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Strongly Interacting Particles with Strongly Singular Potentials

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A statistical system of particles is considered for which interaction potentials are strongly singular so that the standard perturbation theory cannot be used. A regular procedure for constructing a mass operator is suggested, having no ultraviolet divergences and giving the possibility of finding corrections for any approximation chosen. In this procedure, the divergences connected with the potential singularity are eliminated with the help of a smoothing function, for which a simple equation is given and whose properties are analyzed both analytically and numerically. Two effective regularization methods are formulated, eliminating divergences occurring while iterating propagator equations. A continuous iterative procedure is invented for calculating observable quantities and the fast convergence conditions for this procedure are shown to be equivalent to the fixed-point conditions.

1. INTRODUCTION

There exists an old problem in the description of systems modeling condensed matter: the atoms and molecules of which solids or liquids consist are not merely strongly interacting between each other, so that the perturbation theory becomes rather bad, but moreover the interparticle interaction potentials are usually strongly singular, so that the perturbation theory completely loses its sense insofar as all terms of the series diverge. The standard way to solve this problem is to use various decouplings for higher correlation functions or Green functions when taking account of the two-particle correlation to compensate the divergence of the interaction potential. In the case of classical liquids the pair correlation function is defined by the Percus–Yevick or hyperchained equations (Temperley *et al.*,

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1968). For quantum systems the binary Green function may be given by the Bethe–Salpeter equation (Kadanoff and Baym, 1962; Negele, 1982). An approximation is also used in which the form of a pair correlation function is postulated, and the parameters entering into it are found from experiments or from a variational procedure (Abraham, 1979; Miller, 1980). The main deficiency of all these methods is that one does not know how to obtain in consecutive order corrections improving the accuracy of the decoupling chosen.

The aim of the present paper is the construction of a regular procedure combining the merits of the decoupling method and of the perturbation theory, that is, the construction of a procedure without divergences and at the same time allowing one to find subsequent corrections to any initial approximation. Some aspects of this problem were considered earlier (Yukalov, 1973, 1976*a*,*b*, 1987) and applied to the description of quantum crystals (Yukalov, 1977, 1981, 1985; Yukalov and Zubov, 1983). Here, the ideas suggested earlier are developed and generalized, resulting in the formulation of a unified approach.

I explain what is meant by the strongly singular potential in Section 2, and in Section 3 give the basic definitions. In Section 4 a regular procedure for constructing a mass operator is suggested. This procedure has no divergences and at the same time it gives the possibility for defining subsequent corrections to any approximation chosen. As an illustration for the starting point of the procedure, the Kirkwood (1965) decoupling is generalized. Then, the divergences connected with the potential singularity are eliminated due to the presence of a smoothing function containing short-range correlations. In Section 5 a simple equation is proposed for the smoothing function and the properties of the latter are considered analytically as well as numerically for several matters. A solution of the propagator equation is analyzed in Section 6, where two effective regularizations of the propagator powers are formulated in order to remove the arising divergences. The calculation of observable quantities is considered in Section 7. A continuous representation for the iterative procedure is invented, allowing, together with the renormalization group approach, reasonable results for any strongly interacting systems to be obtained. The fast convergence conditions are shown to be equivalent to the fixed-point conditions when the Gell-Mann–Low function is nullified.

2. SINGULAR POTENTIALS

Interactions between particles are often described by singular potentials of the form $\phi(r) \sim r^{-n}$ with $n > 0$. How dangerous this singularity is depends on the integratibility of the interaction potential, that is, on the behavior

of the integral

$$\int \phi(r)\, d\mathbf{r} = 4\pi \int_a^R \phi(r) r^2\, dr$$

in which a and R are the shortest and largest interparticle distances, respectively. Divergences can appear at long or at short distances. The first kind of divergence, i.e., the long-range one, corresponds to the so-called infrared divergences, while the second kind, i.e., the short-range one, corresponds to the ultraviolet divergences in quantum field theory (Bogolubov and Shirkov, 1973). In the considered case the infrared divergence occurs if $0 < n < 3$, when

$$\int_a^R \phi(r) r^2\, dr \sim R^{3-n} - a^{3-n} \to \begin{cases} \infty, & R \to \infty \\ \text{const}, & a \to 0 \end{cases}$$

This divergence is not dangerous for the many-body problem insofar as the former is eliminated by taking into account long-range correlations. For example, in the Coulomb case these correlations yield the Debye screening, renormalizing the potential by the factor $\exp(-r/r_D)$, where r_D is the Debye radius. The screened potential is already integrable:

$$\int_0^\infty \phi_s(r) r^2\, dr = \alpha r_D^2 < \infty, \qquad \phi_s(r) = \frac{\alpha}{r} \exp\left(-\frac{r}{r_D}\right)$$

The ultraviolet divergence appears if $3 < n < \infty$, when

$$\int_a^R \phi(r) r^2\, dr \sim R^{3-n} - a^{3-n} \to \begin{cases} \text{const}, & R \to \infty \\ \infty, & a \to 0 \end{cases}$$

To eliminate this divergence, it is necessary to take into consideration short-range correlations. The marginal case $n = 3$ contains logarithmic divergences at long as well as at short distances,

$$\int_a^R \phi(r) r^2\, dr \sim \ln R - \ln a \to \begin{cases} \infty, & R \to \infty \\ \infty, & a \to 0 \end{cases}$$

This case needs both the long-range and short-range correlations.

In what follows, I concentrate on the strongly singular potentials with $n > 3$ when the short-range correlations are mostly important for eliminating ultraviolet divergences. Dealing with these singular potentials leads to difficulties because the simple perturbation theory is not applicable, while the decoupling methods give no possibility for finding higher approximations. At the same time, potentials of such a strongly singular type are widely used when describing condensed matter; recall, for instance, the quite popular Lennard-Jones potential.

3. BASIC FORMULAS

Consider the many-particle system with the Hamiltonian

$$H(t)=\int \psi^{+}(\mathbf{r},t)\left[-\frac{\nabla^2}{2m}-\mu(\mathbf{r},t)\right]\psi(\mathbf{r},t)\,d\mathbf{r}$$
$$+\tfrac{1}{2}\int \psi^{+}(\mathbf{r},t)\psi^{+}(\mathbf{r}',t)\phi(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}',t)\psi(\mathbf{r},t)\,d\mathbf{r}\,d\mathbf{r}' \tag{1}$$

in which $\hbar\equiv 1$, the field operators satisfy the Heisenberg equation

$$i\frac{\partial}{\partial t}\psi(\mathbf{r},t)=[\psi(\mathbf{r},t),H(t)] \tag{2}$$

and the function $\mu(\mathbf{r},t)$ includes the chemical potential and external fields generally depending on time. The average of an operator $\hat{A}(t)$ is defined by the expression

$$\langle\hat{A}\rangle=\mathrm{Tr}\,\rho(t)\hat{A}(0)=\mathrm{Tr}\,\rho(0)\hat{A}(t) \tag{3}$$

with the statistical operator $\rho(t)$.

It is convenient to use the following abbreviations: for the functions

$$f(12,\ldots,n)\equiv f(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2,\ldots,\mathbf{r}_n,t_n) \tag{4}$$

and differentials

$$d(12,\ldots,n)\equiv\prod_{i=1}^{n}d\mathbf{r}_i\,dt \tag{5}$$

Then, for example, as the function $\mu(\mathbf{r},t)$, the interaction potential, and the delta function one has

$$\mu(1)\equiv\mu(\mathbf{r}_1,t_1)$$
$$\phi(12)\equiv\phi(\mathbf{r}_1,\mathbf{r}_2)\,\delta(t_1-t_2+0)$$
$$\delta(12)\equiv\delta(\mathbf{r}_1-\mathbf{r}_2)\,\delta(t_1-t_2)$$

Define the causal Green functions, propagators, by the following expressions: the one-particle propagator is

$$G(12)\equiv -i\langle\hat{T}\psi(\mathbf{r}_1,t_1)\psi^{+}(\mathbf{r}_2,t_2)\rangle \tag{6}$$

and the two-particle propagator is

$$B(1234)\equiv -\langle\hat{T}\psi(\mathbf{r}_1,t_1)\psi(\mathbf{r}_2,t_2)\psi^{+}(\mathbf{r}_3,t_3)\psi^{+}(\mathbf{r}_4,t_4)\rangle \tag{7}$$

where $\hat{T}$ is the time-ordering operator.

Equations of motion can be written (Yukalov, 1976*a*,*b*) in the form

$$\int G^{-1}(13)G(32)\,d(3)=\delta(12) \tag{8}$$

Here the inverse propagator is

$$G^{-1}(12)=\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}+\mu(1)\right]\delta(12)-\Sigma(12) \tag{9}$$

and the mass operator, or the self-energy part, is

$$\Sigma(12)=\pm i\int \phi(13)B(1334)G^{-1}(42)\,d(34) \tag{10}$$

The upper sign is for Bose statistics, the lower for Fermi statistics.

The solution of any many-particle problem may be separated into the three consecutive stages: (1) construction of the mass operator (10) and its substitution into equation (8); (2) solution of equation (8) for the one-particle propagator; (3) calculation of observables by means of formula (3).

4. MASS OPERATOR

Introduce the vertex function (the triangular vertex)

$$\Gamma(123)\equiv =\delta G^{-1}(12)/\delta\mu(3) \tag{11}$$

and the response function

$$\chi(123)\equiv \delta G(12)/\delta\mu(3) \tag{12}$$

Taking the variational derivative of equation (8) with respect to $\mu(\cdot)$ gives

$$\Sigma(12)=\pm i\delta(12)\int \phi(13)G(33)\,d(3)+i\int \phi(13)G(14)\Gamma(423)\,d(34) \tag{13}$$

where the diagonal one-particle propagator is defined by the expression

$$G(11)\equiv \lim_{\mathbf{r}_2\to\mathbf{r}_1}\lim_{t_2-t_1\to+0} G(12)$$

The triangular vertex (11) and response function (12) are connected with each other:

$$\Gamma(123)=\delta(12)\delta(13)+\int \frac{\partial\Sigma(12)}{\delta G(45)}\chi(453)\,d(45) \tag{14}$$

$$\chi(123)=\int G(14)G(52)\Gamma(453)\,d(45) \tag{15}$$

Comparing (13) with (10), we find the binary propagator-triangular vertex relation

$$B(1223) = G(13)G(22) \pm \int G(14)\Gamma(452)G(53)\, d(45)$$

The latter together with (14) yields the equation for the binary propagator

$$B(1223) = G(13)G(22) \pm G(12)G(23) + \int \Lambda(1453)[B(4225) - G(45)G(22)]\, d(45) \tag{16}$$

in which

$$\Lambda(1234) \equiv \int G(15) \frac{\delta\Sigma(56)}{\delta G(23)} G(64)\, d(56) \tag{17}$$

In place of the binary propagator (7) it is possible to use the dressing function $D(1234)$ defined by the expression (Yukalov, 1987)

$$B(1234) = \int D(1256)G(63)G(54)\, d(56)$$

The dressing function helps us to write down the mass operator (10) in the simpler form

$$\Sigma(12) = \pm i \int \phi(13)D(1324)G(43)\, d(34)$$

The equation for the dressing function results from (16) and its definition:

$$D(1234) = \delta(13)\delta(24) \pm \delta(14)\delta(23) + \int G(17) \frac{\partial\Sigma(73)}{\delta G(58)} G(68)[D(5264) - \delta(56)\delta(24)]\, d(5678)$$

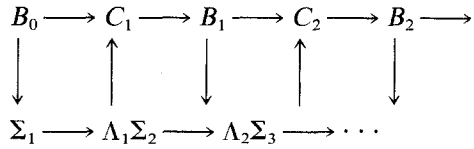
If one solves these equations by means of the iteration beginning with $\Sigma = 0$, as is usually adopted, then, naturally, the ultraviolet divergences arise owing to the strong singularity of the interaction potential. In order to avoid the divergences, we rearrange the equations, introducing the three-point correlator

$$C(123) = \frac{B(1223)}{B(1223) - \int \Lambda(1453)[B(4225) - G(45)G(22)]\, d(45)} \tag{18}$$

Then (16) takes the form

$$B(1223) = C(123)[G(13)G(22) \pm G(12)G(23)] \tag{19}$$

The system of equations (10) and (17)–(19) will be solved following the iteration scheme



As a zeroth approximation here one could take any decoupling for the binary propagator which does not lead to divergences. In the case of an equilibrium classical system Kirkwood (1965) suggested a simple decoupling for the two-particle correlation function

$$f_2(\mathbf{r}, \mathbf{r}') = f_1(\mathbf{r}) f_1(\mathbf{r}') s(|\mathbf{r} - \mathbf{r}'|)$$

where $f_1(\mathbf{r})$ is the one-particle distribution function and $s(r)$ is the function describing short-range interparticle correlations. The Kirkwood decoupling can be generalized to the quantum case for the propagators, taking account of their symmetry properties:

$$B_0(1234) = s(12)[G(14)G(23) \pm G(13)G(24)]$$

Starting from this zeroth iteration and using the iteration scheme given above, one can obtain any consecutive approximations for the mass operator. So, in first order one gets

$$\Sigma_1(12) = \pm i\delta(12) \int \bar{\phi}(13) G(33)\, d(3) + i\bar{\phi}(12) G(12)$$

$$\Lambda_1(1234) = \pm i\delta(23) \int G(15)\bar{\phi}(52) G(54)\, d(5) + iG(12)\bar{\phi}(23) G(34)$$

where the following notation is introduced:

$$\bar{\phi}(12) \equiv s(12)\phi(12) \tag{20}$$

It is important that here as well as at any other iteration step the initial singular potential $\phi(12)$ always stands near the short-range correlation function $s(12)$ that smooths its singularities, making the smoothed potential (20) integrable. Therefore, $s(12)$ may be called the smoothing function. To write down the mass operator in the second approximation, we invoke the formal notation

$$B_0 = sGG, \qquad \Sigma_1 = \pm i\bar{\phi}G, \qquad \Lambda_1 = \pm iG\bar{\phi}G$$

allowing us to simplify the formulas. Then,

$$\Sigma_2 = \frac{\pm i\bar{\phi}GGG}{sGG \pm iG\bar{\phi}G(GG - sGG)}$$

Again we make sure that the interaction potential enters here into the smoothed combination (20).

5. SMOOTHED FUNCTION

Kirkwood (1965) proposed to define the short-range correlation function from experiments on light scattering. However, this inclusion of phenomenological functions into the theory reduces the value of the latter. In what follows I suggest a theoretical construction of the smoothing function.

General properties of the functions describing pair correlations have been thoroughly investigated by Coleman (1963, 1965). In our case, the smoothing function, according to its definition, has to be real and symmetric:

$$s(12) = s^*(12) = s(21) \tag{21}$$

The correlation between particles at large distances should disappear, while at short distances the smoothing function must tend to zero in order to compensate the divergence of the interaction potential:

$$s(12) \simeq \begin{cases} 0, & r_{12} \to 0 \\ 1, & r_{12} \to \infty \end{cases} \qquad (r_{12} \equiv |\mathbf{r}_1 - \mathbf{r}_2|) \tag{22}$$

It is supposed that the interaction potential approaches zero as $r_{12} \to \infty$. This potential usually depends solely on the coordinate difference r_{12},

$$\phi(\mathbf{r}_1, \mathbf{r}_2) = \phi(r_{12})$$

As the properties of the smoothing function are guided by those of the interaction potential, it seems natural to shape the smoothing function in the spherically symmetric form

$$s(12) \times \int |\Psi(12)|^2 r_{12}^2 \, d\Omega_2 = s(r_{12}) \tag{23}$$

where Ω_2 is the spherical angle relative to the coordinate $\mathbf{r}_2$, the function $\Psi(12)$ being defined by minimizing the two-particle energy

$$E_{12} = \int \Psi^*(12) H(12) \Psi(12) \, d\mathbf{r}_1 \, d\mathbf{r}_2 \tag{24}$$

in which

$$H(12) = -\frac{\nabla_1^2}{2m} - \frac{\nabla_2^2}{2m} + \phi(r_{12})$$

is the two-particle Hamiltonian.

Note that $\Psi(12)$ is not the two-particle wave function in the literal meaning, as the extremum condition

$$\delta E_{12}/\delta\Psi^*(12)=0$$

does not include the usual normalization condition. The resulting equation

$$H(12)\Psi(12)=0$$

differs from the Schrödinger equation by the right-hand side. The constants uniquely defining $\Psi(12)$ are to be found from the asymptotic condition (22). In the variables

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2, \qquad \mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$$

the function $\Psi(12)$ factorizes:

$$\Psi(12)=\Psi(\mathbf{R})\,Y(\vartheta,\varphi)\chi(r)/r$$

where $|\Psi(\mathbf{R})|\sim\text{const}$, $Y(\vartheta,\varphi)$ is the spherical function, and $\chi(r)$ is given by the equation

$$\frac{d^2\chi(r)}{dr^2}-m\phi(r)\chi(r)=0 \tag{25}$$

All this yields the smoothing function (23),

$$s(r)=|\chi(r)|^2=\chi^2(r) \tag{26}$$

As an illustration, we make concrete the behavior of the smoothing function for a potential with the asymptotic properties

$$\phi(r)\simeq 4\varepsilon\begin{cases}(\sigma/r)^n, & r\to 0\\ -(\sigma/r)^k, & r\to\infty\end{cases} \qquad (n>k>3)$$

In this case, equation (25) at short distances becomes

$$\frac{d^2\chi}{dr^2}-4m\varepsilon\left(\frac{\sigma}{r}\right)^n\chi\simeq 0 \qquad (r\to 0)$$

The corresponding asymptotic solution is of the form

$$\chi(r)\simeq r^{1/2}Z_\mu^{(x)}$$

where $Z_\mu^{(x)}$ is the cylindrical function with

$$\mu\equiv-\frac{1}{n-2}, \qquad x\equiv -i\left(\frac{\kappa_n}{r}\right)^{(n-2)/2}$$

$$\kappa_n\equiv\sigma\left[\frac{4}{(n-2)\Lambda}\right]^{2/(n-2)}, \qquad \Lambda\equiv(m\varepsilon\sigma^2)^{-1/2}$$

κ_n is the correlation length, and Λ is the De Boer parameter. The cylindrical function

$$Z_\mu^{(x)} = C_1 J_\mu^{(x)} + C_2 N_\mu^{(x)}$$

is a linear combination of the Bessel function $J_\mu(\cdot)$ and the Neumann function $N_\mu(\cdot)$. Owing to the asymptotic condition

$$\begin{aligned} J_\mu(x) &\simeq \left(\frac{2}{\pi x}\right)^{1/2} \cos\left(x - \frac{\mu\pi}{2} - \frac{\pi}{4}\right) \\ N_\mu(x) &\simeq \left(\frac{2}{\pi x}\right)^{1/2} \sin\left(x - \frac{\mu\pi}{2} - \frac{\pi}{4}\right) \end{aligned} \qquad (|x| \gg 1)$$

and choosing the bounded expression for the solution, we get

$$\chi(r) \simeq C r^{n/4} \exp\left[-\left(\frac{\kappa_n}{r}\right)^{(n-2)/2}\right]$$

For the smoothing function (26) we obtain

$$s(r) \simeq C^2 r^{n/2} \exp\left[-2\left(\frac{\kappa_n}{r}\right)^{(n-2)/2}\right] \qquad (r \to 0) \tag{27}$$

At large distances equation (25) transforms into

$$\frac{d^2\chi}{dr^2} + 4m\varepsilon\left(\frac{\sigma}{r}\right)^k \chi \simeq 0 \qquad (r \to \infty)$$

The asymptotic solution of the equation written above is

$$\chi(r) \simeq r^{1/2} \bar{Z}_\nu(z)$$

where

$$\bar{Z}_\nu(z) = C_3 J_\nu(z) + C_4 J_{-\nu}(z)$$

$$\nu \equiv \frac{1}{k-2}, \qquad z \equiv -\left(\frac{\kappa_k}{r}\right)^{(k-2)/2}$$

In accordance with the asymptote

$$J_\nu(z) \simeq \frac{(z/2)^\nu}{\Gamma(1+\nu)}\left[1 - \frac{x^2}{4(1+\nu)}\right] \qquad (|z| \ll 1)$$

in which $\nu < 1$ for $k > 3$ and $\Gamma(\cdot)$ is the gamma function, we have

$$\chi(r) \simeq \bar{C}\left[1 - \frac{k-2}{4(k-1)}\left(\frac{\kappa_k}{r}\right)^{k-2}\right]$$

Condition (22) shows that $\bar{C} = 1$. Therefore, the smoothing function (26) is

$$s(r) \simeq 1 - \frac{k-2}{2(k-1)}\left(\frac{\kappa_k}{r}\right)^{k-2} \qquad (r \to \infty) \tag{28}$$

The constant C in expression (27) can be found when sewing together the solutions for $\chi(r)$ at intermediate distances.

In the theory of condensed matter the Lennard-Jones potential

$$\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^n - \left(\frac{\sigma}{r}\right)^k\right]$$

is often used, having the minimum

$$\phi(r_0) = -4\varepsilon\frac{n-k}{n}\left(\frac{k}{n}\right)^{k/(n-k)}$$

at the point

$$r_0 = \sigma\left(\frac{n}{k}\right)^{1/(n-k)}$$

and for $r \ll r_0$ as well as for $r \gg r_0$ showing the same asymptotic properties as just examined. Especially popular is the potential with $n = 12$, $k = 6$. Then

$$\phi(r_0) = -\varepsilon, \qquad r_0 = 2^{1/6}\sigma \qquad (n = 12,\ k = 6)$$

The asymptotic expressions (27) and (28) for the smoothing function become

$$s(r) \simeq C^2 r^6 \exp\left[-2\left(\frac{\kappa_{12}}{r}\right)^5\right], \qquad (r \ll r_0) \tag{29}$$

and

$$s(r) \simeq 1 - \frac{2}{5}\left(\frac{\kappa_6}{r}\right)^4 \qquad (r \gg r_0) \tag{30}$$

with the correlation lengths

$$\kappa_{12} = \sigma\left(\frac{2}{5\Lambda}\right)^{1/5}, \qquad \kappa_6 = \frac{\sigma}{\sqrt{\Lambda}}$$

To check the behavior of the smoothing function for the whole range of the dimensionless variable r/σ, equation (25) has been solved numerically. The 12-6 Lennard-Jones potential has been taken corresponding to the following inert-group elements and polarized hydrogen, deuterium, and tritium, whose De Boer parameters Λ are written in the parentheses:

^{3}He (0.494), He (0.430), ^{6}He (0.347)

Ne (0.092), Ar (0.029), Kr (0.016), Xe (0.010)

H↑ (0.740), D↑ (0.523), T↑ (0.428)

At short and large distances numerical calculations are in agreement with the asymptotes (29) and (30). At intermediate distances the smoothing function (26) has been found to increase monotonically together with the variable r/σ.

In all the cases considered the smoothing function $s(r)$ exponentially tends to zero as $r \to 0$ when $\phi(r) \to \infty$; this compensates the divergence of the interaction potential, so that the smoothed potential

$$\bar{\phi}(r) = s(r)\phi(r)$$

becomes integrable.

There exist other variational methods for constructing short-range correlation functions. A review of these methods has been done by Guyer (1969). Those methods are based on the minimization of the total N-particle energy of the system, which leads to very complicated equations. The method presented here is much simpler because of the minimization of only the two-particle energy (24). At the same time, the smoothing function found satisfies all conditions needed.

6. PROPAGATOR EQUATION

After the mass operator is constructed according to the previous sections it is to be substituted in the equation of motion (8). The latter may be rewritten in the Dyson form

$$G(12) = G_0(12) + \int \Delta(13) G(32)\, d(3) \tag{31}$$

where

$$\Delta(12) = \int G_0(13)[\Sigma(32) - \Sigma_0(32)]\, d(3) \tag{32}$$

and $\Sigma_0(12)$ is an arbitrary mass operator to which the propagator $G_0(12)$ corresponds.

The standard perturbation theory has to do with the iteration of equation (31) beginning from $\Sigma_0 = 0$ when G_0 is the propagator of free particles. However, for strongly interacting particles this procedure would be wrong. Then, one should take for the zeroth approximation some solvable problem modeling the main physical peculiarities of the considered system. To improve the convergence of the iterative sequence, we define the function

$$R(12) = \frac{G(12)}{G(12) - \int \Delta(13) G(32)\, d(3)} \tag{33}$$

Equation (31) takes the form

$$G(12) = R(12)G_0(12) \tag{34}$$

The system of equations (33) and (34) is to be iterated following the scheme

$$G_0 \to R_1 \to G_1 \to R_2 \to G_2 \to \cdots \tag{35}$$

When iterating according to the scheme (35), some technical difficulties occur. There are divergences similar to those appearing in quantum field theory. Let us explain the origin of these divergences in our case and show how to eliminate them.

Considering an equilibrium system, the propagator of the zeroth approximation is usually represented as the expansion

$$G_0(12) = \int G_0(\varepsilon, t_{12})\psi_\varepsilon(\mathbf{r}_1)\psi_\varepsilon^*(\mathbf{r}_2)J(\varepsilon)\, d\varepsilon \tag{36}$$

over some orthonormalized wave functions forming a complete basis,

$$\int \psi_\varepsilon^*(\mathbf{r})\psi_\varepsilon(\mathbf{r}')J(\varepsilon)\, d\varepsilon = \delta(\mathbf{r}-\mathbf{r}')$$

In expansion (36),

$$G_0(\varepsilon, t) = -i\{\Theta(t)[1 \pm n(\varepsilon)] \pm \Theta(-t)n(\varepsilon)\}\, e^{-i\varepsilon t} \tag{37}$$

and

$$\Theta(t) = \begin{cases} 1, & t > 0 \\ 0, & t < 0 \end{cases}$$

$$n(\varepsilon) = \frac{1}{e^{\beta\varepsilon} \mp 1}, \qquad t_{12} = t_1 - t_2$$

β is the inverse temperature. The iterative procedure (35) involves propagator powers $G_0^m(\varepsilon, t)$, where $m \geq 2$. Integrals containing these powers diverge. The appearance of these divergences is quite understandable. In fact, the propagator $G_0(\varepsilon, t)$ is not the usual function, but is a distribution (generalized function). The power $G_0^m(\varepsilon, t)$ is a product of distributions, and it is known that these products need to be defined correctly. In the quantum-field perturbation theory one eliminates similar divergences by invoking regularization procedures of the Pauli-Willars type (Bogolubov and Shirkov, 1973). For the quantum-statistical perturbation theory it is also possible to define an analogous regularization procedure (Yukalov, 1976*a,b*, 1979) introducing the expression

$$G_0^m(\varepsilon, t) = \lim_{\varepsilon_j \to \varepsilon} \prod_{j=1}^{m} G_0(\varepsilon_j, t) \tag{38}$$

where the limit is supposed to be taken only after the calculation of the corresponding integrals. The regularization with the help of condition (38) leads to rather tedious computations with bulky intermediate expressions. It can be shown (Yukalov, 1981) that there is another way of regulation giving the same results as (38) but in a shorter and more elegant way. The second method is based on the representation of the propagator power by the formula

$$G_0^m(\varepsilon, t) = -\frac{i}{(m-1)!}\frac{d^{m-1}}{d\varepsilon^{m-1}}\{\Theta(t)[1 \pm n(\varepsilon)] \pm \Omega(-t)n(\varepsilon)\}\, e^{-i\varepsilon t} \tag{39}$$

The Fourier transform

$$\tilde{G}_0(\varepsilon, \omega) = \int G_0(\varepsilon, t)\, e^{i\omega t}\, dt$$

for expression (39) gives

$$\tilde{G}_0^m(\varepsilon, \omega) = \frac{1 \pm n(\omega)}{(\omega - \varepsilon + i0)^m} \mp \frac{n(\omega)}{(\omega - \varepsilon - i0)^m} \tag{40}$$

which clarifies the meaning of the product of distributions with coinciding poles.

7. OBSERVABLE QUANTITIES

When the propagators are found in some approximation, it remains to calculate the observable quantities as the averages of the corresponding operators (3). In this section I propose a method allowing one to increase greatly the accuracy of these calculations. This method is especially useful for systems with strong interparticle interactions.

Let us choose for the zeroth approximation of the mass operator Σ_0 an expression containing a set of trial parameters z. Consequently, the zeroth propagator G_0 and all other successive propagators G_k also depend on this set z. Observable quantities calculated by means of these propagators G_k naturally depend on the trial parameters z as well. Introduce the notation $A_{k+1}(z)$ for the approximate value of an observable quantity $\langle \hat{A} \rangle_k$ calculated with the use of the k-time iterated propagator G_k. So the value $A_1(z)$ corresponds to G_0; the value $A_2(z)$, to G_1; etc. In this way we have the sequence $\{A_k(z)\}$ composed of the elements

$$A_{k+1}(z) = \langle \hat{A} \rangle_k \qquad (k = 1, 2, \ldots) \tag{41}$$

The iterative procedure is of course discrete. However, it is possible to generalize it formally to a continuous case by invoking a kind of analytical continuation. For doing this, define the function $A(t, z)$ depending on the

continuous variable $t \in [1, \infty)$ so that when the variable t passes through the discrete points $t = k$; then

$$A(k, z) = A_k(z) \tag{42}$$

Define the function $z(A)$ by the equation

$$A_1(z) = A \tag{43}$$

Introduce the function

$$\bar{A}(t, A) \equiv A(t, z(A)) \tag{44}$$

having by definition (43) the property

$$\bar{A}(1, A) = A \tag{45}$$

The accuracy of calculations for observable quantities in the case of strongly interacting particles can be sufficiently improved when recurrent relations connecting $A_k(z)$ with $A_{k+1}(z)$ are known. Then, one could use the renormalization group method and find renormalized values for observable quantities that are much more correct as compared with the approximation (41) of the simple iterative procedure.

Generally speaking, changing the iterative scheme or zeroth iteration, one is able to reconstruct an iterative procedure in an infinite number of ways. But for any of the ways a common peculiarity holds true (Yukalov, 1988): the terms of a convergent sequence with the first approximation (43) that is close to the exact result approximately satisfy the self-similar recurrent relation

$$\bar{A}(\lambda t, A) = \bar{A}(t, \bar{A}(\lambda, A)) \tag{46}$$

in which $\lambda \geq 1$, $t \geq 1$. It is not difficult to check this statement. Due to the convergence of the iterative procedure, there exists a saturation point t_s such that

$$\bar{A}(\lambda t, A) \cong \bar{A}(t, A) \qquad (\lambda \geq 1, t \geq t_s)$$

Because of the supposition that the first approximation (43) is already close to the saturation point, we have $t_s \approx 1$ and

$$\bar{A}(\lambda, A) \cong A \qquad (\lambda \geq 1, t_3 \approx 1)$$

Thus, we make sure that equation (46) is approximately valid.

Differentiating (46) over t and putting $t \to 1$, $\lambda \to t$, we come to the differential renormalization-group equation

$$\frac{\partial \bar{A}(t, A)}{\partial \ln t} = \beta(\bar{A}(t, A)) \tag{47}$$

in which

$$\beta(A) \equiv \left. \frac{\partial \bar{A}(t, A)}{\partial t} \right|_{t=1} \tag{48}$$

is the Gell-Mann-Low function. Integrating (47), we get

$$\int_A^{\bar{A}} \frac{dA'}{\beta(A')} = \ln t$$

As is usual in the renormalization-group method, the Gell-Mann-Low function can be found only approximately. In our case the continuous derivative with respect to t is to be replaced by the finite difference

$$\frac{\partial \bar{A}(t, A)}{\partial t} \cong \bar{A}([t]+1, A) - \bar{A}([t], A)$$

where $[t]$ means the whole part of t. Therefore,

$$\left. \frac{\partial \bar{A}(t, A)}{\partial t} \right|_{t=1} \cong A(2, z(A)) - A(1, z(A))$$

The Gell-Mann-Low function (48) takes the form

$$\beta(A) \cong A_2(x(A)) - A \tag{49}$$

Here the properties (42)-(45) have been used.

Owing to the assumption about the convergence of the iterative procedure considered, there is a saturation point k_s such that with any preassigned accuracy

$$A_{k_s+1}(z) = A_{k_s}(z)$$

Consequently, when the variable t approaches the saturation point $t_s \approx k_s$, the function $\bar{A}(t, A)$ tends to the value called the fixed point

$$A_s = \bar{A}(t_s, A)$$

not depending on $t \geq t_s$. We have that

$$\frac{\partial \bar{A}(t, A)}{\partial t} \to 0 \qquad (t \to t_s)$$

From this and from equation (47) it follows that the Gell-Mann-Low function taken at the fixed point A_s is equal to zero:

$$\beta(\bar{A}(t_s, A)) = \beta(A_s) = 0$$

Substituting here the representation of the function (49), we obtain

$$A_2(z_s) = A_1(z_s), \qquad z_s \equiv z(A_s) \tag{50}$$

Equation (50) defining in a self-consistent way the trial parameters is the criterion for the initial approximation (43) to be close to the exact result.

Equations equivalent to (50) have been suggested (Yukalov, 1976*a*,*b*) and used for describing quantum crystals (Yukalov, 1977, 1981, 1985; Yukalov and Zubov, 1983). As is evident, these equations may be called, equally either the self-consistency conditions or fast-convergence conditions, as they permit the self-consistent definition of trial parameters z entering into the zeroth approximation of the propagator G_0 guaranteeing by this the fast convergence of the iterative procedure for observable quantities. In particular cases, when z is a set of ν parameters, $z = \{z_i \mid i = 1, 2, \ldots, \nu\}$, it is necessary to impose ν equations of the type (50) for the same number of different operators that are most important in each situation.

The principal novelty of the present section is in the proof that equation (50) has the meaning of the fixed-point condition. It is just this fact that explains why this condition really improves the convergence of the iterative procedure.

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