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Statistical mechanics of strongly nonideal systems

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An alternative approach for treating strongly interacting statistical systems with strongly singular potentials is developed. This approach combines both the advantages of decoupling procedures for Green functions, which eliminate divergences caused by singular potentials, and the advantages of perturbation theory, which is a regular procedure that makes it possible to construct subsequent approximations above the chosen decoupling. The resulting iterative sequence of Green functions generates corresponding sequences of observable quantities. To improve the convergence of the latter sequences a method is suggested based on the renormalization-group ideas. A simple illustration is given.

I. NONIDEAL SYSTEMS

By an "ideal statistical system" is usually understood to be one possessing any of the two following properties: Either there is no particle interaction or there is an absolutely regular space structure. These properties, although quite different, have a common feature that is an idealization of a system. For example, a system with no interparticle interactions is called an ideal gas. A system having an absolutely periodic crystalline lattice is called an ideal crystal.

Systems deviating in a small way from these idealized properties are called weakly nonideal. Thus, a weakly nonideal gas is a system of particles with very weak interactions. A weakly nonideal crystal is a solid with a lattice whose periodicity is slightly disturbed by a small number of defects. The weakly nonideal systems can be treated by perturbation theory starting from a corresponding ideal picture.

When the ideality of a system in one of the two possible meanings is strongly disturbed, the system is called strongly nonideal. Generally, such strongly nonideal systems display at least one of the following five properties: strong interactions between particles, strong singularities of the interaction potentials, strong many-particle correlations, strong fluctuations inside the system, and strong space irregularities. Below, a more detailed explanation of these properties is given.

(i) *Strong particle interactions.* One calls an interaction strong if the mean potential energy of the system E_P is of the order or greater than the mean kinetic energy E_K.

$$|E_P/E_K| \gtrsim 1 .$$

In this situation the standard perturbation theory dealing with the series in powers of the potential energy leads to unreasonable results, unless some resummation techniques are invoked.

(ii) *Strong potential singularities.* Let a system of N particles inside a d-dimensional region $\mathbb{V}$ be described by the set of variables

$$x_i = \{x_i^\alpha \mid \alpha = 1,2,\ldots,d\}, \quad i = 1,2,\ldots,N .$$

Each pair of particles interacts with each other through interaction potential $v(x_i,x_j)$, $i \neq j$. This potential is called strongly singular if it is not integrable in the region with a finite measure, that is, when the integral

$$\left| \int_{\mathbb{V}} v(x_i,x_j)\,dx_i \right| \to \infty$$

diverges for any fixed

$$x_j \in \mathbb{V}, \;\; \text{mes}\;\mathbb{V} < \infty \quad \left[\text{mes}\,\mathbb{V} \equiv \int_{\mathbb{V}} dx_i \right] ,$$

where mes denotes measure. These strongly singular potentials are quite familiar for a number of realistic systems. Examples are the Lennard-Jones, Buckingham and others widely used in statistical mechanics, and the hard-core potentials used in nuclear theory. The small-distance behavior of such potentials in the real space is as $v(r) \sim r^{-n}$ $(n \geq 3)$, which just yields their nonintegrability for the real-space dimension $d = 3$. In the case of strongly singular potentials the standard perturbation theory is of no sense at all as far as all terms of the expansion diverge.

(iii) *Strong pair correlations.* In general, the correlations between particles are described by one of the representations for reduced density matrices $\rho(x_1,x_2,\ldots,x_j)$ $(j \geq 2)$; they may be correlation functions or Green functions. Strong pair correlations mean that the two-particle density matrix cannot be factorized into the product of the single-particle density matrices,

$$\rho(x_i,x_j) \neq \rho(x_i)\rho(x_j) \quad (i \neq j) ,$$

even if this product is symmetrized or antisymmetrized, according to the statistics of particles. It is just such a factorization that leads to divergences when using perturbation theory for strongly singular potentials. Therefore, to treat the latter, it is absolutely necessary to consider strong pair correlations.

(iv) *Strong local fluctuations.* The appearance of strong fluctuations is directly connected with strong interparticle correlations. There are two kinds of fluctuations: homogeneous and heterogeneous. The first kind corresponds to elementary excitations arising above a ground state. For instance, acoustic waves or spin waves are of this kind. These excitations do not change the homogeneity of matter. The role of these fluctuations becomes especially important in the vicinity of instability points and second-order phase transitions. The fluctuations of the second kind are called heterogeneous because they drastically disturb the real-space structure of systems. Heterogeneous fluctuations can be of two types: static and dynamic. The former, often called frozen, are usually due to a large number of defects incorporated into a lattice. The examples of systems with static heterogeneous fluctuations are amorphous solids and spin glasses. The configuration of static fluctuations for each particular system is random in space but does not change in time. The dynamic heterogeneous fluctuations also are random in space but each of their configurations has a finite lifetime. The examples are various structural fluctuations near first-order phase transitions and, generally, fluctuating nuclei of one thermodynamic phase inside another.

(v) *Strong space irregularities.* These irregularities, as is clear, are caused by strong heterogeneous fluctuations. As a result we need to deal with nonuniform, or even with nonequilibrium, systems having a random distribution of structure disturbances in space, and in the case of dynamic fluctuations, in time as well. It goes without saying that all this strongly complicates the description of such systems.

The brief review of features of strongly nonideal systems shows that the properties of the latter are closely interconnected, although different properties may need different mathematical methods for their description. From this point of view one can separate the first three properties from the rest: strong particle interactions, strong potential singularities, and strong pair correlations.

As has been stressed above, in the case of strongly singular potentials the standard statistical perturbation theory[1] loses its sense because of divergences. This situation is relevant to the appearance of the ultraviolet divergence in the quantum-field theory where it can be eliminated by means of the renormalization of interaction constants.[2,3]

The sole known way in statistical mechanics to avoid the divergences due to strongly singular potentials is to invoke one of the variants of the so-called decoupling procedure preserving pair correlations. One decouples whether they are correlation functions, Green functions, or wave functions. We may mention here the decouplings of Green functions yielding the equations of the Bethe-Salpeter and Brueckner-Goldstone types,[4,5] the Kirkwood decoupling of correlation functions,[6] and coupled-cluster[7,8] and Jastrow[7,9] approximations for wave functions.

However, the decoupling is not a regular procedure, that is, it does not give a consistent method for finding out successive corrections to the approximation chosen.

In this paper we suggest an approach for describing strongly interacting statistical systems with strongly singular potentials. The approach combines the advantages of the perturbation theory that is a regular procedure and of the decoupling methods that eliminate divergences. An iterative scheme is constructed that starts from one of the decouplings, taking into account pair correlations, and defines all further subsequent approximations, containing no divergences at any step. The sequences of iterative approximations for observable quantities are considered and a method to improve the convergence of the sequences is advanced. The work has been influenced by renormalization ideas of quantum-field theory. Everywhere below $\hbar \equiv 1$.

II. GREEN FUNCTIONS

Although, for describing statistical systems it is possible to use any many-particle function such as correlation functions, Green functions, or wave functions, we prefer to deal with Green functions whose analytical properties seem to us to be the most convenient for achieving a more elegant theory. In addition, the Green-function technique makes it possible to present in a unified way a general approach to different systems, either at zero or at finite temperature, equilibrium or not.

The Heisenberg representation for the field operators $\psi(x,t)$ will be used where $t \in \mathbb{R}$ is the time variable. All internal degrees of freedom, like spin, isospin, color, etc., can be included into the set x together with space coordinates. In accordance with the Bose-Einstein or Fermi-Dirac statistics, the commutation or anticommutation relations, respectively, are valid

$$[\psi(x,t),\psi^\dagger(x',t)]_\mp = \delta(x-x') \; ,$$

$$[\psi(x,t),\psi(x',t)]_\mp = 0 \; .$$

The Hamiltonian of the system with binary interactions $v(x,x')$ has the form

$$H = \int \psi^\dagger(x,t)[K(x)-\mu(x,t)]\psi(x,t)dx + \tfrac{1}{2}\int \psi^\dagger(x,t)\psi^\dagger(x',t)v(x,x')\psi(x',t)\psi(x,t)dx\,dx' \; , \tag{1}$$

in which $K(x)$ is the kinetic energy operator, and $\mu(x,t)$, the chemical potential including external fields, if any. The two-particle interaction potential $v(x,x')$ is supposed to be strongly singular in the sense defined earlier.

To simplify the expressions to follow we shall use the abbreviation for functions

$$f(1,2,\ldots,n) \equiv f(x_1,t_1;x_2,t_2;\ldots;x_n,t_n)$$

and for differentials

$$d(1,2,\ldots,n) \equiv dx_1dt_1dx_2dt_2 \cdots dx_ndt_n \; ,$$

and introduce the interaction potential

$$v(1,2) \equiv v(x_1,x_2)\delta(t_1-t_2+0) \tag{2}$$

in which

$$\delta(t+0) \equiv \lim_{\epsilon\to 0+} \delta(t+\epsilon) \; .$$

We shall deal with the causal Green functions, the propagators. The single-particle propagator is defined as

$$G(1,2)=-i\langle \hat{T}\psi(1)\psi^{\dagger}(2)\rangle \ , \qquad (3)$$

where $\hat{T}$ is the chronological operator ordering the time variables so that $t_1>t_2$, and the brackets mean the average of an operator $\hat{A}$,

$$\langle \hat{A}\rangle \equiv \mathrm{Tr}\hat{\rho}\hat{A} \ ,$$

$\hat{\rho}$ being the statistical operator. The two-particle, binary propagator is

$$B(1,2,3,4)=-\langle \hat{T}\psi(1)\psi(2)\psi^{\dagger}(3)\psi^{\dagger}(4)\rangle \ ; \qquad (4)$$

here again the chronological operator arranges the time variables in the order $t_1>t_2>t_3>t_4$.

The equation of motion for the single-particle propagator can be written[1] in the form

$$\int G^{-1}(1,3)G(3,2)d(3)=\delta(1,2) \ , \qquad (5)$$

in which the inverse propagator

$$G^{-1}(1,2)=\left[i\frac{\partial}{\partial t_1}-K(1)+\mu(1)\right]\delta(1,2)-\Sigma(1,2) \qquad (6)$$

is connected with the self-energy $\Sigma(1,2)$ defined by the equation

$$\Sigma(1,2)=\pm i\int v(1,3)B(1,3,3,4)G^{-1}(4,2)d(3,4) \ , \qquad (7)$$

the right-hand side of Eq. (5) being the δ function

$$\delta(1,2)\equiv\delta(x_1-x_2)\delta(t_1-t_2) \ .$$

In the quantum-field theory $\Sigma(1,2)$ is called the mass operator.

From Eqs. (5)–(7) it follows that the equation of motion for the single-particle propagator is a functional relation $F_1[G,B]$ between this propagator and the binary one. Analogously, if one writes down the equation of motion for the binary propagator, one obtains a functional relation $F_2[B,G_3]$ between propagator (4) and the three-particle propagator

$$G_3(1,2,3,4,5,6)\equiv i\langle \hat{T}\psi(1)\psi(2)\psi(3)\psi^{\dagger}(4)\psi^{\dagger}(5)\psi^{\dagger}(6)\rangle \ ,$$

in which $t_1>t_2>t_3>t_4>t_5>t_6$, and so on; the equation of motion for the n-particle propagator G_n is a relation $F_n[G_n,G_{n+1}]$ between this propagator and the higher-order one. The infinite set of these equations is called the hierarchical chain. To obtain a self-consistent set of equations one may invoke an additional condition expressing one of the higher-order propagators through the lower-order ones, thus breaking the hierarchical chain. This is just what is called the decoupling procedure that, as is evident, does not formulate a regular way for finding out further approximations. We shall follow another path.

Let us notice that self-energy (7) contains not an arbitrary binary propagator, but a quasidiagonal one $B(1,2,2,3)$. For the latter, using the Schwinger variational technique,[1,4,10] we can get the variational representation

$$B(1,2,2,3)=G(1,3)G(2,2)\mp\frac{\delta G(1,3)}{\delta\mu(2)} \ , \qquad (8)$$

following from definition (4), and defining the diagonal single propagator as

$$G(1,1)\equiv \lim_{x_2\to x_1}\ \lim_{t_2\to t_1+0} G(1,2) \ . \qquad (9)$$

With representation (8) self-energy (7) takes the form

$$\Sigma(1,2)=\pm i\delta(1,2)\int v(1,3)G(3,3)d(3)$$
$$-i\int v(1,3)\frac{\delta G(1,4)}{\delta\mu(3)}G^{-1}(4,2)d(3,4) \ . \qquad (10)$$

Equations (5), (6), and (10) form a closed set of equations which one could solve by means of an iterative procedure. This is what one usually does in the perturbation theory. However, the first term in Eq. (10), corresponding to the Hartree approximation, diverges because of the strong singularity of the potential $v(1,2)$. That is why for such potentials the standard perturbation theory, based on expression (10), makes no sense.

III. SMOOTHING FUNCTION

To overcome the discussed difficulties we need to invoke some additional ideas and definitions. Remember that in the quantum-field theory the elimination of the ultraviolet divergences can be done by rearranging the perturbation series so that just from the initial step we should deal not with the so-called bare coupling constant but with a renormalized one.[2,3] Under such a renormalization the whole structure of the perturbation series changes transforming to an expansion over a renormalized interaction parameter. If an analogous rearrangement of the perturbation series in the statistical mechanics are possible, this would mean that we could construct an iterative procedure whose initial step would take into account particle correlations renormalizing the bare interaction potential, and thus eliminating divergences. As a result of this rearranged iterative procedure we should obtain an expansion in powers of a renormalized interaction potential.

Let us introduce a new function $s(1,2,)$, which will play the role of a renormalizing multiplier for the initial interaction potential. Since this multiplicative renormalization results in the smoothing of the strongly singular potential, we shall call the new object $s(1,2)$ the smoothing function. To eliminate the divergences this function has to make the product $s(1,2)v(1,2)$ integrable, so that

$$\left|\int_{\mathbb{V}} s(1,2)v(1,2)dx_1\right|<\infty \qquad (11)$$

for any fixed $t_1,t_2\in\mathbb{R}$ and $x_2\in\mathbb{V}$. This can be done by defining the smoothing function as a correlation function.

Here, we introduce the one-particle density operator

$$\hat{\rho}(1)\equiv\psi^{\dagger}(1)\psi(1) \qquad (12)$$

and the two-particle density operator

$$\hat{\rho}(1,2)\equiv\psi^{\dagger}(1)\psi^{\dagger}(2)\psi(2)\psi(1) \ . \qquad (13)$$

Operator (12) defines the average number of particles by means of the expression

$$N=\langle\hat N\rangle,\quad \hat N\equiv\int_{\mathbb{V}}\hat\rho(1)dx_1\ . \tag{14}$$

The number-of-particle operator $\hat N$ commutes with Hamiltonian (1); therefore the average number of particles N does not depend on time. The averages of the operators $\hat\rho(1)$ and $\hat\rho(1,2)$ are connected by the equation

$$\langle\hat\rho(1,2)\rangle=\langle\hat\rho(1)\hat\rho(2)\rangle-\delta(1,2)\langle\hat\rho(1)\rangle\ . \tag{15}$$

The average particle density is given by the ratio

$$\rho\equiv N/V\quad(V\equiv\operatorname{mes}\mathbb{V})\ .$$

In general, the smoothing function describing pair correlation can be defined as

$$s(1,2)\equiv\frac{\langle\hat\rho(1,2)\rangle}{\langle\hat\rho(1)\rangle\langle\hat\rho(2)\rangle}\ . \tag{16}$$

Definition (16), to within the normalization, is what one calls the second-order reduced density matrix.

A thorough study of general mathematical properties of reduced density matrices has been done in the framework of the representability problem.[11-16] More concrete features of function (16) depend, of course, on the behavior of the interaction potential. For instance, if the latter satisfies the asymptotic condition

$$v(x_1,x_2)\to\begin{cases}\infty, & |x_1-x_2|\to 0\\ 0, & |x_1-x_2|\to\infty\end{cases} \tag{17}$$

which is usual for potentials of many statistical systems, then one should expect the following properties of function (16). When $v(x_1,x_2)\to\infty$ with $|x_1-x_2|\to 0$, this means that the repulsion between two particles, approaching each other, is infinitely increasing, which must yield the impossibility for these particles to be placed, at the same moment, at the same space point, that is,

$$\lim_{|x_1-x_2|\to 0}\ \lim_{|t_1-t_2|\to 0}\langle\hat\rho(1,2)\rangle=0\ . \tag{18}$$

When $v(x_1,x_2)\to 0$ with $|x_1-x_2|\to\infty$ then we get two noninteracting particles separated by a large distance. The correlation between such particles should disappear, which can be expressed with the help of the Bogoliubov principle of correlation weakening[17] leading to

$$\lim_{|x_1-x_2|\to\infty}\langle\hat\rho(1,2)\rangle=\langle\hat\rho(1)\rangle\langle\hat\rho(2)\rangle \tag{19}$$

for any fixed $t_1,t_2\in\mathbb{R}$. Conditions (18) and (19) determine the asymptotic properties of the smoothing function (16), which are

$$s(1,2)\simeq\begin{cases}0, & |x_1-x_2|\to 0,\quad |t_1-t_2|\to 0\ ,\\ 1, & |x_1-x_2|\to\infty,\quad |t_1-t_2|<\infty\ .\end{cases} \tag{20}$$

An exact expression for the smoothing function is not known, as far as the second-order reduced density matrix $\langle\hat\rho(1,2)\rangle$ cannot be found exactly. One can find out solely an approximate expression for the density matrix after invoking some decoupling for the hierarchical chain of equations discussed in Sec. II. Therefore, a particular choice of the smoothing function corresponds to a particular choice of the decoupling procedure. Several possibilities of constructing the smoothing function with property (20) have been analyzed.[18-20]

IV. DOUBLING FUNCTION

Suppose that after invoking one of the decouplings the smoothing function (16) has been explicitly defined. In order to obtain a regular procedure that could give us the corrections of all desired orders to the decoupling chosen, we need yet to rearrange the equations of Sec. II.

Varying the equation of motion (5) with respect to the chemical potential and using Eq. (8) we get the equation for the quasidiagonal binary propagator

$$\begin{aligned}B(1,2,2,3)={}&G(1,3)G(2,2)\pm G(1,2)G(2,3)\\&+\int G(1,4)G(5,3)\frac{\delta\Sigma(4,5)}{\delta G(6,7)}\\&\times[B(6,2,2,7)\\&-G(6,7)G(2,2)d(4,5,6,7)]\ .\end{aligned} \tag{21}$$

Equations (5)–(7) and (21) form a closed set of equations. However, again we cannot iterate this set, as the first two terms, entering into Eq. (21) and corresponding to the Hartree-Fock approximation, being substituted into Eq. (7), would lead to divergences because of the strong singularity of the interaction potential $v(1,2)$.

The principal step of our approach making it possible to reorganize the equations is the introduction of a new function $D(1,2,3)$ which we shall call the doubling function since its duty is to transform the one-particle propagator to the two-particle one:

$$B(1,2,2,3)\equiv s(1,2)\int D(1,2,4)G(4,3)d(4)\ . \tag{22}$$

Definition (22) separates out the two actions: taking account of correlations with the help of the smoothing function and the doubling procedure realized by means of the doubling function.

The advantage of using the doubling function becomes evident if one rewrites self-energy (7) with definition (22) getting

$$\Sigma(1,2)=\pm i\int\phi(1,3)D(1,3,2)d(3)\ , \tag{23}$$

where the renormalized smoothed potential

$$\phi(1,2)\equiv v(1,2)s(1,2) \tag{24}$$

appears. This potential, owing to the property (11), is already integrable.

Now we need to find out for the doubling function an equation that would allow a consequent iterative procedure to be defined. Substituting Eq. (22) into Eq. (21) and using the equation of motion (5) we have

$$s(1,2)D(1,2,3)=\delta(1,3)G(2,2)\pm G(1,2)\delta(2,3) + \int G(1,4)\frac{\delta\Sigma(4,3)}{\delta G(5,6)}\left[s(5,2)\int D(5,2,7)G(7,6)d(7)-G(5,6)G(2,2)\right]d(4,5,6)\ . \tag{25}$$

Denote the zeroth-order doubling function

$$D_0(1,2,3)=\delta(1,3)G(2,2)\pm G(1,2)\delta(2,3) \tag{26}$$

and introduce the operator $\hat{X}$ whose action on any three-point function $f(1,2,3)$ is given by the equality

$$\hat{X}f(1,2,3)\equiv s(1,2)f(1,2,3)+\int G(1,4)\frac{\delta\Sigma(4,3)}{\delta G(5,6)}\left(G(5,6)G(2,2)-s(5,2)\int f(5,2,7)G(7,6)d(7)\right)d(4,5,6)\ . \tag{27}$$

With Eqs. (26) and (27) Eq. (25) can be written as

$$\hat{X}D(1,2,3)=D_0(1,2,3)\ . \tag{28}$$

Define the operator $\hat{Y}$, left inverse to $\hat{X}$, as

$$\hat{Y}\hat{X}=1\ . \tag{29}$$

Having $\hat{Y}$ acting on Eq. (28) we come to

$$D(1,2,3)=\hat{Y}D_0(1,2,3)\ . \tag{30}$$

Equation (30) will play the major role in constructing an iterative procedure for the doubling function.

V. ITERATIVE PROCEDURE

Considering Eq. (29) as a definition of the formal operator $\hat{Y}=1/\hat{X}$, expand the latter in the Taylor series at the point $\hat{X}=1$, which yields

$$\hat{Y}=\sum_{n=0}^{\infty}(1-\hat{X})^n\ . \tag{31}$$

According to definition (27), the operator $\hat{X}$ is a functional of the self-energy, $\hat{X}=\hat{X}[\Sigma]$. Let $\hat{X}_n$ be the corresponding operator functional of the nth approximation for the self-energy Σ_n, that is,

$$\hat{X}_n\equiv\hat{X}[\Sigma_n]\ . \tag{32}$$

Define the nth approximation for operator (31) by

$$\hat{Y}_n\equiv\sum_{m=0}^{n}(1-\hat{X}_n)^m,\quad \hat{Y}_0\equiv 1\ . \tag{33}$$

As is clear,

$$\hat{Y}=\lim_{n\to\infty}\hat{Y}_n\ .$$

Equations (23) and (30) define the self energy Σ and the doubling function D, respectively, while Eq. (31)–(33) and (27) define the operator $\hat{Y}$. Now we can organize the following succession of approximations:

$$D_0\to\Sigma_1\to\hat{Y}_1\to D_1\to\Sigma_2\to\hat{Y}_2\to D_2\to\cdots\ ,$$

that presents an iterative procedure with the scheme

$$D_n\to\Sigma_{n+1}\to\hat{Y}_{n+1}\to D_{n+1}\quad (n=0,1,2\ldots)\ . \tag{34}$$

Substituting the zeroth-order doubling function (26) into Eq. (23), we have the first-order approximation for the self-energy

$$\Sigma_1(1,2)=\pm i\delta(1,2)\int\phi(1,3)G(3,3)d(3) + i\phi(1,2)G(1,2)\ . \tag{35}$$

Expression (35) is of the Hartree-Fock form, but with the renormalized smoothed potential (24) which is integrable. Thus no divergences appear.

Following scheme (34) further we get

$$\hat{Y}_1=2-\hat{X}[\Sigma_1] \tag{36}$$

and the first-order doubling function

$$D_1(1,2,3)=D_0(1,2,3)[2-s(1,2)]\pm i\int G(4,2)[G(1,4)G(2,3)\phi(4,3)\pm G(1,3)G(2,4)\phi(3,4)]d(4) \mp i\int G(2,2)[G(1,3)G(4,4)\phi(3,4)\pm G(1,4)G(4,3)\phi(4,3)][1-s(4,2)]d(4)\ . \tag{37}$$

Using (37) for Eq. (23), we obtain the second-order approximation for the self-energy

$$\Sigma_2(1,2)=\pm i\delta(1,2)\int\tilde{\phi}(1,3)G(3,3)d(3)+i\tilde{\phi}(1,2)G(1,2) - \int\phi(1,3)G(4,3)[\phi(4,2)G(1,4)G(3,2)\pm\phi(2,4)G(1,2)G(3,4)]d(3,4) + \int\phi(1,3,4)G(4,4)[\phi(2,3)G(1,2)G(3,3)\pm\phi(3,2)G(1,3)G(3,2)]d(3,4)\ , \tag{38}$$

where we have introduced the notation for the twice renormalized potential

$$\tilde{\phi}(1,2)\equiv\phi(1,2)[2-s(1,2)] \\ =v(1,2)s(1,2)[2-s(1,2)] \tag{39}$$

and for the vertex

$$\phi(1,2,3)\equiv\phi(1,3)[1-s(2,3)] \\ =v(1,3)s(1,3)[1-s(2,3)] \; , \tag{40}$$

taking account of triple correlations.

In this way we may find out any approximation for the self-energy, and consequently, for the Green functions; all approximations contain no divergences at any step, as long as the initial interaction potential enters everywhere solely through the renormalized smoothed potential (24). A similar iterative scheme has been used[21] to solve the Bethe-Salpeter equation.

The constructed iterative procedure gives a microscopic justification for the phenomenological method of effective potentials that is sometimes used[22–24] for systems with strongly singular potentials. In this method one chooses some approximation for the self-energy in the form equivalent to one of the approximations in the standard perturbation theory, but replacing the initial singular potential by a phenomenological one, whose parameters are to be defined by comparing calculations for the chosen approximation with experimental data.

VI. OBSERVABLE QUANTITIES

From the equations of motion (5) and (6) it is clear that propagators are functionals of the self-energy, $G=G[\Sigma]$. Really, the self-energy is just a part of the inverse propagator (6). Therefore, the sequence $\{\Sigma_n\}$ of the iterative approximations for the self-energy generates the corresponding sequences $\{G_n\}$ for the propagator approximations $G_n\equiv G[\Sigma_n]$. What can be said about the convergence of such sequences?

Remember that propagators are not usual functions; they are distributions (generalized functions) whose correct mathematical definition can be done through a class of integral functionals, continuous linear forms.[25] In statistical mechanics such a natural class of functionals is a set of observable quantities defined as averages of corresponding operators. Let $\mathcal{A}=\{\hat{A}\}$ be an algebra of operators to observable quantities. The average of any operator $\hat{A}\in\mathcal{A}$, as is known,[1,5,17] can be expressed by means of propagators as an integral functional $\langle\hat{A}\rangle$. Involving the nth approximation for propagators for calculating the average $\langle\hat{A}\rangle_n$ we get the corresponding approximation for this observable quantity,

$$f_n\equiv\langle\hat{A}\rangle_n \; .$$

Thus the sequence of iterative approximations for propagators yields the sequence $\{f_n\}$ for each observable quantity. It is emphasized that the question of convergence of an iterative procedure for propagators has the correct mathematical meaning solely as the question of convergence of sequences $\{f_n\}$ for observable quantities.

The iterative procedure constructed in Sec. V results in the appearance of expansions in powers of the renormalized smoothed potential (24). From the mathematical point of view it is more correct to extract from the potential $\phi(1,2)$ an effective expansion parameter, which is dimensionless, and to consider expansions in powers of this parameter. The latter is usually called the coupling parameter and is defined by the identity

$$\phi(1,2)\equiv g\varphi(1,2) \quad (g=2ma^2\phi_0) \; ,$$

where a is the nearest-neighbor distance and ϕ_0 a characteristic potential strength. The physical meaning of the coupling parameter g is apparent; it is an effective strength of the potential energy.

In this way, each approximation for an observable quantity should be considered as a polynomial of the coupling parameter

$$f_n\equiv f_n(g) \; .$$

Therefore, the question of the convergence of an iterative procedure is to be formulated as the question of the convergence of functional sequences $\{f_n(g)\}$.

Although the potential $\phi(1,2)$, according to (24), is a smoothed potential, this does not necessarily require that the coupling constant g be small. Because of this, the convergence of a sequence $\{f_n(g)\}$ can be either very poor or can be lacking completely. The standard situation is when $\lim_{n\to\infty}f_n(g)$ is an asymptotic series. If we were able to calculate many first approximations $f_n(g)$, then we could invoke some of the known techniques[26] for an effective summation of asymptotic series. In the majority of cases in order to obtain such an effective sum of an asymptotic series with an accuracy of about 1% one needs to know about ten approximations for $f_n(g)$. However, it is technically impossible to calculate so many approximations for strongly nonideal statistical systems. The maximum that one is able to do for practically all real statistical systems is to calculate a pair of approximations. How then can we succeed in obtaining reasonable results in such a complicated situation when only several first terms of a sequence are available and the standard resummation techniques are not applicable? In the next sections we suggest a new method for giving us the possibility to overcome these difficulties.

VII. CONVERGENCE AND SELF-SIMILARITY

Consider a sequence $\{f_n(g)\}$ of approximations for some observable quantity. Generally speaking, this sequence is divergent. In order to make the sequence convergent we have to rearrange it, involving again the renormalization ideas.[2,3] Note that any observable quantity depends, in general, not solely on the coupling constant but, in addition, on a number of other parameters, either entering into the Hamiltonian of the system or being introduced under the process of a decoupling when choosing the initial step of an iterative procedure. Let us select one of these additional parameters, say z, emphasizing that $f_n(g)$ depends on it,

$$f_n(g)\equiv f_n(g,z) \; . \tag{41}$$

Suppose now that there exists a new sequence $\{z_n(g)\}$ of functions $z_n(g)$, such that after the replacement

$$z\to z_n(g), \quad f_n(g)\to f_n(g,z_n(g)) \tag{42}$$

the obtained sequence $\{f_n(g,z_n(g))\}$ becomes convergent. Replacement (42) just implies a rearrangement of the iterative procedure by renormalizing some trial parameters. The functions $z_n(g)$, with $n=0,1,2,\ldots$, govern the convergence of the sequence $\{f_n(g,z_n(g))\}$, that is why we shall call them the governing functions. Let us stress that as far as the choice of the initial step for any iterative procedure contains some arbitrariness, it is always possible to introduce an additional parameter and, therefore, to define the governing functions. A concrete example will be given later.

If the uniform convergence of the sequence $\{f_n(g,z_n(g))\}$ on $g\in\mathbb{R}$ is assumed, then the Cauchy criterion is true:

$$|f_{n+p}(g,z_{n+p}(g))-f_n(g,z_n(g))|<\epsilon \quad (n\geq s, p\geq 0) , \tag{43}$$

in which $s=s(\epsilon)$. We shall call the number $n=s$, beginning from which the approximations f_{n+p} and f_n coincide, with a given accuracy, a saturation number; and we shall write, for brevity,

$$f_{n+p}(g,z_{n+p}(g))\cong f_n(g,z_n(g)) \quad (n\geq s, p\geq 0) , \tag{44}$$

meaning Eq. (43).

The convergence of a sequence may be achieved in many ways. Therefore, in order to concretize the introduction of the governing functions, let us strengthen the requirement imposed on them, demanding that they not merely make the sequence convergent, but that this convergence be as fast as possible. The latter subtends the validity of the fastest-convergence criterion,

$$f_{n+p}(g,z_{n+p}(g))\cong f_n(g,z_n(g)) \quad (n,p\geq 0) , \tag{45}$$

being the general definition for the governing functions.

To extract further information from criterion (45) let us rewrite it in another form. Define the function $g(f)$ by the equation

$$f_0(g,z_0(g))=f \tag{46}$$

and denote the new function

$$\bar{f}_n(f)\equiv f_n(g(f),z_n(g(f))) \tag{47}$$

with the evident condition

$$\bar{f}_0(f)=f , \tag{48}$$

following from Eq. (46). In terms of function (47) the fastest-convergence criterion (45) becomes

$$\bar{f}_{n+p}(f)\cong \bar{f}_n(f) . \tag{49}$$

Putting here $n=0$ and using Eq. (48), one gets $f\cong\bar{f}_p(f)$, the substitution of which into the right-hand side of Eq. (49) causes us to obtain

$$\bar{f}_{n+p}(f)\cong\bar{f}_n(\bar{f}_p(f)) . \tag{50}$$

This equation describes the self-similar functional transformation. Thus, the fastest-convergence criterion (45) is equivalent to the self-similarity relation (50).

VIII. CONTINUOUS ITERATION

Relation (50) can become much more useful if we apply a trick defining a continuous iterative procedure.[27] This can be done in the following way.

Introduce the variable

$$t_n\equiv e^n \quad (n=0,1,2,\ldots) , \tag{51}$$

and the functions

$$\begin{aligned} &z(t_n,g)\equiv z_n(g) , \\ &f(t_n,g,z(t_n,g))\equiv f_n(g,z_n(g)) . \end{aligned} \tag{52}$$

Then, change function (47) for

$$\bar{f}(t_n,f)\equiv\bar{f}_n(f) . \tag{53}$$

Now replace the discrete variable (51) by the continuous variable

$$t_n\to t\in[1,\infty) , \tag{54}$$

and make an analytical continuation of all functions depending on t_n to functions of the continuous variable (54). For instance, for function (53) we get

$$\bar{f}(t,f)=f(t,g(f),z(t,g(f))) , \tag{55}$$

with condition (48) changing for

$$\bar{f}(1,f)=f . \tag{56}$$

The self-similar relation (50) in the continuous representation reads

$$\bar{f}(bt,f)\cong\bar{f}(t,\bar{f}(b,f)) \quad (b\geq 1) . \tag{57}$$

Differentiating Eq. (57) over t and making the substitutions $t\to 1$, $b\to t$, we have

$$\frac{\partial\bar{f}(t,f)}{\partial\ln t}\cong\gamma(\bar{f}(t,f)) , \tag{58}$$

where

$$\gamma(f)\equiv\lim_{t\to 1}\frac{\partial}{\partial t}\bar{f}(t,f) . \tag{59}$$

The obtained differential equation (58) with boundary condition (56) is analogous to the renormalization-group equations for invariant charges in the quantum-field theory,[2] where Eq. (59) is called the Gell-Mann–Low function.

Integration of Eq. (58) over $t\in[t_n,t_s]$ yields

$$\int_{f_n(g)}^{f_s(g)} d\varphi\frac{1}{\gamma(\varphi)}=s-n , \tag{60}$$

where definition (51) is taken into account, $f_n(g)\equiv f_n(g,z_n(g))$, and $f_s(g)$ is the sought self-similar approximation for an effective limit of the sequence $\{f_n(g,z_n(g))\}$.

Defining the Gell-Mann–Low function (59) we have to bear in mind that $\bar{f}(t,f)$, in accordance with Eq. (55), depends on the variable t directly and through the governing function $z(t,g)$. Therefore

$$\frac{\partial \bar{f}(t,f)}{\partial t} = \left[\frac{\partial}{\partial t} f(t,g,z) \right]_z + \left[\frac{\partial}{\partial z} f(t,g,z) \right]_t \frac{\partial z}{\partial t} ,$$

where

$$g=g(f), \quad z=z(t,g(f)) .$$

Everything would be nice if we knew how to define the differentiation over the continuous variable t, since in reality we have only the discrete variable t_n. To surmount this problem we must return to the discrete representation defining the derivatives over t by corresponding finite differences. Thus, we can construct a discrete analog for the Gell-Mann–Low function

$$\gamma_{ns}(f) = \frac{f_s(g,z_n)-f_n(g,z_n)}{s-n} + \frac{z_s-z_n}{s-n} \frac{\partial}{\partial z_n} f_n(g,z_n) , \tag{61}$$

in which

$$g=g(f), \quad z_n=z_n(g(f)), \quad n<s .$$

Substituting Eq. (61) in place of $\gamma(f)$ in Eq. (60), and defining another function,

$$y_{ns}(f) \equiv \frac{1}{(s-n)\gamma_{ns}(f)} = \left[f_s(g,z_n)-f_n(g,z_n)+(z_s-z_n)\frac{\partial}{\partial z_n} f_n(g,z_n) \right]^{-1} \tag{62}$$

we obtain

$$\int_{f_n(g)}^{f_s(g)} y_{ns}(\varphi)\,d\varphi = 1 . \tag{63}$$

This is the main equation defining the self-similar approximation $f_s(g)$ for the sought function.

What we finally need is an explicit equation to determine the governing functions. Their general definition (45) in the continuous representation reads

$$\frac{\partial}{\partial t} \bar{f}(t,f) = 0 , \tag{64}$$

which is the continuous form for the fastest-convergence criterion. Comparing Eqs. (64) and (58) we see that the general definition for the governing functions is

$$\gamma(\bar{f}(t,f)) = 0 . \tag{65}$$

The nullification of the Gell-Mann–Low function is called, in the renormalization-group theory, the fixed-point condition. We could find from Eq. (65) the governing function $z(t,g)$ if we worked in the continuous representation. However, we always have to return to the discrete representation where (and solely where) all our quantities can be explicitly determined. As far as in the discrete representation the derivatives over t have been presented by the two-point finite differences, the discrete analog of the Gell-Mann–Low function (61) contains two governing functions. Consequently, the nullification of $\gamma_{ns}(f)$ would give us a connection between $z_s(g)$ and $z_n(g)$, but not their individual definition. Returning to the discrete representation we are able to find out only relative fixed points, defined not by the zero of the total derivative (64), but by the derivative along a way prescribed by some additional rule. The simplest ways are either when $\bar{f}(t,f)$ is changing with t under fixed $z(t,g)$, which leads to

$$f_s(g,z_n)-f_n(g,z_n)=0 , \tag{66}$$

or when $\bar{f}(t,f)$ is changing with $z(t,g)$ under fixed t, which yields

$$\frac{\partial}{\partial z_n} f_n(g,z_n)=0 . \tag{67}$$

Other ways are possible, each of which may be fixed, for instance, by adding a relation between $z_s(g)$ and $z_n(g)$. Any of these ways gives a relative fixed-point condition from where the governing function $z_n(g)$ is to be found.

The fixed-point conditions of type (66) have been introduced in Refs. 28–30 and later used for describing strongly anharmonic quantum[31–33] and quasiclassical[34] crystals, for calculating the ground-state energy of an anharmonic oscillator[35] and for considering the solid-liquid phase transition.[18] The conditions of the type in Eq. (67) have been applied for calculating the ground-state energy of anharmonic oscillators[36] and of some other models.[37] The method using the conditions of the type in Eqs. (66) or (67) is called the modified perturbation theory.

In Refs. 28–37 the definition of $z_n(g)$ by one of conditions (66) or (67) and its substitution into $f_n(g,z_n(g))$ has been the final result.

Contrary to this, in the approach of the present paper the definition of the governing function $z_n(g)$ with one of the fixed-point conditions is only the initial step, after which three others are to follow, when we have to calculate the function $g(f)$ from Eq. (46), the function $y_{ns}(f)$ given by Eq. (62), and integrate Eq. (63) defining the self-similar approximation $f_s(g)$ for the sought function. This procedure of the renormalization in the vicinity of a relative fixed point must essentially improve the accuracy of results.

Among the two simple fixed-point conditions (66) and (67) the latter seems to be preferable for reducing functions (61) and (62) to simpler forms. Thus, if we adopt Eq. (67) and find $g(f)$ from Eq. (46), we have for the Gell-Mann–Low function (61)

$$\gamma_{ns}(f) = \frac{f_s(g(f),z_n(g(f)))-f_n(g(f),z_n(g(f)))}{s-n} \tag{68}$$

and for function (62)

$$y_{ns}(f) = [f_s(g(f),z_n(g(f)))-f_n(g(f),z_n(g(f)))]^{-1} . \tag{69}$$

Finally, note that when $z_0(g)$ cannot be defined from condition (67), we can put

$$z_0(g)\equiv z_1(g) \ . \tag{70}$$

Now the whole procedure of finding out the self-similar approximation for any observable quantity is completely defined by the scheme

$$z_n(g)\rightarrow g(f)\rightarrow z_n(g(f))\rightarrow y_{ns}(f)\rightarrow f_s(g) \ .$$

The corresponding functions may be calculated with the help of Eqs. (67), (46), (69), and (63).

IX. SIMPLE EXAMPLE

Let us illustrate on a simple model how to calculate observable quantities in the self-similar approximation. Consider the so-called φ^4 model whose Hamiltonian corresponds to the scalar-field theory.[2] This model, as is known, is equivalent to the anharmonic quartic-oscillator model[38,39] with the Hamiltonian

$$H=-\frac{1}{2m}\frac{d^2}{dx^2}+\frac{m\omega^2}{2}x^2+\lambda m^2x^4 \ , \tag{71}$$

in which m, ω, and λ are positive parameters; for simplicity the one-dimensional case is assumed, $x\in(-\infty,+\infty)$. Let us find out the ground-state energy of the model. Note that the standard perturbation theory in powers of λ diverges[38,39] for any λ.

First, we have to introduce the governing functions. As has been discussed in Sec. VII; this can be done by including a trial parameter, for example, incorporating this parameter into the initial form of either the self-energy Σ_0 or the propagator G_0, or what is the same, into the initial approximation for the Hamiltonian H_0. Choose the latter in the form

$$H_0=-\frac{1}{2m}\frac{d^2}{dx^2}+\frac{m\omega_0^2}{2}x^2 \ , \tag{72}$$

in which ω_0 is just the trial parameter. The iterative procedure for the system with Hamiltonian (71), starting from the approximating Hamiltonian (72), is equivalent to the perturbation theory with respect to the effective interaction

$$\Delta H\equiv H-H_0=(m/2)(\omega^2-\omega_0^2)x^2+\lambda m^2x^4 \ . \tag{73}$$

We introduce the dimensionless quantities

$$e(g)\equiv\frac{E}{\omega}, \quad g\equiv\frac{\lambda}{\omega^3}, \quad z\equiv\frac{\omega_0}{\omega} \ , \tag{74}$$

where E is the ground-state energy for Eq. (71). Using perturbation theory over Eq. (73) we get the approximations $e_n(g,z)$ for the dimensionless ground-state energy. Then, according to Eqs. (41) and (42), we come to $e_n(g,z_n)$. Thus, for the approximations up to the second order we obtain

$$\begin{aligned} &e_0(g,z_0)=\tfrac{1}{2}z_0 \ , \\ &e_1(g,z_1)=\frac{3g+z_1+z_1^3}{4z_1^2} \ , \\ &e_2(g,z_2)=\frac{4z_2^3(3g+z_2+z_2^3)-(6g+z_2-z_2^3)^2-6g^2}{16z_2^5} \ , \end{aligned} \tag{75}$$

where $z_n(g)$ are governing functions.

Take $n=1$ and $s=2$ for the formulas of Sec. VIII. The fixed-point condition (67) becomes

$$\frac{\partial}{\partial z_1}e_1(g,z_1)=0 \ , \tag{76}$$

from where the equation for the governing function $z_1(g)$ follows,

$$z_1^3-z_1-6g=0 \ . \tag{77}$$

Seeking for the real solution of this equation we get

$$z_1(g)=\begin{cases}(2/\sqrt{3})\cos(\alpha/3), & g\le g_0\\ A^{+}+A^{-}, & g\ge g_0 \ ,\end{cases} \tag{78}$$

where the notation is used

$$\alpha=\arccos(g/g_0) \ ,$$

$$A^{\pm}=(3g)^{1/3}\left\{1\pm\left[1-\left[\frac{g_0}{g}\right]^2\right]^{1/2}\right\}^{1/3} \ ,$$

$$g_0=\frac{1}{9\sqrt{3}}=0.064\,15 \ .$$

The function $g(f)$ is to be found from Eq. (64) together with Eq. (70), that is, from the equation

$$e_0(g,z_1(g))=f \ , \tag{79}$$

which gives

$$z_1(g)=2f \ . \tag{80}$$

Combining Eqs. (77) and (80), we find

$$g(f)=\frac{f}{3}(4f^2-1) \ . \tag{81}$$

For the function (69) we have

$$y_{12}(f)=[e_2(g(f),z_1(g(f)))-e_1(g(f),z_1(g(f)))]^{-1} \ , \tag{82}$$

from where, involving Eqs. (75), (77), and (81), we come to

$$y_{12}(f)=-768f^3/(4f^2-1)^2 \ . \tag{83}$$

Function (83) should be substituted into Eq. (63), i.e., into the integral

$$\int_{e_1(g)}^{e_s(g)}y_{12}(\varphi)d\varphi=1 \ . \tag{84}$$

in which $e_1(g)\equiv e_1(g,z_1(g))$ and $e_s(g)$ is the sought self-similar approximation for the ground-state energy. Integrating Eq. (84) we obtain

$$\frac{4e_s^2(g)-1}{4e_1^2(g)-1}=\exp\left[\frac{1}{4e_s^2(g)-1}-\frac{1}{4e_1^2(g)-1}-\frac{1}{24}\right] . \tag{85}$$

We analyze the asymptotic behavior of the self-similar approximation $e_s(g)$. As follows from the expression of the governing function (78), the weak-coupling and strong coupling limits correspond to $g \ll g_0$ and $g \gg g_0$, respectively. For the governing function (78) we have

$$z_1(g) \simeq 1+3g-\tfrac{27}{2}g^2+108g^3-\tfrac{8505}{8}g^4 \quad (g \ll g_0) , \tag{86}$$

in the weak coupling limit, and

$$z_1(g) \simeq (6g)^{1/3}+\tfrac{1}{3}(6g)^{-1/3}-\tfrac{1}{81}(6g)^{-5/3} \quad (g \gg g_0) , \tag{87}$$

in the strong coupling limit. Using Eqs. (86) and (87), we obtain from Eq. (85) the asymptotic expressions for the ground-state energy in the self-similar approximation

$$e_s(g) \simeq \tfrac{1}{2}+\tfrac{3}{4}g-\tfrac{75}{32}g^2+\tfrac{3675}{256}g^3-\tfrac{236\,487}{2048}g^4 \tag{88}$$

in the weak coupling limit, when $g \ll g_0$, and

$$e_s(g) \simeq 0.667\,37g^{1/3}+0.150\,03g^{-1/3}-0.012\,72g^{-1} \tag{89}$$

in the strong coupling limit, when $g \gg g_0$.

Compare these asymptotic expressions with the exact expansion

$$e_{\text{ex}}(g) \simeq \tfrac{1}{2}+\tfrac{3}{4}g-\tfrac{21}{8}g^2+\tfrac{333}{16}g^3-\tfrac{30\,885}{128}g^4$$

for the weak-coupling limit,[38,39] when $g \to 0$, and

$$e_{\text{ex}}(g) \simeq 0.667\,986g^{1/3}+0.143\,67g^{-1/3}-0.0088g^{-1}$$

for the strong coupling limit,[40–42] when $g \to \infty$. For a more visual comparison let us rewrite the self-similar asymptotic form for $e_s(g)$ and the exact expansion for $e_{\text{ex}}(g)$ in the weak coupling limit as

$$\begin{aligned} e_s(g) &\simeq \tfrac{1}{2}+\tfrac{3}{4}g-2.344g^2+14.355g^3-115.472g^4 , \\ e_{\text{ex}}(g) &\simeq \tfrac{1}{2}+\tfrac{3}{4}g-2.625g^2+20.813g^3-241.289g^4 , \end{aligned} \tag{90}$$

where $g \to 0$. As is obvious, the asymptotic expressions for the self-similar approximation $e_s(g)$ and for the exact expansion $e_{\text{ex}}(g)$ are very close to each other in both the weak coupling as well as strong coupling limits.

The comparison of numerical results for the self-similar approximation $e_s(g)$, given by Eq. (85) and of exact numerical calculations for $e_{\text{ex}}(g)$, directly following from a numerical solution[41,42] of the Schrödinger equation with Hamiltonian (71), shows that the accuracy of the self-similar approximation is of 0.1% in the whole range of the coupling constant $g \in [0,\infty)$. In the weak coupling limit $g \to 0$, the accuracy asymptotically improves, the error tending to zero.

It is also useful to compare our results with those of the modified perturbation theory[28–37] based on conditions (66) or (67). The accuracy of this theory up to the second order for the anharmonic oscillator has been thoroughly studied.[35–37,43] It has been found that this theory invoking solely the two-order expansion is not less accurate than the methods of the Padé approximants and Borel transformation requiring about ten perturbation terms. The ground-state energy of the anharmonic oscillator, calculated by means of the second-order modified theory, has the best accuracy of 1% for arbitrary coupling constants $g \in [0,\infty)$.

From the latter comparison it follows that, invoking an equal number of perturbation terms, the method of self-similar approximations provides the accuracy by an order better than the modified perturbation theory.

X. DISCUSSION

In the example of the Sec. IX we deliberately have limited ourselves by considering the self-similar approximations only up to the second order. This is not merely because the higher-order approximations involve much more cumbersome expressions, but mainly because our aim has been to construct an accurate method of calculating observable quantities for such complicated systems for which, in principle, we are able to find out solely a few terms of an iterative procedure. For these systems the standard methods[26] (for recent literature see Refs. 44, and 45) of an effective summation of asymptotic series are not applicable at all, since they need to include tens of perturbation terms.

The method of self-similar approximations can be easily generalized to the case where there are several interaction potentials, that is, several coupling parameters $g=\{g^\alpha|\alpha=1,2,\ldots\}$. One of the possible ways[28,29] to do it is as follows. Take the number of observable quantities $f_n^\alpha(g)$ which is equal to the number of coupling constants. Introduce the same number of governing functions $z_n(g)=\{z_n^\alpha(g)\}$, obtaining the set $f_n(g,z_n(g))=\{f_n^\alpha(g,z_n(g))\}$. The governing functions are to be found from one of the conditions like (66) or (67); for example, from the equation

$$f_s^\alpha(g,z_n)-f_n^\alpha(g,z_n)=0 ,$$

or from the condition

$$\frac{\partial}{\partial z_n^\alpha} f_n^\alpha(g,z_n)=0 ,$$

from which we get $z_n^\alpha(g)$. The set of functions $g(f)=\{g^\alpha(f)\}$, where $f=\{f^\alpha\}$, should be found from the set of equations

$$f_0^\alpha(g,z_0(g))=f^\alpha .$$

Analogously, in the place of function (62) we get the set of functions $y_{ns}(f)=\{y_{ns}^\alpha(f)\}$, and in the place of integral (63) the set of integrals

$$\int_{f_n^\alpha(g)}^{f_s^\alpha(g)} y_{ns}^\alpha(\varphi)\,d\varphi^\alpha=1 .$$

In the present paper we have elaborated an alternative general approach to treat strongly interacting systems.

We have not considered here the last two properties of nonideal systems, discussed in Sec. I, that is, strong fluctuations breaking the uniformity of a system, and connected with these fluctuations, strong space irregularities. These questions are related to the problem of heterogeneous fluctuations.[46,47] An original method to deal with such heterogeneous systems has been advanced.[18,48,49] The method also is based on renormalization ideas, making it possible to average over heterogeneous configurations and to obtain a renormalized Hamiltonian corresponding to an effective uniform system. This method has been applied to several systems (for review see Ref. 50) with infinitely long-range interactions. The final version of this method and its application to realistic systems with finite-range interactions is planned to be given in a future paper.

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