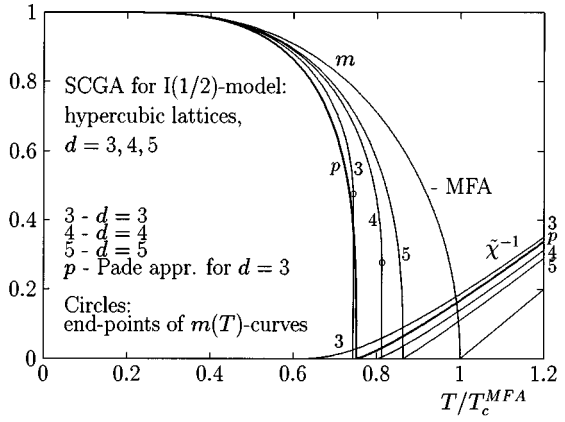

FIG. 3. Temperature dependences of spontaneous magnetization and zero-field susceptibility of the $S=1/2$ Ising model on d-dimensional hypercubic lattices in the SCGA, compared with Padé approximations of Refs. 6,8 for $d=3$.

TABLE I. The values of reduced Curie temperature $\theta_c \equiv T_c / T_c^{\mathrm{MFA}}$ calculated for different classical spin models on different lattices from the upper spinodal boundary of the SCGA equations. The results of other methods are placed below for comparison.

Model (Lattice)	fcc ($z=12$)	bcc ($z=8$)	sc ($z=6$)	Diamond ($z=4$)	fcc-sc ($z=18$)	bcc-sc ($z=14$)	hpc ($4d$) ($z=8$)	hpc ($5d$) ($z=10$)
0(1)	0.808	0.785	0.744	0.673	0.854	0.824	0.812	0.864
(Ising, $S=1/2$)	0.816 17[a]	0.793 85[a]	0.751 72[a]	0.676 0[b]	0.860 9[c]	0.830 7[c]	0.8340 1[d]	0.8769 4[d]
	0.816 20[e]		0.751 00[e]					
	0.816 28[f]							
O(2)	0.797	0.773	0.729	0.651	0.847	0.813	0.810	0.864
(plane rotator)	0.803 3[g]	0.780 2[g]	0.734 3[g]				0.831 9[h]	0.876 2[h]
		0.780 19[i]	0.733 89[i]					
			0.733 2[j]					
O(3)	0.790	0.766	0.719	0.637	0.842	0.807	0.808	0.864
(Heisenberg,	0.794[k]	0.771[k]	0.723[k]		0.850 5[k]	0.814 5[k]	0.829 2[h]	0.874 7[h]
$S=\infty$)	0.794 3[l]	0.770 5[l]	0.721 6[l]					
		0.770 32[i]	0.721 48[i]					
O(4)	0.785	0.761	0.712	0.628	0.839	0.803	0.808	0.864
		0.763 06[i]	0.712 39[i]				0.827 5[h]	0.873 7[h]
			0.712 3[m]				0.821 0[n,o]	
O(5)	0.781	0.757	0.707	0.621	0.837	0.799	0.807	0.864
	0.798[p]	0.771[p]	0.728[p]				0.826 2[h]	0.873 0[h]
O(6)	0.778	0.754	0.704	0.616	0.835	0.797	0.807	0.864
	0.789[p]	0.762[p]	0.717[p]				0.825 3[h]	0.872 4[h]
		0.752 95[i]	0.700 09[i]					
O(8)	0.774	0.749	0.698	0.608	0.832	0.793	0.807	0.864
	0.778[p]	0.751[p]	0.702[p]				0.824 0[h]	0.871 7[h]
		0.746 40[i]	0.692 21[i]					
O(10)	0.771	0.746	0.694	0.603	0.830	0.790	0.806	0.864
	0.771[p]	0.745[p]	0.694[p]				0.824 0[h]	0.871 1[h]
		0.741 84[i]	0.686 80[i]					
O(∞)	0.743 68	0.717 77	0.659 46	0.557 76	0.813 97	0.766 56	0.806 68	0.864 82
(spherical)							0.815 0[h]	0.867 4[h]
Ising, $S=1$	0.844	0.826	0.790	0.727	0.883	0.857	0.853	0.896
	0.851[q]		0.798 93[e]					
	0.852 46[e]							
	0.852 64[f]							
Ising	0.845	0.827	0.792	0.730	0.883	0.858	0.854	0.896
($n=1$ $D=2$)								
Ising, $S=\infty$	0.868	0.853	0.822	0.767	0.902	0.879	0.880	0.916
($n=1$ $D=3$)	0.874[q]		0.831 95[e]					
	0.876 82[e]							
	0.876 98[f]							
x-y, $S=\infty$	0.828	0.808	0.768	0.699	0.871	0.842	0.843	0.890
($n=2$ $D=3$)	0.835 4[g]	0.815 6[g]	0.776 0[g]					

[a]Reference 9.
[b]Reference 56.
[c]Reference 57.
[d]Reference 45.
[e]Reference 12.
[f]Reference 11.
[g]Reference 17.
[h]Reference 46.
[i]Reference 21.
[j]Reference 24.
[k]Reference 14.
[l]Reference 16.
[m]Reference 31.
[n]Reference 25.
[o]Reference 19.
[p]Reference 50.
[q]Reference 7.

tially weaker than the corresponding deviations from the MFA described by the SCGA.

As was mentioned at the end of the preceding section, the SCGA upper spinodal boundary should provide a good estimate of phase transition temperatures of three-dimensional systems. Indeed, the corresponding values of $\theta_c \equiv T_c / T_c^{\mathrm{MFA}}$ listed in Table I differ from the ones obtained by HTSE and other accurate methods generally by (1–0.5)%, which was never achieved by some other closed-form approximation. One can see that for the models with higher spin dimensionalities D, the accordance with HTSE results is better than that for the most critical for the SCGA $S=1/2$ Ising model ($n=D=1$). One can see from Table I, that the SCGA yields for the O(n) models with $n<10$ more accurate results than

the $1/n$ expansion performed for the fcc, bcc, and sc lattices by Okabe and Masutani,[50] who calculated numerically the analytical expressions (the double integrals over the Brillouin zone) obtained by Abe and Hikami.[48,49]

The models with higher lattice dimensionalities d are very important for testing the present approximation, which allows for Gaussian, i.e., noninteracting, fluctuations in the system. The interaction between fluctuations dies out in the spherical limit $D\to\infty$, as well as for $d\geqslant 4$.[47] Thus, one can expect that the SCGA yields rather accurate results for $d\geqslant 4$, whereas the deviations from the MFA described by the SCGA are still appreciable. Indeed, from Fig. 3 one can see that for the $I(1/2)$ model on the $d=4$ hypercubic lattice the distance between upper and lower spinodal boundaries is very small. The latter is due to the fact that the singularity of the function $P(X)$ at $X\to 1$ [see (4.2)] is only logarithmic. The discontinuity of magnetization at T_c is for the $I(1/2)$ model still substantial, but decreases quickly with the increase of the number of spin components D. For $d\geqslant 5$ discontinuities of thermodynamic functions in the SCGA disappear. The value of θ_c for the $I(1/2)$ model in $d=4$ dimensions (see Table I) is over 2% less then the $1/d$ expansion result of Fisher and Gaunt,[45] and this discrepancy diminishes smoothly with the increase of d. This can be seen from the comparison with the θ_c values of Ref. 45 for $d=5,6$ and the recent high-accuracy results of Ref. 10 for $d=6,7$. For $d=6,7$ the SCGA yields the θ_c values 0.894 [0.902 27, (Ref. 45) 0.902 90 (Ref. 10)] and 0.913 [0.919 22, (Ref. 10)] respectively. These values of θ_c are also very close to those for the spherical model (see Table I). With the increase of the spin dimensionality the accuracy of SCGA also increases. In Table I the SCGA results for θ_c for $d=4,5$ are compared with those of the general-n $1/d$ expansion by Gerber and Fisher[46] terminated by the term d^{-5}. Unfortunately the terminated $1/d$ expansion becomes less accurate for larger values of n and does not reproduce, unlike SCGA, the exact results for the spherical model. It should be also noted that for the O(n) models with $d\geqslant 4$ the results for θ_c approach with the increase of n those for the spherical model much faster than in three dimensions. This means that the coefficient in the $1/n$ expansion for θ_c in Refs. 48–50 should be very small in high dimensions.

The values of the energy of three-dimensional spin systems on the upper spinodal boundary of the SCGA equations are also rather close to the series ones. The calculated values of the normalized energy $\tilde{U}(\theta_c)\equiv U(\theta_c)/U(0)$ of the $S=1/2$ Ising model are 0.276 (0.25), 0.298 (0.27), 0.365 (0.33) for the fcc, bcc, and sc lattices, where the HTSE results are placed in brackets for comparison. For the classical Heisenberg model the normalized critical energies are given by 0.237 (0.245), 0.261 (0.265), 0.315 (0.325), respectively. For systems with higher lattice dimensionalities d, the energies are close to the ones for the spherical model, $\tilde{U}(\theta_c)=1-\theta_c$, especially for systems with many spin components. The normalized critical energies in the SCGA of the $I(1/2)$, $H(\infty)$, and spherical models, respectively, are 0.225, 0.198, 0.1933 for $d=4$ and 0.143, 0.135, 0.1352 for $d=5$.

In a magnetic field $H\neq 0$, the SCGA becomes more accurate, because the system is driven away from the critical point $(0,T_c)$, where the SCGA breaks down. The latter leads to the disappearance of the fictitious first-order phase transition in the SCGA starting from the fields, which are much smaller than the exchange interaction [i.e., for $h\equiv H/J_0\ll 1$]. For systems with a continuous spin symmetry (e.g., for the isotropic Heisenberg model) the magnetic field introduces a gap in the spin-wave spectrum and suppresses the singular contribution to magnetization $\propto\theta^{3/2}$ [see (4.7) and the following discussion], which improves the situation in the whole region below T_c. A comparison of the SCGA results for the magnetization in magnetic field $m(H,T)$ of the classical Heisenberg model on the sc lattice with the MC-simulation results of Binder and Müller-Krumbhaar[58] is represented in Fig. 4.

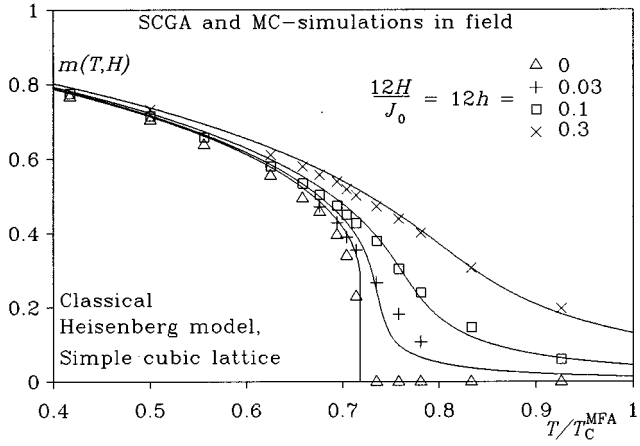

FIG. 4. Temperature dependencies of magnetization in magnetic field $m(H,T)$ for the classical Heisenberg model in the SCGA, compared with MC simulations of Ref. 58.

By application of the SCGA to experimentally investigated magnetic systems one should restrict oneself to the ones with large spin values ($S\gg 1$) and to the temperature range $T\gtrsim T_c/S$, where the whole Brillouin zone is populated by spin waves and the system behaves classically. An attempt to apply the SCGA to the $S=1/2$ Heisenberg model using the Brillouin function with $S=1/2$ [i.e., the Langevin function (3.7) with $D=1$], which corresponds formally to the consideration of the model with $n=3$ and $D=1$, yields for the sc lattice, in addition to the wrong linear behavior of the magnetization at low temperatures, the phase transition point $\theta_c=0.592$, being considerably higher than the HTSE value 0.560.[14] On the other hand, for systems with $S\gg 1$ quantum effects in the range of elevated temperatures are determined by a small parameter[38] $1/(zS)$ and can be partially taken into account in the SCGA by using the Brillouin function B_S. In typical cases this introduces errors that are smaller than the intrinsic inaccuracy of the SCGA. The Heisenberg ferromagnets EuO ($T_c\simeq$ 69 K) and EuS ($T_c\simeq$ 16.6 K) having $S=7/2$ are, perhaps, the most convenient materials for testing the SCGA, and they were extensively studied with NMR (Ref. 59) and neutron scattering[60] methods. EuO and EuS form fcc lattices, and the exchange interaction extends up to the next nearest sc neighbors. The contribution of dipole-dipole interaction (DDI) to T_c^{MFA} is[61] 1.7% for EuO and 4.9% for EuS. With the use of HTSE's it was shown[62] that DDI suppresses to some extent the reduced transition temperatures $\theta_c\equiv T_c/T_c^{\mathrm{MFA}}$ due to its competing

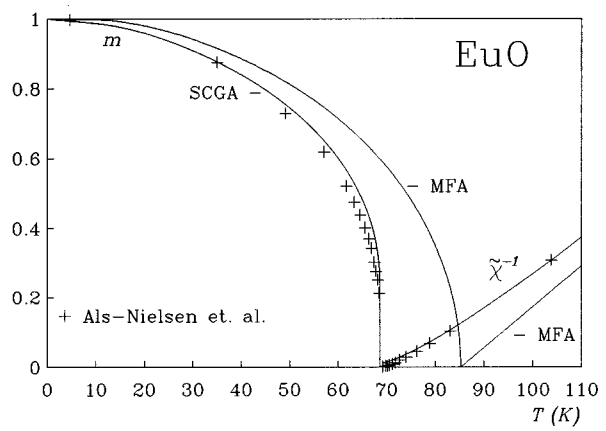

FIG. 5. Temperature dependences of magnetization and zero-field susceptibility of EuO in the SCGA, compared with the neutron scattering data of Ref. 60.

nature. In the SCGA rigorous taking into account DDI requires allowing for correlations between different components of molecular field fluctuations, $l_{\alpha\beta}$ with $\alpha \neq \beta$, which leads to the complication of the formalism and goes beyond the scope of this article. Instead, for a comparison with experimental data on EuO and EuS we take DDI into account in a simplified manner, only through the renormalization of T_c^{MFA} mentioned above. The results of numerical calculations for EuO represented in Fig. 5 show the same accordance of the SCGA results with the neutron scattering data of Ref. 60 as its accordance with the HTSE and MC results demonstrated above. For EuS, due to the negative value of the nnn exchange constant J_2, and hence the reduction of the effective number of interacting neighbors, the level of fluctuations is greater than in EuO, the Watson integral W is close to that for the sc lattice, and the deviation of the results from the MFA, as well as the discrepancy between the SCGA and experimental results, is somewhat larger.

VI. DISCUSSION

The self-consistent Gaussian approximation (SCGA) for classical spin systems described here is a unified theory applicable to a wide class of lattice models investigated currently by different groups with different methods. The SCGA takes into account fluctuations of the molecular field in the simplest way and is sensitive to the lattice dimensionality and structure and to the form of spin interactions. The SCGA yields rather accurate values of the field-dependent magnetization $m(H,T)$ and other thermodynamic functions in the whole plane (H,T) excluding the vicinity of the critical point $(0,T_c)$. In particular, the values of T_c themselves can be determined in the SCGA with an accuracy better than 1%, which makes it already important for practical applications to new lattice and spin Hamiltonian types.

Indeed, the SCGA is more flexible (although less accurate) than series expansions, and consideration of new substances reduces in the simplest case to some modifications of the lattice integral $P(X)$, Eq. (4.1), and of the Gaussian integrals (3.18). This can be exemplified by studying the crossover between fcc, sc, and bcc lattices varying the relative strength of the first and second nearest neighbor interactions J_2/J_1, or the crossover between Ising, Heisenberg, and x-y models varying anisotropy constants. Having solved the SCGA system of equations (3.15), one obtains all quantities of interest as a result of a single calculation. More serious generalizations of the SCGA are required for consideration of systems with DDI or with a transverse field, where nondiagonal correlations of molecular field fluctuations should be taken into account. For systems with many interacting sublattices the number of variables in the SCGA equations increases quadratically with the number of sublattices, and calculations become cumbersome.

Consideration of ferromagnets with a transverse field or antiferromagnets in field in the SCGA can be avoided, if one is interested only in zero-field susceptibilities. The zero-field ferro- and antiferromagnetic susceptibilities can be calculated through the correlation functions of the simplest ferromagnetic model with the longitudinal field. This requires, however, summation of some new diagram sequences and is the subject of a separate work.

Possible improvements of the SCGA should include non-Ornstein-Zernike effects in spin correlation functions (CF's) and non-Gaussian fluctuations of the molecular field. The former seems to be more important, since using Ornstein-Zernike CF's leads, due to singularities of the lattice integral $P(X)$, Eq. (4.2), to the overestimation of fluctuational effects for three-dimensional systems, which results in the breakdown of the SCGA in the critical region. The diagram technique for classical spin systems used for the construction of the SCGA is undoubtfully the best instrument for its further development, because it allows summation of different, more complicated diagram series than those considered here. All other perturbative schemes that do not take explicitly the advantage of classical properties of a system fail to reproduce the SCGA, although the physical picture of Gaussian fluctuations of the molecular field is quite transparent.

One more possible application of the classical spin diagram technique is that to low-dimensional and finite-size systems, where the level of fluctuations is large and an improvement of the SCGA is necessary. The first step in this direction was the calculation of the energy and susceptibility of low-dimensional antiferromagnets in the whole temperature interval[52] and also for a nonzero magnetic field[63] with the use of a $1/D$ expansion. By this calculation, the results of which are rather good even for $D=3$, some diagram series going beyond the SCGA were summed up. This can, in principle, show how to improve the SCGA in a nonperturbative way with respect to D.

The SCGA can be generalized also for inhomogeneous states of magnetics. It turns out, however, that interesting results can be obtained already in the limit $D \to \infty$, where the model (1.1) is analytically soluble but *not* equivalent to the standard spherical model of Berlin and Kac[43] in inhomogeneous situations, even in the isotropic case. The anisotropic spherical model defined by (1.1) in the limit $D \to \infty$ was already applied to domain walls[64] and to thin films.[65]

And, finally, of a principal importance would be to construct the dynamical part of the classical spin diagram technique and to try to generalize the SCGA for dynamics.

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