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The Spectral Density Method Applied to Systems Showing Phase Transitions

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Contents

1. Formulation of the method and some general relations

2. Two-particle interaction — Normal and anomalous Fermi systems

- 2.1 Specification of a model — Connection of the one-particle spectral density $A_{p\gamma}(\omega)$ with the macroscopic quantities of the system
- 2.2 A set of closed relations — Spectral decomposition for $A_{p\gamma}(\omega)$ and its simplest approximation
- 2.3 An improved approximation for $A_{p\gamma}(\omega)$ — Account of quasi-particle scattering
- 2.4 Anomalous coupling of quasi-particles — Generalized Hartree-Fock approximation
- 2.5 Collective modes of the interacting Fermi system — Plasma oscillation and spin wave spectra

3. Interaction of fermions mediated by a Bose field

- 3.1 Specification of the model — Spectral decomposition of one-particle spectral densities
- 3.2 The simplest approximation for the Fermi spectral density $A_{p\gamma}(\omega)$
- 3.3 The simplest approximation for the Bose spectral density $\mathcal{R}_q(\omega)$

4. Application of the spectral density method to special models of statistical physics

- 4.1 Heisenberg-Ising model — Spin wave spectrum
- 4.2 Bardeen-Cooper-Schrieffer model of superconductivity
- 4.3 Electron correlations in narrow energy bands — Interpolating solution of the Hubbard model
- 4.4 Ising model — A set of equations for correlation functions

5. Concluding remarks

References

1. Formulation of the Method and Some General Relations

At present there is a wide variety of methods to calculate the macroscopic quantities of systems of many strongly interacting particles in thermodynamic equilibrium. Not all of them, however, are equal in their capacities and effi-

ciencies. More essentially a number of them encounter actual difficulties as applied to systems (e.g. to a system with strong interaction or in the intermediate density regime) where the usual small parameters are absent for some reason. It is just this sort of problems that is dealt with more and more frequently now in applications. As a rule these are systems of many strongly interacting particles with anomalous behaviour of specific heat, susceptibility, or other thermodynamic quantities what in turn indicates various phase transitions to occur in these systems. Therefore, there is great interest to develop methods going beyond the scope of ordinary perturbation theory since only those provide hope to involve correctly the various anomalies in the thermodynamic behaviour of the above systems.

Some results of such investigations are well known. For example, the possibility of decoupling the set of coupled equations of motion suggested by Bogolyubov and Tyablikov [1] and also a variety of approximate methods for handling the closed set of equations for the Green functions and the diagram technique [2] are being discussed for a long time. The method of functional integration whose fundamental ideas as applied to statistical physics have been developed by Fradkin [3] and Schwinger and Martin [4] also allows to get solutions not obtainable within the scope of ordinary perturbation calculation. Furthermore, Bogolyubov's variational method (cf. [5]) and Wentzel's principle of thermodynamical equivalence [6] are frequently used. There also exist somewhat more heuristic methods, e.g. the linear canonical transformation [7] or the method of mean field [8]. All the above-mentioned methods were and are repeatedly used to investigate various problems of statistical physics, and rather essential results have been obtained with their aid in a number of cases. Great difficulties still remain when there is no actual small parameter, since either the calculations are too complicated or the ways for further improvement of any special approximation are not sufficiently clear. Further investigations are therefore desired in this field.

The spectral density method [9] described below meets to a considerable extent the requirements mentioned above. It is sufficiently simple and effective and can also be successfully applied to systems showing a phase transition. In the framework of this method, the approximations are done on the basis of spectral decompositions of the corresponding spectral densities.

Such a method for calculating the approximations is very convenient since we can always confine ourselves to a few first terms of the corresponding spectral decomposition, irrespective either to the interaction strength or to any other characteristic inherent to the system of interacting particles. The more terms in the spectral decomposition are exactly taken into account, the more correct the approximate solution will be. One fails, however, to indicate exactly the error involved in every specific approximation. This fact is due to the lack of a small parameter in the interacting particle system under consideration and should be regarded as a natural disadvantage of any method of self-consistent calculations when applied to systems like those. The efficiency of a given approximation is to be estimated either via the character of the final results or by comparing it with the next-higher approximation. The latter should only quantitatively affect the physical features of the system found in an initial approximation that has been chosen correctly.

The corresponding spectral densities are defined as a grand-canonical ensemble average of a non-equal-time commutator or anticommutator ($\eta = \mp 1$) of some

operators A and B :

$$\eta \langle [A; B(\tau)]_{\eta} \rangle_{\omega} = \int d\tau \exp(i\omega\tau) \langle \eta \langle [A; B(\tau)]_{\eta} \rangle \rangle, \quad (1.1)$$

and are determined by the exact set of integral relations

$$\int \frac{d\omega}{2\pi} \omega^m \langle \eta \langle [A; B(\tau)]_{\eta} \rangle_{\omega} \rangle = \frac{1}{2} \left\{ \left\langle \left[\underbrace{[H[H \dots [H; A]_{-} \dots]}_{m \text{ times}}; B \right]_{\eta} \right\rangle + \left\langle \left[A; \underbrace{[\dots [B; H]_{-} \dots H]_{-}}_{m \text{ times}} \right]_{\eta} \right\rangle \right\} \quad (1.2)$$

that are a direct consequence of the equation of motion for the operator $B(\tau)$,

$$i \frac{\partial}{\partial \tau} B(\tau) = [B(\tau); H(\tau)]_{-}, \quad (1.3)$$

and of the peculiarities of the statistical averaging. The various correlation functions and the macroscopic quantities of the system can be related to the spectral density (1.1) by use of the spectral decompositions of (1.1). As to the spectral decomposition it can be easily derived under the assumption that the Hamiltonian of the system under consideration has a complete orthonormal set of eigenfunctions, $H|n\rangle = E_n|n\rangle$; $\langle n|n\rangle = 1$; $\sum_n |n\rangle \langle n| = \mathbf{1}$, and has the following well-known form:

$$\eta \langle [A; B(\tau)]_{\eta} \rangle_{\omega} = Z^{-1} \sum_{m,n} (m|A|n) \langle n|B|m\rangle \times \\ \times 2\pi \delta(\omega - E_m + E_n) e^{-\beta E_m} (1 + \eta e^{\beta \omega}), \quad (1.4)$$

where $Z = \text{Tr} [\exp(-\beta H)]$ is the grand partition function¹⁾ of the interacting particle system; $(m|A|n)$ and $\langle n|B|m\rangle$ are the exact matrix elements of the operators A and B taken with the eigenfunctions of the Hamiltonian. Now using the spectral decompositions (1.4), one can easily obtain a simple known expression for the statistical average of the corresponding operators:

$$\langle A B \rangle - \theta(-\eta) \langle A \rangle \langle B \rangle = \int \frac{d\omega}{2\pi} \frac{\eta \langle [A; B(\tau)]_{\eta} \rangle_{\omega}}{\exp(\beta \omega) + \eta}. \quad (1.5)$$

In a somewhat more complicated way implying the use of the equations of motion (1.3), analogous formulae can also be obtained for some higher-order correlation functions. Thus most attention should be paid to the accurate calculation of the corresponding spectral density within the set of relations (1.2), since once the explicit form of the spectral density is found, it is no longer difficult to calculate the macroscopic quantities of the system under investigation.

However, this problem can be solved exactly in exceptional cases only. In the majority of cases, one has to look for an approximate representation of the spectral density within only several first moments. The problem thus outlined becomes naturally non-unique, and one has to determine the spectral density on a class of beforehand chosen functions in order to achieve a unique solution. The class of admissible functions is to be chosen in accordance with the spectral

¹⁾ The chemical potential is supposed to be incorporated into H .

decomposition (1.4) and turns immediately the finite set of relations into a set of equations determining the unknown functional parameters of the spectral density. As a simplest example, the corresponding spectral density is usually approximated by one or a set of δ -functions, the functional parameters connected with the spectral density being then uniquely determined by solving one or a set of non-linear integral equations. For example, the simplest approximation of the one-particle spectral density

$$A_{p\gamma}(\omega) = \langle [a_{p\gamma}^+; a_{p\gamma}(\tau)]_+ \rangle_\omega \quad (1.6)$$

for a Fermi system with pair forces by means of one δ -function,

$$A_{p\gamma}(\omega) = 2\pi \delta(\omega - T_{p\gamma}), \quad (1.7)$$

together with the use of the two first moments immediately results in the following non-linear integral equation:

$$T_{p\gamma} = \varepsilon_{p\gamma} + g \nu(0) n - \frac{g}{V} \sum_k \frac{\nu(p-k)}{\exp(\beta T_{k\gamma}) + 1} \quad (1.8)$$

for the elementary excitation spectrum $T_{p\gamma}$. Equation (1.8) thus obtained is equivalent to the well-known self-consistent equation in the Hartree-Fock approximation. In more complicated cases, a number of important results can also be easily obtained if one uses more complicated approximations for the spectral density and a larger number of the first moments to determine the unknown functional parameters.

On the whole, the method suggested here is simple and useful for practical calculations and enables us to obtain easily significant results also for systems having no effective small parameter. In the subsequent sections we shall show how the method works by solving several special models of statistical physics (see also [10]). A solution of the same problem given from a more formal mathematical point of view can be found in recent papers of other authors [11].

2. Two-Particle Interaction — Normal and Anomalous Fermi Systems

2.1 Specification of a model — Connection of the one-particle spectral density $A_{p\gamma}(\omega)$ with the macroscopic quantities of the system

We shall consider a system of N interacting fermions enclosed in a large but finite volume V . In the final results N and V are supposed to become infinite, the particle density $n = N/V$ being left constant. The particles are assumed to interact via pair forces depending on the interparticle distance only. The dynamic behaviour of such a system is given by a Hamiltonian $H = H(a_{p\gamma}^+, a_{p\gamma})$ which can be easily reduced to the following form in the second quantization representation:

$$H = H_0 + H_{\text{int}}; \quad H_0 = \sum_{p\gamma} \varepsilon_{p\gamma} a_{p\gamma}^+ a_{p\gamma}, \quad (2.1)$$

$$H_{\text{int}} = \frac{g}{2V} \sum_{p_1 \dots p_4} \sum_{\gamma_1 \gamma_2} \delta_{p_1+p_2; p_3+p_4} \nu(p_2 - p_3) a_{p_1 \gamma_1}^+ a_{p_2 \gamma_2}^+ a_{p_4 \gamma_2} a_{p_3 \gamma_1},$$

where $a_{p\gamma}^+$ and $a_{p\gamma}$ are the Fermion creation and annihilation operators, $\varepsilon_{p\gamma}$ is the dispersion law of the free particles with μ involved into it, $\nu(p_2 - p_3) = \nu(|\mathbf{p}_2 - \mathbf{p}_3|)$ is the Fourier transform of the interaction potential, g is a coupling constant.

The thermodynamic and kinetic properties of such a system can be conveniently investigated by means of a one-particle spectral density

$$A_{p\gamma}(\omega) = \langle [a_{p\gamma}^+; a_{p\gamma}(\tau)]_+ \rangle_\omega, \quad (2.2)$$

which is a real and positive function according to its definition. One can easily verify this by analysing the corresponding spectral decomposition of the function (2.2),

$$A_{p\gamma}(\omega) = Z^{-1} \sum_{mn} |(a_{p\gamma}^+)_{mn}|^2 2\pi \delta(\omega + E_n - E_m) e^{-\beta E_m} (1 + e^{\beta \omega}), \quad (2.3)$$

obtained under the only assumption that the Hamiltonian of the system of particles considered has a complete orthonormal set of eigenfunctions. Due to the spectral decomposition (2.3), the formulae connecting the one-particle spectral density with the macroscopic quantities of the system can be also readily derived. For example, after a not complicated transformation of (2.3) one can easily express the average occupation numbers in terms of the spectral density by means of the very simple formula

$$\bar{n}_{p\gamma} = \langle a_{p\gamma}^+ a_{p\gamma} \rangle = \int \frac{d\omega}{2\pi} \frac{A_{p\gamma}(\omega)}{\exp(\beta\omega) + 1}, \quad (2.4)$$

with the aid of which both the equation for determining the chemical potential μ of the system can be easily obtained and the magnetization, the susceptibility, and some other macroscopic quantities can be investigated. In a somewhat more complicated way, by using the equation of motion for the one-particle spectral density,

$$(\omega - \varepsilon_{p\gamma}) A_{p\gamma}(\omega) = \frac{1}{2} \{ \langle [[H_{\text{int}}; a_{p\gamma}^+]_-; a_{p\gamma}(\tau)]_+ \rangle_\omega + \langle [a_{p\gamma}^+; [a_{p\gamma}(\tau); H_{\text{int}}(\tau)]_-]_+ \rangle_\omega \}, \quad (2.5)$$

and calculating the equal-time commutators, it is possible to derive another important formula that enables us to determine the average interaction energy

$$\frac{E_{\text{int}}}{V} = \frac{\langle H_{\text{int}} \rangle}{V} = \frac{1}{2V} \sum_{p\gamma} \int \frac{d\omega}{2\pi} \frac{(\omega - \varepsilon_{p\gamma}) A_{p\gamma}(\omega)}{\exp(\beta\omega) + 1}, \quad (2.6)$$

and the thermodynamic potential

$$\Omega = -\frac{1}{\beta} \ln \text{Tr} [\exp(-\beta H)], \quad (2.7)$$

if we use the usual procedure of differentiating over the coupling constant:

$$\frac{\partial}{\partial g} \left(\frac{\Omega}{V} \right) = \frac{1}{g} \frac{E_{\text{int}}}{V}; \quad \frac{\Omega - \Omega_0}{V} = \int_0^g \frac{dg_1}{g_1} \left(\frac{1}{2V} \sum_{p\gamma} \int \frac{d\omega}{2\pi} \frac{(\omega - \varepsilon_{p\gamma}) A_{p\gamma}(\omega)}{\exp(\beta\omega) + 1} \right). \quad (2.8)$$

There also exists a sufficiently simple formula for the ground state energy:

$$\frac{E}{V} - \mu n = \frac{\langle H \rangle}{V} = \frac{1}{2V} \sum_{p\gamma} \int \frac{d\omega}{2\pi} \frac{(\omega + \varepsilon_{p\gamma}) A_{p\gamma}(\omega)}{\exp(\beta\omega) + 1}, \quad (2.9)$$

which is a direct consequence of (2.4) and (2.6).

Thus, if the one-particle spectral density $A_{p\gamma}(\omega)$ is known, the investigation of the thermodynamic and kinetic properties of the system on the basis of the

formulae obtained above does not present any difficulties. Therefore, in what follows we shall confine ourselves to the methods for calculating the corresponding spectral densities.

2.2 A set of closed relations — Spectral decomposition for $A_{p\gamma}(\omega)$ and its simplest approximation

Using the equation of motion for the field operator $a_{p\gamma}^+(\tau)$, we can easily write down an infinite set of moments for the one-particle spectral density $A_{p\gamma}^+(\omega)$:

$$\int \frac{d\omega}{2\pi} \omega^m A_{p\gamma}(\omega) = \frac{1}{2} \left\{ \left\langle \left[\underbrace{[H; [H \dots [H; a_{p\gamma}^+]_- \dots]_-}_{m \text{ times}}; a_{p\gamma} \right]_+ \right\rangle + \left\langle \left[a_{p\gamma}^+; [\dots [a_{p\gamma}; \underbrace{H_- \dots H_-}_{m \text{ times}}]_- \right]_+ \right\rangle \right\}, \quad (2.10)$$

which, if the Hamiltonian of the system is known and the right-hand side of (2.10) can be calculated in an explicit form, enables us to obtain in a certain way an explicit form of $A_{p\gamma}(\omega)$. For example, in the trivial case of free fermions which are described by the Hamiltonian (2.1) at $g = 0$, the set (2.10) is easily calculated:

$$\int \frac{d\omega}{2\pi} A_{p\gamma}(\omega) = 1; \quad \int \frac{d\omega}{2\pi} (\omega - \varepsilon_{p\gamma})^m A_{p\gamma}(\omega) = 0; \quad m = 1, 2, \dots, \quad (2.11)$$

and its solution has the very simple form

$$A_{p\gamma}(\omega) = 2\pi \delta(\omega - \varepsilon_{p\gamma}). \quad (2.12)$$

In more complicated cases, however, it is extremely difficult to solve this problem exactly. Therefore, in most cases the corresponding spectral density is obtained approximately within the set of the few first moments. Naturally, in the general form this problem has no single-values solution. The latter can be achieved only if the functional form of the one-particle spectral density is postulated beforehand in correspondence with its spectral decomposition. For normal Fermi systems a corresponding spectral decomposition can be taken in the following equivalent form:

$$A_{p\gamma}(\omega) = \text{---} \textcircled{J_2} \text{---} \times \textcircled{J_2} \text{---} + \textcircled{J_4} \text{---} \times \textcircled{J_4} \text{---} + \textcircled{J_6} \text{---} \times \textcircled{J_6} \text{---} \quad (2.13)$$

in which the first graph corresponds to the pole approximation, i.e. to the non-scattered propagation of a quasi-particle, the other graphs including scattering processes. The spectral decomposition of $A_{p\gamma}(\omega)$, equation (2.13), permits to develop step-by-step approximations for the one-particle spectral density, which already in a simple approximation lead to plausible results irrespective either of the strength of interaction or of any other specific characteristics of the investigated system of interacting particles.

For example, the simplest approximation for $A_{p\gamma}(\omega)$ corresponds to keeping only the first graph in the spectral decomposition (2.13),

$$A_{p\gamma}(\omega) = |\mathcal{J}_2|^2 2\pi \delta(\omega - T_{p\gamma}), \quad (2.14)$$

and to determining the corresponding functional parameters $|\mathcal{F}_2|^2$ and $T_{p\gamma}$ within the set of the first two momenta,

$$\begin{aligned} \int \frac{d\omega}{2\pi} A_{p\gamma}(\omega) &= 1; \quad \int \frac{d\omega}{2\pi} (\omega - \varepsilon_{p\gamma}) A_{p\gamma}(\omega) = \\ &= \frac{1}{2} \{ \langle [[H_{\text{int}}; a_{p\gamma}^+]; a_{p\gamma}]_+ \rangle + \langle [a_{p\gamma}^+; [a_{p\gamma}; H_{\text{int}}]_-]_+ \rangle \} = \\ &= g \nu(0) n - \frac{g}{V} \sum_q \nu(p-q) \bar{n}_{q\gamma}. \end{aligned} \quad (2.15)$$

In this case, we find after a simple algebra that $|\mathcal{F}_2|^2 = 1$, and the one-particle elementary excitation spectrum $T_{p\gamma}$ is determined as a solution of the well-known self-consistent integral equation

$$T_{p\gamma} = \varepsilon_{p\gamma} + g \nu(0) n - \frac{g}{V} \sum_q \frac{\nu(p-q)}{\exp(\beta T_{q\gamma}) + 1}, \quad (2.16)$$

which is derived by a direct calculation of the first momentum of $A_{p\gamma}(\omega)$, (2.14) and (2.4) being included.

In spite of its simplicity, this approximation leads to phase transitions, i.e. it is far from being trivial. We shall explain this by considering the example of a magnetic ordering in a system of interacting fermions, i.e., we shall investigate the possibility of spontaneous magnetization $R = (n_\uparrow - n_\downarrow)/n$ in this system at sufficiently low temperatures. The starting point for obtaining the self-consistent equation determining R can be the expression for the average occupation numbers,

$$\bar{n}_{p\gamma} = \left\{ \exp \beta \left[(\varepsilon_{p\gamma} + g \nu(0) n) - \frac{g}{V} \sum_q \nu(p-q) \bar{n}_{q\gamma} \right] + 1 \right\}^{-1}, \quad (2.17)$$

which is easily obtained with the aid of (2.4), (2.14), and (2.16). If we now express the average occupation numbers $\bar{n}_{p\gamma}$ in terms of the spin density \bar{s}_p and the particle density \bar{n}_p by means of the formulae $\bar{n}_p + \bar{s}_p = \bar{n}_{p\uparrow}$ and $\bar{n}_p - \bar{s}_p = \bar{n}_{p\downarrow}$, and assume that $\varepsilon_{p\gamma} = \varepsilon_p$, we easily obtain after some simple algebra the following self-consistent equation:

$$\begin{aligned} \frac{n R}{2} = \frac{1}{V} \sum_q \bar{s}_p; \quad \bar{s}_p = \\ = \frac{\sinh \frac{\beta g}{V} \sum_q \nu(p-q) \bar{s}_q}{\cosh \beta \left[(\varepsilon_p + g \nu(0) n) - \frac{g}{V} \sum_q \nu(p-q) \bar{n}_q \right] + \cosh \frac{\beta g}{V} \sum_q \nu(p-q) \bar{s}_q} \end{aligned} \quad (2.18)$$

which determines the possibility for a spontaneous magnetization R to appear in the system. Equation (2.18) is a complicated non-linear integral equation which, apart from the trivial solution $\bar{s}_p \equiv 0$, has, generally speaking, a solution different from zero. A full analysis of this equation (see, for example, [12]) is beyond the scope of this review and, therefore, we shall only schematically outline its trend. The non-trivial solution of (2.18) arises in the vicinity of a bifurcation point which can be determined by linearization of the original equation. Since the linearization leads to a homogeneous Fredholm equation

of the second kind, the question of existence of a non-trivial solution becomes thus equivalent to that for the linearized equation, and can be easily answered within the standard theory of integral equations. Thus, under certain conditions, (2.18) has a non-trivial solution, i.e., the system undergoes a phase transition. As it can be easily shown, the latter is a second-order transition which results in a non-zero spontaneous magnetization and in a finite discontinuity in the specific heat.

In conclusion of what has been said above, we may state that the choice of the spectral density $\Lambda_{p\gamma}(\omega)$ in the form (2.14), which is an attempt to replace the true spectrum of elementary excitations by the undamped effective one-particle spectrum, leads to reasonable and non-trivial results and may always be recommended for calculations as the simplest approximation for $\Lambda_{p\gamma}(\omega)$. A more complicated approximation for $\Lambda_{p\gamma}(\omega)$ taking account of quasi-particle scattering is considered below.

2.3 An improved approximation for $\Lambda_{p\gamma}(\omega)$ — Account of quasi-particle scattering

The need to improve the simplest approximation for the one-particle spectral density is not only due to the desire to obtain better results in concrete calculations, but also to physical considerations, since in actual systems quasi-particles, though slowly, do damp in time.

Quasi-particle damping is explained by the scattering which has not been taken into account in the simplest approximation since all the terms in the spectral decomposition (2.13) responsible for such processes were omitted. The scattering would be taken into account by keeping the terms with more complicated intermediate states in the spectral decomposition (2.13), the simplest of which contains two quasi-particles and one quasi-hole in the intermediate state and can be represented (account taken of the spin structure) by the following two graphs:

$$(2.19)$$

In this approximation, i.e. if one omits all the subsequent terms of the spectral decomposition (2.13) except the pole term and that written down above, the one-particle spectral density is represented as

$$\begin{aligned} \Lambda_{p\gamma}(\omega) = & Z_{p\gamma}^{-1} \left\{ 2\pi \delta(\omega - T_{p\gamma}) + \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1\gamma; p\gamma}^{q_1\gamma; q_2\gamma}|^2 \times \right. \\ & \times \frac{2\pi \delta(\omega - T_{q_1\gamma} - T_{q_2\gamma} + T_{k_1\gamma})}{(T_{q_1\gamma} + T_{q_2\gamma} - T_{k_1\gamma} - T_{p\gamma})^2} + \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1-\gamma; p\gamma}^{q_1-\gamma; q_2\gamma}|^2 \times \\ & \left. \times \frac{2\pi \delta(\omega - T_{q_1-\gamma} - T_{q_2\gamma} + T_{k_1-\gamma})}{(T_{q_1-\gamma} + T_{q_2\gamma} - T_{k_1-\gamma} - T_{p\gamma})^2} \right\}, \end{aligned} \quad (2.20)$$

where $Z_{p\gamma}$ is the function responsible for the normalization of $\Lambda_{p\gamma}(\omega)$, $T_{p\gamma}$ is the real effective one-particle spectrum of elementary excitations, $|U_{k_1\gamma; p\gamma}^{q_1\gamma; q_2\gamma}|^2$

is a reduced matrix element squared permitting the following parametrization:

$$|U_{k_1\gamma; q_2\gamma}^{q_1\gamma}|^2 = |\mathcal{J}_{k_1\gamma; p\gamma}^{q_1\gamma; q_2\gamma}|^2 \{(1 - \bar{n}_{q_1\gamma})(1 - \bar{n}_{q_2\gamma})\bar{n}_{k_1\gamma} + \bar{n}_{q_1\gamma}\bar{n}_{q_2\gamma}(1 - \bar{n}_{k_1\gamma})\}. \quad (2.21)$$

However, we should not restrict ourselves to this representation of the one-particle spectral density since the possibility of repeated scattering into the same intermediate states is not properly taken into account. The latter can approximately be accounted for by summing the function (2.20) into the exponential form

$$\begin{aligned} A_{p\gamma}(\tau) = & Z_{p\gamma}^{-1} \exp \left\{ -i T_{p\gamma} \tau + \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1\gamma; p\gamma}^{q_1\gamma; q_2\gamma}|^2 \times \right. \\ & \times \frac{\exp[-i(T_{q_1\gamma} + T_{q_2\gamma} - T_{k_1\gamma} - T_{p\gamma})\tau]}{(T_{q_1\gamma} + T_{q_2\gamma} - T_{k_1\gamma} - T_{p\gamma})^2} + \\ & \left. + \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1-\gamma; p\gamma}^{q_1-\gamma; q_2\gamma}|^2 \frac{\exp[-i(T_{q_1-\gamma} + T_{q_2\gamma} - T_{k_1-\gamma} - T_{p\gamma})\tau]}{(T_{q_1-\gamma} + T_{q_2\gamma} - T_{k_1-\gamma} - T_{p\gamma})^2} \right\}, \end{aligned} \quad (2.22)$$

after which the functional form of $A_{p\gamma}(\omega)$ is regarded as given while the unknown functional parameters are determined from the set of the few first moments. So within the zero and first moments one can determine the unknown functions $Z_{p\gamma}$:

$$\begin{aligned} Z_{p\gamma} = & \exp \left\{ \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1\gamma; p\gamma}^{q_1\gamma; q_2\gamma}|^2 (T_{q_1\gamma} + T_{q_2\gamma} - T_{k_1\gamma} - T_{p\gamma})^{-2} + \right. \\ & \left. + \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1-\gamma; p\gamma}^{q_1-\gamma; q_2\gamma}|^2 (T_{q_1-\gamma} + T_{q_2\gamma} - T_{k_1-\gamma} - T_{p\gamma})^{-2} \right\}, \end{aligned} \quad (2.23)$$

and the effective one-particle spectrum of elementary excitations:

$$\begin{aligned} T_{p\gamma} = & M_{p\gamma}^{(1)} - \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1\gamma; p\gamma}^{q_1\gamma; q_2\gamma}|^2 (T_{q_1\gamma} + T_{q_2\gamma} - T_{k_1\gamma} - T_{p\gamma})^{-1} - \\ & - \frac{1}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} |U_{k_1-\gamma; p\gamma}^{q_1-\gamma; q_2\gamma}|^2 (T_{q_1-\gamma} + T_{q_2\gamma} - T_{k_1-\gamma} - T_{p\gamma})^{-1}, \end{aligned} \quad (2.24)$$

and, after the second-order semi-invariant being calculated:

$$\begin{aligned} Q_{p\gamma}^{(2)} = & [M_{p\gamma}^{(2)} - (M_{p\gamma}^{(1)})^2]; \quad Q_{p\gamma}^{(2)} = \frac{g^2}{V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} v^2 (p - q_2) \times \\ & \times \{(1 - \bar{n}_{q_1-\gamma})(1 - \bar{n}_{q_2\gamma})\bar{n}_{k_1-\gamma} + \bar{n}_{q_1-\gamma}\bar{n}_{q_2\gamma}(1 - \bar{n}_{k_1-\gamma})\} + \frac{g^2}{2V^2} \sum_{k_1 q_1 q_2} \delta_{p+k_1; q_1+q_2} \times \\ & \times [v(p - q_1) - v(p - q_2)]^2 \{(1 - \bar{n}_{q_1\gamma})(1 - \bar{n}_{q_2\gamma})\bar{n}_{k_1\gamma} + \bar{n}_{q_1\gamma}\bar{n}_{q_2\gamma}(1 - \bar{n}_{k_1\gamma})\}, \end{aligned} \quad (2.25)$$

it is easy to find the corresponding expressions for the vertex functions:

$$|\mathcal{J}_{k_1-\gamma; p\gamma}^{q_1-\gamma; q_2\gamma}|^2 = g^2 v^2 (p - q_2); \quad |\mathcal{J}_{k_1\gamma; p\gamma}^{q_1\gamma; q_2\gamma}|^2 = \frac{g^2}{2} [v(p - q_1) - v(p - q_2)]^2. \quad (2.26)$$

Thus, after all the transformations are carried out, the one-particle spectral density is approximated here by the following simple expression:

$$\begin{aligned}
 A_{p\gamma}(\tau) = & \exp \left\{ -i M_{p\gamma}^{(1)} \tau + \right. \\
 & + \left(\frac{g}{V} \right)^2 \sum_{qk\sigma} \nu(p-k) [v(p-k) - \delta_{\gamma;\sigma} v(k-q)] [\bar{n}_{q\sigma} (1 - \bar{n}_{k\gamma} - \bar{n}_{p+q-k,\sigma}) + \\
 & + \bar{n}_{k\gamma} \bar{n}_{p+q-k,\sigma}] \left(\frac{\exp[-i(T_{p+q-k,\sigma} + T_{k\gamma} - T_{q\sigma} - T_{p\gamma})\tau] - 1}{(T_{p+q-k,\sigma} + T_{k\gamma} - T_{q\sigma} - T_{p\gamma})^2} - 1 + \right. \\
 & \left. \left. + \frac{i\tau}{T_{p+q-k,\sigma} + T_{k\gamma} - T_{q\sigma} - T_{p\gamma}} \right) \right\}, \quad (2.27)
 \end{aligned}$$

and satisfies exactly the set of the first three moments, provided that the two-particle correlation functions determining the second moment (see also formula (2.25)) are calculated in the self-consistent approximation

$$\langle a_{p\gamma}^+ a_{k\sigma}^+ a_{p+k-q,\sigma} a_{q\gamma} \rangle = (\delta_{q;p} - \delta_{k;q} \delta_{\gamma;\sigma}) \bar{n}_{k\sigma} \bar{n}_{p\gamma}. \quad (2.28)$$

It should be noted for comparison that the simplest approximation for the one-particle spectral density by one δ -function does not satisfy the second moment with any reasonable coupling of the two-particle correlation functions.

As to the elementary excitation spectrum and damping of quasi-particles, the one-particle spectral density in the region of large τ (i.e. after all scattering processes have happened) is responsible for them. Transition into the asymptotic region is guided by the formula

$$\left[\frac{\exp(-i\varepsilon\tau) - 1}{\varepsilon^2} + \frac{i\tau}{\varepsilon} \right]_{\tau \rightarrow \pm\infty} \rightarrow \frac{\partial}{\partial\varepsilon} \left(p \frac{1}{\varepsilon} \pm i\delta(\varepsilon) \right) + i\tau \left(p \frac{1}{\varepsilon} \pm i\delta(\varepsilon) \right), \quad (2.29)$$

which is easily verified in the sense of generalized functions. With (2.27) this transition leads to the following result:

$$\begin{aligned}
 A_{p\gamma}(\tau \rightarrow \pm\infty) = & \exp \left[\left(\frac{\partial \operatorname{Re} \tilde{\Sigma}(p\gamma; \omega)}{\partial\omega} \right)_{\omega=T_{p\gamma}} \right] \times \\
 & \times \exp \left\{ -i(M_{p\gamma}^{(1)} + \operatorname{Re} \tilde{\Sigma}(p\gamma; T_{p\gamma})) \tau - \right. \\
 & \left. - |\tau| \left[\operatorname{Im} \tilde{\Sigma}(p\gamma; T_{p\gamma}) + \Gamma_{p\gamma} \left(\frac{\partial \operatorname{Re} \tilde{\Sigma}(p\gamma; \omega)}{\partial\omega} \right)_{\omega=T_{p\gamma}} \right] \right\}, \quad (2.30)
 \end{aligned}$$

where by definition the new functions $\operatorname{Re} \tilde{\Sigma}(p\gamma; \omega)$ and $\operatorname{Im} \tilde{\Sigma}(p\gamma; \omega)$ are equal, respectively, to the following expressions:

$$\left. \begin{aligned}
 \operatorname{Re} \tilde{\Sigma}(p\gamma; \omega) = & \left(\frac{g}{V} \right)^2 P \sum_{qk\sigma} \nu(p-k) \frac{[v(p-k) - \delta_{\gamma;\sigma} v(k-q)]}{\omega + T_{q\sigma} - T_{k\gamma} - T_{p+q-k,\sigma}} \times \\
 & \times [\bar{n}_{q\sigma} (1 - \bar{n}_{k\gamma} - \bar{n}_{p+q-k,\sigma}) + \bar{n}_{k\gamma} \bar{n}_{p+k-q,\sigma}], \\
 \operatorname{Im} \tilde{\Sigma}(p\gamma; \omega) = & \pi \left(\frac{g}{V} \right)^2 \sum_{qk\sigma} \nu(p-k) [v(p-k) - \delta_{\gamma;\sigma} v(k-q)] \times \\
 & \times [\bar{n}_{q\sigma} (1 - \bar{n}_{k\gamma} - \bar{n}_{p+q-k,\sigma}) + \bar{n}_{k\gamma} \bar{n}_{p+k-q,\sigma}] \times \\
 & \times \delta(\omega - T_{p+q-k,\sigma} + T_{q\sigma} - T_{k\gamma}).
 \end{aligned} \right\} \quad (2.31)$$

In the derivation, a small term of the type $(\partial \text{Im } \tilde{\Sigma}(p\gamma; \omega)/\partial \omega)_{\omega=T_{p\gamma}}$ is omitted as usual. Comparing now the expression (2.30) with the standard form of the one-particle spectral density in the asymptotic region,

$$A_{p\gamma}(\tau \rightarrow \pm \infty) = Z_{p\gamma}^{-1} \exp \{ -i T_{p\gamma} \tau - \Gamma_{p\gamma} |\tau| \}, \quad (2.32)$$

we immediately obtain the corresponding expressions both for the spectrum of quasi-particles and for their damping:

$$\left. \begin{aligned} T_{p\gamma} &= M_{p\gamma}^{(1)} + \text{Re } \tilde{\Sigma}(p\gamma; T_{p\gamma}), \\ \Gamma_{p\gamma} &= \frac{\text{Im } \tilde{\Sigma}(p\gamma; T_{p\gamma})}{1 - \left(\frac{\partial \text{Re } \tilde{\Sigma}(p\gamma; \omega)}{\partial \omega} \right)_{\omega=T_{p\gamma}}} \end{aligned} \right\} \quad (2.33)$$

The quasi-particles thus obtained are interpreted further as the effective one-particle excitations of the considered system of particles.

The self-consistent equation (2.33) for the determination of the elementary excitation spectrum is the generalization of results obtained by a number of authors [13] and corresponds to a rather complicated summation of graphs within the ordinary perturbation theory. Moreover, the expression obtained here for the damping of quasi-particles, due to a more accurate account of the elementary excitation spectrum, has a correct behaviour on the Fermi surface which is not always guaranteed by approximate calculations within the other methods.

Thus, within the spectral density method, it is easy to make the simplest approximation for the corresponding spectral density and to improve it step by step as well. For each approximation we shall obtain a new self-consistent equation to determine the effective spectrum of elementary excitations, but not the corrections to the results of the previous approximation, this feature being particularly important for the investigation of thermodynamic and kinetic properties of a system of interacting particles subject to a phase transition.

2.4 Anomalous coupling of quasi-particles — Generalized Hartree-Fock approximation

Though the above approximations of the one-particle spectral density lead to far not trivial results for normal Fermi systems, they are of little use to describe the thermodynamic and kinetic properties of the so-called anomalous Fermi systems. Since at low temperatures the latter have a qualitatively different behaviour of the spectrum of elementary excitations, a more careful choice of the functional form of the one-particle spectral density is required.

Below the simplest approximation of the one-particle spectral density for anomalous Fermi systems with superconducting coupling is considered. Since in this case an effective attraction of two quasi-particles with opposite momenta near the Fermi surface is responsible for the formation of bound states, it is convenient to make use of the matrix technique to determine in an appropriate way the new matrix operators:

$$\gamma_{p\gamma} = \begin{pmatrix} a_{p\gamma} \\ a_{-p-\gamma}^+ \end{pmatrix}, \quad \gamma_{p\gamma}^+ = (a_{p\gamma}^+, a_{-p-\gamma}), \quad (2.34)$$

and to calculate in terms of them the one-particle spectral density

$$\mathbf{\Lambda}(p \gamma; \omega) = \begin{pmatrix} \langle [a_{p\gamma}^+; a_{p\gamma}(\tau)]_+ \rangle_\omega & \langle [a_{p\gamma}^+; a_{-p-\gamma}^+(\tau)]_+ \rangle_\omega \\ \langle [a_{-p-\gamma}; a_{p\gamma}(\tau)]_+ \rangle_\omega & \langle [a_{-p-\gamma}; a_{-p-\gamma}^+(\tau)]_+ \rangle_\omega \end{pmatrix}, \quad (2.35)$$

defined in the usual way. For this spectral density there is an infinite set of matrix relations analogous to (2.10) on the basis of which we can carry out calculations restricting ourselves to some set of first moments and assuming the corresponding functional form of $\mathbf{\Lambda}(p \gamma; \omega)$.

For example, consider in more detail the simplest approximation of the one-particle spectral density by means of one matrix δ -function:

$$\mathbf{\Lambda}(p \gamma; \omega) = 2 \pi \delta(\omega - \mathbf{T}(p \gamma)), \quad (2.36)$$

provided that $\bar{n}_{p\gamma} = \bar{n}_{-p-\gamma}$. In this case, to determine the unknown matrix $\mathbf{T}(p \gamma)$, it is sufficient to know the set of the two first moments which are easily calculated and have the following simple form:

$$\int \frac{d\omega}{2\pi} \mathbf{\Lambda}(p \gamma; \omega) = \mathbf{I}, \quad \int \frac{d\omega}{2\pi} (\omega - \varepsilon_{p\gamma} \boldsymbol{\sigma}_3) \mathbf{\Lambda}(p \gamma; \omega) = \tilde{\mathbf{M}}^{(1)}(p \gamma); \quad (2.37)$$

$$\boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\tilde{\mathbf{M}}^{(1)}(p \gamma) = \begin{pmatrix} g v(0) n - \frac{g}{V} \sum_q v(p-q) \bar{n}_{q\gamma} & \frac{g}{V} \sum_q v(p-q) \langle a_{q\gamma}^+ a_{-q-\gamma}^+ \rangle \\ \frac{g}{V} \sum_q v(p-q) \langle a_{-q-\gamma} a_{q\gamma} \rangle & -g v(0) n + \frac{g}{V} \sum_q v(p-q) \bar{n}_{q\gamma} \end{pmatrix}.$$

The solution of the set (2.37) involving (2.36) is uniquely determined:

$$\mathbf{T}(p \gamma) = \varepsilon_{p\gamma} \boldsymbol{\sigma}_3 + \tilde{\mathbf{M}}^{(1)}(p \gamma), \quad (2.38)$$

thus solving in principle the formulated problem. To obtain a more explicit form of the solution, however, some further transformations of purely mathematical origin are needed connected with special realization of the function of the matrix. Nevertheless these transformations are elementary in this case and we are immediately led from the theory of superconductivity to the well-known representation for the one-particle spectral density in the following form:

$$\mathbf{\Lambda}(p \gamma; \omega) = \pi \begin{pmatrix} 1 + \frac{T_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} & \frac{\Delta_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} \\ \frac{\Delta_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} & 1 - \frac{T_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} \end{pmatrix} \delta(\omega - \sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}) + \\ + \begin{pmatrix} 1 - \frac{T_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} & \frac{-\Delta_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} \\ \frac{-\Delta_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} & 1 + \frac{T_{p\gamma}}{\sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}} \end{pmatrix} \pi \delta(\omega + \sqrt{\Delta_{p\gamma}^2 + T_{p\gamma}^2}), \quad (2.39)$$

where by definition $T_{p\gamma}$ and $\Delta_{p\gamma}$ are respectively equal to the following expres-

sions:

$$\left. \begin{aligned} T_{p\gamma} &= (\varepsilon_{p\gamma} + g\nu(0)n) - \frac{g}{V} \sum_q \nu(p-q) \bar{n}_{q\gamma}, \\ \Delta_{p\gamma} &= \frac{g}{V} \sum_q \nu(p-q) \langle \alpha_{-q-\gamma} \alpha_{q\gamma} \rangle, \end{aligned} \right\} \quad (2.40)$$

and the necessary self-consistent equations

$$\left. \begin{aligned} T_{pq} &= (\varepsilon_{pq} + g\nu(0)n) - \frac{g}{2V} \sum_q \nu(p-q) \left[1 - \frac{T_{q\gamma}}{\sqrt{\Delta_{q\gamma}^2 + T_{q\gamma}^2}} \tanh \frac{\beta \sqrt{\Delta_{q\gamma}^2 + T_{q\gamma}^2}}{2} \right], \\ \Delta_{p\gamma} &= -\frac{g}{2V} \sum_q \frac{\nu(p-q)}{\sqrt{\Delta_{q\gamma}^2 + T_{q\gamma}^2}} \tanh \frac{\beta \sqrt{\Delta_{q\gamma}^2 + T_{q\gamma}^2}}{2} \end{aligned} \right\} \quad (2.41)$$

are easily obtained from (2.40) if the operator averages involved are expressed through the above explicit expression for the one-particle spectral density by the ordinary formulae.

Thus, within the Hamiltonian of two-particle interaction (2.1), approximating the one-particle spectral density by one matrix δ -function, it is possible to obtain at once all the results of the usual theory of superconductivity [14] based on the exact solution of the Bardeen-Cooper-Schrieffer model. Assuming a more complicated form of $\Lambda(p\gamma; \omega)$, this solution can be consistently improved. The calculations, however, are not traced in this review.

2.5 Collective modes of the interacting Fermi system — Plasma oscillation and spin wave spectra

It is well known that though the calculation of the one-particle spectral density $\Lambda_{p\gamma}(\omega)$ provides exhaustive information of the macroscopic properties of a many-particle system, it does not solve a sum of problems arising in the study of some special physical problems. In many cases, therefore, it is necessary to calculate higher-order spectral densities whose singularities provide information not only about one-particle excitations of the system, but on collective modes as well. The latter are particularly important for the interpretation of various experimental results, since most physical experiments, such as scattering of fast electrons and slow neutrons in solids, scattering of neutrons in liquid helium, etc., are sources of information about the collective modes in such systems. Collective modes also play a determining role in the theory of phase transitions since they stabilize the systems below the point of phase transition and, what is most probable, determine the character of singularities of the corresponding thermodynamic quantities.

Within the spectral density method, the collective modes of the system should be investigated with the aid of an appropriately determined higher-order spectral density, the functional form of which is chosen subject to the corresponding spectral decomposition. The unknown functional parameters are derived from the set of a finite number of first moments. Below we shall present a detailed investigation of the plasma oscillation spectrum in a many-fermion system with Coulomb interaction, and in conclusion we shall briefly touch upon the spin wave theory.

Consider now the simplest approximation of the spectral density-density function:

$$K_q(\omega) = -\langle [\varrho_q^+; \varrho_q(\tau)]_- \rangle_\omega; \quad \varrho_q = \frac{1}{\sqrt{V}} \sum_{k\sigma} a_{k\sigma}^\dagger a_{k+q, \sigma}, \quad (2.42)$$

whose singularities in the case of the long-range interaction correspond to plasma oscillations. For a non-interacting system of particles (see formula (2.1) for $g = 0$), the spectral function (2.42) is easily calculated exactly:

$$K_q(\omega) = \frac{1}{V} \sum_{k\sigma} (\bar{n}_{k\sigma} - \bar{n}_{k+q, \sigma}) 2\pi \delta(\omega - \varepsilon_{k+q, \sigma} + \varepsilon_{k\sigma}). \quad (2.43)$$

However, it does not contain an isolated singularity, but only has a cut along the real axis ω , corresponding to the propagation of a non-interacting particle-hole pair. As soon as the interaction is switched on, the situation will change radically, since the interaction causes a coherent superposition of quasi-particle-quasi-hole pairs which in turn must lead to isolated singularities in the spectral density (2.42). Of course, apart from the appearance of isolated singularities, the regular part of $K_q(\omega)$ will be changed essentially. However if q is small, considerable simplifications are possible here since it is well known that many-pair excitations and non-coherent excitations of quasi-particle-quasi-hole pairs determining the regular term in $K_q(\omega)$ in the region of small momenta are substantially suppressed, i.e., in a long-wave region $K_q(\omega)$ can be approximated by isolated singularities only. Following the spectral decomposition of the function (2.42),

$$K_q(\omega) = Z^{-1} \sum_{mn} e^{-\beta E_m} |(\varrho_q^+)_{mn}|^2 \{ \delta(\omega - \omega_{nm}) - \delta(\omega + \omega_{nm}) \}, \quad (2.44)$$

and taking into account that $K_q(\omega) = -K_q(-\omega)$, we make sure that two isolated singularities symmetric in ω exist. In accordance with this, the simplest approximation of the function $K_q(\omega)$ has the following form:

$$K_q(\omega) = 2\pi \psi_q \{ \delta(\omega - \omega_q) - \delta(\omega + \omega_q) \}, \quad (2.45)$$

where the unknown functional parameters ψ_q and ω_q are assumed to depend on the modulus q only and to be determined from the set of the first four moments:

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} K_q(\omega) &= 0, \\ \int \frac{d\omega}{2\pi} \omega K_q(\omega) &= n \frac{q^2}{m}, \\ \int \frac{d\omega}{2\pi} \omega^2 K_q(\omega) &= 0, \\ \int \frac{d\omega}{2\pi} \omega^3 K_q(\omega) &= n \frac{q^2}{m} \left(\frac{q^2}{2m} \right)^2 + \frac{3q^2}{m} \frac{1}{V} \sum_{k\gamma} \frac{(\mathbf{q} \cdot \mathbf{k})^2}{m^2} \bar{n}_{k\gamma} + \\ &\quad + \frac{g}{V} \sum_k v(k) \frac{(\mathbf{q} \cdot \mathbf{k})^2}{m^2} [\langle \varrho_{k+q}^+ \varrho_{k+q} \rangle - \langle \varrho_k^+ \varrho_k \rangle]. \end{aligned} \right\} (2.46)$$

The latter represent a set of exact relations and are obtained after a direct calculation of the equal-time commutator of the Fourier component of the density

operator with the Hamiltonian of the system (2.1). We assume here that $\varepsilon_{p\gamma} = p^2/(2m) - \mu$. Substituting (2.45) into (2.46), it is easy to find both functional parameters and the corresponding spectrum of collective modes:

$$\left. \begin{aligned} \psi_q &= n \frac{q^2}{2 \omega_q m}, \\ \omega_q^2 &= \left(\frac{q^2}{2m} \right)^2 + \frac{3}{nV} \sum_{k\gamma} \left(\frac{\mathbf{q} \cdot \mathbf{k}}{m} \right)^2 \bar{n}_{k\gamma} + \\ &+ \frac{m}{n q^2} \frac{g}{V} \sum_k \nu(k) \left(\frac{\mathbf{q} \cdot \mathbf{k}}{m} \right)^2 [\langle \varrho_{k+q}^+ \varrho_{k+q} \rangle - \langle \varrho_k^+ \varrho_k \rangle], \end{aligned} \right\} \quad (2.47)$$

which for the long-range Coulomb interaction potential $\nu(k) = 1/k^2$ corresponds to plasma oscillations.

Further transformations of the expression (2.47) are connected with the approximation of the correlation density-density function for which we use here the simplest approximate expression

$$\langle |\varrho_q^+|^2 \rangle = \delta_{q,0} V n^2 + \frac{1}{V} \sum_{p\gamma} \bar{n}_{p+q,\gamma} (1 - \bar{n}_{p\gamma}), \quad (2.48)$$

equivalent to the usual decoupling of higher correlation functions. Then with (2.48) taken into account, the collective excitation spectrum (2.47) at small q takes the form of the well-known spectrum of plasma oscillations:

$$\omega_q^2 = \frac{g n}{m} + \frac{3}{V n} \sum_{k\gamma} \left(\frac{\mathbf{q} \cdot \mathbf{k}}{m} \right)^2 \bar{n}_{k\gamma} - \frac{m}{n q^2} \frac{g}{2V} \sum_{p k \gamma} \frac{[\mathbf{q}(\mathbf{k} - \mathbf{p})]^2}{m^2 |\mathbf{p} - \mathbf{k}|} \left(\mathbf{q} \frac{\partial \bar{n}_{k\gamma}}{\partial \mathbf{k}} \right) \left(\mathbf{q} \frac{\partial \bar{n}_{p\gamma}}{\partial \mathbf{p}} \right), \quad (2.49)$$

which was obtained in [15] by more complicated calculations, whereas our calculations are elementary.

As for the spin waves, the calculations are essentially analogous. Consider the higher spectral density in terms of the spin operators:

$$\mathcal{F}_q(\omega) = -\langle [S_q^-; S_q^+(\tau)]_- \rangle_\omega; \quad S_q^\pm = \frac{1}{\sqrt{V}} \sum_k a_{k+q}^\pm a_{k\pm}, \quad (2.50)$$

and with the aid of the explicit form of the Hamiltonian (2.1) of the system, several first moments are calculated for this function. Adopting the simplest approximation for $\mathcal{F}_q(\omega)$ by one δ -function, it is sufficient to calculate the two first moments

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} \mathcal{F}_q(\omega) &= n R, \\ \int \frac{d\omega}{2\pi} \omega \mathcal{F}_q(\omega) &= \frac{q^2}{2m} n, \end{aligned} \right\} \quad (2.51)$$

after which it is possible to restore unambiguously the well-known expression for the spin wave spectrum (see, for example, [16]):

$$\mathcal{F}_q(\omega) = 2\pi n R \delta(\omega - \omega_q); \quad \omega_q = \frac{q^2}{2m R}, \quad (2.52)$$

being valid below the temperature of ferromagnetic ordering. If necessary, the result of the simplest approximation may be improved consistently.

On the whole, without going into further details of calculations, there is every reason to believe that the spectral density method may be successfully applied not only to calculate the one-particle spectrum, but also to investigate the spectrum of collective modes in the system of many strongly interacting particles, the calculations being also simple and effective.

3. Interaction of Fermions Mediated by a Bose Field

3.1 Specification of the model — Spectral decomposition of one-particle spectral densities

Interaction of fermions mediated by a Bose field will be considered within the generalized model

$$H = \sum_{k\sigma} \varepsilon_{k\sigma} a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_q \omega_q b_q^{\dagger} b_q + \sum_{qk\sigma} g(q) \left(\frac{\omega_q}{2V} \right)^{1/2} a_{k+q,\sigma}^{\dagger} a_{k\sigma} (b_q + b_{-q}^{\dagger}), \quad (3.1)$$

where $\varepsilon_{k\sigma}$ is the dispersion law for free fermions, containing in the usual way a chemical potential μ , ω_q is the dispersion law for free phonons, and $g(q) = g(|\mathbf{q}|)$ is the matrix element of the interaction between fermions and the Bose field. The system is considered to be placed in a large but finite volume V , with a subsequent transition to the thermodynamical limit in the final results.

Using the spectral density method, we shall consider in this section some versions of approximate calculations of the one-particle spectral functions of both Fermi- and Bose-type which can help to investigate the thermodynamic and kinetic properties of such a system.

The one-particle spectral density of Fermi-type is by definition analogous to the function (2.2):

$$A_{p\gamma}(\omega) = \langle [a_{p\gamma}^{\dagger}; a_{p\gamma}(\tau)]_{+} \rangle_{\omega}. \quad (3.2)$$

However, it has a somewhat different spectral expansion:

$$A_{p\gamma}(\omega) = \text{---} \bigcirc \text{---} \times \bigcirc \text{---} + \text{---} \bigcirc \text{---} \times \bigcirc \text{---} \text{---} \text{---} \text{---} \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \times \bigcirc \text{---} \text{---} \text{---} \text{---} \bigcirc \text{---} \quad (3.3)$$

due to the change in the character of interaction. Furthermore, apart from the function $A_{p\gamma}(\omega)$ it is necessary to determine the one-particle spectral density of Bose-type

$$R_q(\omega) = -\langle [b_q^{\dagger}; b_q(\tau)]_{-} \rangle_{\omega}, \quad (3.4)$$

whose spectral representation is easily found to be

$$R_q(\omega) = Z^{-1} \sum_{m,n} |(b_q^{\dagger})_{mn}|^2 2\pi \delta(\omega + E_n - E_m) e^{-\beta E_m} (e^{\beta \omega} - 1); \quad (3.5)$$

and the corresponding spectral decomposition is

$$R_q(\omega) = \text{---} \bigcirc \text{---} \times \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \times \bigcirc \text{---} \text{---} \text{---} \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} \times \bigcirc \text{---} \text{---} \text{---} \text{---} \bigcirc \text{---} \quad (3.6)$$

under the same assumptions adopted for the Hamiltonian of the system as in the derivation of the spectral representation for $A_{p\gamma}(\omega)$.

The singularities of these functions provide exhaustive information about the elementary excitation spectra of both Bose- and Fermi-type either of which can be used to determine the average interaction energy:

$$\left. \begin{aligned} \frac{E_{\text{int}}}{V} &= \frac{1}{V} \sum_{p\gamma} \int \frac{d\omega}{2\pi} \frac{(\omega - \varepsilon_{p\gamma}) A_{p\gamma}(\omega)}{\exp(\beta\omega) + 1}, \\ \frac{E_{\text{int}}}{V} &= \frac{2}{V} \sum_q \int \frac{d\omega}{2\pi} \frac{(\omega - \omega_q) \mathcal{R}_q(\omega)}{\exp(\beta\omega) - 1}, \end{aligned} \right\} \quad (3.7)$$

and, therefore, the thermodynamical potential of the system.

3.2 The simplest approximation for the Fermi spectral density $A_{p\gamma}(\omega)$

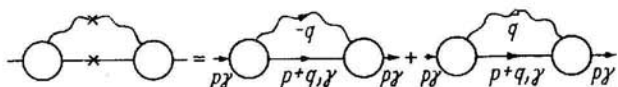
According to the general rules, the approximation for the one-particle spectral density $A_{p\gamma}(\omega)$ is based on the spectral decomposition (3.3) with a subsequent determination of the unknown functional parameters within a finite number of first moments. For our purpose it is quite sufficient to have a set of the first three moments which, under the assumption that $\langle b_{-q} b_q \rangle = \langle b_q^+ b_{-q}^+ \rangle = 0$, take the following simple form:

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} A_{p\gamma}(\omega) &= 1, \\ \int \frac{d\omega}{2\pi} (\omega - \varepsilon_{p\gamma}) A_{p\gamma}(\omega) &= 0, \\ \int \frac{d\omega}{2\pi} (\omega - \varepsilon_{p\gamma})^2 A_{p\gamma}(\omega) &= \sum_q g^2(q) \frac{\omega_q}{2V} (1 + 2\bar{v}_q). \end{aligned} \right\} \quad (3.8)$$

Analysing further the set of relations (3.8), we see that approximating $A_{p\gamma}(\omega)$ only by the pole term in the spectral decomposition (3.3) yields a trivial result:

$$A_{p\gamma}(\omega) = 2\pi \delta(\omega - T_{p\gamma}); \quad T_{p\gamma} = \varepsilon_{p\gamma}. \quad (3.9)$$

Therefore we shall include at once the contribution of scattering processes, confining ourselves to the first approximation. The latter means that besides the pole term of the spectral decomposition (3.3), the term corresponding to the simplest scattering process is also kept:



$$\quad (3.10)$$

whereas the remaining terms corresponding to more complicated scattering processes are ignored. Therefore, if account is taken of the processes of repeated scattering into the same intermediate states, the one-particle spectral density $A_{p\gamma}(\omega)$ must be approximated by the following simple expression:

$$\begin{aligned} A_{p\gamma}(\tau) &= Z_{p\gamma}^{-1} \exp \left\{ -i T_{p\gamma} \tau + \frac{1}{V} \sum_q \frac{\exp[-i(T_{p+q,\gamma} - T_{p\gamma} + \omega_q)\tau]}{(T_{p+q,\gamma} - T_{p\gamma} + \omega_q)^2} \times \right. \\ &\quad \left. \times |\tilde{U}_{p\gamma}(-q)|^2 + \frac{1}{V} \sum_q \frac{\exp[-i(T_{p+q,\gamma} - T_{p\gamma} - \omega_q)\tau]}{(T_{p+q,\gamma} - T_{p\gamma} - \omega_q)^2} |U_{p\gamma}(q)|^2 \right\}, \quad (3.11) \end{aligned}$$

where $|U_{p\gamma}(q)|^2$ and $|\tilde{U}_{p\gamma}(-q)|^2$ are the squares of the reduced matrix elements with the following parametrization:

$$\left. \begin{aligned} |U_{p\gamma}(q)|^2 &= |\mathcal{F}(q)|^2 [(1 - \bar{n}_{p+q,\gamma}) \bar{v}_q + \bar{n}_{p+q,\gamma} (1 + \bar{v}_q)], \\ |U_{p\gamma}(-q)|^2 &= |\mathcal{F}(q)|^2 [(1 - \bar{n}_{p+q,\gamma}) (1 + \bar{v}_q) + \bar{n}_{p+q,\gamma} \bar{v}_q]. \end{aligned} \right\} \quad (3.12)$$

The unknown functional parameters are determined by the relations (3.8) and are equivalent to the following expressions:

$$\left. \begin{aligned} Z_{p\gamma} &= \exp \left\{ \frac{1}{V} \sum_q |\tilde{U}_{p\gamma}(-q)|^2 (T_{p+q,\gamma} - T_{p\gamma} + \omega_q)^{-2} + \right. \\ &\quad \left. + \frac{1}{V} \sum_q |U_{p\gamma}(q)|^2 (T_{p+q,\gamma} - T_{p\gamma} - \omega_q)^{-2} \right\}, \\ T_{p\gamma} &= \varepsilon_{p\gamma} - \frac{1}{V} \sum_q |\tilde{U}_{p\gamma}(-q)|^2 (T_{p+q,\gamma} - T_{p\gamma} + \omega_q)^{-1} - \\ &\quad - \frac{1}{V} \sum_q |U_{p\gamma}(q)|^2 (T_{p+q,\gamma} - T_{p\gamma} - \omega_q)^{-1}, \\ |\mathcal{F}(q)|^2 &= g^2(q) \frac{\omega_q}{2}. \end{aligned} \right\} \quad (3.13)$$

Using (3.13), the explicit form of the one-particle spectral density $A_{p\gamma}(\omega)$ may be rewritten in a more convenient form:

$$\begin{aligned} A_{p\gamma}(\tau) &= \exp \left\{ -i \varepsilon_{p\gamma} \tau + \frac{1}{V} \sum_q \left(\frac{\exp[-i(T_{p+q,\gamma} - T_{p\gamma} + \omega_q)\tau] - 1}{(T_{p+q,\gamma} - T_{p\gamma} + \omega_q)^2} + \right. \right. \\ &\quad \left. \left. + \frac{i\tau}{T_{p+q,\gamma} - T_{p\gamma} + \omega_q} \right) |\tilde{U}_{p\gamma}(-q)|^2 + \frac{1}{V} \sum_q |U_{p\gamma}(q)|^2 \times \right. \\ &\quad \left. \times \left(\frac{\exp[-i(T_{p+q,\gamma} - T_{p\gamma} - \omega_q)\tau] - 1}{(T_{p+q,\gamma} - T_{p\gamma} - \omega_q)^2} + \frac{i\tau}{T_{p+q,\gamma} - T_{p\gamma} - \omega_q} \right) \right\}. \end{aligned} \quad (3.14)$$

Then going over to the asymptotic region, i.e. taking τ to be infinite, we obtain for the one-particle spectral density $A_{p\gamma}(\tau)$ according to (2.29) the following limiting expression:

$$\begin{aligned} A_{p\gamma}(\tau \rightarrow \pm \infty) &= \\ &= \exp \left[\left(\frac{\partial \operatorname{Re} \Sigma(p\gamma; \omega)}{\partial \omega} \right)_{\omega=T_{p\gamma}} \right] \exp \left\{ -i(\varepsilon_{p\gamma} + \operatorname{Re} \Sigma(p\gamma; T_{p\gamma})) \tau - \right. \\ &\quad \left. - |\tau| \left[\operatorname{Im} \Sigma(p\gamma; T_{p\gamma}) + \Gamma_{p\gamma} \left(\frac{\partial \operatorname{Re} \Sigma(p\gamma; \omega)}{\partial \omega} \right)_{\omega=T_{p\gamma}} \right] \right\}, \end{aligned} \quad (3.15)$$

in the derivation of which a small term of the type $(\partial \operatorname{Im} \Sigma(p\gamma; \omega)/\partial \omega)_{\omega=T_{p\gamma}}$ was omitted, and the new functions $\operatorname{Re} \Sigma(p\gamma; \omega)$ and $\operatorname{Im} \Sigma(p\gamma; \omega)$ are respec-

tively equal to

$$\left. \begin{aligned} \operatorname{Re} \Sigma(p\gamma; \omega) &= \frac{P}{V} \sum_q g^2(q) \frac{\omega_q}{2} \left(\frac{1 - \bar{n}_{p+q, \gamma} + \bar{v}_q}{\omega - T_{p+q, \gamma} - \omega_q} + \frac{\bar{n}_{p+q, \gamma} + \bar{v}_q}{\omega - T_{p+q, \gamma} + \omega_q} \right) \\ \text{and} \\ \operatorname{Im} \Sigma(p\gamma; \omega) &= \frac{\pi}{V} \sum_q g^2(q) \frac{\omega_q}{2} \left[(1 - \bar{n}_{p+q, \gamma} + \bar{v}_q) \delta(\omega - T_{p+q, \gamma} - \omega_q) + \right. \\ &\quad \left. + (\bar{n}_{p+q, \gamma} + \bar{v}_q) \delta(\omega - T_{p+q, \gamma} + \omega_q) \right]. \end{aligned} \right\} \quad (3.16)$$

Comparing the limiting expression obtained for $A_{p\gamma}(\tau)$ with the standard functional form of the one-particle spectral density in the asymptotic region, we obtain the expression both for the elementary excitation spectrum of quasi-particles and for their damping:

$$\left. \begin{aligned} T_{p\gamma} &= \varepsilon_{p\gamma} + \operatorname{Re} \Sigma(p\gamma; T_{p\gamma}), \\ \Gamma_{p\gamma} &= \frac{\operatorname{Im} \Sigma(p\gamma; T_{p\gamma})}{1 - \left(\frac{\partial \operatorname{Re} \Sigma(p\gamma; \omega)}{\partial \omega} \right)_{\omega=T_{p\gamma}}}. \end{aligned} \right\} \quad (3.17)$$

Thus the problem is completely solved and the results obtained differ advantageously from those known earlier (see, for example, [17]) by a more consistent inclusion of the spectrum of elementary excitations $T_{p\gamma}$, in the corresponding self-consistent equations.

3.3 The simplest approximation for the Bose spectral density $R_q(\omega)$

As in the previous case, the simplest approximation for the spectral density $R_q(\omega)$ must involve scattering processes, since the approximation by only one pole term of the spectral decomposition (3.6) is trivial. Apart from the pole term, one graph will be included which corresponds to the simplest scattering process into an intermediate state with two quasi-particles:



$$(3.18)$$

All the rest, i.e., more complicated scattering processes, will be ignored. When repeated scattering processes into the same intermediate states are taken into account, the spectral density $R_q(\omega)$ in this approximation has the following functional form:

$$R_q(\tau) = Z_q^{-1} \exp \left\{ -i \Omega_q \tau + \frac{1}{V} \sum_{p\gamma} |Q_{p\gamma}(q)|^2 \frac{\exp[-i(T_{p+q, \gamma} - T_{p\gamma} - \omega_q)\tau]}{(T_{p+q, \gamma} - T_{p\gamma} - \omega_q)^2} \right\}, \quad (3.19)$$

where $|Q_{p\gamma}(q)|^2$ is a reduced square of the matrix element with the parametrization

$$|Q_{p\gamma}(q)|^2 = |\mathcal{F}(q)|^2 [(1 - \bar{n}_{p+q, \gamma}) \bar{n}_{p\gamma} - \bar{n}_{p+q, \gamma} (1 - \bar{n}_{p\gamma})]. \quad (3.20)$$

Here $|\mathcal{F}(q)|^2$ is the same function as in (3.12). The determination of the unknown functional parameters within the first three moments,

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} \mathcal{R}_q(\omega) &= 1, \\ \int \frac{d\omega}{2\pi} (\omega - \omega_q) \mathcal{R}_q(\omega) &= 0, \\ \int \frac{d\omega}{2\pi} (\omega - \omega_q)^2 \mathcal{R}_q(\omega) &= \frac{1}{V} \sum_{p\gamma} g^2(q) \frac{\omega_q}{2} (\bar{n}_{p\gamma} - \bar{n}_{p+q, \gamma}), \end{aligned} \right\} \quad (3.21)$$

leads to the following expressions:

$$\left. \begin{aligned} Z_q &= \exp \left\{ \frac{1}{V} \sum_{p\gamma} |Q_{p\gamma}(q)|^2 [T_{p+q, \gamma} - T_{p\gamma} - \omega_q]^{-2} \right\}, \\ \Omega_q &= \omega_q - \frac{1}{V} \sum_{p\gamma} |Q_{p\gamma}(q)|^2 [T_{p+q, \gamma} - T_{p\gamma} - \omega_q]^{-1}, \\ |\mathcal{F}(q)|^2 &= g^2(q) \frac{\omega_q}{2}. \end{aligned} \right\} \quad (3.22)$$

Thus, the one-particle spectral density in this approximation has the following simple functional form:

$$\begin{aligned} \mathcal{R}_q(\tau) &= \exp \left\{ -i \omega_q \tau + \frac{1}{V} \sum_{p\gamma} |Q_{p\gamma}(q)|^2 \times \right. \\ &\times \left. \left(\frac{\exp[-i(T_{p+q, \gamma} - T_{p\gamma} - \omega_q)\tau] - 1}{(T_{p+q, \gamma} - T_{p\gamma} - \omega_q)^2} + \frac{i\tau}{T_{p+q, \gamma} - T_{p\gamma} - \omega_q} \right) \right\}, \end{aligned} \quad (3.23)$$

and after having gone over to the asymptotic region $\tau \rightarrow \pm \infty$ and determined the new functions

$$\left. \begin{aligned} \text{Re } H(q; \omega) &= \frac{P}{V} \sum_{p\gamma} g^2(q) \frac{\omega_q}{2} \frac{\bar{n}_{p\gamma} - \bar{n}_{p+q, \gamma}}{\omega - T_{p+q, \gamma} + T_{p\gamma}} \\ \text{and} \\ \text{Im } H(q; \omega) &= \frac{\pi}{V} \sum_{p\gamma} g^2(q) \frac{\omega_q}{2} [\bar{n}_{p\gamma} - \bar{n}_{p+q, \gamma}] \delta(\omega - T_{p+q, \gamma} + T_{p\gamma}), \end{aligned} \right\} \quad (3.24)$$

one easily obtains the corresponding expressions both for the elementary excitation spectrum of quasi-particles and for their damping:

$$\left. \begin{aligned} \Omega_q &= \omega_q + \text{Re } H(q; \omega_q), \\ \Gamma_q &= \frac{\text{Im } H(q; \omega_q)}{1 - \left(\frac{\partial \text{Re } H(q; \omega)}{\partial \omega} \right)_{\omega=\omega_q}}. \end{aligned} \right\} \quad (3.25)$$

Thus the problem is completely solved.

4. Application of the Spectral Density Method to Special Models of Statistical Physics

4.1 Heisenberg-Ising model — Spin wave spectrum

The spin wave spectrum in magnetically ordered systems is at present under intense theoretical and experimental investigation. The interest in this problem increased considerably after the papers of Dyson [18] and other authors [19] who showed that at low temperatures it is mainly the spin wave spectrum that is responsible for all thermodynamic and kinetic properties of those systems. Fundamental theoretical results in this field were obtained for ferromagnetics in the classical works by Bloch [20], Holstein and Primakoff [21], and for anti-ferromagnetics by Anderson [22] and Kubo [23]. For recent results, reference should be made to the monographs of Tyablikov [5] and of Akhieser et al. [24]. Until recently these systems were treated on the basis of the Bose formalism suggested by Dyson and Maleev [25], and only not long ago calculation methods directly in terms of spin operators [26] appeared. However, these methods, just like the usual decoupling of the equations of motion for the Green functions in terms of spin operators (see, for example, [5]), in the general case are still rather complicated and require further improvement. The main difficulty hampering to obtain a simple and effective method of calculations in the framework of magnetically ordered systems is due to the peculiarity of the commutation relations of the spin operators. In view of this it would be particularly interesting to apply the spectral density method to such systems where the above mentioned difficulty has no principle meaning.

Below we shall restrict ourselves to consider the spin wave spectrum within the anisotropic Heisenberg model

$$H = \sum_{i,m} I_{i,m} \{ \rho (S_i^x S_m^x + S_i^y S_m^y) + g S_i^z S_m^z \} - \hbar \sum_j S_j^z \quad (4.1)$$

for spin 1/2 in an external magnetic field. Calculations will be made for a model with ferromagnetic ordering implying the nearest-neighbour interaction only. The spin wave spectrum is to be determined as a singularity of the one-particle spectral density,

$$\mathcal{F}_{\mu\nu}(\omega) = -\langle [S_{\mu}^{-}; S_{\nu}^{+}(\tau)]_{-} \rangle_{\omega}, \quad (4.2)$$

expressed directly in terms of the spin operators $S_{\mu}^{\pm} = S_{\mu}^x \pm i S_{\mu}^y$, which in the simplest approximation, according to the general procedure of the spectral density method, can be approximated by one δ -function term:

$$\mathcal{F}_{\mu\nu}(\omega) = \psi_{\mu\nu} 2\pi \delta(\omega - \omega_{\mu\nu}). \quad (4.3)$$

Provided the spectrum is found in a self-consistent way, this approximation is interpolating for all temperatures and must lead to a correct temperature dependence of the spin wave spectrum at rather low temperatures since in this case the spin waves are practically undamped excitations. The unknown functional parameters $\psi_{\mu\nu}$ and $\omega_{\mu\nu}$ are determined from the set of the two first

moments,

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} \mathcal{F}_p(\omega) &= R, \\ \int \frac{d\omega}{2\pi} (\omega - h) \mathcal{F}_p(\omega) &= \left(g \frac{I(p)}{I(0)} - \varrho \right) \frac{2}{M} \sum_k I(k) \bar{n}_k + \\ &+ \left(\varrho \frac{I(p)}{I(0)} - g \right) \frac{4}{M} \sum_k I(k) \langle S^z S^z \rangle_k; \\ \bar{n}_k &= \langle S^- S^+ \rangle_k, \quad R = 2 \langle S_\mu^z \rangle, \end{aligned} \right\} \quad (4.4)$$

and, according to (4.3), have the simple form

$$\left. \begin{aligned} \psi_p &= R, \\ \omega_p &= h + \frac{1}{R} \left(g \frac{I(p)}{I(0)} - \varrho \right) \frac{2}{M} \sum_k I(k) \bar{n}_k + \\ &+ \frac{1}{R} \left(\varrho \frac{I(p)}{I(0)} - g \right) \frac{4}{M} \sum_k I(k) \langle S^z S^z \rangle_k; \quad R \neq 0. \end{aligned} \right\} \quad (4.5)$$

Further calculations in the framework of (4.5) make use both of the spectral representation for the function (4.2),

$$\mathcal{F}_p(\omega) = Z^{-1} \sum_{m,n} |(S_p^+)_{m,n}|^2 2\pi \delta(\omega - E_m + E_n) e^{-\beta E_m} (e^{\beta\omega} - 1), \quad (4.6)$$

a direct consequence of which is the formula for the average magnon occupation numbers,

$$\bar{n}_p = \int \frac{d\omega}{2\pi} \frac{\mathcal{F}_p(\omega)}{\exp \beta \omega - 1}, \quad (4.7)$$

and of the spectral representation for higher-order correlation functions analogous to (4.6). The latter representation makes it possible to convert the equation of motion for the one-particle spectral density $\mathcal{F}_{\mu\nu}(\omega)$ and to obtain the expression for the correlation function $\langle S_k^z S_k^z \rangle$ through $\mathcal{F}_k(\omega)$ without the usual procedure of decoupling of higher correlation functions:

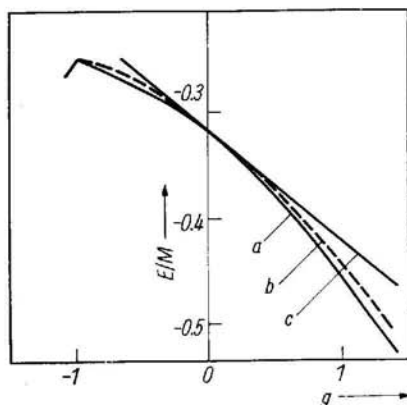
$$\frac{4g}{M} \sum_k I(k) [\langle S_k^z S_k^z \rangle - \langle S_k^z \rangle \langle S_k^z \rangle] = \frac{2}{M} \sum_k \int \frac{d\omega}{2\pi} \frac{(\omega - h) \mathcal{F}_k(\omega)}{\exp \beta \omega - 1} - \frac{2\varrho}{M} \sum_k I(k) \bar{n}_k. \quad (4.8)$$

Equations (4.7) and (4.8) permit a self-consistent calculation of the spin wave spectrum, which, after all the simple algebra within (4.5), is determined as a solution of the rather complicated non-linear self-consistent equation

$$\begin{aligned} \omega_p &= h + g \frac{I(p)}{I(0)} (1 - \kappa^2) \frac{1}{M} \sum_k \frac{I(k)}{I(0)} \coth \frac{\beta \omega_k}{2} + R (\varrho I(p) - g I(0)) \times \\ &\times \frac{1 + (1 - \kappa^2) (1/M \sum_k (I(k)/I(0)) \coth (\beta \omega_k)/2)^2}{1 - (R \kappa)/M \sum_k (I(k)/I(0)) \coth (\beta \omega_k)/2}; \quad \kappa = \frac{\varrho}{g}, \end{aligned} \quad (4.9)$$

and considerably differs from the results of analogous calculations making use of all other approximate methods except the variational method [27]. The calculations of [27], however, are carried out only for the isotropic model and are, therefore, of limited applicability.

Fig. 1. Dependence of the ground state energy on g for the one-dimensional Heisenberg-Ising model ($\varrho = 1$). (a) Method of spectral densities (identical with the exact solution); (b) method of linear canonical transformation; (c) Hartree-Fock approximation



The renormalization of the spin wave spectrum obtained here is a direct consequence of the more accurate handling with the higher correlation functions inherent to the spectral density method and, compared with the results of the method of the mean field, leads to a more correct temperature dependence both for the spin wave spectrum and the spontaneous magnetization.

Note that for the one-dimensional model, due to the possibility to replace the spin operators exactly by Fermi operators, equation (4.1) takes the form

$$H = \frac{Mg}{4} - \sum_p (\varrho \cos p + g) a_p^+ a_p + \frac{g}{M} \sum_{p_1 \dots p_4} \delta_{p_1 + p_2; p_3 + p_4} \cos(p_2 - p_3) a_{p_1}^+ a_{p_2}^+ a_{p_3} a_{p_4}. \quad (4.10)$$

The corresponding calculations are easily made also up to more complicated approximations. For example, for the Hamiltonian (4.10) one succeeds to develop in a rather simple way an approximation of the one-particle spectral density by two δ -functions [9], what corresponds to antiferromagnetic ordering. The numerical results obtained in this approximation were compared with those of the other approximate methods. It was shown that the spectral density method fits the exactly known ground state energy of this model better than any other known method (see Fig. 1).

4.2 Bardeen-Cooper-Schrieffer model of superconductivity

We shall proceed from a rather simple and well-known model Hamiltonian [28]

$$H = \sum_k \varepsilon_k a_k^+ a_k + \frac{g}{2V} \sum_{p,k} V_{p;k} a_p^+ a_{-p}^+ a_{-k} a_k, \quad (4.11)$$

which is the basis of the Bardeen-Copper-Schrieffer theory of superconductivity [14] and is developed by some other authors (see, for example, [29]). This model can be solved exactly [30] and is of particular interest since it clears up the possibilities of various approximate methods. The exact solution of this model will be presented below in a rather simple way via the spectral density method, thus demonstrating the efficiency of this method when applied to an essentially non-trivial model of statistical physics.

As in Section 2.4 of the present review, the calculations will make use of the matrix technique. The one-particle spectral density is defined in the

form of a 2×2 matrix:

$$\mathbf{\Lambda}(k; \omega) = \begin{pmatrix} \langle [a_k^+; a_k(\tau)]_+ \rangle_\omega & \langle [a_k^+; a_{-k}^+(\tau)]_+ \rangle_\omega \\ \langle [a_{-k}; a_k(\tau)]_+ \rangle_\omega & \langle [a_{-k}; a_{-k}^+(\tau)]_+ \rangle_\omega \end{pmatrix}, \quad (4.12)$$

containing the normal and anomalous spectral functions and satisfying the matrix system of the corresponding moments.

Let us find the solution of this model in the simplest approximation, i.e., approximating the one-particle spectral density by one matrix δ -function:

$$\mathbf{\Lambda}(k; \omega) = 2\pi \delta(\omega - \mathbf{M}^{(1)}(k)), \quad (4.13)$$

and determining the unknown functional parameters within the set of the two first moments:

$$\int \frac{d\omega}{2\pi} \mathbf{\Lambda}(k; \omega) = \mathbf{I}, \quad \int \frac{d\omega}{2\pi} \omega \mathbf{\Lambda}(k; \omega) = \mathbf{M}^{(1)}(k);$$

$$\mathbf{M}^{(1)}(k) = \varepsilon_k \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 0 & +\frac{g}{V} \sum_p V_{k;p} \langle a_p^+ a_{-p}^+ \rangle \\ +\frac{g}{V} \sum_p V_{k;p} \langle a_{-p} a_p \rangle & 0 \end{pmatrix}.$$

It can be easily seen by comparison with the known results that the solution thus obtained is exact. In fact, estimating the eigenvalues of the matrix $\mathbf{M}^{(1)}(k)$, we immediately obtain the well-known expression for the elementary excitation spectrum:

$$E_k = \sqrt{\Delta_k^2 + \varepsilon_k^2}; \quad \Delta_k = +\frac{g}{V} \sum_p V_{k;p} \langle a_{-p} a_p \rangle, \quad (4.14)$$

and representing the function of the matrix in an explicit form, we find the known expression for both the normal and anomalous spectral densities:

$$\mathbf{\Lambda}(k; \omega) = \pi \begin{pmatrix} 1 + \frac{\varepsilon_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} & \frac{\Delta_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} \\ \frac{\Delta_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} & 1 - \frac{\varepsilon_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} \end{pmatrix} \delta(\omega - \sqrt{\Delta_k^2 + \varepsilon_k^2}) +$$

$$+ \pi \begin{pmatrix} 1 - \frac{\varepsilon_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} & -\frac{\Delta_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} \\ -\frac{\Delta_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} & 1 + \frac{\varepsilon_k}{\sqrt{\Delta_k^2 + \varepsilon_k^2}} \end{pmatrix} \delta(\omega + \sqrt{\Delta_k^2 + \varepsilon_k^2}). \quad (4.15)$$

The self-consistent equation determining the energy gap in the elementary excitation spectrum is a direct consequence of the spectral properties of the function (4.13) and has the usual form

$$\Delta_k = -\frac{g}{2V} \sum_p \frac{V_{k;p} \Delta_p}{\sqrt{\Delta_p^2 + \varepsilon_p^2}} \tanh \frac{\beta \sqrt{\Delta_p^2 + \varepsilon_p^2}}{2}. \quad (4.16)$$

One can convince oneself that this is an exact solution also by calculating the subsequent moments for the one-particle spectral density and substituting the above solution into them. In practice it is sufficient to prove that with a reasonable decoupling of the higher correlation functions, several subsequent

moments are satisfied. This is just the case for this model and, therefore, from this point of view it may also be stated that this solution is in accord with the exact one.

Thus we see that the exact solution of the Bardeen-Cooper-Schrieffer model of superconductivity corresponds to the simplest approximation of the spectral density method, whereas, for example, the usual perturbation treatment of this model is quite helpless.

4.3 Electron correlations in narrow energy bands — Interpolating solution of the Hubbard model

Explanation of ferromagnetism (antiferromagnetism) and of the electron behaviour in narrow energy bands has been a subject of investigation by a number of authors [32]. The interest in these problems increased even more after the metal-dielectric transition was discovered in some oxides of transition metals (for example Ti_2O_3 , VO, V_2O_3 , etc.) and qualitatively considered by Mott [33]. Actually at low temperatures a substance exhibits the properties of the antiferromagnet and dielectric (semiconductor), but as the temperature increases, the magnetic ordering is broken at a certain point T_{cr} . This occurs practically at the same point where the conductivity sharply increases, i.e., the substance becomes a metal. This phenomenon cannot be explained by a simplified band theory since the oxides of the transition metals have their d-shells not completely occupied and must be metals. In fact, however, for a substance whose crystal lattice has a large distance between ions (narrow conductivity bands), this generally takes place at high temperatures only. As the temperature decreases, a strong Coulomb repulsion leads to the electron localization in the centres and the substance becomes a dielectric (semiconductor). Thus, the electron correlations must be taken into account when describing the electron behaviour in narrow energy bands, and a physical model to be comparable with experiment therefore cannot be constructed without taking electron correlations into account.

A realistic model involving electron correlations and being not too complicated mathematically was recently suggested by Hubbard [34] and was further developed in a number of papers (see, for example, [35], [36], and [37]). In the second quantization representation, the Hamiltonian of this model is easily reduced to the following form:

$$H = \sum_{p\gamma} \varepsilon_p \gamma a_{p\gamma}^+ a_{p\gamma} + \frac{g}{M} \sum_{p_1 \dots p_4} \delta_{p_1+p_2; p_3+p_4} a_{p_1\uparrow}^+ a_{p_2\downarrow}^+ a_{p_3\downarrow} a_{p_4\uparrow}, \quad (4.17)$$

where ε_p is the dispersion law for free electrons in the energy band, summation is everywhere carried out within the band, M is the number of centres in the crystal lattice, g is the strength of the Coulomb interaction between two electrons with opposite spins at the same centre. It is convenient to assume that $\varepsilon_p = \varrho \eta_p - \mu$ where μ is the chemical potential of the system, ϱ is a constant, and $\eta_p = \sum_{i=1}^t \cos p^{(i)}$. Such a choice of the dispersion law is rather realistic in

most cases and, besides, it leads to considerable mathematical simplifications. The aim of this section is to construct an interpolating solution for this model with the aid of the spectral density method, and to compare it with the known approximate results and in some limiting cases with exact solutions. The most attention is paid to take consistently into account all possible pair correlations,

which are not small in this model and are mainly responsible for all the quantitative results. We shall restrict ourselves below to consider the ferromagnetic ordering or paramagnetic phase taking account only of one-particle excitations. The solution obtained here is valid in the whole temperature range and for any ratio of coupling constants as well as for any density n (n is the number of electrons at a centre). Moreover, in the free electron limit $g = 0$ and in the Heitler-London limit $\varrho = 0$ this solution becomes exact. In all the intermediate region, this solution gives a simplest interpolation approximation.

Exact solutions for both the limiting cases within this model are easily found, and their simplest interpolation is the approximation of the one-particle spectral density $A_{p\uparrow}(\omega)$ through a set of two different δ -functions:

$$A_{p\uparrow}(\omega) = \pi (1 + \gamma_{p\uparrow}) \delta(\omega - E_{p\uparrow}^{(1)}) + \pi (1 - \gamma_{p\uparrow}) \delta(\omega + E_{p\uparrow}^{(2)}), \quad (4.18)$$

with a subsequent determination of the functional parameters within the set of the first four moments:

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} A_{p\uparrow}(\omega) &= 1, \\ \int \frac{d\omega}{2\pi} (\omega - \varepsilon_p) A_{p\uparrow}(\omega) &= g n_{\downarrow}, \\ \int \frac{d\omega}{2\pi} (\omega - \varepsilon_p)^2 A_{p\uparrow}(\omega) &= g^2 n_{\downarrow}, \\ \int \frac{d\omega}{2\pi} (\omega - \varepsilon_p)^3 A_{p\uparrow}(\omega) &= g^3 n_{\downarrow} - 2g^2 n_{\downarrow} (1 - n_{\downarrow}) \varrho \psi_{p\uparrow}. \end{aligned} \right\} \quad (4.19)$$

This set in the chosen class of the approximating functions is easily transformed into a set of corresponding equations:

$$\left. \begin{aligned} E_{p\uparrow}^{(1,2)} &= E_{p\uparrow} \pm U_{p\uparrow}; \\ E_{p\uparrow} &= \sqrt{\left[\varrho \psi_{p\uparrow} - \frac{g}{2} (1 - 2n_{\downarrow}) \right]^2 + g^2 n_{\downarrow} (1 - n_{\downarrow})}, \\ \gamma_{p\uparrow} &= \frac{\varrho \psi_{p\uparrow} - (g/2) (1 - 2n_{\downarrow})}{E_{p\uparrow}}, \quad U_{p\uparrow} + \varrho \psi_{p\uparrow} = \varepsilon_p + \frac{g}{2}, \end{aligned} \right\} \quad (4.20)$$

connecting the elementary excitation spectrum with exact correlation functions. The latter enter (4.20) through the parameter ψ_p , which, after easy calculations, using equal-time commutation relations and the explicit expression for the one-particle spectral density, can be represented as

$$\begin{aligned} 2n_{\downarrow} (1 - n_{\downarrow}) \psi_{p\uparrow} &= 2n_{\downarrow} (1 - n_{\downarrow}) C_{\uparrow} + n_{\downarrow} \eta_p + \\ &+ \frac{1}{M^2} \sum_{p_1 \dots p_4} \delta_{p_1+p_2; p_3+p_4} \eta_{p_1+p-p_2} \langle a_{p_1\downarrow}^+ a_{p_2\downarrow}^+ a_{p_3\downarrow} a_{p_4\downarrow} \rangle + \\ &+ \frac{1}{M^2} \sum_{p_1 \dots p_4} \delta_{p_1+p_2; p_3+p_4} (\eta_{p_2+p-p_1} + \eta_{p_3+p_4-p}) \langle a_{p_1\uparrow}^+ a_{p_2\downarrow}^+ a_{p_3\downarrow} a_{p_4\uparrow} \rangle, \end{aligned} \quad (4.21)$$

where by definition $2n_{\downarrow} (1 - n_{\downarrow}) C_{\uparrow} = t [(1 - 2n_{\uparrow}) u_{\downarrow} + 2n_{\uparrow} (1 - n_{\uparrow}) \vartheta_{\downarrow}]$ and

the new functions u_{\downarrow} and ϑ_{\downarrow} have the following form:

$$u_{\downarrow} = \frac{1}{tM} \sum_p \eta_p \bar{n}_{p\downarrow}, \quad \vartheta_{\downarrow} = \frac{g}{tM} \sum_p \eta_p \frac{F_{p\downarrow}}{E_{p\downarrow}}; \quad (4.22)$$

$$F_{p\downarrow} = \frac{1}{2} \frac{\sinh \beta E_{p\downarrow}}{\cosh \beta U_{p\downarrow} + \cosh \beta E_{p\downarrow}}.$$

The approximation of the one-particle spectral density thus obtained corresponds, for the density of states, to the two-band approximation with sharp boundaries and satisfies the qualitative picture of the phenomenon in this point. The success of further calculations, however, crucially depends on an accurate handling of the two-particle correlation functions determining the parameter $\psi_{p\uparrow}$.

These functions will be calculated here within the one-particle approach which, though ignoring collective modes, takes consistently account of the corresponding one-particle excitations. The simple decoupling of the binary correlation functions in (4.21) would be much worse in this respect.

In view of what has been said above, let us now define the three two-particle spectral densities:

$$\left. \begin{aligned} A_{p_1\downarrow; p_1\uparrow}^{(1)}(\omega) &= \sum_{p_2; p_3} \delta_{p_1+p_2; p_3+p_1} \langle [a_{p_1\uparrow}^+ a_{p_2\downarrow}^+ a_{p_3\downarrow}; a_{p_1\uparrow}(\tau)]_+ \rangle_{\omega}, \\ A_{p_1\downarrow; p_1\uparrow}^{(2)}(\omega) &= \sum_{p_2; p_3} \delta_{p_1+p_2; p_3+p_1} \langle [a_{p_1\uparrow}^+ a_{p_2\downarrow}^+ a_{p_3\downarrow}; a_{p_1\uparrow}(\tau)]_+ \rangle_{\omega}, \\ A_{p_1\downarrow; p_1\downarrow}^{(3)}(\omega) &= \sum_{p_2; p_3} \delta_{p_1+p_2; p_3+p_1} \langle [a_{p_1\downarrow}^+ a_{p_2\downarrow}^+ a_{p_3\downarrow}; a_{p_1\downarrow}(\tau)]_+ \rangle_{\omega}, \end{aligned} \right\} \quad (4.23)$$

after the estimation of which it is easy to find the parameter $\psi_{p\uparrow}$. In accordance with the choice made for $A_{p\uparrow}(\omega)$, the functional forms of all the three spectral densities are the same:

$$A_{p\gamma; k\sigma}^{(\nu)}(\omega) = \pi \mathcal{R}_{p\gamma; k\sigma}^{(\nu)} \{ (1 + b_{p\gamma; k\sigma}^{(\nu)}) \delta(\omega - E_{k\sigma}^{(1)}) + (1 - b_{p\gamma; k\sigma}^{(\nu)}) \delta(\omega + E_{k\sigma}^{(2)}) \}, \quad (4.24)$$

as well as all the further calculations of the functional parameters $\mathcal{R}_{p\gamma; k\sigma}^{(\nu)}$ and $b_{p\gamma; k\sigma}^{(\nu)}$ are. Therefore, we shall present here a detailed calculation of one of the two-particle spectral densities (the most complicated), and for the remaining two we shall give only the final results (see, for example, the appendix of [31]).

Specific calculations will be given for the function $A_{p_1\downarrow; p_1\downarrow}^{(3)}(\omega)$ within the set of the first two moments which are easily calculated and have rather a simple form:

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} A_{p_1\downarrow; p_1\downarrow}^{(3)}(\omega) &= \bar{n}_{p_1\downarrow} - M n_{\downarrow} \delta_{p_2; p_1}; \\ Z_{p\gamma; k\sigma}^{(\nu)} &= \int \frac{d\omega}{2\pi} \frac{A_{p\gamma; k\sigma}^{(\nu)}(\omega)}{\exp(\beta\omega) + 1}, \\ \int \frac{d\omega}{2\pi} (\omega - \varepsilon_{p_1}) A_{p_1\downarrow; p_1\downarrow}^{(3)}(\omega) &= -\frac{g}{M} \sum_{k_2 k_3} \delta_{p_1+k_2; k_3+p_1} Z_{k_2\uparrow; k_3\uparrow}^{(4)} + \\ &\quad + \int \frac{d\omega}{2\pi} \frac{\omega - \varepsilon_{p_2}}{\exp(\beta\omega) + 1} A_{p_2\downarrow}(\omega). \end{aligned} \right\} \quad (4.25)$$

This set of relations is however not closed and for the sake of self-consistency, we have to consider one more two-particle spectral density:

$$A_{p_1 \uparrow; p_4 \uparrow}^{(4)}(\omega) = \sum_{p_2 p_3} \delta_{p_1 + p_2; p_3 + p_4} \langle [a_{p_1 \uparrow}^+ a_{p_2 \downarrow}^+ a_{p_3 \downarrow}; a_{p_4 \uparrow}(\tau)]_+ \rangle_{\omega}, \quad (4.26)$$

which is also determined from the set of the first two moments,

$$\left. \begin{aligned} \int \frac{d\omega}{2\pi} A_{p_1 \uparrow; p_4 \uparrow}^{(4)}(\omega) &= \delta_{p_1; p_4} M n_{\downarrow}, \\ \int \frac{d\omega}{2\pi} (\omega - \varepsilon_{p_1}) A_{p_1 \uparrow; p_4 \uparrow}^{(4)}(\omega) &= g n_{\downarrow} - \frac{g}{M} \sum_{k_2 k_3} \delta_{p_1 + k_2; k_2 + p_4} Z_{k_2 \downarrow; k_2 \downarrow}^{(3)}, \end{aligned} \right\} \quad (4.27)$$

according to (4.24).

Now the set of relations (4.25) and (4.27) is closed and after the auxiliary spectral density $A_{p_1 \uparrow; p_4 \uparrow}^{(4)}(\omega)$ is eliminated, one can obtain a simple integral equation for the unknown function $Z_{p_2 \downarrow; p_4 \downarrow}^{(3)}$:

$$\frac{E_{p_2 \downarrow}}{F_{p_2 \downarrow}} Z_{p_2 \downarrow; p_4 \downarrow}^{(3)} = Q_{p_2 \downarrow; p_4 \downarrow}^{(3)} + d_{\uparrow} \frac{g}{M} \sum_{k_2 k_3} \delta_{p_2 + k_2; p_4 + k_2} Z_{k_2 \downarrow; k_2 \downarrow}^{(3)}, \quad (4.28)$$

the exact solution of which is rather simple:

$$\frac{E_{p_2 \downarrow}}{F_{p_2 \downarrow}} Z_{p_2 \downarrow; p_4 \downarrow}^{(3)} = Q_{p_2 \downarrow; p_4 \downarrow}^{(3)} + \frac{d_{\uparrow}}{1 - d_{\uparrow} d_{\downarrow}} \frac{g}{M} \sum_{k_2 k_3} \delta_{p_2 + k_2; p_4 + k_2} \frac{F_{k_2 \downarrow}}{E_{k_2 \downarrow}} Q_{k_2 \downarrow; k_2 \downarrow}^{(3)}. \quad (4.29)$$

The new functions d_{\uparrow} and $Q_{p_2 \downarrow; p_4 \downarrow}^{(3)}$ were obtained in the solution procedure to be

$$\left. \begin{aligned} d_{\uparrow} &= \frac{g}{M} \sum_p \frac{F_{p \uparrow}}{E_{p \uparrow}}, \\ Q_{p_2 \downarrow; p_4 \downarrow}^{(3)} &= \delta_{p_2; p_4} M n_{\downarrow} \left(g n_{\downarrow} d_{\uparrow} - \frac{E_{p_2 \downarrow}}{F_{p_2 \downarrow}} \bar{n}_{p_2 \downarrow} \right) - \\ &\quad - g n_{\downarrow} d_{\uparrow} + g^2 n_{\uparrow} (1 - n_{\uparrow}) \frac{F_{p_2 \downarrow}}{E_{p_2 \downarrow}} + \frac{E_{p_2 \downarrow}}{F_{p_2 \downarrow}} \bar{n}_{p_2 \downarrow} \bar{n}_{p_4 \downarrow}. \end{aligned} \right\} \quad (4.30)$$

If now the spectral properties of the function $A_{p_2 \downarrow; p_4 \downarrow}^{(3)}(\omega)$ are taken into account it is easy to derive the validity of the following expression:

$$\frac{1}{M^2} \sum_{p_1 \dots p_4} \delta_{p_1 + p_2; p_3 + p_4} \eta_{p_1 + p - p_2} \langle a_{p_1 \downarrow}^+ a_{p_2 \downarrow}^+ a_{p_3 \downarrow} a_{p_4 \downarrow} \rangle = \frac{1}{M^2} \sum_{p_2 p_4} \eta_{p_2 + p - p_2} Z_{p_2 \downarrow; p_4 \downarrow}^{(3)}, \quad (4.31)$$

which enables us to find a part of the function $\psi_{p \uparrow}$ in a self-consistent way (see formula (4.31)). The function $\psi_{p \uparrow}$ can be completely calculated in a closed form if the remaining two-particle spectral densities are dealt with in an analogous way.

All the calculations being made, the function $\psi_{p \uparrow}$ turns out to be representable as a sum of the two other functions, i.e. $\psi_{p \uparrow} = C_{p \uparrow} + \theta_{\uparrow} \eta_p$, the function θ_{\uparrow} being

of the following simple form:

$$\theta_{\uparrow} = \frac{1}{2} \left\{ 1 - \frac{\vartheta_{\uparrow} u_{\downarrow}}{n_{\downarrow} (1 - n_{\downarrow})} \left(\frac{n R}{1 - d_{\uparrow}} + \frac{1 - n}{1 + d_{\uparrow}} \right) + \frac{u_{\downarrow}}{n_{\downarrow} (1 - n_{\downarrow})} \left(\frac{u_{\downarrow}}{1 - d_{\uparrow} d_{\downarrow}} + \frac{2 u_{\uparrow}}{1 - d_{\uparrow}^2} \right) + \frac{n_{\uparrow} (1 - n_{\uparrow})}{n_{\downarrow} (1 - n_{\downarrow})} \left(\frac{\vartheta_{\downarrow}}{1 - d_{\uparrow} d_{\downarrow}} + \frac{2 d_{\uparrow} \vartheta_{\uparrow}}{1 - d_{\uparrow}^2} \right) \vartheta_{\downarrow} \right\}. \quad (4.32)$$

When obtaining the solution (4.32), we need not impose any limitations on the coupling constant g (g can be either positive or negative) and the temperature T . This solution is valid under the only additional requirement $n_{\uparrow} (1 - n_{\uparrow}) d_{\downarrow} = n_{\downarrow} (1 - n_{\downarrow}) d_{\uparrow}$, which is easily obtained by considering the simple operator equality

$$\begin{aligned} & \frac{1}{M^2} \sum_{p_1, \dots, p_4} \delta_{p_1+p_2; p_3+p_4} \langle a_{p_1 \uparrow}^+ a_{p_2 \downarrow}^+ a_{p_3 \downarrow} a_{p_4 \uparrow} \rangle = \\ & = \frac{1}{M^2} \sum_{p_1, \dots, p_4} \delta_{p_1+p_2; p_3+p_4} \langle a_{p_1 \downarrow}^+ a_{p_2 \uparrow}^+ a_{p_3 \uparrow} a_{p_4 \downarrow} \rangle \end{aligned} \quad (4.33)$$

and expressing both its parts through the one-particle spectral density. The self-consistent equations determining u_{\downarrow} and ϑ_{\downarrow} are easily obtained with the aid of (4.22) and the explicit form of the one-particle spectral density. However, since the thermodynamic properties of the system are not investigated in this section, we shall not write down their explicit form.

It is of interest now to compare the above equation for the function θ_{\uparrow} (see equation (4.35)) with the analogous equation of [36] obtained within the limit $g \rightarrow \infty$ and under the assumption that electrons occupy the low levels which it can most readily reach, in other words at $\beta \rightarrow \infty$. A complete agreement between both self-consistent equations can be obtained if we take into account the above assumptions and simplify (4.32) with the aid of the following approximate expressions:

$$\left. \begin{aligned} \vartheta_{\uparrow} &\approx \frac{u_{\uparrow}}{1 - n_{\downarrow}}, & d_{\uparrow} &\approx \frac{n_{\uparrow}}{1 - n_{\downarrow}}; \\ n_{\uparrow} &= \frac{1 - n_{\downarrow}}{M} \sum_p [\exp(-\beta E_{p \uparrow}^{(2)}) + 1]^{-1}, \end{aligned} \right\} \quad (4.34)$$

but in $E_{p \uparrow}^{(2)}$ it is necessary to keep only the lower terms of the expansion in ϱ/g . It should be noted, however, that the expression (4.34) is not a direct expansion of the exact expressions, for example with respect to ϱ/g or to $1/\beta$, though the fact that these parameters are small is essential. The expression (4.34) rather reflects a certain summation of this or that kind of diagrams in this limiting case. Thus all the results of [36] are contained in the solution (4.32) found above which, being more general, provides their consistent improvement.

Further the comparison is worth being discussed of the solution obtained here with the exact solution in the one-dimensional case found by Lieb and Wu [37]. Comparison of the corresponding expressions showed (see Fig. 2) a rather good coincidence in the whole region of g at $\varrho \neq 0$ ($\varrho = -2$) between the exact expression for the energy of the ground state and the corresponding

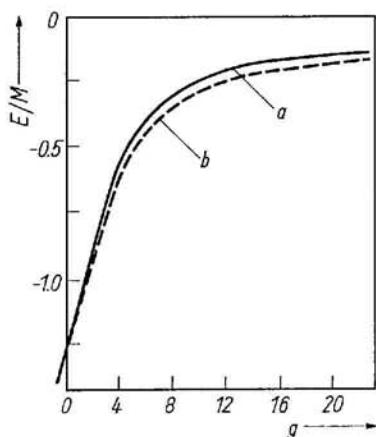


Fig. 2. Dependence of the ground state energy on g for the one-dimensional Hubbard model ($q = -2$). (a) Exact solution; (b) method of spectral densities

expression following from the above formulae at $n = 1$, $n_{\uparrow} = n_{\downarrow}$, and $T = 0$,

$$\frac{E}{M} = \frac{g}{4} + \frac{g^2 k}{4 \pi \theta^2} \left(1 - \frac{\theta}{2}\right) K(k) - \frac{4 E(k)}{\pi k}; \quad k = \frac{1}{\sqrt{1 + g^2/(16 \theta^2)}}, \quad (4.35)$$

where $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kind, respectively, and the parameter θ is defined as a solution of the c-numerical self-consistent equation

$$\theta = \frac{1}{2} \left(1 + \frac{12 u^2}{1 - d^2}\right); \quad d = \frac{g k}{2 \pi \theta} K(k), \quad u = \frac{E(k)}{\pi k} - \frac{g^2 k}{16 \pi \theta^2} K(k). \quad (4.36)$$

Thus, according to what has been said we can be sure that the solution obtained here, at least in what concerns the macroscopic properties, corresponds to the true situation, i.e. takes a rather effective account of binary correlations and, therefore, can be recommended as a basis for further calculations.

As a whole, the method suggested here to construct interpolating solutions within the spectral density method can be useful and effective when being applied to concrete calculations.

4.4 Ising model — A set of equations for correlation functions

The Ising model is a rough attempt to describe the properties of a real physical substance showing a tendency to magnetic ordering. Ising [39] was the first to suggest this model to explain ferromagnetism, and to solve it exactly in the one-dimensional case. Further, this model was developed by a large number of authors. At present most fundamental results are obtained for various two-dimensional Ising lattices in the absence of an external field [40], the simplest of which was solved exactly by Onsager [41] after the paper of Kramers and Wannier [42]. As to two-dimensional Ising lattices in an external field and three-dimensional lattices even in the absence of an external field, there is no exact solution for any of them. The point is that the main methods for investigating (see, for example, [43]) this model are to a considerable extent heuristic and only suited to solve various two-dimensional Ising lattices in the absence of an external field. The application of more general methods of statistical physics

to solve this model provides an easy obtaining of a number of approximate solutions for any case. However, this method is less resultative in the limit of a removed external field.

In this connection the application of the spectral density method to this model is of particular interest now. On the one hand, being exactly solved in many not-trivial cases, this model enables us to control the efficiency of approximate solutions within the framework of the latter; on the other hand, since this method is equally efficient in any case irrespective either of the dimensionality of the model or of the presence of an external field, we may hope to extend the known results by means of this method.

Below, irrespective of the dimensionality of the model, we shall obtain a number of exact results concerning the functional form of the corresponding spectral densities and, as a straightforward consequence of these results, exact finite difference equations for the correlation functions will be written. For the one-dimensional Ising model in an external field one can easily obtain exact expressions both for the partition function and for all correlation functions.

Our starting point is the well-known model Hamiltonian

$$H = -h \sum_f S_f^z + g \sum_{m,f} I_{m,f} S_m^z S_f^z, \quad (4.37)$$

where h is the external field, g is the coupling constant, S_f^z is the z -component of the spin operator located at the f -site. We restrict ourselves here only to the cubic t -dimensional lattice with nearest-neighbour interaction:

$$I_{\mu\nu} = \sum_{m=0}^t \delta_{\mu_1; \nu_1} \cdots \frac{1}{2} (\delta_{\mu_m; \nu_{m+1}} + \delta_{\mu_{m+1}; \nu_m}) \cdots \delta_{\mu_t; \nu_t}. \quad (4.38)$$

Besides it is convenient to replace the spin operators by the Fermi operators

$$S_\mu^z = n_\mu - \frac{1}{2}; \quad n_\mu = a_\mu^+ a_\mu, \quad (4.39)$$

in terms of which the Hamiltonian (4.37) has the simple form

$$H = C + \sum_f \varepsilon n_f + g \sum_{m,f} I_{m,f} n_m n_f; \quad (4.40)$$

$$C = \frac{Nt}{2} \left(h + t \frac{g}{2} \right), \quad \varepsilon = -(h + tg),$$

and has been conveniently prepared for investigation with the aid of the spectral density method.

The thermodynamic quantities of (4.40) are conveniently investigated with the aid of the one-particle spectral density

$$A_\mu(\omega) = \langle [a_\mu^+; a_\mu(\tau)]_+ \rangle_\omega, \quad (4.41)$$

which can be easily calculated in a closed form for this model since the particle number density operators commute with the Hamiltonian of the system:

$$A_\mu(\tau) = \left\langle \exp \left\{ -i \left(\varepsilon + 2g \sum_\nu I_{\mu\nu} n_\nu \right) \tau \right\} \right\rangle. \quad (4.42)$$

Using further the definition of $I_{\mu\nu}$ (cf. equation (4.38)), we can write down the

infinite set of moments for $A_\mu(\omega)$ in form of a single recurrence relation:

$$\int \frac{d\omega}{2\pi} (\omega - \varepsilon)^r A_\mu(\omega) = g^r \sum_{m=0}^{2t} m^r d_{\mu|m}^{2t}; \quad r = 0, 1, \dots; \quad (4.43)$$

$$d_{\mu|m}^{2t} = \sum_{p=m}^{2t} (-1)^{m+p} \binom{p}{m} \langle II_p^{2t}(\mu) \rangle; \quad \binom{p}{m} = \frac{p!}{m!(p-m)!},$$

where $II_p^{2t}(\mu)$ is the sum of all possible combinations of the particle number density operators of the $2t$ nearest neighbours over p of the lattice point (μ) . The spectral density satisfying the whole infinite set of moments has the very simple form

$$A_\mu(\omega) = \sum_{m=0}^{2t} d_{\mu|m}^{2t} 2\pi \delta(\omega - \varepsilon - mg) \quad (4.44)$$

and solves the problem in principle if the coefficients $d_{\mu|m}^{2t}$ can be calculated in explicit form. In virtue of the translational invariance the quantities $d_{\mu|m}^{2t}$ evidently do not depend on the number of the lattice point (μ) and if they are known, the investigation of the thermodynamic properties of the system encounters no difficulties. For example, the average occupation numbers and the thermodynamic potential for the system are respectively given by the simple expressions

$$\bar{n} = \sum_{m=0}^{2t} \frac{d_m^{2t}}{\exp[\beta(\varepsilon + mg)] + 1} \quad \left. \vphantom{\sum_{m=0}^{2t}} \right\} \quad (4.45)$$

$$\text{and} \quad \frac{\Omega - \Omega_0}{Nt} = t \frac{g}{4} + \frac{1}{2} \int_0^g dg_1 \sum_{m=0}^{2t} \frac{(m-2t) d_m^{2t}}{\exp[\beta(\varepsilon + mg)] + 1}, \quad \left. \vphantom{\int_0^g} \right\}$$

where the thermodynamic potential of the system, Ω_0 , for $g = 0$ usually can be easily calculated.

For studying the correlation functions it is necessary to consider the μ -particles spectral density

$$A_{i_\mu \dots i_1}(\omega) = \langle [n_{i_\mu} \dots n_{i_1} a_{i_1}^+; a_{i_1}(\tau)]_+ \rangle_\omega, \quad (4.46)$$

where it is essential that $i_1 \neq (i_\mu \dots i_2)$. In analogy to $A_\mu(\omega)$, the infinite system of moments for the spectral density (4.46) can also be written down in form of a single recurrence relation:

$$\int \frac{d\omega}{2\pi} (\omega - \varepsilon)^r A_{i_\mu \dots i_1}(\omega) = g^r \sum_{m=0}^{2t} m^r d_{i_\mu \dots i_1|m}^{2t}, \quad (4.47)$$

and then we can directly verify that the solution of the set (4.47) is given by a spectral density of the following form:

$$A_{i_\mu \dots i_1}(\omega) = \sum_{m=0}^{2t} d_{i_\mu \dots i_1|m}^{2t} 2\pi \delta(\omega - \varepsilon - mg), \quad (4.48)$$

where $d_{i_\mu \dots i_1 | m}^{2t}$ are the natural generalizations of expression (4.43):

$$d_{i_\mu \dots i_1 | m}^{2t} = \sum_{m=p}^{2t} (-1)^{m+p} \binom{p}{m} \langle n_{i_\mu} \dots n_{i_1} II_p^{2t}(i_1) \rangle. \quad (4.49)$$

Now, utilizing the spectral properties of the function (4.46), we define the μ -particle correlation function:

$$W_{i_\mu \dots i_1} = \langle n_{i_\mu} \dots n_{i_1} \rangle = \int \frac{d\omega}{2\pi} \frac{A_{i_\mu \dots i_1}(\omega)}{\exp \beta \omega + 1}, \quad (4.50)$$

for which, using the explicit form of the spectral density (4.48), the simple set of equations can be easily obtained:

$$W_{i_\mu \dots i_1} = \sum_{m=0}^{2t} \frac{d_{i_\mu \dots i_1 | m}^{2t}}{\exp [\beta (\varepsilon + m g)] + 1}. \quad (4.51)$$

These equations form the basic set for determining the correlation functions of the Ising model with an arbitrary number of dimensions. Here we restrict ourselves to an exact solution of this set for the one-dimensional model with the topology of a closed ring.

In this case the set (4.51) has a very simple form and after substituting in accordance with (4.49), the explicit form of the coefficients $d_{i_\mu \dots i_1 | m}^{2t}$

$$\left. \begin{aligned} d_{i_\mu \dots i_1 | 0}^2 &= W_{i_\mu \dots i_2, i_1-1, i_1+1} + W_{i_\mu \dots i_2} - (W_{i_\mu \dots i_2, i_1-1} + W_{i_\mu \dots i_2, i_1+1}), \\ d_{i_\mu \dots i_1 | 1}^2 &= (W_{i_\mu \dots i_2, i_1+1} + W_{i_\mu \dots i_2, i_1-1}) - 2 W_{i_\mu \dots i_2, i_1+1, i_1-1}, \\ d_{i_\mu \dots i_1 | 2}^2 &= W_{i_\mu \dots i_2, i_1+1, i_1-1}, \end{aligned} \right\} \quad (4.52)$$

reduces to the following equations:

$$W_{i_\mu \dots i_1} + s (W_{i_\mu \dots i_2, i_1-1} + W_{i_\mu \dots i_2, i_1+1}) = \frac{W_{i_\mu \dots i_2}}{\exp (\beta \varepsilon) + 1} + r W_{i_\mu \dots i_2, i_1+1, i_1-1}, \quad (4.53)$$

where s and r are known functions:

$$\left. \begin{aligned} s &= \left(\frac{1}{\exp (\beta \varepsilon) + 1} - \frac{1}{\exp [\beta (\varepsilon + g)] + 1} \right), \\ r &= \left(\frac{1}{\exp (\beta \varepsilon) + 1} - \frac{2}{\exp [\beta (\varepsilon + g)] + 1} + \frac{1}{\exp [\beta (\varepsilon + 2g)] + 1} \right). \end{aligned} \right\} \quad (4.54)$$

We note that (4.53) is valid if $i_1 \neq (i_\mu \dots i_2)$, and is the basic equation for the one-dimensional Ising model.

If the external field is switched off, we have $r = 0$, and the set of equations (4.53) is decoupled into closed equations of a more simple form:

$$W_0 | i_\mu \dots i_1 + s_0 (W_0 | i_\mu \dots i_1-1 + W_0 | i_\mu \dots i_1+1) = \frac{W_0 | i_\mu \dots i_2}{\exp (-\beta g) + 1}, \quad (4.55)$$

where s_0 is the value of s for $h = 0$. In what follows we denote the quantities corresponding to a switched-off external field by the subscript zero. Further, without loss of generality we can assume that $i_\mu > i_{\mu-1} > \dots > i_1$ since the particle number density operators (cf. equation (4.50)) commute; in what follows this condition will be essentially exploited. In virtue of translational invariance, the correlation function depends only on the differences between the

subscripts, i.e., $W_0|_{i_\mu \dots i_1} = W_0(\gamma_{\mu-1} \dots \gamma_1)$, where $\gamma_l = i_{l+1} - i_l$, and one can easily verify that the solution which has a correct behaviour for $N \rightarrow \infty$ has the following form:

$$W_0(\gamma_{\mu-1} \dots \gamma_1) = \bar{n}_0 \sigma_0(\gamma_{\mu-1}) \dots \sigma_0(\gamma_1), \quad (4.56)$$

i.e., in the limit $N \rightarrow \infty$ the μ -particle correlation function is represented in a multiplicative form with the aid of the simple functions

$$\sigma_0(\gamma) = \frac{1}{2} \left[1 + (-1)^\gamma \left(\tanh \frac{\beta g}{4} \right)^\gamma \right]. \quad (4.57)$$

Now we proceed to consider the case $\hbar \neq 0$. In this case $r \neq 0$ and it is necessary to solve the complete set of equations. If $N \rightarrow \infty$, however, it can be shown that the correlation functions retain as before their multiplicative form (4.56), and so we obtain again a simple equation for $\sigma(\gamma)$:

$$\sigma(\gamma) + s[\sigma(\gamma+1) + \sigma(\gamma-1)] = [\exp(\beta \varepsilon) + 1]^{-1} + r \sigma(\gamma-1) \sigma(2), \quad (4.58)$$

which must be solved in accordance with the boundary conditions for $\sigma(\gamma)$: $\sigma(0) = 1$; $\sigma(\gamma)|_{\gamma \rightarrow \infty} \rightarrow \text{const.}$ Now, provided the solution of the equation (4.58) is written down as follows:

$$\sigma(\gamma) = b x^\gamma + \kappa, \quad (4.59)$$

one can obtain the set of coupled non-linear equations for the three functions:

$$\left. \begin{aligned} b + \kappa &= 1, & x + s(x^2 + 1) &= r(b x^2 + \kappa), \\ \kappa(1 + 2s) - r\kappa(b x^2 + \kappa) &= [\exp(\beta \varepsilon) + 1]^{-1}, \end{aligned} \right\} \quad (4.60)$$

which are solved in the usual manner. For this it is needed to introduce the new variables $\kappa = \frac{1}{2}(1 + R)$, $b = \frac{1}{2}(1 - R)$, and to carry out a fractional-linear transformation of the simple form

$$\frac{R - \tanh(\beta \hbar/2)}{R + \tanh(\beta \hbar/2)} = x. \quad (4.61)$$

Then the first equation of the set (4.60) is reduced to a degenerate quadratic equation which is easily solved:

$$R^2 = \frac{\sinh^2(\beta \hbar/2)}{\sinh^2(\beta \hbar/2) + \exp(\beta g)}. \quad (4.62)$$

By a direct substitution we verify now that the second equation of the set (4.60) is satisfied identically and for x and R the following expressions hold:

$$\left. \begin{aligned} x &= \frac{\cosh(\beta \hbar/2) - \sqrt{\sinh^2(\beta \hbar/2) + \exp(\beta g)}}{\cosh(\beta \hbar/2) + \sqrt{\sinh^2(\beta \hbar/2) + \exp(\beta g)}}, \\ R &= \frac{\sinh(\beta \hbar/2)}{\sqrt{\sinh^2(\beta \hbar/2) + \exp(\beta g)}}. \end{aligned} \right\} \quad (4.63)$$

Thus, the function $\sigma(\gamma)$ is completely determined, and then, according to (4.56) we have an expression for all the correlation functions of the system for $\hbar \neq 0$ and $N \rightarrow \infty$.

Now we proceed to consider the thermodynamic quantities of this system. According to the formulae (4.45), in order to determine all the thermodynamical properties of the system it is sufficient to know the quantities $d_{m_i}^2$ which according to (4.43) have the following form:

$$d_0^2 = 1 + W(2) - 2\bar{n}, \quad d_1^2 = 2(\bar{n} - W(2)), \quad d_2^2 = W(2), \quad (4.64)$$

i.e., we see that all the thermodynamic quantities of the system are determined by the single correlation function $W(2)$.

First of all we calculate average occupation numbers for which in accordance with (4.45) one can obtain the following expression:

$$\bar{n} = \frac{1}{(1 + 2s) [\exp(\beta \varepsilon) + 1]} + \frac{r}{1 + 2s} W(2), \quad (4.65)$$

where r and s are the functions determined earlier (cf. equation (4.54)). Comparing this expression with the second expression of the set (4.60) and taking into account that $W(2) = \bar{n}(bx^2 + \kappa)$, we find that $\bar{n} = \kappa = \frac{1}{2}(1 + R)$.

Further, defining the magnetization per unit spin by the expression $(2/N) \sum_{i=1}^N \langle S_i^z \rangle$ we easily verify, utilizing (4.39), that the previously defined quantity R is the magnetization of the system. In view of its importance we reproduce it explicitly once again:

$$R = \frac{\sinh(\beta h/2)}{\sqrt{\sinh^2(\beta h/2) + \exp(\beta g)}}. \quad (4.66)$$

Thus we see that when the external field is switched off, the magnetization of the system vanishes, i.e., the one-dimensional Ising lattice does not exhibit any spontaneous magnetization.

Further it is of interest to calculate the thermodynamic potential, which in this case is merely the free energy. Using the formulae (4.45) and (4.46) we find after straightforward transformations the following expression:

$$\frac{F - F_0}{N} = \frac{g}{4} - \int_0^g dg_1 \left(\frac{1 + W(2) - 2\bar{n}}{\exp(\beta \varepsilon) + 1} + \frac{\bar{n} - W(2)}{\exp[\beta(\varepsilon + g_1)] + 1} \right), \quad (4.67)$$

which after simple calculations is reduced to an integral over the coupling constant:

$$\frac{F - F_0}{N} = \frac{g}{4} - \int_0^g \frac{dg_1 \exp(\beta g_1)}{2 \sqrt{\sinh^2(\beta h/2) + \exp(\beta g_1)} [\cosh(\beta h/2) + \sqrt{\sinh^2(\beta h/2) + \exp(\beta g_1)}]}. \quad (4.68)$$

The integral (4.68) and F_0 (the free energy for $g = 0$) are evaluated in an elementary manner and we finally obtain the well known result [44]

$$\frac{F}{N} = \frac{g}{4} - \frac{1}{\beta} \ln \left[\cosh \frac{\beta h}{2} + \sqrt{\sinh^2 \frac{\beta h}{2} + \exp(\beta g)} \right]. \quad (4.69)$$

Thus we can see that the solution of the set of equations for the correlation functions is efficient enough, for it enables us to find not only the thermodynamical potential, but also all the correlation functions of the system in view. Unfortunately, the solution of the analogous equations for the two- and three-dimensional Ising lattice encounter at present some difficulties of mathematical origin.

5. Concluding Remarks

In this review article we confined ourselves to present the spectral density method and to illustrate the efficiency of its lowest approximations as applied to various problems and models of statistical physics. Particular attention was paid throughout the paper to self-consistent calculations since it is only with the help of them that one may expect to describe in an accurate and efficient enough way the various anomalies in the macroscopic quantities of the systems subject to phase transitions.

The procedures for the self-consistent calculations suggested here are all of quasi-particle origin, i.e., the damping is considered to be small everywhere. It would thus be meaningless to treat it in a self-consistent manner. It is the elementary excitation spectrum that is found within the self-consistent scheme, the damping being estimated after the corresponding self-consistent equations have been solved.

It is worth noting that the sequence of approximations in the spectral density method considerably differs from that of the ordinary methods insofar as every new approximation implies new self-consistent equations and not corrections to the previous solution. Such a feature makes it possible to examine the efficiency of the chosen approximation even for systems with no ordinary small parameters. The sequence of approximations may be considered to be satisfactory if every new approximation preserves the qualitative features of the previous one.

In conclusion, we should point out some problems that are thought of as being especially important for further development of the spectral density method and its applications. Those are the presentation of the variational method via the spectral densities, the search for scale-invariant solutions in various models of statistical physics, and the further specification of the approximations given above to include efficiently the quasi-particle damping.

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