Derivation of effective field theories

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A general self-consistency approach allows for a thorough treatment of the corrections to the mean-field approximation (MFA). The natural extension of standard MFA with the help of a cumulant expansion leads to a point of view on the effective field theories. The proposed approach can be used for a systematic treatment of fluctuation effects of various length scales and, perhaps, for the development of a coarse-graining procedure. We outline and justify our method by some preliminary calculations. Results are given for the critical temperature and the Landau parameters of the ϕ^4 theory—the field counterpart of the Ising model. An important unresolved problem of the modern theory of phase transitions—the problem for the calculation of the true critical temperature—is considered within the framework of the present approach. A comprehensive description of the ground-state properties of many-body systems is also demonstrated.

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I. INTRODUCTION

This investigation is focused on the correspondence between microscopic models of phase transitions and their quasimacroscopic (field-theoretic) counterparts. Here we shall outline a self-consistency approach to a more accurate derivation of effective field theories from microscopic models defined on lattices.

Our method is general and can be used for a wide class of microscopic models but for a concreteness here we shall illustrate our approach with the Ising model (IM), given by

$$\mathcal{H}(s) = -\frac{1}{2}\sum_{ij}^{N} J_{ij}s_i s_j, \tag{1}$$

where $s \equiv \{s_i\}$ denotes a lattice "field," $s_i = \pm 1$, and the interaction constant of ferromagnetic type $J_{ij}=J(|i-j|)>0$ depends on the intersite distance $|i-j|$ in a regular D-dimensional lattice of N sites ("spins" or pseudospins). Note, that $J(0) \equiv J_{ii}=0$.

We shall follow the main path of the phase transition theory, where the effective (quasimacroscopic) field Hamiltonians [alias Ginzburg-Landau (GL) free energies] are derived with the help of two systematic methods: (i) Hubbard-Stratonovich transformations (HST) and, (ii) a mean-field-(MF-) like procedure [1–3]. Here we propose a more thorough approach based on a convenient generalization of (ii).

The known field theories exhibit both success and failure in the description of many-body systems defined by microscopic models. For example, we believe that the renormalization group methods of the modern theory of phase transitions [1] based on the ϕ^4 theory yield a quite convenient description of the scaling and universality properties of IM but we cannot be certain that the field theory satisfactorily describes important nonuniversal properties, such as, for example, the critical temperature T_c and the lower critical dimensionality D_L (for IM, $D_L=1$, whereas within the ϕ^4 theory, $D_L=2$). In fact the field theory fails along this line of studies. For example, the fluctuation shift $(\Delta T_c)_f$ of T_c predicted within the one-loop approximation for the ϕ^4 theory is very small and, hence, unrealistic, while in the higher orders of the loop expansion this shift turns out to be infinite and its calculation needs a special renormalization. As a result, the problem for the value of T_c within the framework of the present field theory of phase transitions remains unresolved. Here we shall show the genesis of this problem and present a satisfactory solution.

The reason for the mentioned difficulties of the field-theory approach is in the quite simplified coarse-graining procedures used in the derivation of the GL effective Hamiltonians from microscopic models. HST is applied together with the long-wavelength approximation (LWLA), namely, $(ka_0) \ll \pi$, where $k=|\boldsymbol{k}|$ is the magnitude of the wave vector $\boldsymbol{k}=(k_1,\ldots,k_D)$, a_0 is either the lattice constant or, generally, the mean interparticle distance. LWLA leads to a correct expression for the Ornstein-Zernicke correlation function but cuts the short-range [high-energy, $\epsilon(k) \sim k^2$, $\Lambda < k < \phi/a_0$] interparticle correlations of fluctuation type that have the main contribution to the shift $(\Delta T_c)_f$; $\Lambda \ll \pi/a_0$ is the upper cutoff for k within LWLA.

Within the approach (ii) we usually mention that we neglect the fluctuations of the physical quantities from their equilibrium values. This, is not entirely true. It seems important to emphasize that the latter are values in MF approximation (MFA) and, hence, they are incorrect. Thus, the fluctuations are defined towards incorrect statistical averages, and their contribution to the free energy of the system cannot be accepted as an entire fluctuation effect. The latter can be correctly evaluated, if we are able to define the fluctuations as variations towards exact statistical averages calculated by the Hamiltonian (1). This task seems unsolvable, but the present paper makes a step for improvement of the theory along the same direction.

Note, that the methods (i) and (ii), no matter of the difference between them, lead to the same GL effective field theory. Both methods use LWLA. For the method (ii) LWLA seems to me obligatory because of the following important argument. HST can be applied only to positively definite

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matrices (J_{ij}) but this condition is not satisfied by quite important lattice models, such as the nearest-neighbor (NN) IM. In LWLA, however, the same interaction matrix $J_{ij;nn}$ of IM is modified to a form that is positively definite. Besides, in both methods, LWLA is used to help the derivation of the quasimacroscopic (fluctuation) and macroscopic (thermodynamic) properties, i.e., the LWLA is a tool of a "coarse-graining" procedure for the many-body system. But in both cases (i) and (ii), the microscopic and mesoscopic interparticle correlations are ignored. Here we shall use a generalization of the method (ii) in order to improve this disadvantage of the theory. In this way we shall present more accurate calculation of the LG parameters (vertices) of the effective field theory of Ising systems. Besides, we shall show explicitly the mechanism of "statistical correlation" which leads from the two-site $(i-j)$ trivial correlation presented by the initial interaction J_{ij} to short-scale, mesoscale, and large-scale effective multiparticle correlations of fluctuation type—fluctuation correlations. Thus, we shall establish and develop a "coarse-graining" procedure, and this is the main aim of our paper. Besides, we shall show that the GL parameters of the ϕ^4 theory acquire $(1/z)$ corrections for both short-range and long-range interactions $J(|i-j|)$ [1]. These corrections will be presented to second order in $(1/z)^2$.

The $1/z$ expansion has been introduced by Brout [4] and applied in calculations of T_c and thermodynamic susceptibilities [5–13]. We are not aware of another relevant work along this line of research except for our recent investigation [2,3]; the latter will be used in our investigation. Remember, that the (Brout) approach is a development of an older method—the Kirkwood method of cumulants (semi-invariants) [14]; hence, we shall follow a cumulant expansion which is well known.

We shall generalize the Brout approach in a way that makes it possible to derive effective field theories, and this will allow us to reveal surprising features of many-body systems. In the Brout scheme, the mean ("molecular") field is spatially (i) independent. We find that there are no physical reasons for this assumption and extend the "mean-field concept." Within our approach, the so-called mean field is spatially dependent up to the moment when one should find the actual ground state. Then the fluctuation phenomena occur with respect to this ground state. In our approach the GL parameters and, hence, the ground state have a more precise evaluation.

Our consideration has been performed for interactions $J(|i-j|)$ of a quite general type, namely for all interactions that can be presented by the equality,

$$\sum_j J_{ij} = zJ_0 \equiv J, \tag{2}$$

where J_0 is an effective exchange constant, and z is an effective "coordination" number (number of interacting neighbors). In particular cases our results will be referred to as the most common case of NN interactions (then $n=2D$ for simple lattices). For a simplicity, here we shall assume that IM is defined by a simple cubic (sc) lattice. The consideration can be easily expended to other types of regular lattices, as well as to irregular lattices with certain forms of quenched disorder, for example, random potential [1]. We introduce the interaction radius by $R_{\text{int}} \approx z^{1/D}$—a quantity, which is equal to the so-called zero-temperature correlation length (see Sec. II). Let us emphasize that our results can be rederived without difficulties in the presence of an external field $\{h_i\}$ conjugate to the lattice field $\{s_i\}$.

Other theories intended to improve the coarse-graining procedures of many-body systems are, for example, the hierarchical reference theory [15] and a method of collective variables [16]. The former is based on a particular renormalization procedure and yields interesting results for the effective critical exponents of continuous phase transitions. The latter theory uses a variant of cumulant expansion and collective variables which, in certain limit, form the order parameter field. In these features the collective variable theory [16] resembles our approach but, generally, in contrast to the latter, it significantly departs from the original Brout idea. The mentioned theories do not use $1/z$ expansion and for this reason and apart from some common aims and general ideas, cannot easily be compared with the present approach, which is a very direct extension of the many-body theory beyond the standard mean-field ("tree") approximation.

In Sec. II we present a general approach to the treatment of fluctuation correlations at various length scales and discuss aspects of the usual theory that corresponds to the lowest-order approximation of a perturbation expansion of cumulant type. In Sec. III we investigate the higher orders of the mentioned perturbation expansion and demonstrate several features of the effective field theory. Our main results are summarized and discussed in Secs. III D–III G.

II. PRESENT STATUS OF THE EFFECTIVE FIELD THEORY

A. General scheme

The equilibrium free energy of IM as a function of the temperature T and the field configuration $h=\{h_i\}$ is given by

$$G(T) = -\beta^{-1} \ln\{\text{Tr}\, e^{-\beta\mathcal{H}(s)}\}, \tag{3}$$

where $\beta^{-1}=k_BT$, and the Trace is over the allowed lattice configurations $s=\{s_i\}$. Note, that the equilibrium values of the physical quantities are calculated as averages with respect to the statistical ensemble based on the Hamiltonian (1) and, in particular, the statistical averages of type $\langle s_i \cdots s_j \rangle$ are obtained as derivatives of the partition sum whereas the irreducible averages $\langle\langle s_i \cdots s_j \rangle\rangle = \langle (s_i - \langle s_i \rangle) \cdots (s_j - \langle s_j \rangle) \rangle$ are obtained as derivatives of the Gibbs free energy (3).

Let us introduce the shift

$$s_i = \phi_i + \delta s_i, \tag{4}$$

where the lattice field ϕ_i is an arbitrary (auxiliary) field configuration that is not necessarily associated with the averaged spin $\langle s_i \rangle$ at site i, and the "fluctuation" δs_i is merely the difference $(s_i - \phi_i)$. The identification of ϕ_i with a statistical average $\langle \cdots \rangle$ over the full Hamiltonian (1), or, with a statistical average $\langle \cdots \rangle_0$ corresponding to another ensemble as well as the interpretation of δs_i as a fluctuation around $\langle s_i \rangle$ (or $\langle s_i \rangle_0$) may be a matter of further considerations. At this

stage ϕ_i and δs_i are auxiliary variables which obey Eq. (4) and are not referred to as concrete physical quantities.

Following a standard procedure (see, e.g., Refs. [1,2]) we obtain the following effective nonequilibrium free energy:

$$\mathcal{H}(\phi) = \mathcal{H}_0(\phi) + \mathcal{H}_f(\phi), \tag{5}$$

with $\phi \equiv \{\phi_i\}$,

$$\mathcal{H}_0(\phi) = \frac{1}{2}\sum_{ij} J_{ij}\phi_i\phi_j - \beta^{-1}\sum_i \ln[2\,\mathrm{ch}(\beta a_i)]. \tag{6}$$

Here

$$a_i = \sum_j J_{ij}\phi_j \tag{7}$$

is the "mean" (molecular) field, and

$$\mathcal{H}_f(\phi) = -\beta^{-1}\ln\left\langle \exp\left[\frac{\beta}{2}\sum_{ij} J_{ij}(s_i-\phi_i)(s_j-\phi_j)\right]\right\rangle_0 \tag{8}$$

is the "fluctuation" part. As usual, we shall often call the free energy (5) an "effective Hamiltonian" (see, also, Ref. [17]).

In Eq. (8), $\langle\cdots\rangle_0$ denotes a statistical average over an ensemble defined by the auxiliary ("MF") Hamiltonian

$$\mathcal{H}_a(\phi,s) = -\sum_i a_i s_i; \tag{9}$$

the respective partition function and (nonequilibrium) free energy are given by $\mathcal{Z}_a(\phi)=\mathrm{Tr}[\exp(-\beta\mathcal{H}_a)]$, and $G_a(\phi)=-\beta^{-1}\ln\mathcal{Z}_a(\phi)$. For this simple ensemble, we have

$$\langle s_i\rangle_0 = \mathrm{th}[\beta a_i(\phi)]. \tag{10}$$

The calculation of averages of type $\langle s_i\cdots s_j\rangle_0$ as well as "irreducible" averages of type $\langle\langle \delta s_i\cdots\delta s_j\rangle\rangle_0$ is also straightforward. These averages represent a form of fluctuation correlations, but they are just an auxiliary theoretical tool rather than real objects. In contrast, the real objects, namely, (full) statistical averages $\langle\cdots\rangle$ and $\langle\langle\cdots\rangle\rangle$ within the total Hamiltonian (1) cannot be exactly calculated.

B. Usual theory

In the framework of the usual theory, the "fluctuation" term $\mathcal{H}_f$ is ignored. This is the MFA. In the present general format of the theory, we have N (self-consistency) equations of state $(\partial\mathcal{H}/\partial\phi_i)=0$ at fixed T (and $h=\{h_i\})=0$—one equation per lattice vertex i,

$$\sum_j J_{ij}\{\bar{\phi}_j - \mathrm{th}[\beta a_j(\bar{\phi})]\} = 0, \tag{11}$$

where $\bar{\phi}=\{\phi_i\}$. It is easy to see that the number $(z-1)$ of nonzero terms $(i\neq j)$ in all N sums (11) is equal to the number of nonzero interaction constants acting on the site i: $J(|i-j|)>0$ for $a_0\leqslant|i-j|\leqslant R_{\mathrm{int}}$; $J(|i-j|=0$ for $|i-j|\equiv R > R_{\mathrm{int}}$. The "equations of state" (11) can be written in the simple form

$$\bar{\phi}_i = \mathrm{th}[\beta a_i(\bar{\phi})]. \tag{12}$$

The equivalence of Eqs. (11) and (12) can be easily proven for any number $N\geqslant 1$.

From Eqs. (10) and (12) we obtain

$$\langle\bar{s}_i\rangle_0 = \mathrm{th}[\beta a_i(\bar{\phi})] = \bar{\phi}_i. \tag{13}$$

Thus in this quite general form of MFA ($\mathcal{H}_f\approx 0$), we have $\langle s_i\rangle_0=\bar{\phi}_i$, $\langle\cdots\rangle=\langle\cdots\rangle_0$, and $G(T,h)=\mathcal{H}_0(\bar{\phi})$ is the equilibrium free energy that corresponds to extrema (including minima) $\bar{\phi}$ of $\mathcal{H}(\phi)\approx\mathcal{H}_0(\phi)$—the nonequilibrium MF free energy given by the nonequilibrium (arbitrary) order parameter field ϕ_i. By $\bar{\phi}_i$ from Eq. (11) we denote the equilibrium configuration of the latter; hereafter the "bar" of the equilibrium value $\bar{\phi}_i$ of ϕ_i will be often omitted. Now one may perform a Landau expansion for small $\bar{\phi}_i$ in order to obtain other known forms of the MF theory.

However, at the present stage of consideration we are interested in some more generality and for this reason we continue our discussion of the nonequilibrium free-energy functional

$$\tilde{G}(T/\phi) \equiv \mathcal{H}(T/\phi) \approx \mathcal{H}_0(T/\phi) \tag{14}$$

as given by Eq. (6). In Eq. (14), the dependence of the nonequilibrium free energy $\tilde{G}$ on ϕ is denoted by "$/\phi$" because of the more special role of this variable, namely, the variation $\delta\tilde{G}$ should be zero at thermal equilibrium and from this condition one obtains the possible thermal equilibria $\bar{\phi}$ (alias "self-consistency condition").

The expansion of the logarithm term in Eq. (6) up to fourth order in ϕ_i yields the known result for the lattice ϕ_i^4 theory of the Ising model,

$$\mathcal{H}_0(\phi) = \frac{1}{2}\sum_{ij} J_{ij}\phi_i\phi_j - \frac{\beta}{2}\sum_{ijk} J_{ij}J_{ik}\phi_j\phi_k + \frac{\beta^3}{12}\sum_{ijklm} J_{ij}J_{ik}J_{il}J_{im}\phi_j\phi_k\phi_l\phi_m. \tag{15}$$

One may apply LWLA to this form of the theory but we shall follow a different path.

C. Continuum limit

Using the rule

$$\sum f_i = \rho\int d^D x f(\boldsymbol{x}) \equiv \rho\int d\boldsymbol{x} f(\boldsymbol{x}), \tag{16}$$

where $\rho=(N/V)$, we can write Eq. (2) in the form

$$J = \rho\int d^D R J(R), \tag{17}$$

with $R=|\boldsymbol{R}|$; $\boldsymbol{R}=(\boldsymbol{x}-\boldsymbol{y})$. Note, that the factor ρ in Eqs. (19)–(21) can be avoided and this is the usual practice. In the latter case the physical dimension of the respective physical quantity is changed by a factor $[V]\sim[L]^D$; for example,

$[L]^D[f_i]=[f(\boldsymbol{x})]$. Of course, one may use both variants.

In the continuum limit the effective Hamiltonian (6) corresponding to a zero external field ($h=0$) takes the form

$$\mathcal{H}_0 = \frac{\rho}{2}\int d^D x \phi(\boldsymbol{x}) I[\phi(\boldsymbol{x})] - \rho\beta^{-1}\int d^D x \ln \mathrm{ch}\{\beta^{-1} I[\phi(\boldsymbol{x})]\}, \tag{18}$$

where

$$I[\phi(\boldsymbol{x})] = \rho\int d^D y J(R)\phi(\boldsymbol{y}). \tag{19}$$

Now we apply LWLA in the form

$$[\phi(\boldsymbol{x}) - \phi(\boldsymbol{y})]^2 \ll |\phi(\boldsymbol{x})\phi(\boldsymbol{y})| \tag{20}$$

and under this assumption truncate the Taylor expansion

$$\phi(\boldsymbol{y}) = \phi(\boldsymbol{x}) + \sum_{\alpha=1}^{D}\frac{\partial\phi(\boldsymbol{x})}{\partial x_\alpha}R_\alpha + \frac{1}{2}\sum_{\alpha,\beta=1}^{D}\frac{\partial^2\phi(\boldsymbol{x})}{\partial x_\alpha \partial x_\beta}R_\alpha R_\beta + \cdots \tag{21}$$

to the second order in $\boldsymbol{R}=\{R_\alpha\}$.

Using the approximation (20) and (19) becomes

$$I[\phi(\boldsymbol{x})] = J\phi(\boldsymbol{x}) + \frac{\tilde{J}}{2D}\nabla^2\phi(\boldsymbol{x}), \tag{22}$$

where J is given by Eq. (17), and

$$\tilde{J} = \rho\int d^D R J(R) R^2. \tag{23}$$

Now we substitute Eq. (22) in Eq. (18). We perform the expansion up to order $\phi^4(\boldsymbol{x})$ and to second order in $\nabla\phi(\boldsymbol{x})$. Besides, we should keep in mind, that in expansion in powers of ϕ_i we cannot distinguish between T and T_{c0} except for the ϕ_i^2 term where the difference between T and T_{c0} should be kept only to the lowest nonvanishing order; in our case, this is the first order in $(T-T_{c0})$: see, e.g., Ref. [1]. Following these notes, we perform at a certain stage of the calculation an integration by parts with the convenient boundary condition $\nabla\phi(\boldsymbol{x})=0$ and obtain the well-known GL effective Hamiltonian

$$\mathcal{H}_0 = \rho\int d^D x\left(\frac{\tilde{c}_0}{2}[\nabla\phi(\boldsymbol{x})]^2 + \frac{r_0}{2}\phi^2(\boldsymbol{x}) + u_0\phi^4(\boldsymbol{x})\right), \tag{24}$$

with

$$c_0 = \frac{R_{\mathrm{int}}^2}{2D}J, \quad r_0(T) = k_B(T-T_{c0}), \quad u_0 = \frac{J}{12}. \tag{25}$$

Here $T_{c0}=(J/k_B)$ and terms of order $t_0=(T-T_{c0})/T_{c0}\ll 1$ have been neglected in c_0 and u_0 [2], i.e., these two parameters are calculated at T_{c0} [1,2].

To clarify the results in Eqs. (24) and (25) we shall mention that $J(R)$ for $R>R_{\mathrm{int}}$ is very small and can be ignored. Setting $J(R)\sim J_0$ in Eq. (17), comparing the result with $J=zJ_0$ from Eq. (2), and noticing that $\rho=1/v\sim a_0^D$, one obtains $z\sim(R_{\mathrm{int}}/a_0)^D$ as should be, and $J\approx J_0 R_{\mathrm{int}}^D$. In the same way, one obtains $\tilde{J}\approx JR_{\mathrm{int}}^2$.

The results (24) and (25) show that the energy of the spatially dependent configurations of the field depends on the interaction radius. The latter serves as a coherence (correlation) length of the field $\phi(\boldsymbol{x})$; see the parameter c_0 given in Eq. (25). In order to clarify this point, let us consider the so-called zero-temperature correlation length [1], defined by $\xi_0\equiv\xi(T=0)=[-c_0/r_0(0)]^{1/2}$. Using Eq. (25) and $T_{c0}=J/k_B$ we obtain $\xi_0=R_{\mathrm{int}}\sqrt{2D}$.

D. Discussion

Note that the temperature range of validity of these considerations is $t_0(T)\ll 1$ and $(ka_0)\ll\pi$. The spatially dependent fluctuations correspond to a higher energy than the uniform configuration, and hence the latter contains the deepest (global) minima $\bar{\phi}$ of the effective free energy nevertheless we have written N "equations of state" as a result of the minimization of the effective Hamiltonian. Now one can easily show that the variation of the Hamiltonian (24) with respect to the field will give again spatially dependent solutions but in the usual theory they are interpreted as "spatially dependent fluctuations" which, together with the uniform fluctuation $\delta\phi=(\phi-\bar{\phi})$ towards the stable state $\bar{\phi}$, are all fluctuations in the system in LWLA. But we know that this picture contains the approximation $\langle s_i\rangle\sim\langle s_i\rangle_0=\bar{\phi}$.

Our point of view is the following. The averages $\langle\cdots\rangle_0$ should not be taken very seriously. They are an auxiliary tool in our consideration, and are not the final aim of our investigation. We have used these averages only because they appear along our way of obtaining an effective Hamiltonian $\mathcal{H}$ (or $\mathcal{H}_0$ in the lowest order of the theory) in which the statistical degree of freedom ϕ_i varies in a wide range of values $(-\infty<\phi_i<\infty)$. This is the only consistent interpretation of our consideration performed so far. We can assume that up to now we have obtained nothing else but an effective free energy (effective lattice Hamiltonian) in terms of the lattice field ϕ_i. In a clear approximation, this effective model is given by Eq. (6); for the expansion in powers of ϕ_i, see Eq. (15).

Another important aspect of our consideration is that the Hamiltonian contains more ij interactions than the original model (1). The mathematical form of Eq. (15) gives a clear physical interpretation of these interactions: The first $\phi_i\phi_j$ term on the right-hand side (rhs) of Eq. (15) describes an interaction that is quite similar to the original interspin interaction in Eq. (1) whereas the second term of the same type in Eq. (15) describes an indirect two-site jk interaction that is mediated by the "i spins." This means that the latter interaction $J_{ij}J_{ik}$ has 2 times larger radius of action than the original J_{ij} exchange. The four-point interaction given by the third term on the rhs of Eq. (15) can also be described in the above style.

Therefore, even at this early stage of consideration ($\mathcal{H}\approx\mathcal{H}_0$) we see that the effective free energy exhibits effects of "statistical extension of the original interparticle correlations (interactions)." This "principle of growth of statistical correlations" is well known in the general phase-transition theory. Here we show the concrete mechanism of the respective phenomenon and a systematic way of description of growth of

statistical correlations. This point will become more clear from the results in the next section. We shall see that the investigation along this path leads to a quite unexpected and intriguing picture.

III. BEYOND THE STANDARD THEORY

A. Perturbation series

Here we consider the ϕ contributions to the effective free energy (Hamiltonian) $\mathcal{H}(\phi)$ which are generated by the term $\mathcal{H}_f(\phi)$. For obvious reasons, terms that are ϕ_i independent will be omitted.

It seems convenient to rearrange our theory by introducing the auxiliary variables $\Delta_i=(s_{i0}-\phi_i)$, and $\sigma_i=(s_i-s_{i0})$, where $s_{i0}\equiv\langle s_i\rangle_0$. Then $\mathcal{H}$ can be written as an infinite perturbation series in powers of the (perturbation) Hamiltonian part

$$S_f(s,\phi)=-\frac{1}{2}\sum_{ij}J_{ij}\sigma_i\sigma_j-\sum_{ij}\Delta_i\sigma_j. \tag{26}$$

The respective series can be presented in the form

$$\mathcal{H}_f(\phi)=-\frac{1}{2}\sum_{ij}J_{ij}\Delta_i\Delta_j+\sum_{l=1}^{\infty}\mathcal{H}_f^{(l)}(\phi), \tag{27}$$

where

$$\mathcal{H}_f^{(l)}(\phi)=\frac{(-\beta)^{l-1}}{l!}\langle S_f^l(s,\phi)\rangle_{0c}, \tag{28}$$

$\langle\cdots\rangle_{0c}$ denotes the so-called connected averages [1]; for example, the average $\langle S_f^2\rangle_0\langle S_f^2\rangle_0$ is excluded from the connected $\langle S_f^4\rangle_{0c}$. For this cumulant (semi-invariant), expansion rules, similar to the Wick theorem in the perturbation theory of propagator type, are not available and one should perform the calculations with some caution. The term $\mathcal{H}_f^{(1)}$ is equal to zero, and this leads to a reduction of some infinite series in the next orders of the theory $(l>1)$.

B. Lowest-order correction

Let us consider the first term on the rhs of Eq. (27) and neglect all others. This yields $\mathcal{H}=(\mathcal{H}_0+\mathcal{H}_f)$ in the form

$$\mathcal{H}\approx\frac{\beta}{2}\sum_{ijk}J_{ij}J_{ik}\phi_j\phi_k-\frac{\beta^2}{2}\sum_{ijkl}J_{ij}J_{ik}J_{jl}\phi_k\phi_l-\frac{\beta^3}{4}\sum_{ijklm}J_{ij}J_{ik}J_{il}J_{im}\phi_j\phi_k\phi_l\phi_m+\frac{\beta^4}{3}\sum_{ijklmn}J_{ij}J_{jk}J_{il}J_{im}J_{in}\phi_k\phi_l\phi_m\phi_n. \tag{29}$$

Performing this straightforward calculation one readily sees a very important property of the present theory, namely, that the first term on the rhs of Eq. (15) is totally compensated by a respective counterterm coming from the contribution $(\sim\Delta_i\Delta_j)$ to the effective free energy. Besides, another term twice compensates the second term in Eq. (15) so that the term of type $JJ\phi\phi$ now appears with a positive sign. The ϕ^4 part of the effective free energy also undergoes a drastic change due to the $\Delta\Delta$ correction coming from Eq. (28).

The same result can be obtained in a more general and, perhaps, more convenient way, if we add the $\Delta\Delta$ term in Eq. (27) to $\mathcal{H}_0$ from Eq. (6) before doing the expansion of Landau type. Then, within the same lowest-order approximation for the series (27) we obtain a more general result for $\mathcal{H}$, namely

$$\mathcal{H}=-\frac{1}{2}\sum_{ij}J_{ij}\,\mathrm{th}(\beta a_i)\mathrm{th}(\beta a_j)+\sum_{ij}J_{ij}\phi_i\,\mathrm{th}(\beta a_j)-\beta^{-1}\sum_i\ln[2\,\mathrm{ch}(\beta a_i)]. \tag{30}$$

This form of $\mathcal{H}$ clearly shows the lack of the simple $J_{ij}\phi_i\phi_j$ term describing the direct two-site exchange. In our further considerations we shall be faced only with interparticle interactions (correlations), which are extended at distances larger than R_{int}. In order to obtain Eq. (29) one must expand the transcendental functions in Eq. (30); $(\beta a_i)\ll 1$.

The forms (29) and (30) of the effective free energy describe only indirect two-site interactions because the direct two-site interaction disappeared from our consideration. Now we are at a stage of description of correlations which extend up to $2R_{ij}$ and larger distances. The tendency of the growing length scale of the interactions included in our effective free energy will be the main and unavoidable feature of our further consideration.

Another very important feature of our findings is that in the simplest variant of the theory when the field is uniform $(\phi_i\equiv\phi)$ as well as in the GL variant in LWLA given by Eq. (24) the values of the Landau coefficients c_0, r_0, and u_0 do not change within the framework of accuracy of the effective ϕ^4-field theory, where terms (Landau invariants) of order $O(t^3)$ are ignored; $t=(T-T_c)/T_c$. This property seems to exist for any order of the expansion (27) in the limit of an infinite-range $(z\to\infty)$ initial interaction J_{ij}. The $1/z$ corrections to the parameters (c_0, r_0, u_0) of the effective field theory are obtained from the $(l>1)$ terms in the series (27).

C. High-energy corrections of higher order

We have already mentioned that the $(l=1)$ term in Eq. (27) is zero. A calculation of the next two terms $(l=2,3)$ in Eq. (27) has been carried out in Ref. [2]. Following Ref. [2] we can write $\mathcal{H}_f^{(2)}$ in the form

$$\mathcal{H}_f^{(2)}=-\frac{\beta}{4}\sum_{ij}\frac{J_{ij}^2}{\mathrm{ch}^2(\beta a_i)\mathrm{ch}^2(\beta a_j)}-\frac{\beta}{2}\sum_{ijk}J_{ij}J_{ik}\frac{\Delta_j\Delta_k}{\mathrm{ch}^2(\beta a_i)}. \tag{31}$$

The result (31) gives the first $(1/z)$ corrections to the parameters c_0, r_0, and u_0. Adding the result (31) to $\mathcal{H}(\phi)$ we obtain a form of the effective Hamiltonian $\mathcal{H}(\phi)$ which is more precise than the preceding ones. Let us write this quite lengthy expression of the effective Hamiltonian as

$$\mathcal{H} = \frac{\beta^2}{2}\sum_{ijkl} J_{ij}J_{ik}J_{jl}\phi_k\phi_l + \frac{\beta^3}{2}\sum_{ijkl} J_{ij}^2 J_{ik}J_{il}\phi_k\phi_l$$
$$- \frac{\beta^3}{2}\sum_{ijklm} J_{ij}J_{ik}J_{jl}J_{km}\phi_l\phi_m + \frac{\beta^3}{4}\sum_{ijklm} J_{ij}J_{ik}J_{il}J_{im}\phi_j\phi_k\phi_l\phi_m$$
$$- \beta^4\sum_{injklm} J_{in}J_{ij}J_{ik}J_{il}J_{nm}\phi_j\phi_k\phi_l\phi_m$$
$$+ \frac{\beta^5}{3}\sum_{inpjklm} J_{in}J_{ip}J_{nj}J_{nk}J_{nl}J_{pm}\phi_j\phi_k\phi_l\phi_m$$
$$+ \frac{\beta^5}{2}\sum_{inpjklm} J_{in}J_{ip}J_{ij}J_{ik}J_{nl}J_{pm}\phi_j\phi_k\phi_l\phi_m$$
$$- \frac{\beta^5}{3}\sum_{injklm} J_{in}^2 J_{ij}J_{ik}J_{il}J_{im}\phi_j\phi_k\phi_l\phi_m$$
$$- \frac{\beta^5}{4}\sum_{injklm} J_{in}^2 J_{ij}J_{ik}J_{il}J_{im}\phi_j\phi_k\phi_l\phi_m. \quad (32)$$

The result (32) shows that the indirect two-point interactions of type $JJ\phi\phi$ available in the effective Hamiltonian (29) do not exist in this higher accuracy of the theory. The interactions of type $JJJ\phi\phi$ and $JJJJ\phi\phi$ presented in the effective Hamiltonian (32) extend up to distances $3R_{\rm int}$. The same is valid for the four-point interactions included in Eq. (32).

Within LWLA, Eq. (32) yields

$$\mathcal{H} = \frac{1}{2}\sum_{\boldsymbol{k}} (r + ck^2)|\phi(\boldsymbol{k})|^2$$
$$+ \frac{u}{N}\sum_{(\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3)} \phi(\boldsymbol{k}_1)\phi(\boldsymbol{k}_2)\phi(\boldsymbol{k}_3)\phi(-\boldsymbol{k}_1-\boldsymbol{k}_2-\boldsymbol{k}_3). \quad (33)$$

In Eq. (33),

$$c = \left(1+\frac{5}{z}\right)c_0, \quad r = \left(1+\frac{3}{z}\right)\tilde{r}_0, \quad u = \left(1+\frac{4}{z}\right)u_0, \quad (34)$$

where $\tilde{r}_0 = k_B(T - T_c)$ is given by the "true" (renormalized) critical temperature

$$T_c = T_{c0}\left(1 - \frac{1}{z}\right). \quad (35)$$

In deriving this lattice version of the effective Hamiltonian we have performed the lattice summations in Eq. (32) in the reciprocal ($\boldsymbol{k}$) space with the help of LWLA, $J(k) \approx (J - c_0k^2)$.

The present results demonstrate a type of renormalization of the GL parameters (c_0, r_0, u_0) of the effective Hamiltonian due to $1/z$ corrections. By a suitable choice of units, one of these parameters can be kept invariant, for example, equal to unity. Therefore, within a suitable normalization of the theory, the field $\phi(\boldsymbol{x})$ acquires a $1/z$ correction as well [2].

The term $\mathcal{H}_f^{(3)}$ in Eq. (27) has the form

$$\mathcal{H}_f^{(3)} = -\frac{\beta^2}{3}\sum_{ij} J_{ij}^3 \frac{\mathrm{th}(\beta a_i)\mathrm{th}(\beta a_j)}{\mathrm{ch}^2(\beta a_i)\mathrm{ch}^2(\beta a_j)}$$
$$- \frac{\beta^2}{6}\sum_{ijl} \frac{J_{ij}J_{il}J_{jl}}{\mathrm{ch}^2(\beta a_i)\mathrm{ch}^2(\beta a_j)\mathrm{ch}^2(\beta a_l)}$$
$$- \beta^2\sum_{ijl} J_{ij}^2 J_{jl} \frac{\Delta_l \mathrm{th}(\beta a_j)}{\mathrm{ch}^2(\beta a_i)\mathrm{ch}^2(\beta a_j)}$$
$$- \frac{\beta^2}{2}\sum_{ijln} J_{ij}J_{il}J_{jn} \frac{\Delta_l\Delta_n}{\mathrm{ch}^2(\beta a_i)\mathrm{ch}^2(\beta a_j)}$$
$$- \frac{\beta^2}{3}\sum_{ijln} J_{ij}J_{il}J_{in} \frac{\Delta_j\Delta_l\Delta_n \mathrm{th}(\beta a_i)}{\mathrm{ch}^2(\beta a_i)}. \quad (36)$$

Let us consider the contribution of the term $\mathcal{H}_f^{(3)}$ to the quadratic (ϕ^2) part of the effective Hamiltonian (33). In performing the calculations for both short range (NN) and long range ($R_{\rm int} \gg a_0$) we must evaluate again several lattice sums. Here we shall mention a particular sum, namely,

$$\frac{1}{N}\sum_{ijl} J_{ij}J_{il}J_{jl}, \quad (37)$$

which is equal to zero for NN interactions but gives a contribution ($\approx J^3/z$) for interaction radius $R_{\rm int} > a_0$. Thus we introduce the following interpolation formula: $E = \kappa(z)/z$, where $0 \leqslant \kappa(z) \leqslant 1$ is an interpolation parameter which is supposed to be a smooth function of the coordination number z. The limiting case $\kappa = 0$ corresponds to NN interactions and the limiting case $\kappa = 1$ corresponds to interactions of larger size. We suppose that the shape of the function $\kappa(z)$ depends on details of the function $J(R)$.

Bearing in mind these notes, we have calculated the quadratic ($\phi_i\phi_j$) contribution to the effective Hamiltonian $\mathcal{H}(\phi)$ which comes from the Hamiltonian part $\mathcal{H}_f^{(3)}(\phi)$ given by Eq. (36). Here we present the results for the parameters T_{c0}, c, and r which define the quadratic part $\mathcal{H}_2$ of $\mathcal{H}$,

$$\mathcal{H}_2(\phi) = \frac{1}{2}\sum_{\boldsymbol{k}} G_0^{-1}(k)|\phi(\boldsymbol{k})|^2, \quad (38)$$

with the (bare) correlation function

$$G_0^{-1}(k) = \mathcal{D}_1(z)[T - T_c + \mathcal{D}_2(z)T_c\rho^2k^2]. \quad (39)$$

Here

$$T_c = \left(1 - \frac{1+\kappa}{z} - \frac{1+3\kappa}{3z^2}\right)T_{c0}, \quad (40)$$

$$\mathcal{D}_1(z) = 1 + \frac{3+4\kappa}{z} + \frac{22+60\kappa+30\kappa^2}{3z^2}, \quad (41)$$

and

$$\mathcal{D}_2(z) = 1 + \frac{2+3\kappa}{z} + \frac{14+30\kappa+9\kappa^2}{3z^2}. \quad (42)$$

The result (35) for $T_c(z)$ has been presented [3] in the case of NN interactions ($\kappa = 0$); note, that there are errors in Ref. [3] for the functions $\mathcal{D}_1(z)$ and $\mathcal{D}_2(z)$.

The functions $\mathcal{D}_1(z)$ and $\mathcal{D}_2(z)$ renormalize the field $\phi(\boldsymbol{k})$ and the vertices c_0, and r_0. For a total renormalization of the parameters of the theory up to the second order in the $1/z$ expansion we need to know the $(1/z)^2$ correction to the vertex u_0. We suppose that the calculation of this correction can be accomplished in the manner described above; this "z renormalization" has been discussed to first order in $(1/z)$ in Ref. [2]. Here we wish to stress that within our extension of the theory the magnetic susceptibility $G_0(0)$ is $\mathcal{D}_1$ times smaller than the known MF susceptibility corresponding to $\mathcal{D}_1(\infty)=1$.

The numerical coefficients in Eqs. (40)–(42) indicate that real numbers z of NN like $n=2,4,6$ for simple lattices of spatial dimensionalities $D=1,2,3$, respectively, give a good expansion parameter $1/z$. The $1/z$ corrections are more substantial for the case of short-range interactions ($R_{\text{int}} \sim a_0$), and one may suppose that for such interactions the $(1/z)$ series (40)–(42) are asymptotic; for the case of T_c, see a discussion of this topic in Ref. [8]. But even in the case of asymptotic types of these series they may give more reliable results than the "bare" values (c_0, r_0, u_0) of the Landau parameters; see arguments presented in Ref. [8].

D. Critical temperature

The critical temperature T_c given by Eq. (40) can be compared with exact and reliable numerical (MC) results. Let us consider NN interactions ($\kappa=0$). For one-dimensional (1D) IM, we know that $T_c=0$, MFA predicts $T_c=2J_0/k_B$ (in this case, $z=2D=2$), and Eq. (40) yields $T_c=5J_0/6k_B$. This is a quite good result for 1D systems with very strong fluctuation effects. In two-dimensional (2D) systems the fluctuations are not so strong and we find that Eq. (40) reproduces the exact Onsager result ($T_c=2.27J_0/k_B$) with an error of 22%, i.e., we have $T_c=35J_0/12k_B$. For three-dimensional (3D) systems our result is $T_c=89J_0/18k_B$, whereas the best series analysis and MC results yield a difference of 9%, $T_c=4.5J_0/k_B$ (see, e.g., Refs. [18,19]). Our results seem quite reliable. Let us emphasize, that the $1/z$ series, as almost all most-relevant series known in theoretical physics, is an asymptotic series. Therefore, one may expect, that the results for T_c will be worsened after some order in $1/z$, for example, fourth order for T_c(3D), and third, or, even second order for T_c(2D).

E. Ground state

The $1/z^2$ correction to the vertex u_0 has not been calculated as yet, although this calculation does not present difficulties. In this situation we shall give notion for the ground-state energy by using the first-order corrections to r_0 and u_0. The equilibrium free energy per site $f=(F/N)$ is given by $F=\mathcal{H}$ and Eq. (33) for the $(k=0)$ Fourier amplitude $\phi(0)$, which minimizes f. Denote for convenience $\phi(0)=\sqrt{N}\varphi\neq 0$ for the low-temperature ordered phase. From Eq. (33) we obtain $f=-(r^2/16u)<0$ whereas the "unrenormalized free energy is $f_0=(\mathcal{H}_0/N)=-(r_0^2/16u_0)<0$. Thus, using Eq. (34), we have $f(T)=(1+2/z)f_0(T)$, which means that the effective theory has a lower energy of the ordered phase. This is true also in the case of $T=0$, where $r_0=-k_BT_{c0}=-J$. For the zero temperature (ground) state we have $f_0(0)=-3J/4$ and $f(0)=-3(1+2/z)J/4$. This result is also along the correct direction because the MF theories ($\mathcal{H}_0$) give unreliable high values of the ground-state energy. The order parameter $\varphi^2(T)=(-r/4u)$ is $(1-z)$ times smaller than the respective quantity $\varphi_0^2(T)=(-r_0/4u_0)$ in the usual theory based on $\mathcal{H}_0$.

F. Effective interactions and growing of fluctuation correlations

We have explicitly shown the phenomenon of the growing length size of the interparticle correlations in a classic system of interacting particles. To see this we have already introduced a interpretation of the terms in the effective Hamiltonian (see Sec. II D). Let us consider the terms present in $\mathcal{H}$ as terms describing certain intersite interactions. While the initial interaction J_{ij} in IM ensures only two-site correlations (interactions), the effective Hamiltonians (15), (29), and (32) contain multisite effective interactions. In contrast to the usual theory (15), where only extremely short-range effective correlations are contained, the more precise effective Hamiltonians contain long-range two-site $(\phi_i\phi_j)$ and four-site $(\phi_i\phi_j\phi_k\phi_l)$ correlations, and all of these correlations are indirect, i.e., the correlation, for example, between two sites (ij) is mediated by one or more other sites $(k,\ldots)$. A direct (J_{ij}) interaction is presented by the first term on the rhs of Eq. (15) but also the system exhibits two indirect correlations of type $\phi_i\phi_j$ and $\phi_i\phi_j\phi_k\phi_l$ given by the last two terms on the rhs of Eq. (15). In the more precise variants of the theory, where a larger portion of the initial partition function has been calculated, the direct intersite interaction vanishes, and the particles are correlated only by indirect effective interactions. The length scale of these correlations grows in a monotonous way with the increase of the accuracy of the calculation, i.e., with the increase of the number l of the terms in the series (27). If we take the two-site correlations in the NN IM as an example, the maximal length of extension of these correlations in Eq. (1) is a_0; in Eq. (15), $2a_0$; in Eq. (29), $3a_0$; in Eq. (32), $4a_0$, i.e., $(p-1)a_0$, where p is the maximal number of the summation indices in terms of type $\phi_i\phi_j$ in a given effective Hamiltonian. Surely, the number p tends to N. This means that the most accurate effective field theory of many-body systems will correspond to (almost-) infinite range of correlations.

The origin of these correlations is purely statistical. This effect is known and has both general formulation and application in many-body physics. Here we have established and described in details the concrete mechanism of this effect and, moreover, we have performed a demonstration of the remarkable picture of successive growth of the correlation length scale.

G. Final remarks

Obviously the $(1/z)$ corrections are not the main point of discussion at the end of this paper. Let us mention that the growth of the correlations discussed in Sec. III F is not related to the $1/z$ corrections. It exists for any z, even in the "MF limiting case" of $z\to\infty$, when the GL parameters keep their "initial" values (c_0, r_0, u_0). This effect follows from the fact that the terms in the initial Hamiltonian are compensated by the first "fluctuation" correction; see the first term on the

rhs of Eq. (27). At the next level of accuracy of the calculation, terms coming from the $(l=2)$ term in Eq. (27) compensate the available terms and this process continues up to the incorporation of all particles in the correlation phenomenon; remember that the term corresponding to $l=1$ is equal to zero.

Here we emphasize that the terms in $\mathcal{H}_0$, actually one of the most often used Hamiltonians, does not exist at all. They vanish just after the inclusion of the first correction to the usual theory; see $\Delta_i\Delta_j$ correction in Eq. (27). In place of these terms, other terms with more complex structure come from the perturbation series (27). The outlined picture clearly indicates, that the terms which finally remain in the ϕ^4 theory, are terms of type

$$\tfrac{1}{2}(\beta^{M-1}J^M - \beta^M J^{M+1})\phi^2, \quad M \sim N, \tag{43}$$

where obvious notations have been introduced; for example, $\beta^1 J^2$ denotes the first term on the rhs of Eq. (29). The ϕ^4 terms behave differently, because a lowest-order term in J, namely, a term of type $\beta^3 J^4 \phi^4$ appear at any step of development of the series (27).

At any stage of this surprising picture of the infinite series of successive modifications of the Hamiltonian, both ϕ^2 and ϕ^4 terms keep their numerical coefficients equal to that in the usual GL Hamiltonian $\mathcal{H}_0$. This is true within the whole scope of validity of the expansion in powers of ϕ.

An important note should be emphasized is the following. While the sum (2) is invariant with respect to the site i in regular lattices, the sum (7) depends on the site i. The reason is that the field configuration $\{\phi_i\}$ which takes part in Eq. (7) is not the equilibrium field. For the equilibrium field $\bar{\phi}_i$ the sum (7) will not depend on the site i. This is consistent with the general notion that the equilibrium order in the volume of a homogeneous system in lack of effects of external fields, should be uniform.

Our consideration justifies the GL fluctuation Hamiltonian. However, we have presented a quite surprising picture of the interparticle correlations, which reveals remarkable properties of the GL theory. Apart from the $1/z$ corrections to the GL parameters, the structure of this theory is absolutely comprehensive as a tool for investigation of large-scale correlation phenomena in many-body systems. We are certain that our findings have an application beyond the field of phase transitions.

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[17] Remember that the thermodynamic states represented by the variable ("lattice field") ϕ in Eq. (5) correspond to stable, metastable or (absolutely) unstable thermodynamic equilibria, ϕ_0, given by the variation condition $\delta\mathcal{H}(\phi_0)=0$. In this interpretation of Eq. (5) both equilibrium (ϕ_0) and nonequilibrium $(\phi \neq 0)$ states can participate in the function $\mathcal{H}(\phi)$. For this reason, the latter can be referred to as "nonequilibrium free energy" with equilibrium part, given by $\mathcal{H}(\phi_0)$.
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