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# *THE METHOD OF SPECTRAL DENSITIES IN QUANTUM STATISTICAL MECHANICS*

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A system of equations for the spectral densities is proposed for the purpose of solving problems in quantum statistical mechanics. The effectiveness of this method is demonstrated by solving the BCS model of superconductivity and the one-dimensional quantum Ising model with anisotropic interaction. In the latter instance the solution obtained here is an essential improvement over results derived previously by means of other methods.

## 1. INTRODUCTION

THE use of methods from quantum field theory in quantum statistical mechanics and many-body theory has witnessed a considerable development. This refers in the first place to the Green's function technique (in momentum space) in quantum statistics.[1] Since in this case all thermodynamic properties are determined from the one-particle Green's function, the fundamental problem reduces to finding a sufficiently accurate approximation for this function. The system of equations for the Green's functions is an infinite coupled system of equations, expressing the n-particle Green's function in terms of the Green's functions of higher numbers of particles. Therefore, in attempting to solve this system, one must truncate it, and in each stage of truncation the system turns out to be incomplete; only an approximation procedure, expressing the Green's spectral function in terms of lower order functions completes this truncated system. This can be done consistently only in those cases when the problem involves a smallness parameter permitting the separation and summation of essential diagrams and leading to a good approximation for the one-particle Green's function (or the mass operator). In those cases when the problem does not have a small parameter, the problem of obtaining a finite system of approximating equations which is closed has not yet been solved.

In this connection, the method of spectral densities, to be discussed below, may prove to be of considerable interest. The reason for this is the fact that in the final count all interesting quantities can be expressed in terms of the spectral density of the Green's functions. In particular, all thermodynamic characteristics of the system can be expressed in terms of the spectral density of the one-particle Green's function in a simple manner (cf. Eqs. (2.6), (2.7) and (2.10)). On the other hand, in quantum statistical mechanics there exists a close connection between the various expectation values of field operators in the grand canonical ensemble[1,2]. This circumstance allows one, taking into account the Hamiltonian of the system, to derive for these fundamental quantities (spectral densities of the one-particle Green's function) a closed system of exact equations, giving in integral form a relation between the various moments of the spectral densities and the equal-time commutators of the field operators with the Hamiltonian of the system (cf. (2.11)), thus reflecting the exact dynamics of the model under consideration. In terms of these relations all known approximation methods (the Hartree-Fock, method, the method of canonical transformations, etc.) could be reclassified according to the form of the spectral density and the number of exact relations in the system of moments of the spectral density satisfied by these methods. The principle for selecting the best approximation for the spectral density can be formulated in the following form: an approximation for the spectral function will be better if number of exact relations it satisfies rigorously is larger. Thus, the Hartree-Fock method corresponds to solving the equations in the class of functions which approximate the spectral density by means of a single delta function (cf. (2.20)), the first two moments of the spectral density being rigorously satisfied (the normalization condition involves the zeroth and first moments). Further, considering the solution for the spectral density in the class of two delta functions, one obtains that for the model Hamiltonian (cf. Sec. 3 and the end of Sec. 4) this is equivalent to the method of linear canonical transformations. However, in the general case of a four-fermion interaction the results obtained are considerably better than those guaranteed by the method of linear canonical transformations (cf. Sec. 4). In this case the spectral density satisfies rigorously three relations in the system of moments, as compared to two for the Hartree-Fock approximation.

In the present paper we expose the essence of the method (Sec. 2) and concrete applications to solving the BCS model of superconductivity (Sec. 3) and the one-dimensional quantum Ising model with anisotropic interaction (Sec. 4).

## 2. THE METHOD OF SPECTRAL DENSITIES (A CLOSED SYSTEM OF EQUATIONS)

We consider a system of interacting fermions in a volume V. The dynamical behavior of the system is defined by giving the Hamiltonian $H = H(a^+_{p,\gamma}; a_{p,\gamma})$, where $a^+_{p,\gamma}$ and $a_{p,\gamma}$ are the field operators satisfying the canonical anticommutation relations associated to Fermi statistics. We shall be interested in the sequel in systems with binary interactions for which the Hamiltonian conserves the total particle number.

The thermodynamic properties of such a system are conveniently investigated by means of a function of the form

$$\Lambda_{p,\gamma}(\tau) = \langle [\overset{+}{a}_{p,\gamma};\, a_{p,\gamma}(\tau)]_{+} \rangle, \tag{2.1}$$

which we shall from now on call the first spectral density, or simply spectral density. The expectation value everywhere is understood to be over the Gibbs grand canonical ensemble; $a_{p,\gamma}$ is the field operator in the Heisenberg picture. Taking the Fourier transform of the spectral density $\Lambda_{p,\gamma}(\tau)$ and assuming that the Hamiltonian admits a complete set of eigenstates, i.e., that $H|n\rangle = E_n|n\rangle$ and $\langle n|n\rangle = 1$, one can write a spectral representation of the function $\Lambda_{p,\gamma}(\omega)$ in terms of the variable $\omega$. Transforming directly the definition of the spectral density (2.1), we obtain

$$\Lambda_{p,\gamma}(\omega) = \sum_{m,n} \langle n|\overset{+}{a}_{p,\gamma}|m\rangle \langle m|a_{p,\gamma}|n\rangle e^{-\beta E_n} 2\pi\delta(\omega + E_m - E_n)(1 + e^{\beta\omega}). \tag{2.2}$$

Thus, $\Lambda_{p,\gamma}(\omega)$ is a real positive definite quantity. Analyzing Eq. (2.2) one can see that the average occupation numbers are easily expressed in terms of the spectral density:

$$\bar{n}_{p,\gamma} = \langle \overset{+}{a}_{p,\gamma} a_{p,\gamma} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\Lambda_{p,\gamma}(\omega)}{1 + e^{\beta\omega}}. \tag{2.3}$$

We now show that for the case of a pair interaction the energy of the equilibrium state with given density of physical particles is easily expressed in terms of the spectral density. Indeed, let the Hamiltonian of the system have the form:

$$H = H_0 + H_{int}, \qquad H_0 = \sum_{p,\gamma} \varepsilon_{p,\gamma} \overset{+}{a}_{p,\gamma} a_{p,\gamma}, \tag{2.4}$$

where $\epsilon_{p,\gamma}$ is an arbitrary real function containing in the usual manner the chemical potential $\mu$ of the system. Then, using the equation of motion for the Heisenberg field operators, one obtains for the spectral density the equation

$$\left(i\frac{\partial}{\partial\tau} - \varepsilon_{p,\gamma}\right)\Lambda_{p,\gamma}(\tau) = \langle [[H_{int};\, \overset{+}{a}_{p,\gamma}]_{-};\, a_{p,\gamma}(\tau)]_{+} \rangle. \tag{2.5}$$

Utilizing in the right-hand side of (2.5) the spectral representations obtained in a form analogous to (2.2), then for the case of a pair interaction one can assert that the following formulas are valid even if the concrete form of $H_{int}$ is not specified:

$$\frac{E_{int}}{V} = \frac{\langle H_{int} \rangle}{V} = \frac{1}{2V} \sum_{p,\gamma} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{(\omega - \varepsilon_{p,\gamma})\Lambda_{p,\gamma}(\omega)}{1 + e^{\beta\omega}} \tag{2.6}$$

and similarly, after a simple manipulation

$$\frac{E - \mu N}{V} = \frac{\langle H \rangle}{V} = \frac{1}{2V} \sum_{p,\gamma} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{(\omega + \varepsilon_{p,\gamma})\Lambda_{p,\gamma}(\omega)}{1 + e^{\beta\omega}}. \tag{2.7}$$

The formulas are easily verified to be true by directly calculating the right-hand side of (2.5) and using for $H_{int}$, e.g., the expression:

$$H_{int} = \frac{g}{V} \sum_{\gamma_1;\, p_1 \dots p_4;\, \gamma_2} \delta_{p_1+p_2;\, p_3+p_4}\, \varphi(p_2 - p_3)\, \overset{+}{a}_{p_1,\gamma_1} \overset{+}{a}_{p_2,\gamma_2} a_{p_3,\gamma_2} a_{p_4,\gamma_1}, \tag{2.8}$$

where g is a coupling constant taking arbitrary real values and $\varphi(p_2 - p_3) = \varphi(p_3 - p_2)$ is the arbitrary real function which defines the interaction. A sufficiently large number of practically interesting problems leads to $H_{int}$ of the form (2.8); however in the derivation of (2.6) and (2.7) only the pair character of the interaction is essential, and not its concrete form.

In a similar manner one can derive the other equations which are important for a study of the thermodynamic properties of the system, e.g., an expression for the (Helmholtz) thermodynamic potential $\Omega = -\beta^{-1} \ln Z$ can be obtained in terms of the spectral density, $\Lambda_{p,\gamma}(\omega)$ where

$$Z = \mathrm{Sp}\, e^{-\beta H}. \tag{2.9}$$

In this computation we assume that Eq. (2.6) is valid and we do not specify the explicit form of $H_{int}$; we also assume that $\epsilon_{p,\gamma}$ does not depend on g (cf. (2.8)), although the generalization to that case is obvious. Differentiating $\Omega$ with respect to g and then integrating, we derive the following formulas:

$$\frac{\partial}{\partial g}\left(\frac{\Omega}{V}\right) = \frac{1}{g}\left(\frac{E_{int}}{V}\right),$$

$$\left(\frac{\Omega - \Omega_0}{V}\right) = \frac{1}{2V} \sum_{p,\gamma} \int_0^g \frac{dg_1}{g_1} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{(\omega - \varepsilon_{p,\gamma})\Lambda_{p,\gamma}(\omega)}{1 + e^{\beta\omega}}, \tag{2.10}$$

where $\Omega_0$ is the thermodynamic potential for g = 0, a quantity one can usually easily calculate.

Thus, for the determination of all thermodynamic characteristics of the system it suffices to know the spectral density $\Lambda_{p,\gamma}(\omega)$. If the spectral density is known, the remainder of the investigation does not present any difficulty.

We now indicate a method which allows one to calculate the spectral density, given the Hamiltonian of the system. In this case, using the definition of $\Lambda_{p,\gamma}(\omega)$ and the equation of motion for the Heisenberg field operators, we obtain the following infinite system of moments:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^m \Lambda_{p,\gamma}(\omega) = \langle [[H, \dots [H, \overset{+}{a}_{p,\gamma}]]_{-}^{m};\, a_{p,\gamma}]_{+} \rangle, \quad m = 0, 1, \dots, \tag{2.11}$$

i.e., knowing the explicit form of the Hamiltonian of the system we can in principle calculate the right-hand sides of the equations (2.11), giving the moments of the spectral density $\Lambda_{p,\gamma}(\omega)$. However even in this case there remains a problem, since the expressions obtained in this manner have to be made self-consistent, i.e., expressed in terms of the $\Lambda_{p,\gamma}(\omega)$, and only in this case will the system be closed and we have the possibility to find the exact explicit form of the first spectral density. This method allows one to solve a series of classical problems, and also problems for which the number of independent commutators is finite. Nevertheless, for the majority of practically important problems this way of posing the problem is unrealistic, in view of the absence of recurrence relations among the various moments and the complicated form of the expressions obtained in this manner.

However one can always indicate a closed system of relations for the spectral density $\Lambda_{p,\gamma}(\omega)$. Indeed, assuming the validity of the expression (2.4) for the total Hamiltonian we obtain an operator expression for the first moment of the system (2.11):

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon_{p,\gamma}) \Lambda_{p,\gamma}(\omega) = \langle [[H_{int};\, \overset{+}{a}_{p,\gamma}]_{-};\, a_{p,\gamma}]_{+} \rangle. \tag{2.12}$$

If $H_{int}$ is given explicitly (cf. (2.8)) it is easy to compute this expression, and we find that the zeroth and first moments are of the form

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Lambda_{p,\gamma}(\omega) = 1,$$

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon_{p,\gamma}) \Lambda_{p,\gamma}(\omega) = 2g\varphi(0)n - \frac{2g}{V} \sum_{p_1} \varphi(p - p_1) \bar{n}_{p_1}, \quad (2.13)$$

where we assume that $\varphi(0)$ is a finite quantity, otherwise one must make the Hamiltonian of the system more precise. These two relations are self-consistent, since $\bar{n}_{p,\gamma}$ is easily expressed in terms of $\Lambda_{p,\gamma}(\omega)$ (cf. (2.3)) and is exact.

Further, we compute the second moment of the spectral density $\Lambda_{p,\gamma}(\omega)$. Using (2.4) one can write the following operator expression:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon_{p,\gamma})^2 \Lambda_{p,\gamma}(\omega) = \langle [[H_{int}; \overset{+}{a}_{p,\gamma}]_-; [a_{p,\gamma}; H_{int}]_-]_+ \rangle. \quad (2.14)$$

One can evaluate this expression explicitly for $H_{int}$ in the form (2.8). Indeed, simple transformations of the equal-time commutators leads to

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon_{p,\gamma})^2 \Lambda_{p,\gamma}(\omega) = L(\beta | g)$$

$$+ \left(\frac{2g}{V}\right) \sum_{p_1} \varphi(p - p_1) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon_{p_1,\gamma}) \Lambda_{p_1,\gamma}(\omega) \operatorname{th} \frac{\beta\omega}{2}. \quad (2.15)$$

In the derivation of (2.15) we have used the spectral properties of $\Lambda_{p,\gamma}(\omega)$ and the equation of motion (2.5), and have expressed some of the two-particle correlation functions in a self-consistent manner. However at this stage the second moment of $\Lambda_{p,\gamma}(\omega)$ is still not self-consistent, since the effective constant of the problem is not expressed in terms of the first spectral density for an arbitrary potential. In order to obtain a closed set of relations for the case in which one considers the second moment of the spectral density (cf. (2.15)) it is necessary to introduce into consideration the higher spectral densities, for which the explicit form is selected according to the form of $H_{int}$. For a $H_{int}$ of the form (2.8) it is convenient to select the second spectral density in the form

$$A_{p_1,\gamma_1;\, p_4,\gamma_1}(\tau) = \sum_{p_2,\, p_3;\, \gamma_2} \delta_{p_1+p_2;\, p_3+p_4} \langle [\overset{+}{a}_{p_1,\gamma_1} a_{p_2,\gamma_2} a_{p_3,\gamma_2}; a_{p_4,\gamma_1}(\tau)]_+ \rangle. \quad (2.16)$$

In the same manner as in the case of the first spectral density $\Lambda_{p,\gamma}(\omega)$ one can write an infinite system of moments for $A_{p_1,\gamma_1;\, p_4,\gamma_1}(\omega)$ analogous to the system (2.11). This is not necessary, however, since the first two moments are completely sufficient for our purposes. Utilizing the explicit form of $H_{int}$ (cf. (2.8)), we obtain the following expressions:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_{p_1,\gamma_1;\, p_4,\gamma_1}(\omega) = (Vn\delta_{p_1,\, p_4} - \bar{n}_{p_1,\gamma_1}),$$

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon_{p_4,\gamma_1}) A_{p_1,\gamma_1;\, p_4,\gamma_1}(\omega) = 2gn\varphi(p_1 - p_4)$$

$$- \frac{2g}{V} \sum_{p_3} \varphi(p_1 - p_3) \bar{n}_{p_3,\gamma_1} + \left(\frac{2g}{V}\right)$$

$$\times \sum_{k_2,\, k_3;\, \gamma_3} \delta_{p_4+k_2;\, k_3+p_1} [\varphi(k_2 - k_3) - \varphi(p_4 - k_3)\delta_{\gamma_1,\gamma_3}] \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_{k_2,\gamma_3;\, k_3,\gamma_3}(\omega)}{1 + e^{\beta\omega}}$$

$$- \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\Lambda_{p_1,\gamma_1}(\omega)(\omega - \varepsilon_{p_1,\gamma_1})}{1 + e^{\beta\omega}}. \quad (2.17)$$

and now the effective coupling constant of the problem can be written in terms of $A_{p_1,\gamma_1;\, p_4,\gamma_1}(\omega)$ in the form

$$L(\beta | g) = \left(\frac{2g}{V}\right)^2 \sum_{p_1, p_2; \gamma_2} \varphi^2(p_1 - p_2) \bar{n}_{p_2,\gamma_2}$$

$$+ \left(\frac{2g}{V}\right)^2 \sum_{p_1,\, \gamma_1;\, p_4} \varphi^2(p_1 - p_4) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_{p_1\gamma_1;\, p_4\gamma_1}(\omega)}{1 + e^{\beta\omega}}$$

$$- 2g\varphi(0)n \left(\frac{2g}{V}\right) \sum_{p_1} \varphi(p - p_1). \quad (2.18)$$

The fact that the system (2.13), (2.15), (2.17) and (2.18) is again closed is remarkable, however now, in distinction from the first set of relations (2.13) this system effectively takes into account the two-particle correlations which appear when the interaction is switched on.

Further, if we do not restrict ourselves to considering only two-particle correlations, but are also interested in, e.g., three-particle correlation functions, it becomes necessary to consider the third moment of the first spectral density, which for the Hamiltonian (2.4) has the form

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (\omega - \varepsilon_{p,\gamma})^3 \Lambda_{p,\gamma}(\omega) = \langle [[[H_0; H_{int}]_-; a_{p,\gamma}{}^+]_-; [a_{p,\gamma}; H_{int}]_-]_+ \rangle$$

$$+ \langle [[H_{int}; [H_{int}; \overset{+}{a}_{p,\gamma}]]_-; [a_{p,\gamma}; H_{int}]_-]_+ \rangle. \quad (2.19)$$

However, the calculations for an arbitrary potential, even if $H_{int}$ is represented in the form (2.8), are sufficiently complicated, although for concrete special cases (cf. Sec. 3, Eq. (3.17)) they are entirely feasible. Nevertheless it is clearly visible that at each stage of the calculation one obtains a closed system of relations. Indeed, computing (2.19) for a system with pair interactions one can verify the appearance of three-particle correlation functions (the remainder will be self-consistent on the basis of the preceding stage of calculations). Then it is necessary to compute a system of moments for the three-particle correlation functions, or more correctly, the first two moments, which can be expressed in a self-consistent manner in terms of the same functions.

Thus the system of relations will again be self-consistent, exact, and closed, with the three-particle correlation functions taken into account exactly. In a similar way one can increase steadily the total number of relations considered for the first spectral density, relations which at each stage of the calculation will be self-consistent and closed, a feature which is absent from the usual Green's function method. The approximation to the spectral density $\Lambda_{p,\gamma}(\omega)$ will be the better, the higher the number of relations which it satisfies simultaneously. It now becomes necessary to indicate how the system of closed relations can be converted into a system of closed equations, and how to construct the simplest approximations to the spectral density $\Lambda_{p,\gamma}(\omega)$. It turns out that for this it suffices to assume a class of functions which can be selected for approximating $\Lambda_{p,\gamma}(\omega)$; within that class of functions we obtain a closed set of equations which can be solved by means of the usual methods.

Indeed, consider the system of equations (2.13) and assume that

$$\Lambda_{p,\gamma}(\omega) = 2\pi\delta(\omega - \omega_{p,\gamma}), \tag{2.20}$$

where $\omega_{p,\gamma}$ is the spectrum of one-particle elementary excitations, which has to be determined; then the second equation implies that $\omega_{p,\gamma}$ satisfies the integral equation

$$\omega_{p,\gamma} = (\varepsilon_{p,\gamma} + 2g\varphi(0)n) - \frac{2g}{V}\sum_{p_1}\frac{\varphi(p-p_1)}{1+\exp(\beta\omega_{p_1,\gamma})}, \tag{2.21}$$

which is typical for the Hartree-Fock approximation. This is understandable, since the selection of the spectral density in the form (2.20) corresponds to an attempt of replacing the real spectrum of elementary excitations by an effective undamped spectrum for the one-particle excitations. It is important that we can always control the selected approximation for the spectral density. Indeed, for this it is necessary to analyze the consecutive enlarged system of relations for the class of selected functions, i.e., in this case we must verify whether the equations (2.15) and (2.17) are valid, whether the spectral density is of the form (2.20) and the spectrum of elementary excitations satisfies the equation (2.21). We note that for the higher spectral density this will correspond to the usual decoupling (clustering), i.e.,

$$A_{p_1,\gamma_1;\,p_4,\gamma_1} = (Vn\delta_{p_1,\,p_4} - \bar{n}_{p_1,\gamma_1})2\pi\delta(\omega - \omega_{p_1,\gamma_1}), \tag{2.22}$$

and the enlarged system of relation will not be valid for an arbitrary potential and $g \neq 0$.

Thus the Hartree-Fock approximation for the Hamiltonian with pair interaction of the form (2.8) can be qualitatively justified only as a rough approximation, although in a series of cases it does not yield bad results. One must therefore treat ordinary perturbation theory with caution, though it yields in a first approximation the indicated result.

Further, it is easy to indicate a Hamiltonian for which the solution for the spectral density of the form (2.20) may be selected as a zero order approximation. In distinction from (2.8) this Hamiltonian has the form

$$H_{int} = \frac{g}{V}\sum_{p_1,\gamma_1;\,p_2;\gamma_2}[\varphi(0) - \varphi(p_1 - p_2)\delta_{\gamma_1,\gamma_2}]\,\overset{+}{a}_{p_1,\gamma_1}\overset{+}{a}_{p_2,\gamma_2}a_{p_2,\gamma_2}a_{p_1,\gamma_1}. \tag{2.23}$$

It is not hard to verify that for a Hamiltonian of the form (2.23) the equation (2.13) for the first spectral density remains valid; consequently the solution (2.20) is also valid, but now the second moment of the spectral density has a completely different form, namely

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega - \varepsilon_{p,\gamma})^2\Lambda_{p,\gamma}(\omega) = \left(\frac{2g}{V}\right)^2\sum_{p_1\gamma_1;\,p_2,\gamma_2}[\varphi(0) - \varphi(p - p_1)\delta_{\gamma,\gamma_1}] \times [\varphi(0) - \varphi(p - p_2)\delta_{\gamma,\gamma_2}]\langle n_{p_1,\gamma_1}n_{p_2,\gamma_2}\rangle. \tag{2.24}$$

This expression is obtained by direct calculation according to Eq. (2.24), utilizing the explicit form of the Hamiltonian $H_{int}$ (cf. (2.23)).

It is now sufficient to assume that $\langle n_{p_1,\gamma_1}n_{p_2,\gamma_2}\rangle \approx \bar{n}_{p_1,\gamma_1}\bar{n}_{p_2,\gamma_2}$ and it can be seen by direct substitution that the spectral density in the form (2.20) satisfies the second moment; and since the indicated factorization of the two-particle correlation function is usually valid for $|g| \ll 1$ (cf., e.g., the anisotropic quantum Ising model, Eq. (4.34)), one can definitely state that for the model with $H_{int}$ of the form (2.23) one can successfully use perturbation theory, where as a zeroth approximation one uses the spectral density in the form (2.20).

Thus we have demonstrated on the simplest example how to analyze the equations and their solution, as well as control methods. Further there arises the natural desire to improve the approximation for the spectral density $\Lambda_{p,\gamma}(\omega)$ in such a manner that it satisfies simultaneously the enlarged system of equations (2.13)–(2.17). For this it is important to enlarge the class of functions on which a new self-consistency equation can be derived by using the relations (2.13)–(2.17).

Based on physical considerations one could think that the simplest spectral density satisfying the formulated conditions will be of the form

$$\Lambda_{p,\gamma}(\omega) = \pi(1+\gamma_{p,\gamma})\delta(\omega - \omega_{p;\gamma}) + \pi(1-\gamma_{p,\gamma})\delta(\omega + \omega_{p,\gamma}), \tag{2.25}$$

where $\omega_{p,\gamma}$ and $\gamma_{p,\gamma}$ are unknown functions which have to be determined in the process of solution. The spectrum of elementary excitations obtained in this manner will effectively take into account the correlation among the interacting particles, i.e., the occurrence of collective excitations which, of course, is physically better justified than the Hartree-Fock approximation. The higher spectral density satisfying the system of relations (2.17) in the new class of functions may be selected in the form

$$A_{p_1;\gamma_1;\,p_4,\gamma_1}(\omega) = \pi(Vn\delta_{p_1,\,p_4} - \bar{n}_{p_1,\gamma_1})(1 + \nu_{p_1,\gamma_1;\,p_4,\gamma_1})\delta(\omega - \omega_{p_4,\gamma_1}) + \pi(Vn\delta_{p_1,\,p_4} - \bar{n}_{p_1,\gamma_1})(1 - \nu_{p_1,\gamma_1;\,p_4,\gamma_1})\delta(\omega + \omega_{p_4,\gamma_1}), \tag{2.26}$$

where $\nu_{p_1,\gamma_1;\,p_4,\gamma_1}$ are unknown functions which have to be determined, $\omega_{p,\gamma}$ is the spectrum of elementary excitations (cf. supra). Substituting now the expressions (2.25) and (2.26) into the extended system of relations (2.13) and (2.17), one can again obtain a system of closed integral equations for the determination of the spectrum of elementary excitations and of the function $\nu_{p_1,\gamma_1;\,p_4,\gamma_1}$, which determines the higher spectral density. However, in the general case such a program runs into computational difficulties and we shall realize it on concrete examples, to which we now proceed.

## 3. THE BCS MODEL OF SUPERCONDUCTIVITY

We start from a model Hamiltonian of the form

$$H = \sum_k \varepsilon_k a_k{}^+ a_k + \frac{g}{2V}\sum_{k_1,k_2} I(k_1,k_2)\,a_{k_1}{}^+\overset{+}{a}_{-k_1}a_{-k_2}a_{k_2}. \tag{3.1}$$

where $k = (p, \sigma)$, $-k = (-p, -\sigma)$; $\sigma$ is the spin index taking the values $\pm\frac{1}{2}$; p is the momentum; $\overset{+}{a}_k$, $a_k$ are operators satisfying the usual anticommutation relations of Fermi statistics; $I(k_1, k_2)$ is a real function satisfying the relations

$$I(k_1,k_2) = I(k_2,k_1), \quad I(-k_1,k_2) = -I(k_1,k_2). \tag{3.2}$$

The properties of the model can be studied by means of the spectral density defined in the usual manner (cf. (2.1)). Using the explicit form of the Hamiltonian one can write out the first three moments of the spectral density $\Lambda_k(\omega)$

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Lambda_k(\omega) = 1, \qquad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega - \varepsilon_k)\Lambda_k(\omega) = 0,$$

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega - \varepsilon_k)^2\Lambda_k(\omega) = \left(\frac{g}{V}\right)^2\sum_{k_1,k_2}I(k,k_1)I(k,k_2)\langle a_{k_1}{}^+\overset{+}{a}_{-k_1}a_{-k_2}a_{k_2}\rangle. \tag{3.3}$$

On the basis of the spectral properties in the variable $\omega$, $\Lambda_k(\omega)$ is a positive definite quantity. Then the left-hand side of the second moment is positive definite and it is convenient to use the notation

$$L_k^2 = \left(\frac{g}{V}\right)^2 \sum_{k_1,k_2} I(k, k_1) I(k, k_2) \langle a_{k_1}{}^+ a_{-k_1}^+ a_{-k_2} a_{k_2} \rangle. \tag{3.4}$$

Following the general method one should look for the solution of the system (3.3) in the form $\Lambda_k(\omega) = 2\pi\delta(\omega - \omega_k)$. However the first two equations yield $\omega_k = \epsilon_k$ and the second moment is not satisfied for any values of g except g = 0. Consequently this solution can only be a rough approximation. We note that a perturbative solution will lead to the solution indicated above if one does not sum over diagrams.

Further, in order to satisfy all the moments of the system (3.3), the spectral density must have the form

$$\Lambda_k(\omega) = \pi(1 + \gamma_k)\delta(\omega - \omega_k) + \pi(1 - \gamma_k)\delta(\omega + \omega_k), \tag{3.5}$$

and a direct substitution into the system (3.3) leads to the relations

$$\gamma_k = \varepsilon_k / \omega_k, \quad \omega_k = \sqrt{L_k^2 + \varepsilon_k^2}. \tag{3.6}$$

In order to determine $L_k^2$ it becomes necessary to consider the higher spectral density defined as follows

$$A_{k_1, k_2}(\tau) = \langle [a_{k_1}{}^+ a_{-k_1}{}^+ a_{-k_2}; \quad a_{k_2}(\tau)]_+ \rangle. \tag{3.7}$$

Utilizing the equations of motion for the field operators and the explicit form of the model Hamiltonian, we find that the first two moments of the higher spectral density (3.7) have the form

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_{k_1, k_2}(\omega) = 0,$$

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega A_{k_1, k_2}(\omega) = \frac{g}{V} \sum_{k_3} I(k_3, k_2) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_{k_1, k_3}(\omega)}{1 + e^{\beta\omega}}, \tag{3.8}$$

and their solution can be written in the form

$$A_{k_1, k_2}(\omega) = 2\pi\Gamma_{k_1, k_2}(\delta(\omega - \omega_{k_2}) - \delta(\omega + \omega_{k_2})), \tag{3.9}$$

where $\omega_k$ is the spectrum of elementary excitations, a known function (cf. (3.6)). After substituting into the system (3.8) we derive the integral equation for $\Gamma_{k_1, k_2}$:

$$\omega_{k_2}\Gamma_{k_1,k_2} = -\frac{g}{2V}\sum_{k_3} I(k_2, k_3)\Gamma_{k_1,k_3} \operatorname{th}\frac{\beta\omega_{k_3}}{2}. \tag{3.10}$$

One may seek the solution of Eq. (3.10) in the form $\omega_{k_2}\Gamma_{k_1, k_2} = \nu_{k_1} h_{k_2}$ (the multiplicative nature of the solution suggests that (3.10) involves a free index).

Then we obtain for $h_k$ the equation

$$h_k = -\frac{g}{2V}\sum_{k_3} \frac{I(k, k_3) h_{k_3}}{\omega_{k_3}} \operatorname{th}\frac{\beta\omega_{k_3}}{2}. \tag{3.11}$$

We now show that the function $\nu_k$ is easily expressed in terms of $h_k$. For this purpose we find for the energy gap the expression:

$$L_k^2 = -\left(\frac{g}{V}\right)^2 \sum_{k_1,k_2} \frac{I(k, k_1) I(k, k_2) \nu_{k_1} h_{k_2}}{\omega_{k_2}} \operatorname{th}\frac{\beta\omega_{k_2}}{2}. \tag{3.12}$$

where we have utilized the spectral properties and explicit form of $A_{k_1, k_2}(\omega)$, cf. (3.9).

We further note that the substitution $k_1 \leftrightarrow k_2$ in Eq. (3.4) does not lead to a change of this result; consequently, a similar picture is valid in the explicit form of $L_k^2$ (cf. (3.12), which for a general potential $I(k_1, k_2)$ is equivalent to the condition

$$\nu_k = \text{const}\cdot\frac{h_k}{\omega_k}\operatorname{th}\frac{\beta\omega_k}{2}. \tag{3.13}$$

The constant in (3.13) can be easily reconstructed by comparing, e.g., the expressions for the interaction energy computed by means of the first and second spectral densities, respectively. However, in principle, the presence of the constant is not important in order to derive the self-consistency equation for the energy gap, since (3.11) is homogeneous in $h_k$. Substituting (3.13) into (3.12) and using (3.11), we obtain the well-known self-consistency equation for the energy gap in the form

$$L_k = -\frac{g}{2V}\sum_{k_3} \frac{I(k, k_3) L_{k_3}}{\sqrt{L_{k_3}{}^2 + \varepsilon_{k_3}{}^2}} \operatorname{th}\frac{\beta\omega_{k_3}}{2}. \tag{3.14}$$

Thus the assumption that the spectral density $\Lambda_k(\omega)$ is of the form (3.5), and the solution of the equations for this model leads to an exact solution. The fact that this solution is indeed exact (up to 1/N) can be checked easily computing the third moment of the spectral density $\Lambda_k(\omega)$ and then substituting into it the solution obtained above. For the model under consideration the third moment is relatively easy to compute, and after making it self-consistent by means of the second spectral density $A_{k_1, k_2}(\omega)$ which has the explicit expression

$$A_{k_1, k_2}(\omega) = -\pi\frac{L_{k_1}L_{k_2}}{2\omega_{k_1}\omega_{k_2}} \operatorname{th}\frac{\beta\omega_{k_1}}{2}(\delta(\omega - \omega_{k_2}) - \delta(\omega + \omega_{k_2})), \tag{3.15}$$

we obtain the relatively simple expression:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}(\omega - \varepsilon_k)^3 \Lambda_k(\omega) = -2\varepsilon_k L_k^2 + 2L_k\left(\frac{g}{V}\right)\sum_{k_3} I(k, k_3) L_{k_3}\bar{n}_{k_3}$$
$$-2\left(\frac{g}{V}\right)^3 \sum_{k_1 \ldots k_3} I(k, k_1) I(k, k_2) I(k, k_3) \langle a_{k_3}^+ a_{-k_3}^+ a_{k_2}^+ a_{k_2} a_{-k_1} a_{k_1} \rangle. \tag{3.16}$$

Computing the integral in the left-hand side of (3.16) with the aid of the explicit form of the first spectral density, we find a condition which has to be satisfied if the solution we have found is exact. This condition has the form

$$L_k\left(\frac{g}{V}\right) \sum_{k_3} I(k, k_3) L_{k_3}\bar{n}_{k_3}$$
$$= \left(\frac{g}{V}\right)^3 \sum_{k_1 \ldots k_3} I(k, k_1) I(k, k_2) I(k, k_3) \langle a_{k_3}{}^+ a_{-k_3}^+ a_{k_2}{}^+ a_{k_2} a_{-k_1} a_{k_1} \rangle. \tag{3.17}$$

We note that the condition (3.17) is identically satisfied if the following equality holds

$$\langle a_{k_3}{}^+ a_{-k_3}{}^+ a_{-k_1} a_{k_1} a_{k_2}{}^+ a_{k_2} \rangle = \bar{n}_{k_2} \langle a_{k_3}{}^+ a_{-k_3}{}^+ a_{-k_1} a_{k_1} \rangle. \tag{3.18}$$

The latter equation is easily tested by introducing the three-particle spectral density, writing down its first two moments and solving in the class of two delta functions; consequently one might think that all subsequent relations will be satisfied, and then the solution obtained in this manner is exact (with accuracy 1/N).

Thus, we have not only solved the problem, but have effectively controlled the accuracy of the solution obtained.

## 4. THE ONE-DIMENSIONAL QUANTUM ISING MODEL

We consider a model of N interacting spins localized at the sites of a one-dimensional closed chain. Each of the spins interacts only with its nearest neighbor in an anisotropic manner. The Hamiltonian of the model has the form

$$H=\sum_{j=1}^{N}\left(S_j{}^xS_{j+1}^x+S_j{}^yS_{j+1}^y+\rho S_j{}^zS_{j+1}^z\right), \qquad (4.1)$$

where $S_j^k$ is the k-th component of the spin operator at the site j. Introducing the field operators $a_p^+$ and $a_p$ with the usual commutation relations of Fermi statistics, simple transformations lead to the Hamiltonian in the second-quantized representation:

$$H=\frac{N\rho}{4}-\sum_{p=-\pi}^{\pi}(\cos p+\rho)a_p{}^+a_p$$
$$+\frac{\rho}{N}\sum_{p_1\ldots p_4}\delta_{p_1+p_2;\,p_3+p_4}\cos(p_2-p_3)a_{p_1}{}^+a_{p_2}{}^+a_{p_3}a_{p_4}, \qquad (4.2)$$

where p is the momentum, $\rho$ is the anisotropy parameter, which can take arbitrary real values (cf.[3] for more details).

We introduce the chemical potential $\mu$, since in the sequel we wish to study states with definite particle number, and for convenience use the notation $\epsilon_p = -(\cos p + \rho + \mu)$. Defining the spectral density in the usual manner (2.1) we write down the explicit expression for the first three moments:

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Lambda_p(\omega)=1, \qquad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega-\varepsilon_p)\Lambda_p(\omega)=2\rho n$$
$$-\frac{2\rho}{N}\sum_{p_1}\cos(p-p_1)\bar n_{p_1}, \qquad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega-\varepsilon_p)^2\Lambda_p(\omega)=L$$
$$+\frac{2\rho}{N}\sum_{p_1}\cos(p-p_1)\int_{-\infty}\frac{d\omega}{2\pi}(\omega-\varepsilon_{p_1})\Lambda_{p_1}(\omega)\,\mathrm{th}\frac{\beta\omega}{2}, \qquad (4.3)$$

where $\bar n_p = \langle a_p^+ a_p\rangle$. We have introduced the convenient notations:

$$n=\frac{1}{N}\sum_p\bar n_p,$$
$$L=\left(\frac{2\rho}{N}\right)^2\sum_{p_1\ldots p_4}\delta_{p_1+p_2;\,p_3+p_4}\cos^2(p_2-p_3)\langle a_{p_1}{}^+a_{p_4}a_{p_2}{}^+a_{p_3}\rangle. \qquad (4.4)$$

Proceeding according to the general method exposed above we solve the system of relations obtained in this manner for the spectral density $\Lambda_p(\omega)$. We investigate the solution of the system of moments (4.3) for $\Lambda_p(\omega) = 2\pi\delta(\omega - \omega_p)$, i.e., in the Hartree-Fock approximation. In this case the spectral density satisfies exactly only the first two moments (4.3) and the spectrum of elementary excitations $\omega_p$ is determined up to an effective constant $\alpha$, which must be found by solving the self-consistency equations. We have

$$\omega_p=2\rho\left(n-\frac{1}{2}\right)-\mu-(1+\alpha)\cos p, \quad \alpha=\frac{2\rho}{N}\sum_p\frac{\cos p}{1+e^{\beta\omega_p}}, \qquad (4.5)$$

where we have assumed that $\omega_p = \omega_{-p}$. Using the general formulas (2.3) and (2.7) one can derive an equation for the determination of the chemical potential and the expression of the energy of the system which have the forms

$$n=\frac{1}{N}\sum_p\frac{1}{1+e^{\beta\omega_p}}, \qquad \frac{E}{N}=-\frac{1}{4\rho}(\alpha^2+2\alpha)+\rho\left(n-\frac{1}{2}\right)^2. \qquad (4.6)$$

respectively.

It is further necessary to solve the self-consistency equations and to determine $\alpha$. However, for arbitrary $\beta$ this is a sufficiently complicated problem, therefore we shall solve the self-consistency equations in the quantum-mechanical limit $\beta \to \infty$. In this case the solution is easily found and we obtain the expression for the energy:

$$\frac{E}{N}=-\frac{1}{\pi}\sin\pi n-\frac{\rho}{\pi^2}\sin^2\pi n+\rho\left(n-\frac{1}{2}\right)^2. \qquad (4.7)$$

It is interesting to find the ground state energy, i.e., such a function n = n($\rho$) which minimizes the energy of the system for given $\rho$. Then, using the necessary condition for the extremum of the function n = n($\rho$) we derive the equation:

$$2\rho\left(n-\frac{1}{2}\right)=\cos\pi n\left(1+\frac{2\rho}{\pi}\sin\pi n\right). \qquad (4.8)$$

It is relatively difficult to find all the solutions of Eq. (4.8) but it is clear that n = ½ is a solution of this equation for arbitrary $\rho$. In order to find out for what values of $\rho$ this solution indeed corresponds to the ground state it is necessary to verify the sufficient condition for an extremum. Simple computations show that the antiferromagnetic state n = ½ in fact corresponds to the ground state only if $\rho = -\pi/4$, and the energy of that state is

$$\frac{E}{N}=-\frac{1}{\pi}-\frac{\rho}{\pi^2}, \qquad (4.9)$$

although it is usually assumed that the expression (4.9) corresponds to the ground state energy for arbitrary $\rho$. In reality, for $\rho < -\pi/4$ the expression for the ground state energy has a completely different form.

We now determine a more accurate solution for the spectral density, satisfying the system involving the first three moments. This function has the form

$$\Lambda_p(\omega)=\pi(1+\gamma_p)\delta(\omega-\omega_p)+\pi(1-\gamma_p)\delta(\omega+\omega_p). \qquad (4.10)$$

A direct substitution of the spectral density of the form (4.10) into the system of moments (4.3) leads to the expression

$$\gamma_p=\frac{(2\rho n+\varepsilon_p)-\alpha\cos p}{\omega_p},$$
$$\omega_p=\left[(L+\lambda\cos p)+2\varepsilon_p(2\rho n-\alpha\cos p)+\varepsilon_p{}^2\right]^{1/2}, \qquad (4.11)$$

where we have introduced the notation

$$\alpha=\frac{2\rho}{N}\sum_p\cos p\bar n_p, \quad \lambda=\frac{2\rho}{N}\sum_p\cos p\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega-\varepsilon_p)\Lambda_p(\omega)\,\mathrm{th}\frac{\beta\omega}{2}; \qquad (4.12)$$

where we have required $\bar n_p = \bar n_{-p}$. Since the dependence of the momentum p of the spectrum of elementary excitations is known, we can investigate its form. Assuming that $(1 + 2\alpha) > 0$ (the following computations confirm this assumption) we find the minimum of the spectrum of elementary excitations (the Fermi momentum) and the value at the minimum (the energy gap). The corresponding equations have the form

$$\cos p_0=\frac{(4\rho n-\lambda)-2(1+\alpha)(\rho+\mu)}{2(1+2\alpha)}$$

$$\Delta=L-(\rho+\mu)[4\rho n-(\rho+\mu)]$$
$$-[(4\rho n-\lambda)-2(1+\alpha)(\rho+\mu)]^2/4(1+2\alpha). \qquad (4.13)$$

We investigate the antiferromagnetic state, corresponding to $p_0 = \pm\pi/2$ and $n = 1/2$. According to (4.13) this state is realized if the following condition holds

$$(4\rho n - \lambda) - 2(1+\alpha)(\rho+\mu) = 0. \qquad (4.14)$$

We prove that to this condition corresponds $\mu = 0$. For this purpose we write the equation which determines $\mu$. According to the general formulas (2.3) and making use of the explicit form (4.10) of the spectral density and of the expression (4.11) for $\gamma_p$ we obtain

$$\left(n - \frac{1}{2}\right) = \frac{1}{2N}\sum_p \frac{[(1+\alpha)\cos p + \mu - 2\rho(n - 1/2)]}{\omega_p}\,\mathrm{th}\frac{\beta\omega_p}{2}. \qquad (4.15)$$

For the antiferromagnetic state the expression (4.15) simplifies, and we obtain an equation for the determination of $\mu$:

$$\frac{1}{2N}\sum_p \frac{(1+\alpha)\cos p}{\omega_p}\,\mathrm{th}\frac{\beta\omega_p}{2} = -\mu\frac{1}{2N}\sum_p \frac{\mathrm{th}(\beta\omega_p/2)}{\omega_p}. \qquad (4.16)$$

If, however, one takes into account the fact that if (4.14) is satisfied the spectrum of elementary excitations contains only $\cos^2 p$ and not cos p, in distinction from the general case (Eq. (4.11)), then it is easy to show that the expression in the left-hand side of (4.16) vanishes identically, owing to the presence of cos p in the numerator, whereas the coefficient of $\mu$ in the right-hand side of (4.16) differs from zero. Consequently $\mu$ vanishes, as required. Thus, for the antiferromagnetic state the elementary excitation spectrum has a simple form:

$$\omega_p = [(L - \rho^2) + (1+2\alpha)\cos^2 p]^{1/2}. \qquad (4.17)$$

Now it is necessary to construct the self-consistency equation for the determination of L, $\alpha$, and to show that the condition (4.14) is not contradictory.

Making use of the definition of $\alpha$ and expressing $\bar{n}_p$ in terms of the spectral density (2.3), considering the condition (4.14) and the fact that $\mu = 0$, we find

$$\frac{\alpha}{1+\alpha} = \frac{\rho}{N}\sum_p \frac{\cos^2 p\,\mathrm{th}(\beta\omega_p/2)}{[(L-\rho^2) + (1+2\alpha)\cos^2 p]^{1/2}}. \qquad (4.18)$$

We now prove that the condition (4.14) is noncontradictory. Using the definition of $\alpha$ and $\lambda$ it is necessary to show that the condition $\lambda + 2\rho\alpha = 0$ is satisfied if $n = 1/2$ and the elementary excitation spectrum has the form (4.17). Making use of the definition (4.12) of $\lambda$, of the explicit form of the spectral density, of the condition $n = 1/2$ and of the explicit form of the elementary excitation spectrum, we find

$$\lambda\left(1 - \frac{2\rho}{N}\sum_p \frac{\cos^2 p}{\omega_p}\,\mathrm{th}\frac{\beta\omega_p}{2}\right) = \rho(\alpha - 1)\frac{2\rho}{N}\sum_p \frac{\cos^2 p}{\omega_p}\,\mathrm{th}\frac{\beta\omega_p}{2}. \qquad (4.19)$$

Solving this equation with respect to $\lambda$ and using Eq. (4.18) for the determination of $\alpha$ it is easy to show that the condition $\lambda + 2\rho\alpha = 0$ is identically satisfied.

It is further necessary to construct a self-consistency scheme for L (cf. (4.4)). Using the commutation relations of the field operators one can show that

$$\Lambda_1 = (L - \rho^2) = \left(\frac{2\rho}{N}\right)^2 \sum_{p_1 \ldots p_4} \delta_{p_1+p_2, p_3+p_4} \cos^2(p_2 - p_3)\langle a_{p_1}^+ a_{p_2}^+ a_{p_3} a_{p_4}\rangle. \qquad (4.20)$$

We introduce the higher spectral density defined as

$$A_{p_1, p_4}(\tau) = \sum_{p_2, p_3} \delta_{p_1+p_2, p_3+p_4}\langle [a_{p_1}^+ a_{p_2}^+ a_{p_3}; a_{p_4}(\tau)]_+\rangle. \qquad (4.21)$$

Using the equal-time commutation relations we find the first two moments of the spectral density:

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A_{p_1, p_4}(\omega) = (N\delta_{p_1, p_4}n - \bar{n}_{p_1}),$$

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega - \varepsilon_{p_4})A_{p_1, p_4}(\omega) &= 2\rho n\cos(p_1 - p_4) - \alpha\cos p_1 \\ &- \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\Lambda_{p_1}(\omega)(\omega - \varepsilon_{p_1})}{1 + e^{\beta\omega}} + \frac{2\rho}{N}\sum_{p_5, p_6}\delta_{p_4+p_5; p_6+p_1}[\cos(p_5 - p_6) \\ &- \cos(p_4 - p_6)]\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{A_{p_5, p_6}(\omega)}{1 + e^{\beta\omega}}. \end{aligned} \qquad (4.22)$$

The derivation of Eqs. (4.22) involved the spectral properties in the variable $\omega$ of the functions $\Lambda_p(\omega)$ and $A_{p_1, p_4}(\omega)$.

The spectral density satisfying the system of moments (4.22) has the form

$$\begin{aligned}A_{p_1, p_4}(\omega) &= \pi\varkappa_{p_1, p_4}(1 + \nu_{p_1, p_4})\delta(\omega - \omega_{p_4}) \\ &+ \pi(1 - \nu_{p_1, p_4})\varkappa_{p_1, p_4}\delta(\omega + \omega_{p_4}), \end{aligned} \qquad (4.23)$$

where $\nu_{p_1, p_4}$ is a function to be determined, $\omega_{p_4}$ is the spectrum of elementary excitations (4.17) and $\kappa_{p_1, p_4} = (N\delta_{p_1, p_4}n - \bar{n}_{p_1})$.

Substituting the spectral density $A_{p_1, p_4}(\omega)$ in the form (4.23) into the second equation of the system (4.22) we obtain the integral equation

$$\begin{aligned}\sigma_{p_1, p_4} &= -\left(\omega_{p_4}^{-1}\,\mathrm{th}\frac{\beta\omega_{p_4}}{2}\right)^{1/2} U_{p_1, p_4} \\ &- \cos(p_1 - p_4)\frac{\rho}{N}\sum_{p_5, p_6}\delta_{p_4+p_5, p_6+p_1}\left(\omega_{p_4}^{-1}\omega_{p_6}^{-1}\,\mathrm{th}\frac{\beta\omega_{p_4}}{2}\,\mathrm{th}\frac{\beta\omega_{p_6}}{2}\right)^{1/2}\sigma_{p_5, p_6} \\ &+ \frac{\rho}{N}\sum_{p_5, p_6}\delta_{p_4+p_5, p_6+p_1}\cos(p_5 - p_1)\cdot\left(\omega_{p_4}^{-1}\omega_{p_6}^{-1}\,\mathrm{th}\frac{\beta\omega_{p_6}}{2}\,\mathrm{th}\frac{\beta\omega_{p_6}}{2}\right)^{1/2}\sigma_{p_5, p_6}, \end{aligned} \qquad (4.24)$$

where we have defined a new function

$$\sigma_{p_1, p_4} = \left(\omega_{p_4}\Big/\mathrm{th}\frac{\beta\omega_{p_4}}{2}\right)^{1/2}\left(1 - \nu_{p_1, p_4}\,\mathrm{th}\frac{\beta\omega_{p_4}}{2}\right)\varkappa_{p_1, p_4}. \qquad (4.25)$$

The function $U_{p_1, p_4}$ in (4.24) is known and has the form:

$$\begin{aligned}U_{p_1, p_4} &= 2\rho n\cos(p_1 - p_4) - \alpha\cos p_1 - \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\Lambda_{p_1}(\omega)(\omega - \varepsilon_{p_1})}{1 + e^{\beta\omega}} \\ &- \varkappa_{p_1, p_4}\frac{\omega_{p_4}}{\mathrm{th}(\beta\omega_{p_4}/2)} + \varkappa_{p_1, p_4}\varepsilon_{p_4}. \end{aligned} \qquad (4.26)$$

The equations (4.21)–(4.26) is valid in the general case.

We consider in the sequel the antiferromagnetic state defined above, cf. (4.14). Using the spectral representation in the variable $\omega$ of the function $A_{p_1, p_4}(\omega)$ for this state and also the definition (4.25) of $\sigma_{p_1, p_4}$ we obtain for the energy gap the expression

$$\Delta_0 = \frac{1}{2}\left(\frac{2\rho}{N}\right)^2\sum_{p_1, p_4}\cos^2(p_1 - p_4)\left(\omega_{p_4}^{-1}\,\mathrm{th}\frac{\beta\omega_{p_4}}{2}\right)^{1/2}\sigma_{p_1, p_4}. \qquad (4.27)$$

Owing to the fact that the spectrum of elementary excitations contains only $\cos^2 p$ (cf. (4.17)) and does not contain the first power of cos p as in the general situation (4.11), one can find a solution for the energy gap $\Delta_0$ in the form of an infinite series by using the specific form of the interaction potential. For this it suffices to note that the following formula holds:

$$\frac{1}{2}\left(\frac{2\rho}{N}\right)^2 \sum_{p_1,\,p_4} \cos^m(p_1-p_4)\left(\omega_{p_4}^{-1}\,\mathrm{th}\,\frac{\beta\omega_{p_4}}{2}\right)^{1/2} \sigma_{p_1,\,p_4}$$

$$= -\frac{1}{2}\left(\frac{2\rho}{N}\right)^2 \sum_{p_1,\,p_4} \cos^m(p_1-p_4)\,\omega_{p_4}^{-1}\,\mathrm{th}\left(\frac{\beta\omega_{p_4}}{2}\right) U_{p_1,\,p_4}$$

$$- d\left[\frac{1}{2}\left(\frac{2\rho}{N}\right)^2 \sum_{p_1,\,p_4} \cos^{(m+1)}(p_1-p_4)\left(\omega_{p_4}^{-1}\,\mathrm{th}\,\frac{\beta\omega_{p_4}}{2}\right)^{1/2} \sigma_{p_1,\,p_4}\right]. \qquad (4.28)$$

The validity of the latter is easily checked by means of the integral equation (4.24). We have used the notation

$$d = \frac{\rho}{N} \sum \omega_p^{-1}\,\mathrm{th}\,\frac{\beta\omega_p}{2}. \qquad (4.29)$$

Taking into account (4.28) we obtain the expression for the energy gap

$$\Delta_0 = \sum_{m=0}^{\infty} (-1)^{m+1} d^m \left[\frac{1}{2}\left(\frac{2\rho}{N}\right)^2 \sum_{p_1,\,p_4} \cos^{(m+2)}(p_1-p_4)\,\omega_{p_4}^{-1}\,\mathrm{th}\,\frac{\beta\omega_{p_4}}{2} U_{p_1,\,p_4}\right]. \qquad (4.30)$$

The series (4.30) is meaningful if $|d| < 1$. In this case the series can be summed and yields the more compact expression

$$\Delta_0 = -\frac{1}{2}\left(\frac{2\rho}{N}\right)^2 \sum_{p_1,\,p_4} \frac{\cos^2(p_1-p_4)}{1+d\cos(p_1-p_4)}\,\omega_{p_4}^{-1}\,\mathrm{th}\,\frac{\beta\omega_{p_4}}{2} U_{p_1,\,p_4}. \qquad (4.31)$$

Utilizing the explicit expression (4.26) of $U_{p_1,p_4}$, and also the expression for the spectral density $\Lambda_p(\omega)$, the computation of a few simple integrals leads to the final result:

$$\Delta_0 = \frac{A}{B},$$

$$A = \frac{\rho^2}{d^2}\left(\frac{1}{\sqrt{1-d^2}} - 1\right) - \left(\frac{\rho}{N}\right)^2 \sum_{p_1,\,p_4} \frac{\alpha\cos^2(p_1-p_4)\cos^2 p_1}{1+d\cos(p_1-p_4)}$$

$$\times\, \omega_{p_1}^{-1}\omega_{p_4}^{-1}\,\mathrm{th}\,\frac{\beta\omega_{p_1}}{2}\,\mathrm{th}\,\frac{\beta\omega_{p_4}}{2},$$

$$B = 1 + \left(\frac{\rho}{N}\right)^2 \sum_{p_1,\,p_4} \frac{\cos^2(p_1-p_4)}{1+d\cos(p_1-p_4)}\,\omega_{p_1}^{-1}\,\omega_{p_4}^{-1}\,\mathrm{th}\,\frac{\beta\omega_{p_1}}{2}\,\mathrm{th}\,\frac{\beta\omega_{p_4}}{2}. \qquad (4.32)$$

Thus, for self-consistency it is necessary to solve simultaneously the system of two integral equations with respect to $\alpha$ and $\Delta_0$, cf. (4.18) and (4.32).

In spite of the complicated character of these equations, one can find the asymptotic behavior for $|\rho| \to 0$ of $\alpha$ and $\Delta_0$ in the quantum-mechanical limit $\beta \to \infty$. For $|\rho| \to 0$, Eqs. (4.18) and (4.32) together with the definition (4.29) of d show that in lowest order in $\rho$ the quantities $\alpha$ and $\Delta_0$ have the form

$$\alpha \cong 2\rho/\pi, \quad \Delta_0 \cong \rho^2/2, \quad |\rho| \to 0. \qquad (4.33)$$

We note that such a behavior for the energy gap can be obtained by assuming that the higher spectral density (4.21) has the form

$$A_{p_1,\,p_4}(\omega) \cong (V\delta_{p_1,\,p_4}n - \bar{n}_{p_1})\Lambda_{p_4}(\omega). \qquad (4.34)$$

A higher spectral density $A_{p_1,p_4}(\omega)$ of the form (4.34) satisfies only the zeroth moment of the system (4.22) and corresponds to the usual decoupling (clustering) for the higher correlation functions. However, computing the energy gap with the help of this density shows that the gap does not depend on temperature and coincides with the exact result for $|\rho| \ll 1$. Thus, if we are interested in the asymptotic behavior of the energy gap for $|\rho| \ll 1$ and $\beta \to \infty$, the expression (4.34) for the higher spectral density is quite acceptable, a fact which simplifies the calculations considerably.

We show further that the energy gap does not vanish anywhere. For this we notice that for arbitrary $\rho$ for which the solution we have found is valid, the following inequality must hold: $\Delta_0 > \alpha^2$. This inequality follows from an analysis of the spectral properties of $\Lambda_p(\omega)$. We recall that $\Lambda_p(\omega)$ must be real and positive definite. Let us now assume that for a certain $\rho$ the energy gap vanishes, then $\alpha^2 = 0$ and consequently the spectral density becomes equal to the free spectral density, as required by the explicit form of $\Lambda_p(\omega)$; but this happens only for $\rho = 0$.

After solving the self-consistency equations the spectral density $\Lambda_p(\omega)$ is completely determined and the computation of the physical quantities does not present any difficulties. For example the energy of the equilibrium state is, on the basis of the general formulas (2.71)

$$\frac{E_0}{N} = -\frac{\alpha}{4\rho} - \frac{1}{4N}\sum_p [\Delta_0 + (1+2\alpha)\cos^2 p]^{1/2}\,\mathrm{th}\,\frac{\beta\omega_p}{2}. \qquad (4.35)$$

The energy of the antiferromagnetic state (4.35), and also the solutions of the self-consistency equations (4.18) and (4.32) for zero, temperatures have been determined numerically on a computer. The result for the energy of the antiferromagnetic state has been compared with the energy of the exact ground state of the system[3] over the interval $-0.5 \le \rho \le 1.4$ and no deviations in excess of the accuracy of the machine computations have been observed. At the same time it is clear that the solution obtained by means of a canonical transformation[3] is a much poorer approximation to the energy of the ground state (cf. Fig. 1).

We note that in solving the problem by means of linear canonical transformations one must consider different transformations for $\rho > 0$ and $\rho < 0$, whereas the solution described above describes both these regions in a unified manner. Further, it is easy to show that the method of linear canonical transformations is contained in the method described above, if the spectral density is selected in the form of two delta functions, but only the model Hamiltonian is considered in place of the total Hamiltonian. The elementary excitation spectrum for the solution determined above effectively takes into account the collective excitations, the occurrence of which is due to all possible correlations. This, in particular, made it possible to find a uniform solution for both regions. Furthermore, it turns out that the

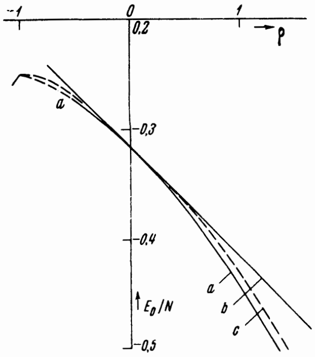

FIG. 1. The dependence of the ground state energy on $\rho$: a – from the method of spectral densities (coincides with the exact solution), b – from the Hartree-Fock approximation, c – from the method of linear canonical transformations.

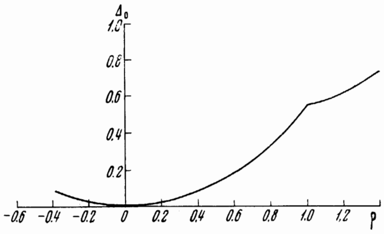

FIG. 2. The dependence of the energy gap on $\rho$.

asymptotic behavior of the energy gap for these two regions has a completely different character, for $|\rho| \to 0$.

In the earlier work[3] the energy gap exhibited an essential singularity for $|\rho| \to 0$, here we have an analytic behavior, cf. (4.33). As regards the agreement with the behavior of the energy gap in the exact solution, one must remark that for $\rho = 1$, when an energy gap appears in the exact solution, the energy gap we found suffers a fracture (discontinuity of derivative), cf. Fig. 2.

Thus, we have demonstrated on a nontrivial and practically interesting problem the proposed method and the results have turned out to be much better, both qualitatively and quantitatively, than results obtained earlier.

In conclusion we would like to express our thanks to L. V. Pariĭskaya for the large amount of computational work she has done in solving the self-consistency equations of the quantum one-dimensional Ising model.

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