

Analytical methods of calculating correlation functions in quantum statistical physics

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A brief but clear and complete account is given for two analytical methods of calculating correlation functions in quantum statistical physics from first principles—the widely used method of two-time temperature Green's functions (the GF method) and a new, "direct algebraic" (DA) method. The mathematical and technical clarity and simplicity of the DA method and its resulting practical value are demonstrated for the five most widely used models in quantum statistical physics. Since the DA method is an exactly self-consistent method (in the sense that the expansion coefficients in the equations of motion are chosen from the requirement that the Jacobi operator identity be satisfied exactly), it in principle affords the possibility of an internal check, which is not possible in the GF method. Like the GF method, the DA method permits calculation of the spectra of possible elementary excitations and, hence, of the density of single-particle energy states corresponding to them.

INTRODUCTION

One of the main tasks of statistical physics is to calculate the correlation functions of the systems under study, since they contain all the necessary information about their observable properties. Therefore, the development of analytical methods of calculating the correlation functions is always a pertinent and extremely important methodological problem in statistical physics.

Of the more or less simple analytical methods of calculating correlation functions in statistical physics, the most widely used is clearly that of the equations of motion for the two-time temperature Green's functions (the GF method), which was introduced by Bogolyubov and Tyablikov in 1959.¹ Mathematically this method is based on the equations of motion for the Fourier time transforms of the Green's functions and the so-called "spectral theorem," which permits one to express the spectral intensity of the correlation functions, which is all that is required for their complete calculation, in terms of the boundary values of the retarded and advanced Green's functions as their argument, the complex energy, approaches the real axis from above and below, respectively. In this theory the spectral intensity can be expressed solely in terms of the boundary value of the imaginary part of the retarded Green's function or solely in terms of the boundary value of the imaginary part of the advanced Green's function, and so in practical calculations it is sufficient to use only the retarded two-temperature Green's function, for example. From a technical standpoint the Bogolyubov–Tyablikov method is always much simpler than all the other methods of calculating correlation functions in quantum statistical physics. However, it suffers from a fundamental computational shortcoming, viz., that within the framework of this method there is no systematic way of breaking the ordinarily infinite chain of equations of motion for the Green's function, and so there is no internal way of checking the accuracy of the decoupling that is done. Nevertheless, this method has come into widespread use as a technically rather simple method, particularly after the review by Zubarev² and the papers by Hubbard^{3–5} stimulated by it on the use of this method for quantitative analysis of the

model he proposed. However, it was the widespread use by authors abroad of the method of two-time Green's functions that revealed for the first time, the difficulties^{6–9} in using the "spectral theorem" of this method in specific calculations. The true cause of these difficulties was established by the present author¹⁰ (who had discovered them independently much later) as being due to the incorrect use of the "spectral theorem" in this method (incidentally, this incorrect treatment apparently sprang from the same widely cited paper by Zubarev,² who gave an example of its use in unrestricted (and, essentially, incorrect) form, see Eq. (3.28) in Ref. 2). In the same paper¹⁰ I also gave a critical analysis of the different ways that had been proposed by various authors abroad for overcoming these difficulties within the framework of the GF method.

On closer inspection the GF method, besides lacking regularity, is also asymmetric with respect to the use of commutator or anticommutator Green's functions in it: the correct calculation of the spectral intensity of the correlation functions sought always requires calculating the anticommutator Green's functions,^{9,10} although there are cases when it is sufficient to use just the commutator Green's functions alone (these cases, however, can be identified only after calculation of the anticommutator Green's functions). Consequently, until a simple criterion is found for identifying these cases, the correct use of the commutator Green's functions for calculating the correlation functions in this method will always be technically unfavorable, and therefore the choice of the commutator or anticommutator Green's functions for practical calculations is actually not solely a matter of convenience. In Ref. 10 I found a very simple, but unfortunately only a necessary, condition for the nonclosure of the GF method by the commutator Green's functions alone. With the use of the anticommutator Green's functions the GF method is always closed (i.e., just the anticommutator Green's functions alone are sufficient for calculating the spectral intensities of the correlation functions), but the calculation is cumbersome if the commutators of the operators used to construct the Green's function of the problem are simple, in which case their anticommutators are complex.

To eliminate this asymmetry in the GF method I pro-

posed¹⁰ to replace the Green's functions in the equation-of-motion (EOM) method by the so-called "half" Green's functions: the introduction of the Green's functions in the Green's-function EOM method was motivated by the fact that ensuring the correct analytical properties of their Fourier time transforms also allows one to take into account automatically the initial conditions on the temporal equations of motion for the Green's functions, something that it seemed to be hard to achieve in the equations of motion directly for the correlation functions themselves. From this standpoint the proposed replacement actually constitutes a transition from analysis of the equations of motion for the Green's functions to analysis of the equations of motion directly for the correlation functions while preserving all the advantages deriving from the analytical properties of the Green's functions (incidentally, the spectral theorem in the method based on the equations of motion of the half Green's functions has an extremely simple form and is therefore impossible to use incorrectly).

The equation-of-motion method for the Green's functions (GF EOM) or half Green's functions (HGF EOM) works as follows:

1) the chain of equations of motion for the Fourier time transforms is decoupled by some arbitrary simple procedure without any very convincing justification, and the resulting closed system of algebraic equations for these transforms is solved;

2) their discontinuities across the real axis are calculated;

3) the spectral intensities of the correlation functions sought are calculated from these discontinuities with the use of the "spectral theorem;"

4) an inverse Fourier transformation using the calculated spectral intensities is done to obtain the ordinary correlation functions.

For certain models (e.g., the Ising model) the system of equations of motion breaks off by itself by virtue of the internal properties of the model, but this fact does not necessarily attain the final goal of the EOM method: the resulting system of equations for the desired correlation functions can still turn out to be infinite. Ordinarily the EOM method leads to an infinite system even for the equations of motion themselves, and so one must decouple it in the first step; this can give rise to various internal inconsistencies and contradictions. To avoid difficulties of this nature, Hewson and ter Haar¹¹ and (independently) Dembinski^{12,13} proposed the following roundabout approach in the GF EOM method: first perform correctly the necessary decoupling in the correlation function itself which corresponds to the Green's function in the infinite chain of equations of motion for the Green's functions where it is necessary to break a link, and then use the "spectral theorem" to convert this decoupling of the correlation function into the correct decoupling of the Green's function corresponding to it. There are other reasons as well why decoupling in the correlation functions themselves is generally more acceptable than decoupling in the intermediate functions used to calculate the correlation functions.

In 1968, i.e., almost ten years after the paper of Bogolyubov and Tyablikov,¹ a very important paper was published by Roth,¹⁴ in which she proposed a universal self-consistent method for decoupling the infinite chain of

equations of motion for the Green's functions. Variational arguments in favor of this decoupling scheme, in addition to those given by Roth herself, were advanced by Sadawa¹⁵ and Young.¹⁶ The principal shortcoming of this scheme is the necessity of making additional approximations (i.e., going beyond the inherent approximations of this scheme) which, moreover, cannot be monitored within the scheme itself.

Around 1980 the present author began developing a new analytical method of calculating the correlation functions in quantum statistical physics that, like the Green's function method, proceeded from first principles; this is the so-called "direct algebraic" (DA) method.¹⁷⁻²² The DA method, like the GF method, does not involve perturbation theory; mathematically the DA method is based on the "dressing-undressing" method and an exact self-consistency procedure.

The dressing-undressing method (in an extremely simple form this method was used by the present author much earlier²³) plays the same role in the DA method as do the equations of motion in the GF method, but here it yields algebraic equations for the desired correlation functions immediately (i.e., directly, and hence the name). Thus the dressing-undressing method completely exhausts all the calculational possibilities of the method of the GF EOM method. The analytical basis of the dressing-undressing method is the exact undressing formula using the F matrix of the problem.

The analytical basis of the second part of the DA method—the exact self-consistency procedure—is the Jacobi operator identity. The procedure of making an exactly self-consistent decoupling of the problem is completely independent of the first part of the DA method, i.e., the dressing-undressing method, and it can of course be used in any other method of calculating correlation functions, in particular, in the GF EOM method when the equations of motion are "linearized" by the Roth procedure.

The main technical and fundamental differences between the DA and GF methods are as follows:

1) The DA method is direct and purely algebraic, i.e., it deals only with operators, traces of their different zero-time or two-time products (i.e., the usual zero-time or two-time correlation functions), and algebraic equations for these traces.

2) The DA method is extremely simple from the mathematical and technical standpoints, making it exceptionally clear and very practical.

3) The DA method is exactly self-consistent in the sense that it requires that the Jacobi operator identity be satisfied exactly, and it is therefore regular (i.e., it in principle affords the possibility of an internal check).

The DA method, like the GF method, can be used to calculate not only correlation functions but also the energy spectra of possible elementary excitations and, hence, the densities of single-particle energy states corresponding to them.

The main goal of this article is to demonstrate the exceptional simplicity, technical efficacy, and inherent capabilities of the DA method for studying the most diverse problems of statistical physics. For the five most important problems all the main correlation functions are obtained in closed form. The subsequent use of these expressions for the correlation functions is limited to analysis of particular cases

for which simple analytical solutions can be obtained for the physical properties.

This article is based primarily on the work of Bogolyubov, Tyablikov, Zubarev, Roth, and the present author.

1. METHOD OF TWO-TIME TEMPERATURE GREEN FUNCTIONS

1.1. Analytical formulation of the method

In this method the time dependence of the system operators is assigned in the Heisenberg picture

$$\hat{A}[t] \equiv \exp(iHt)\hat{A}\exp(-iHt), \quad (1.1.1)$$

and they therefore satisfy the equation of motion

$$\frac{d}{dt}\hat{A}[t] = [\hat{A}[t], H]_- = e^{iHt}[\hat{A}, H]_- e^{-iHt}, \quad (1.1.2)$$

and their average values

$$\langle \hat{A}[t] \rangle \equiv \text{Sp}(e^{-\beta H}\hat{A}[t])(\text{Sp}e^{-\beta H})^{-1} = \langle \hat{A} \rangle$$

are independent of time by virtue of the cyclic invariance of the trace, while averages of the form

$$\langle \hat{B}[t_2]\hat{A}[t_1] \rangle = \langle \hat{B}[t]\hat{A} \rangle, \quad t = t_2 - t_1, \quad (1.1.3)$$

are two-time correlation functions which for the same reason depend only on the difference of the times at which these operators are taken. The Hamiltonian of the system, which is almost always most convenient to have in the representation based on the occupation numbers of single-particle states, can include the chemical potential of the particles being described.

The idea of the GF method is that the Fourier time transform or, what is the same, the spectral intensity

$$\langle \hat{B}[t]\hat{A} \rangle_E \equiv J_{BA}(E) = \int_{-\infty}^{\infty} \langle \hat{B}[t]\hat{A} \rangle e^{iEt} dt \quad (1.1.4)$$

of the ordinary correlation function (1.1.3) is expressed in terms of the Fourier time transforms

$$\langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_E^{\mp} \equiv \lim_{\epsilon \rightarrow +0} \frac{1}{2\pi} \int_{-\infty}^{\infty} J_{BA}(E') \frac{1 \mp \exp(-\beta E')}{E - E' - i\epsilon} dE' \quad (1.1.5)$$

of the two-time temperature Green's functions (the commutator or anticommutator Green's functions)

$$\langle \langle \hat{B}[t] | \hat{A} \rangle \rangle^{\mp} \equiv i\theta(-jt)\langle [\hat{B}[t], \hat{A}]_{\mp} \rangle, \quad (1.1.6)$$

whose practical calculation, i.e., the calculation of expressions (1.1.6) themselves or their transforms (1.1.5), is assumed to be simpler than the direct calculation of the correlation functions (1.1.3) or their transforms (1.1.4). This idea is implemented with the help of the spectral theorem of the GF method:

$$\begin{aligned} \lim_{\epsilon \rightarrow +0} (\langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_{E+i\epsilon}^{\mp} - \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_{E-i\epsilon}^{\mp}) &\equiv C_{\kappa} \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_z^{\mp} \\ &= -iJ_{BA}(E)[1 \mp \exp(-\beta E)] \\ &= 2i \text{Im} \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_{\mp}^{\text{ret}} = -2i \text{Im} \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_{\mp}^{\text{adv}}. \end{aligned} \quad (1.1.7)$$

The Green's functions (1.1.6) or their transforms (1.1.5) are to be calculated from their equations of motion. In prac-

tice it is ordinarily more convenient to use the equations of motion for the transforms (1.1.5):

$$E \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_E^{\mp} = \langle [\hat{B}, \hat{A}]_{\mp} \rangle + \langle \langle [\hat{B}[t], H]_- | \hat{A} \rangle \rangle_E^{\mp}, \quad (1.1.8)$$

which have the same form for the retarded ($j = -$) and advanced ($j = +$) Green's functions. The desired correlation functions (1.1.3) are calculated from the formula for the inverse Fourier transformation

$$\langle \hat{B}[t]\hat{A} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} J_{BA}(E) e^{-iEt} dE, \quad (1.1.9)$$

since the spectral intensity is now known from the spectral theorem (1.1.7). To obtain the transforms (1.1.5) of the Green's functions one needs a correlation function that is transposed in comparison with (1.1.9). It is easily found from (1.1.9) by making use of the cyclic invariance of the trace of the product of operators. It gives

$$\langle \langle \hat{A} | \hat{B}[t] \rangle \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} J_{BA}(E) e^{-i(t-i\beta)E} dE. \quad (1.1.10)$$

Formulas (1.1.9) and (1.1.10) are sufficient for obtaining (1.1.5) by proceeding from their definition

$$\langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_E \equiv \int_{-\infty}^{\infty} \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle e^{iEt} dt \quad (1.1.11)$$

as Fourier transforms and from the definition (1.1.6) of the two-time Green's functions. Here, however, one will obtain integrals that do not exist in the strict sense. They are usually evaluated in the Poisson-Abel generalized sense²⁴

$$\int_0^{\infty} f(x) dx \rightarrow \lim_{\epsilon \rightarrow +0} \int_0^{\infty} f(x) e^{-\epsilon x} dx,$$

if the latter limit exists. From definitions (1.1.3) and (1.1.6) we see that there is an important difference between the correlation functions and Green's functions—the latter are not defined at zero time argument, since there the Heaviside step function is undefined. The spectral theorem of the GF method is easily obtained by using expression (1.1.5) and one of the particular representations of the delta function²⁵

$$-2\pi i \delta(x) \equiv \lim_{\epsilon \rightarrow +0} \left(\frac{1}{x + i\epsilon} - \frac{1}{x - i\epsilon} \right) \equiv C_{\kappa} \left(\frac{1}{z} \right). \quad (1.1.12)$$

1.2. Concerning the correct use of the spectral theorem

Ordinarily, without any reservations, formula (1.1.9) is written with the help of the spectral theorem (1.1.7) in the form

$$\langle \hat{B}[t]\hat{A} \rangle = \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{C_{\kappa} \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_z^{\mp}}{t \mp \exp(-\beta E)} e^{-iEt} dE \quad (1.2.1)$$

(see, e.g., Eq. (3.28) in Ref. 2), which is, generally speaking, incorrect.¹⁰ Indeed, suppose that

$$H = \bar{B} \sum_f \hat{S}_f^z, \quad \bar{B} \equiv -\lambda B.$$

Then it quickly follows from the equation of motion (1.1.8) that the commutator Green's function

$$\langle \langle \hat{S}_f^- [t] | \hat{S}_f^+ \rangle \rangle_E = 0 \rightarrow C_\kappa \langle \langle \dots \rangle \rangle_z = 0 \rightarrow \langle \hat{S}_f^z \hat{S}_f^z \rangle = 0,$$

even though, for example, in the case of half-integral spin the longitudinal diagonal zero-time correlation function is equal to one-fourth. However, if we are interested in the transverse correlation function, then formula (1.2.1), even for the case of the commutator Green's functions, gives the exact result

$$\langle \hat{S}_f^- \hat{S}_f^+ \rangle = [1 + \exp(-\beta \bar{B})]^{-1}.$$

The reason lies in the incorrect solution of algebraic equation (1.1.7) for the spectral intensity: its formal solution in the case of the commutator Green's function in general requires an additional term proportional to the delta function, since one has identically (see Sec. 1 of the Appendix for details)

$$[1 - \exp(\pm \beta E)] \delta(E) \equiv 0.$$

Thus the correct use of the spectral theorem of the GF method for the case of the commutator Green's functions gives the following formula for the spectral intensity:

$$J_{BA}(E) = \text{V.p.} \frac{i C_\kappa \langle \langle \dots \rangle \rangle_z^-}{1 - \exp(-\beta E)} + f_{BA} \delta(E),$$

which clearly turns the spectral theorem of the GF method into a correct identity. If this expression is substituted into (1.1.5), then one can obtain the limits⁹

$$\lim_{E \rightarrow 0} E \langle \langle \hat{B}[t] | \hat{A} \rangle \rangle_E^\mp = (1 \mp 1) f_{BA}, \quad (1.2.2)$$

i.e., the exact anticommutator Green's functions and commutator Green's functions respectively do and do not admit a pole at $E = 0$, and, according to (1.2.2), the residue of the exact anticommutator Green's function at that point determines the unknown function f_{BA} multiplying the delta function.⁹ In practice this refinement of the accuracy of the analytical properties of the exact Green's functions is very important also because any of the approximately calculated Green's functions can admit this pole. Then the pole in the approximately calculated Green's functions must be removed by imposing a suitable condition for this, and the residue of the anticommutator Green's function at this pole gives the coefficient multiplying the delta function in the spectral intensity. The limit (1.2.2) is what makes the GF method asymmetric with respect to the use of the anticommutator or commutator Green's functions in specific calculations, since in actuality it is always necessary to know the exact value of the limit (1.2.2) for the anticommutator Green's function before calculating any physical properties of the system under study with the aid of the approximately calculated commutator or anticommutator Green's functions. Thus the correct form of (1.2.1) is

$$\langle \hat{B}[t] | \hat{A} \rangle = \frac{1}{2} (1 \mp 1) f_{BA} + \text{the right-hand side of (1.2.1)}. \quad (1.2.3)$$

1.3. Analytical continuation of the Green's functions

From expressions (1.1.5) and the equations of motion (1.1.8) we see that the retarded and advanced Green's functions can be combined into one generalized Green's function of complex argument:

$$y(z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} J_{BA}(E) \frac{1 \mp \exp(-\beta E)}{z - E} dE. \quad (1.3.1)$$

This Green's function by definition coincides with the analytical continuation of the retarded (advanced) Green's function into the upper (lower) half plane if the argument of the generalized Green's function takes on values in the upper (lower) half-plane. The Green's function defined as in (1.3.1) is analytic everywhere except the real axis.¹ This axis is outside of its domain of definition, and it is on this axis that any poles or other singularities will occur, if at all. Generally speaking the retarded and advanced Green's functions cannot be regarded as different branches of this generalized Green's function, since they are not analytical continuations of each other except in cases when the only singularities are poles. If the Green's function (1.3.1) has singularities other than poles, this means that the retarded and advanced Green's functions have, as a minimum, complex poles in the "wrong" half-planes. In specific calculations the equations of motion (1.1.8) are most often written for the generalized Green's function (1.3.1), although, as can be seen from (1.1.7), one may use only the retarded or only the advanced Green's function. Irrespective of this choice, the equations of motion in practice admit an approximate solution. Therefore, the Green's functions obtained in such a process can have incorrect analytical properties, and then these properties must be brought into agreement with the above-noted properties of the exact Green's functions by imposing suitable ancillary conditions on the approximate expressions obtained for the Green's functions. This is one of the main reasons for introducing the spectral representations of the Green's functions—expressions of the type (1.1.5) and (1.3.1), which thus play the role of a "procrustean bed" for correcting the approximate Green's functions (generalized, retarded, advanced) calculated by any possible means! For example, in the trivial case considered in Sec. 1.2, the discussion concerned the correct solution of the equation of motion (1.1.8), which for the Green's function $\langle \langle \hat{S}_f^- [t] | \hat{S}_f^+ \rangle \rangle_z^\mp$ has the form

$$(z + \lambda B) \langle \langle \hat{S}_f^- [t] | \hat{S}_f^+ \rangle \rangle_z^\mp = 1,$$

with respect to this Green's function. Formally, the solution of this equation is

$$\langle \langle \hat{S}_f^- [t] | \hat{S}_f^+ \rangle \rangle_z^\mp = (z + \lambda B)^{-1}. \quad (1.3.2)$$

Here, generally speaking, we must add a term $f_{S-S+} \delta(z + \lambda B)$ to the right-hand side of (1.3.2), as we did when solving Eq. (1.1.7) for the spectral intensity, since such an expression for (1.3.2) satisfies the preceding equation. However, the delta function of complex argument $\delta(z)$ has two poles lying off the real axis [at the points $z = \pm i\epsilon$; see expression (1.1.12) with the replacement $\delta(x) \rightarrow \delta(z)$], and therefore the coefficient f_{S-S+} multiplying the delta function must be set equal to zero. Otherwise the analytical properties of the generalized Green's function (1.3.2) constructed in this manner would not correspond to the properties of the exact Green's function, which does not have singularities off the real axis. Thus expression (1.3.2) for the Green's function is correct. The limiting (on approach to the

real axis $\varepsilon \rightarrow +0$) values of this Green's function, i.e., of the function $1/(E + \lambda B \pm i\varepsilon)$, give the retarded and advanced Green's functions of real argument. However, if the calculation is done using only the retarded (advanced) Green's function analytically continued into the upper (lower) half-plane, then obviously the delta-function term should again be absent, since the first (second) does not have singularities in the upper (lower) half-plane. In the case of the solution of equation (1.1.7) for the spectral intensity the question of whether or not to include a delta-function term must be answered each time with the help of (1.2.2) or (1.4.7).

1.4. Method of half Green's functions

Instead of the method of two-time Green's functions, which is internally asymmetric with respect to the anticommutator and commutator Green's functions, the present author has proposed¹⁰ a method of half Green's functions:

$$\widehat{B}[t|\widehat{A}] \equiv i\theta(-t)\widehat{B}[t|\widehat{A}]. \quad (1.4.1)$$

The Fourier time transform of these half Green's functions coincides with (1.1.5) if the expression $[1 \mp \exp(-\beta E)]$ in it is replaced by unity. The equations of motion for the half Green's functions is

$$z\widehat{B}[t|\widehat{A}]_z = \widehat{B}\widehat{A} + \widehat{B}[t, H]_-\widehat{A}_z. \quad (1.4.2)$$

The "spectral theorem" here looks extremely simple,

$$C_k\widehat{B}[t|\widehat{A}]_z = -iJ_{BA}(E), \quad (1.4.3)$$

and does not need to be solved for the spectral intensity. The ordinary time correlation functions are calculated by the formulas

$$\widehat{B}[t|\widehat{A}] = \frac{i}{2\pi} \int_{-\infty}^{\infty} e^{-iEt} C_k\widehat{B}[t|\widehat{A}]_z dE, \quad (1.4.4)$$

$$\widehat{A}\widehat{B}[t] = \frac{i}{2\pi} \int_{-\infty}^{\infty} e^{-i(t-i\beta)E} C_k\widehat{B}[t|\widehat{A}]_z dE, \quad (1.4.5)$$

which follows directly from the "spectral theorem" (1.4.3) and formulas (1.1.9) and (1.1.10), respectively. The identity (2.1.1) also implies the following relation among the anticommutator, commutator, and half Green's functions:

$$\langle\langle\widehat{B}[t|\widehat{A}]\widehat{A}\rangle\rangle_E^+ + \langle\langle\widehat{B}[t|\widehat{A}]\widehat{A}\rangle\rangle_E^- = 2\widehat{B}[t|\widehat{A}]\widehat{A}_E, \quad (1.4.6)$$

which is why these are called "half" Green's functions. From (1.4.6) we readily obtain

$$f_{BA} = \lim_{E \rightarrow 0} (E\widehat{B}[t|\widehat{A}]\widehat{A})_E. \quad (1.4.7)$$

If one insists on using the Green's functions rather than the half Green's functions, this rule for calculating the function f_{BA} in practice is always significantly simpler than rule (1.2.2), since, as can be seen from (1.4.6), the intermediate calculations do not involve terms which are going to drop out in the limit $E \rightarrow 0$ anyway.

1.5. On the postulate of correlation damping

Here we will discuss a new physical postulate, viz., that the time correlations are damped; this postulate was advanced⁸ in order to overcome the difficulties of the GF method (these difficulties actually stemmed from the incor-

rect use of the spectral theorem of the GF method; see Eq. (3.28) of Zubarev's paper²). Analytically this postulate is formulated as⁸

$$\lim_{|t| \rightarrow \infty} \widehat{B}[t|\widehat{A}] = \widehat{A}\widehat{B}. \quad (1.5.1)$$

This postulate was used by the authors of Ref. 8 to determine an additional term in their formula

$$\widehat{B}[t|\widehat{A}] = \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{\exp(-iEt)dE}{1 - \exp(-\beta E)} C_k\langle\langle\cdots\rangle\rangle_z + f_{BA},$$

which can be compared with (1.2.3). The fact that this postulate is rather ineffective for these purposes can easily be seen just by taking the discontinuity in the form¹⁰

$$C_k\langle\langle\widehat{B}[t|\widehat{A}]\rangle\rangle_z = a\delta(E) + \sum_j a_j\delta(E - E_j),$$

which is most often encountered in specific calculations.

What is more important and interesting, however, is that this postulate is evidently responsible for the so-called "Lebowitz zero" (Refs. 26–28). Essentially, the Lebowitz zero consists in the following. According to Kubo theory, the kinetic coefficients are of the form²⁹

$$L_{ik} = \frac{\beta}{2} \int_{-\infty}^{\infty} \langle\dot{\alpha}_k(t)\dot{\alpha}_i\rangle dt. \quad (1.5.2)$$

Lebowitz calculates these coefficients analytically:

$$L_{ik} = \frac{\beta}{2} \langle \langle \int_{-\infty}^{\infty} d\alpha_k \dot{\alpha}_i \rangle \rangle = \frac{\beta}{2} \lim_{|T| \rightarrow \infty} \langle (\alpha_k(T) - \alpha_k(-T))\dot{\alpha}_i \rangle = 0 \quad (1.5.3)$$

by virtue of postulate (1.5.1). Lebowitz himself, according to Norman and Polak²⁷ (the original paper²⁶ is quite difficult to get hold of), assumed that the quantities in (1.5.2) are nonzero only in the thermodynamic limit. However, this assumption of Lebowitz is at odds with the results of calculations of the kinetic coefficients by the same Kubo formulas in the method of molecular dynamics (MMD), where, of course, only finite systems are considered. Qualitatively the difference between Lebowitz's and the MMD results were attributed²⁷ to the fact that Lebowitz's calculations were done for reversible trajectories, whereas in the MMD, where the calculations were done on a computer, it was necessary to use trajectories that satisfied Newton's equations of motion only approximately. However, Norman and Polak²⁷ did not report Lebowitz's indications of the particular place in the chain (1.5.3) that he believed the finiteness of the system is used (they also said nothing about this question), nor did they give their own indications of where they believed Lebowitz used the reversibility of the equations of motion in the chain (1.5.3). Without going into a detailed discussion of Ref. 27, which in any case does not bear directly on the GF method, here I will only point out a general inconsistency of postulate (1.5.1), which has a more direct bearing on the GF method. The exact expression (1.1.9) is first differentiated with respect to time and then integrated over time from zero to infinity, the left-hand side of (1.1.9) being transformed in the integration with the help of (1.5.1):

$$\int_0^{\infty} \langle \hat{B}[t] | \hat{A} \rangle dt = \lim_{T \rightarrow \infty} \left\langle \int_0^T d\hat{B}[t] | \hat{A} \right\rangle = \langle \hat{A} | \hat{B} \rangle - \langle \hat{B} \hat{A} \rangle.$$

The right-hand side of (1.1.9) is evaluated exactly:

$$\begin{aligned} & \frac{1}{2\pi i} \int_{-\infty}^{\infty} EJ_{BA}(E) dE \int_0^{\infty} \exp(-iEt) dt \\ &= -\frac{1}{2\pi} \int_{-\infty}^{\infty} J_{BA}(E) dE = -\langle \hat{B} \hat{A} \rangle. \end{aligned}$$

Thus one obtains the result

$$\langle \hat{A} | \hat{B} \rangle - \langle \hat{B} \hat{A} \rangle = -\langle \hat{B} \hat{A} \rangle,$$

which is true only in the particular case $\langle \hat{A} | \hat{B} \rangle = 0$. Therefore, it is not ruled out that the true cause of the "Lebowitz zero" is postulate (1.5.1). Incidentally, if the system under consideration is such that postulate (1.5.1) nevertheless does hold, then it follows from the last relation that the system must lack not only kinetic processes but even such equilibrium properties as magnetic order (if one takes $\langle \hat{S}_j^z \rangle = 0$ in the Heisenberg model), superconductivity (if one takes $\langle \hat{b}_k \rangle = 0$ in the BCS model), etc.

2. DIRECT ALGEBRAIC METHOD

2.1. K matrix of the problem

The starting objects for the DA method are the operators of the system and its Hamiltonian, which may include the chemical potential, and it is always more convenient for practical calculations to have it in the representation of occupation numbers of single-particle states. It is assumed that the commutation relations between operators, i.e., their commutators or anticommutators, are specified. The relation between the commutators and anticommutators is given by the identity

$$[\hat{A}, \hat{B}]_{\pm} = 2\hat{A}\hat{B} - [\hat{A}, \hat{B}]_{\pm}, \quad (2.1.1)$$

which is valid for any linear operators (which are the only kind used in quantum mechanics).

The pairwise commutators of any three linear operators are connected by a single relation: the Jacobi identity

$$[1, [2, 3]_{\pm}]_{\pm} + [2, [3, 1]_{\pm}]_{\pm} + [3, [1, 2]_{\pm}]_{\pm} = 0. \quad (2.1.2)$$

Sometimes it is more convenient to have one of the mixed commutator-anticommutator forms of the Jacobi identity

$$-[1, [2, 3]_{\pm}]_{\pm} + [2, [3, 1]_{\pm}]_{\pm} + [3, [1, 2]_{\pm}]_{\pm} = 0,$$

$$[1, [2, 3]_{\pm}]_{\pm} - [2, [3, 1]_{\pm}]_{\pm} + [3, [1, 2]_{\pm}]_{\pm} = 0,$$

$$[1, [2, 3]_{\pm}]_{\pm} + [2, [3, 1]_{\pm}]_{\pm} - [3, [1, 2]_{\pm}]_{\pm} = 0,$$

which are obtained from the main identity (2.1.2) with the help of (2.1.1) by successively replacing the commutator that does not contain the first, second, and third operators in pure form by the corresponding anticommutator.

Two more identities are very useful in practice:

$$[1, 23]_{\mp} \equiv 2 \cdot [1, 3]_{\mp} + [1, 2]_{\pm} \cdot 3,$$

$$[12, 3]_{\mp} \equiv 1 \cdot [2, 3]_{\mp} \pm [1, 3]_{\pm} \cdot 2.$$

The Bose and Fermi operators for the creation (annihil-

ation) of particles in single-particle states satisfy the same commutation relation as the occupation-number operators for these states:

$$[\hat{A}_f^{\pm}, \hat{n}_f]_{\pm} = \mp \hat{A}_f^{\pm} \delta_{ff'}, \quad \hat{n}_f \equiv \hat{A}_f^{\dagger} \hat{A}_f$$

The basic consequence of the cyclic invariance of the trace of a product of operators is the identity

$$\langle \hat{A}_2[t] | \hat{A}_1 \rangle = \begin{cases} \langle \hat{A}_1 | \beta | \hat{A}_2[t] \rangle, \\ \langle \hat{A}_1 | \hat{A}_2[t + i\beta] \rangle, \end{cases} \quad (2.1.3)$$

which bears the main burden in the "dressing-undressing" method. The process of "dressing" an operator \hat{A} is to subject it to a nonunitary transformation of the form

$$\begin{aligned} \exp(\beta H) \hat{A} \exp(-\beta H) &\equiv \hat{A}[\beta] \\ &= \hat{A} - \beta [\hat{A}, H]_{\pm} + \frac{\beta^2}{2!} [[\hat{A}, H]_{\pm}, H]_{\pm} - \dots \end{aligned} \quad (2.1.4)$$

and is effected, for example, as

$$\langle \hat{B} \hat{A} \rangle = \begin{cases} \langle \hat{A} | \hat{B}[-\beta] \rangle, \\ \langle \hat{A} | \beta | \hat{B} \rangle; \end{cases} \quad (2.1.5)$$

where the shorthand notation $\hat{A}[\mp i\beta]$ is introduced for $\hat{A}[\pm\beta]$.

According to the equations of motion (1.1.2), the evolution of an operator in time is determined by its commutator with the Hamiltonian of the system. Therefore, even the relations between the commutator itself and its explicit value are usually called equations of motion.

If in a system under study an operator \hat{A} is found such that it satisfies the two conditions

$$[\hat{A}, H]_{\pm} = \hat{B}\hat{A}, \quad [\hat{B}, H]_{\pm} = 0, \quad (2.1.6)$$

then with respect to this operator the system is "operator-oscillatory." A very important case is when \hat{B} in (2.1.6) is not an operator, i.e., $\hat{B} = B$. Then \hat{A} is called an "eigen" operator of the system. In particular, all operators that commute with the Hamiltonian of the system are eigen operators for it. Of particular importance are eigen operators with nonzero eigenvalues, since they create and annihilate elementary excitations of the system.^{30,31} The average values of these eigen operators must vanish:

$$\langle \hat{A} \rangle = \langle \hat{A}[\beta] \rangle = \exp(-\beta B) \langle \hat{A} \rangle = 0.$$

There are no nonoperator-oscillatory systems of practical importance, and one actually must deal with nonoperator-oscillatory systems of a more general form:

$$[\hat{A}_j, H]_{\pm} = \sum_{j'=1}^n K_{jj'} \hat{A}_{j'}. \quad (2.1.7)$$

A tenable way out of (2.1.7), at least in the zeroth order approximation, might be to find a way of constructing the shortest possible expansion (binomial), i.e., it would be necessary to find a two-dimensional operator basis that is closed with respect to the operation of commutation with the system Hamiltonian.

It is known³² that such an expansion will be unique if the set of operators in which the expansion is done is a linearly independent system. Linear operators in a specific basis

have the form of matrices. The set of matrices forms a linear space.³³ Therefore, the concepts of linear dependence (independence) of matrices and, hence, of linear operators have the same definition as the corresponding concepts for vectors of a linear space.

If the K matrix can somehow be found, then one can "linearize" any problem of quantum statistical physics:

1) by diagonalizing it, one can obtain the eigen operators of the system and their eigenvalues, which give the spectra of possible elementary excitations of the system;

2) in the EOM method for two-time temperature Green's functions the exact equations of motion (1.1.8) can be "linearized" by replacing the commutator of the second Green's function by the expansion (2.1.7);

3) the same can be done in the exact equations of motion for (1.4.2);

4) finally, in the "dressing-undressing" method one can undress the dressed operator (2.1.5), i.e., one can obtain the exact sum of the series (2.1.4) in closed form as a linear combination of the "bare" operators of the basis of the expansion with the aid of the F matrix of the problem:

$$\hat{A}_j[\beta] = \sum_{j'=1}^n F_{jj'}(\beta; K) \hat{A}_{j'}. \quad (2.1.8)$$

Here the operators that are most simply undressed are those satisfying relation (2.1.6):

$$\hat{A}[\beta] = \exp(-\beta B) \hat{A}. \quad (2.1.8')$$

At the present time the best-known method of calculating the K matrix is the self-consistent scheme of Roth, which has as its goal the unification of the decoupling of the equations of motion in the GF method by a suitable "linearization" of the equations of motion themselves. Roth proposed to calculate the K matrix in terms of two intermediate matrices E and N according to the scheme

$$\begin{aligned} \langle [\hat{A}_j, H]_-, \hat{A}_j^+ \rangle &\equiv E_{jj} \\ &= \sum_{j''} K_{jj''} \langle [\hat{A}_{j''}, \hat{A}_j^+] \rangle \equiv \sum_{j''} K_{jj''} N_{j''j}; \end{aligned} \quad (2.1.9)$$

where $\langle \dots \rangle$ denotes a statistical or quantum-mechanical averaging over the ground state of the system. In this scheme the matrices E and N are self-adjoint, while the K matrix may not be, but it is assumed (explicitly or implicitly) that it can always be calculated exactly in the framework of (2.1.9) (provided, of course, that the matrix N is nondegenerate). In practice, however, scheme (2.1.9) does not ordinarily permit one to obtain "calculable" quantities for all E_{jj} without additional approximations in these quantities themselves, i.e., without introducing an additional and almost unmonitorable error in the K matrix that is sought, which deprives this scheme not only of its inherent regularity but also its self-consistency. In fact, the best thing about the Roth scheme is the matrix relation

$$NK^+ = KN, \quad (2.1.10)$$

which follows from (2.1.9) but apparently went unnoticed by Roth. Incidentally, relation (2.1.10) immediately implies the curious similarity transformation

$$K^+ = N^{-1}KN, \quad (2.1.11)$$

which will be useful later on.

It is pertinent to note here that instead of the "complete" Roth scheme (2.1.9) one can just as successfully introduce a "half" scheme (in complete analogy with the aforementioned possibility of introducing "half" Green's functions):

$$\langle [\hat{A}_j, H]_-, \hat{A}_j^+ \rangle \equiv \bar{E}_{jj} = \sum_{j''} K_{jj''} \langle \hat{A}_{j''}, \hat{A}_j^+ \rangle \equiv \sum_{j''} K_{jj''} \bar{N}_{j''j}, \quad (2.1.12)$$

where the matrices \bar{E} and \bar{N} are also self-adjoint. Therefore, if the matrix N of a system is positive definite then so will be the matrix \bar{N} . Definition (2.1.12) directly implies the matrix relation

$$\bar{N}K^+ = K\bar{N}, \quad (2.1.13)$$

which is completely analogous to (2.1.10).

An exactly self-consistent scheme of calculating the K matrix can be arrived at as follows. For simplicity and clarity of exposition let us consider the two-operator case of expansion (2.1.7); this is the most important and frequently encountered approximation in practical calculations. As a rule, it is sensible to represent the commutator of any single-particle operator \hat{A} of a system with its Hamiltonian in the form of an exact decomposition

$$[\hat{A}_1, H]_- = K_{11} \hat{A}_1 + K_{12} \hat{A}_2, \quad (2.1.14)$$

where the coefficients K_{11} and K_{12} are known by construction. This expansion, except in rare specific cases, will be nonlinear (the concept of "nonlinear equations of motion" will be clarified later). We propose to "force fit" the commutator of the second operator of this expansion into the exact operator basis of the first commutator,

$$[\hat{A}_2, H]_- = K_{21} \hat{A}_1 + K_{22} \hat{A}_2, \quad (2.1.15)$$

and then to calculate the unknown coefficients K_{21} and K_{22} from the condition of exact satisfaction of the Jacobi operator identity. It is known that this imposes one (generally speaking) operator relation on the pairwise commutators of any three linear operators, and its use in expansion (2.1.15) is therefore not only a natural and most suitable procedure but is even simply indispensable. In practice this procedure consists of substituting expansions of the type (2.1.14), (2.1.15) into identity (2.1.2) to eliminate or at least reduce the arbitrariness in imposing the "forced" expansion (2.1.15).

If the two-operator basis is specified in a general form (\hat{A}_1 and \hat{A}_2) only two triples of operators are possible for using the Jacobi identity. These are the triples \hat{A}_1, \hat{A}_2, H and $\hat{A}_1, \hat{A}_2^+, H$. The use of the first triple leads directly to the result

$$[[\hat{A}_1, \hat{A}_2]_-, H]_- = (\text{Sp } K) [\hat{A}_1, \hat{A}_2]_-,$$

i.e., the commutator of the basis operators is an eigen operator with an eigenvalue equal to the trace of the K matrix. The use of the second triple leads to matrix conditions (2.1.10) and (2.1.13).¹⁹ Of particular importance from a practical standpoint is the two-operator case in which both matrices N and \bar{N} are real; then the K matrix will also be real. In this case

the matrix conditions (2.1.10) and (2.1.13) lead to two simple formulas for the unknown elements of the K matrix:¹⁹

$$K_{21} = K_{12} \frac{N_{12}\bar{N}_{22} - \bar{N}_{12}N_{22}}{\bar{N}_{11}N_{12} - N_{11}\bar{N}_{12}}, \quad (2.1.16)$$

$$K_{22} = K_{11} + K_{12} \frac{\bar{N}_{11}N_{22} - N_{11}\bar{N}_{22}}{\bar{N}_{11}N_{12} - N_{11}\bar{N}_{12}}. \quad (2.1.17)$$

Here the trivial case in which both matrices N and \bar{N} are diagonal is excluded.

In considering specific problems (see, e.g., the analysis of the BCS problem below) the number of substantially different triples can turn out to be much larger, even in the case of a two-operator basis: the Jacobi identity is indeed a truly indispensable instrument in practice for extracting a large number of exact analytical relations inherent in a problem, but because it is not at all obvious at first (or even second) glance, it has remained "in the shadows" in other approaches.

2.2. Nonlinear "linearization"

The procedure of obtaining explicit expansions of the type (2.1.14), (2.1.15) is usually called linearization of the initial problem. By this convention the present procedure should be called exact linearization, although it is more correctly called a scheme of exact self-consistency, since true linearization presupposes that only terms which are linear in some aspect are kept in the right-hand sides. This aspect is apparently most reasonably taken to be the partial order of the operator standing to the left in the commutator. However, such representations in the proposed method in general cannot be called linearized, since in practice the operator basis generally consists of operators of different order; otherwise the decomposition of the first commutator cannot in general be exact. Therefore, expansions of the type (2.1.14), (2.1.15) actually contain something more than truly linearized equations of motion.

How close the solutions of these nonlinear equations of motion are to the exact solution of the original problem depends on the method used actually to calculate K_{21} and K_{22} , but the method should always permit one in practice to carry out the exact self-consistency procedure to the end. Otherwise the regularity is immediately lost if it was in fact, at least in principle, present. This is what happens with the Roth scheme in practice: it is impossible to carry out the entire calculation exactly to the end (of course we mean "exactly" in the framework of the scheme itself), even though, on a fundamental level, the Roth scheme is regular (the latter is due to the possibility of gradually expanding the operator basis) and in a variational sense gives the best solution of the eigenvalue equations of motion

$$[\hat{A}, H]_- = \omega \hat{A},$$

if the eigen operator \hat{A} is sought in the form of an expansion

$$\hat{A} = \sum_j a_j \hat{A}_j$$

in the operator basis that appears in expansion (2.1.7).¹⁴⁻¹⁶ At the same time, it is apparently always possible to achieve exact satisfaction of the Jacobi identity, and since the basic matrix condition (2.1.10) of the Roth scheme is a conse-

quence of the Jacobi identity,¹⁹ the solution obtained with the help of the Jacobi identity cannot be inferior to the solution that could in principle be obtained from the Roth scheme.

Here it is pertinent to ask whether it is possible in principle to obtain an exact solution of the original problem in the framework of a *finite* operator basis, e.g., a two-operator one, even though direct and formally exact calculations lead, as they always do in the many-body problem, to an infinite-dimensional basis. This question is justified by two facts:

1) The energy of interacting particles can be expressed in the form of an exact formula using only a single-particle Green's function (see, e.g., Ref. 34 for the case of the ground state and Ref. 35 for the case of finite temperature); granted, there is at present no analogous formula for the energy in terms of the single-particle density matrix.

2) One can introduce a model system of noninteracting electrons in an external local field, with an energy and electron density equal to those for the same system but with the interaction turned on. This assertion forms the essence of the so-called "electron density functional theory," which is based on the theorem of Hohenberg and Kohn³⁶ for the ground state. In the case of finite temperatures the analogous theorem for the thermodynamic potential was proved by Mermin.³⁷

In the first case, of course, the exact single-particle Green's function, and in the second case the exact form of the electron density functional remain unknown. But in the case of an operator expansion of commutators it is unclear even whether it is possible in principle for such an expansion to be finite, to say nothing of how the coefficients of such a finite expansion (if one is possible in principle) might be calculated to obtain an exact solution.

The choice of the first commutator (2.1.14) of the system under study cannot be made unique, but this shortcoming is not specific to the scheme under discussion—this non-uniqueness is always present in some form or other in the theory of many interacting bodies. In fact, in an attempt to use in a mathematically correct way the "working" methods of solving classical (i.e., the simplest, original) problems in problems pertaining to systems of many interacting bodies, all that remains of these methods are only their former (classical) names. This is the case, for example, for the GF method in many-body theory, which has penetrated here from the theory of linear differential equations, where the classical Green's function satisfies specifically a linear equation of motion, whereas in many-body theory the equations of motion for the "local" Green's functions are essentially nonlinear (provided, of course, that the interaction of the bodies of the system is taken explicitly into account). This is also the case for perturbation theory (which, incidentally, is apparently the mathematically most satisfactory method for approximate solution of problems in systems of many interacting particles): in the classical theory of solving equations by this method the zeroth order approximation is always uniquely determined, since the means of choosing it is contained within the method itself, whereas in many-body theory the separation of the Hamiltonian of the problem into an unperturbed (zeroth order approximation) and a perturbed part is far from being a unique operation (and the different possible variants of such a separation are far from being equally good from the standpoint of efficiency and correct-

ness of calculating the concrete physical properties of a system), and the name "zeroth order" approximation here is justified only by the fact that, as in the case of the classical theory, the "zeroth order" problem admits an exact solution (in accordance with the terms of the separation). The same is true for the procedure of exact "linearization"—for the operator basis here one always chooses the exact basis of the first commutator, i.e., the zeroth order approximation is exact.

2.3. Some properties of the K matrix

The real parts of the poles of the Green's functions in the GF EOM method give the energy of the possible elementary excitations of the system under study.^{2,35} The damping of excitations due to the presence of an interaction in the system is given by the imaginary part of the corresponding complex pole. This microscopic information can also be obtained directly from the K matrix: it is contained in its eigenvalues. Indeed, if the K matrix admits diagonalization by a similarity transformation

$$(S^{-1}KS)_{jj'} = (K')_{jj'}\delta_{jj'},$$

which, as we know from the theory of matrices,³⁸⁻⁴⁰ is possible only in cases where the original matrix has special properties (is either self-adjoint, unitary, or symmetric, or all its eigenvalues are different), then, by transforming to the new operators

$$\hat{A}_j \rightarrow \hat{A}'_j \equiv \sum_{j'} [S^{-1}]_{jj'} \hat{A}_{j'},$$

one can see that these new operators are eigen operators,

$$[\hat{A}'_j, H]_- = K'_j \hat{A}'_j,$$

and, hence, the quantities K'_j give the spectra of possible elementary excitations of the system.^{30,31}

The eigenvalues of a K matrix of order n are calculated from the secular equation

$$\det(\lambda - K) \equiv D(\lambda) = \lambda^n - E_1 \lambda^{n-1} + E_2 \lambda^{n-2} - \dots + (-1)^n E_n = 0; \quad (2.3.1)$$

where E_p is the sum of the principal minors of order p of the K matrix. The number of these minors is C_n^p . It should be recalled that $E_1 = \text{Sp}K$, $E_n = \det K$, and the characteristic polynomials $\det(\lambda - K)$ and $\det(K - \lambda)$ are related by

$$\det(K - \lambda) = (-1)^n \det(\lambda - K).$$

For a K matrix of order two, Eq. (2.3.1) has the form

$$\lambda^2 - T\lambda + D = 0,$$

and the eigenvalues are

$$\lambda_{1,2} = \frac{1}{2} (T \pm R) \equiv E_k^{1,II}. \quad (2.3.2)$$

Having the spectra of possible elementary excitations, one can in principle calculate the corresponding densities of single-particle energy states by proceeding from their definition

$$\begin{aligned} \rho(E) &= \sum_k \delta(E - E_k) = \int_{\omega_k} \frac{dk}{|\omega_k|} \delta(E - E_k) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dt - e^{iEt} \int_{\omega_k} \frac{dk}{|\omega_k|} e^{-itE_k}, \end{aligned} \quad (2.3.3)$$

where ω_k is the cell proper (i.e., the first Brillouin zone) and $|\omega_k|$ is its volume.

For a matrix of order three the secular equation (2.3.1) takes the form

$$\lambda^3 - T\lambda^2 + E_2\lambda - D = 0. \quad (2.3.4)$$

It is unprofitable to write out the formulas for the eigenvalues (and hence for the spectra of possible elementary excitations) in general form for this case because of their awkwardness. It is simpler to obtain them as needed from (2.3.4) for each specific case.

Assuming (and this is not a very strong assumption) that the "true" matrix N is positive definite, one can obtain the important result that in this case all the eigenvalues of the K matrix must be real-valued,⁴¹ i.e., in such a system damping is absent completely. Indeed, by applying the following perfectly obvious elementary transformations

$$K - \lambda = N^{1/2}(N^{1/2}EN^{-1/2} - \lambda)N^{-1/2}$$

to Eq. (2.1.12), written in matrix form

$$E = KN \rightarrow K = NEN^{-1},$$

we see that the secular equation for the K matrix is the same as the secular equation for the self-adjoint matrix $N^{-1/2}EN^{-1/2}$, since E is a self-adjoint matrix.

Further, by successively taking the determinant and trace in matrix relations (2.1.10) and (2.1.13), we obtain the completely general result that the determinant and trace of the K matrix must always be real-valued provided only that the determinant of the matrix N (and hence $\det \bar{N}$) is nonzero.

2.4. The F matrix of the problem

A fact that is of fundamental importance is that for any finite number of terms in expansion (2.1.7), one can easily find the exact form of the F matrix that performs the "undressing" in Eq. (2.1.8). Therefore, the dressing-undressing method itself is an exact analytical method of calculating the correlation functions, and all the approximations, if any were made in solving the problem, reside only in its K matrix. The analytical formulation of the dressing-undressing method is extremely simple. In fact, suppose the dressed operator (2.1.5) is undressed according to formula (2.1.8), where the K matrix is known from expansion (2.1.7). Then, using the dressing-undressing method, we can readily obtain an exact and closed algebraic system of equations directly for the desired correlation functions by the following procedure:

1) first the "bare" operator is "dressed" according to (2.1.5) by making use of the cyclic invariance of the trace of a product of operators, as expressed by relations (2.1.3);

2) then the "dressed" operator is quickly "undressed" by using the "undressing" formula (2.1.8), which gives

$$\langle \widehat{B} \widehat{A}_j \rangle = \langle \widehat{A}_j | \beta | \widehat{B} \rangle = \sum_j F_{jj'}(\beta; K) \langle \widehat{A}_j | \widehat{B} \rangle. \quad (2.4.1)$$

This relation is a system of algebraic equations with respect to the desired correlation functions, since the matrix elements $F_{jj'}$ will be known if the matrix elements $K_{jj'}$ appearing in expansion (2.1.7) are known. The system of equations (2.4.1) will, of course, always be finite and closed if expansion (2.1.7) is finite.

The case when the desired correlation functions are time-dependent will clearly not require introducing any additional changes in this method of calculation, except for the conversion of β into β' .

For the case of a two-operator expansion (2.1.14), (2.1.15), i.e., for the case of a K matrix of order two, the F matrix has the form^{18,19}

$$F = \exp(-\beta K) \\ = \exp\left(-\frac{1}{2}\beta T\right) \left[\frac{T-2K}{R} \operatorname{sh}\left(\frac{1}{2}\beta R\right) + \operatorname{ch}\left(\frac{1}{2}\beta R\right) \right], \quad (2.4.2)$$

and its matrix elements are therefore

$$\begin{aligned} \exp\left(\frac{1}{2}\beta T\right) F_{11} &= \operatorname{ch}\left(\frac{1}{2}\beta R\right) + Q \operatorname{sh}\left(\frac{1}{2}\beta R\right), \\ \exp\left(\frac{1}{2}\beta T\right) F_{12} &= -2R^{-1}K_{12} \operatorname{sh}\left(\frac{1}{2}\beta R\right), \\ \exp\left(\frac{1}{2}\beta T\right) F_{21} &= -2R^{-1}K_{21} \operatorname{sh}\left(\frac{1}{2}\beta R\right), \\ \exp\left(\frac{1}{2}\beta T\right) F_{22} &= \operatorname{ch}\left(\frac{1}{2}\beta R\right) - Q \operatorname{sh}\left(\frac{1}{2}\beta R\right). \end{aligned}$$

For this matrix it is easy to find its trace directly:

$$\operatorname{Sp} F = 2 \exp\left(-\frac{1}{2}\beta T\right) \operatorname{ch}\left(\frac{1}{2}\beta R\right). \quad (2.4.3)$$

In these formulas we have used the notation

$$\begin{aligned} T &\equiv \operatorname{Sp} K, \quad Q \equiv (K_{22} - K_{11})R^{-1}, \\ R &\equiv ((K_{11} - K_{22})^2 + 4K_{12}K_{21})^{1/2}. \end{aligned}$$

In order to give the reader a clear understanding of the technical and computational efficiency of the dressing-undressing method, even at this early stage in the discussion, we need only calculate some correlation function of a nonoperator-oscillatory system (any system in which the interaction is not taken into account explicitly) by any of the familiar methods and by the method under study. One can also look at the very detailed comparative calculation of all the correlation functions of the Ising model by the GF (or HGF) EOM method and the dressing-undressing method in Ref. 18.

The F matrix itself is very simply expressed in terms of the K matrix (see Appendices 1 and 2 of my earlier paper²⁰):

$$F(\beta; K) = \exp(-\beta K). \quad (2.4.4)$$

This yields the important practical formula⁴²

$$\det F = \exp(-\beta \operatorname{Sp} K). \quad (2.4.5)$$

In the general case for the trace of the F matrix there is no such simple formula as there is for its determinant (2.4.5), but an integral representation in terms of the trace of the

auxiliary matrix $(z - K)^{-1}$ can be written

$$\operatorname{Sp} F = \operatorname{Sp} e^{-\beta K} = \frac{1}{2\pi i} \oint dz e^{-\beta z} \operatorname{Sp} \left(\frac{1}{z - K} \right); \quad (2.4.6)$$

here the integration contour encloses all the eigenvalues of the K matrix, which should remain to the left as they are passed around. This integral representation, which, by the way, can also be useful in a direct calculation of the partition function, i.e., the trace of the operator $\exp(-\beta H)$, follows from the general formula⁴³

$$F = e^{-\beta K} = \frac{1}{2\pi i} \oint dz e^{-\beta z} \frac{1}{z - K}, \quad (2.4.7)$$

obtained with the use of the residue theorem for the case of the exponential function of a matrix argument (see Appendix). Experience in actual calculations shows that this formula provides the simplest way of obtaining the matrix elements of the F matrix:

$$F_{jj'} = (e^{-\beta K})_{jj'} = \frac{1}{2\pi i} \oint dz e^{-\beta z} \left(\frac{1}{z - K} \right)_{jj'}, \quad (2.4.8)$$

and is especially valuable in the case of an operator basis of order three or higher. In the two-operator approximation the auxiliary matrix is

$$(z - K)^{-1} \equiv K^{-1}(z) = D(z) \begin{pmatrix} z - K_{22} & K_{12} \\ K_{21} & z - K_{11} \end{pmatrix},$$

$$D(z) = z^2 - Tz + D \equiv \det(z - K) \equiv \det K(z) = \det(K - z).$$

In the three-operator approximation it is

$$D(z)K^{-1}(z) = \begin{pmatrix} \left| \begin{matrix} z - K_{22} - K_{32} \\ -K_{23}z - K_{33} \end{matrix} \right| \cdot \left| \begin{matrix} K_{12}K_{32} \\ K_{13}K_{33} - z \end{matrix} \right| \cdot \left| \begin{matrix} -K_{12}z - K_{22} \\ -K_{13} - K_{23} \end{matrix} \right| \\ \left| \begin{matrix} K_{21}K_{31} \\ K_{23}K_{33} - z \end{matrix} \right| \cdot \left| \begin{matrix} z - K_{11} - K_{31} \\ -K_{13}z - K_{33} \end{matrix} \right| \cdot \left| \begin{matrix} K_{11} - zK_{21} \\ K_{13}K_{23} \end{matrix} \right| \\ \left| \begin{matrix} -K_{21} - K_{31} \\ z - K_{22} - K_{32} \end{matrix} \right| \cdot \left| \begin{matrix} K_{11} - zK_{31} \\ K_{12}K_{32} \end{matrix} \right| \cdot \left| \begin{matrix} z - K_{11} - K_{21} \\ -K_{12}z - K_{22} \end{matrix} \right| \end{pmatrix},$$

where

$$\begin{aligned} D(z) &= z^3 - z^2T + zE_2 - D \\ &\equiv \det(z - K) \equiv \det K(z) = -\det(K - z), \end{aligned}$$

$$\begin{aligned} E_2 &= K_{11}K_{22} - K_{12}K_{21} + K_{11}K_{33} \\ &\quad - K_{13}K_{31} + K_{22}K_{33} - K_{23}K_{32}. \end{aligned}$$

In practice the inversion of a given matrix is done in three steps:

1) the matrix $\widetilde{K}(z)$, which is the transpose of $K(z)$, is written out;

2) each element $\widetilde{K}_{jj'}(z)$ is replaced by its algebraic complement;

3) a factor $1/D(z)$ is appended to the resulting matrix, where $D(z)$ is the determinant of the matrix $K(z)$.

It quickly follows from (2.4.5) that the determinant of the F matrix will be real. Finally, it is easy to show that in this case the trace of the F matrix will also be real, since it follows from (2.4.4) and (2.1.11) that the similarity transformation (2.1.11) is also valid for the F matrix, so that its trace will in fact be real.

2.5. Regularity of the method

Formally the regularity (i.e., the possibility of making an internal check) of the DA method derives from its exact self-consistency. In fact, if a method is exactly self-consistent through the use of some universal analytical condition (such as the Jacobi identity), e.g., in a two-operator basis, then in principle one can expand the original basis to a three-operator basis and again achieve self-consistency with the help of the same condition, since it is universal. Then the first equation of motion remains unchanged, the second equation of motion is represented in the form of an exact expansion in three operators now, the first two of which formed the basis for the two-operator expansion, and the third equation of motion is fitted into this three-operator basis, which is exact for the first two equations of motion by construction, with the help of the Jacobi identity.

In the case of nonoperator expansions (e.g., expansion of an arbitrary state vector in an incomplete basis), an analogous gradual enlargement of the incomplete basis leads to a strictly monotonic approach to the exact results corresponding to expansion in the complete basis. This statement is the content of the Hylleraas–Undheim–MacDonald “separation theorem” (see, e.g., Ref. 44). It is reasonable to expect the same result in the case of operator expansions, since they are ultimately just another way of writing the same procedure for solving the Schrödinger equation.

Thus, as desired (or as necessary) one can refine the physical results of the exact two-operator self-consistency, i.e., at a fundamental level the proposed scheme of exact “linearization” admits a regular means of estimating the accuracy of a chosen operator approximation; this possibility is not afforded by the EOM method for the two-time temperature Green’s functions (and this is its principal computational shortcoming) or even by the constructive scheme of Roth (since it is not possible in practice to calculate exactly the E matrix of that scheme).

3. EXAMPLES

3.1. Bogolyubov model

For studying the ground and lowest excited states of a slightly nonideal Bose gas, Bogolyubov proposed to use the Hamiltonian³⁴

$$H = \frac{1}{2} N^2 V_0 + \sum_{\mathbf{k} \neq 0} H_{\mathbf{k}},$$

$$H_{\mathbf{k}} \equiv (\epsilon_{\mathbf{k}} + NV_{\mathbf{k}}) \hat{n}_{\mathbf{k}} + \frac{1}{2} NV_{\mathbf{k}} (\hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} + \hat{a}_{-\mathbf{k}}^+ \hat{a}_{\mathbf{k}}^+), \quad (3.1.1)$$

which admits an exact analytical solution. The solution is ordinarily constructed with the aid of canonical transformations of the initial operators to new operators and is called upon to reduce (3.1.1) to diagonal form. For this problem the DA method is doubly favored, since the basic equations of motion turn out to be linear from the start, i.e., it is easy to write the exact K matrix for (3.1.1) and so it is not necessary to carry out the most complicated and laborious part of the DA method, viz., the exact self-consistency procedure. Thus, the basic equations of motion here have the form

$$[\hat{a}_{\mathbf{k}}, H_{\mathbf{k}}]_- = \omega_0 \hat{a}_{\mathbf{k}} + \omega_1 \hat{a}_{-\mathbf{k}}^+,$$

$$[\hat{a}_{-\mathbf{k}}^+, H_{\mathbf{k}}]_- = -\omega_1 \hat{a}_{\mathbf{k}} - \omega_0 \hat{a}_{-\mathbf{k}}^+,$$

where we have introduced the Kittel notation³⁴

$$\omega_0 \equiv \epsilon_{\mathbf{k}} + NV_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \omega_1, \quad \epsilon_{-\mathbf{k}} = \epsilon_{\mathbf{k}}, \quad V_{-\mathbf{k}} = V_{\mathbf{k}}, \quad V_{\mathbf{k}}^* = V_{\mathbf{k}}.$$

Thus the K matrix is of the form

$$K = \begin{pmatrix} \omega_0 & \omega_1 \\ -\omega_1 & -\omega_0 \end{pmatrix}.$$

Here it should be emphasized once again that even though the exact form of the K matrix of the problem is known, the Bogolyubov method nevertheless requires a canonical transformation, whereas the DA method allows one to calculate immediately all the necessary correlation functions by the dressing-undressing method if the K matrix is known. First, however, one can extract the possible spectra (2.3.2) and then, using them, find the corresponding densities of single-particle energy states (2.3.3). The spectrum in this case has the form

$$E_{\mathbf{k}} = (\omega_0^2 - \omega_1^2)^{1/2},$$

while the integral (2.3.3) for the density of states cannot be evaluated in terms of elementary functions. Using formula (2.4.1) we can easily write algebraic equations for any correlation functions. For example, for the main correlation functions these equations have the form

$$\langle \hat{n}_{\mathbf{k}} \rangle \equiv \langle \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}} \rangle = \langle \hat{a}_{\mathbf{k}} | \beta | \hat{a}_{\mathbf{k}}^+ \rangle = F_{11} \langle \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{k}}^+ \rangle + F_{12} \langle \hat{a}_{-\mathbf{k}}^+ \hat{a}_{\mathbf{k}}^+ \rangle,$$

$$\langle \hat{a}_{-\mathbf{k}}^+ \hat{a}_{\mathbf{k}}^+ \rangle = \langle \hat{a}_{-\mathbf{k}}^+ | \beta | \hat{a}_{\mathbf{k}}^+ \rangle = F_{21} \langle \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{k}}^+ \rangle + F_{22} \langle \hat{a}_{-\mathbf{k}}^+ \hat{a}_{\mathbf{k}}^+ \rangle.$$

We can now easily find the diagonal correlation function

$$\langle \hat{n}_{\pm \mathbf{k}} \rangle = \frac{1}{2} \left[\frac{2K_{11}}{R} \operatorname{cth} \left(\frac{1}{4} \beta R \right) - 1 \right] = \frac{1}{2} \left[\frac{\omega_0}{E_{\mathbf{k}}} \operatorname{cth} \left(\frac{1}{2} \beta E_{\mathbf{k}} \right) - 1 \right]. \quad (3.1.2)$$

In working with formulas for the average occupation numbers it is useful to keep in mind the identities

$$\frac{1}{2} (1 - \operatorname{th} \frac{x}{2}) \equiv (e^x + 1)^{-1},$$

$$\frac{1}{2} (\operatorname{cth} \frac{x}{2} - 1) \equiv (e^x - 1)^{-1}.$$

The off-diagonal correlation function is

$$\langle \hat{a}_{-\mathbf{k}}^+ \hat{a}_{\mathbf{k}}^+ \rangle = \frac{K_{21}}{R} \operatorname{cth} \left(\frac{1}{4} \beta R \right) \equiv \frac{K_{21}}{2E_{\mathbf{k}}} \operatorname{cth} \left(\frac{1}{2} \beta E_{\mathbf{k}} \right).$$

The overall temperature dependence of the number of particles of the condensate is obtained from (3.1.2):

$$N_0 \equiv N - \sum_{\mathbf{k} \neq 0} n_{\mathbf{k}}, \quad \frac{N_0}{N} = \frac{3}{2} - \frac{1}{2} \frac{1}{N} \sum_{\mathbf{k} \neq 0} \frac{\omega_0}{E_{\mathbf{k}}} \operatorname{cth} \left(\frac{1}{2} \beta E_{\mathbf{k}} \right).$$

For the case of an ideal Bose gas this formula gives

$$\frac{N_0}{N} = \frac{3}{2} - \frac{1}{2} \frac{1}{N} \sum_{\mathbf{k} \neq 0} \operatorname{cth} \left(\frac{1}{2} \beta \epsilon_{\mathbf{k}} \right). \quad (3.1.3)$$

The critical temperature of an ideal Bose gas is determined from the condition that below the transition point the left-hand side of (3.1.3) is finite:

$$\frac{1}{N} \sum_{\mathbf{k} \neq 0} \operatorname{cth} \left(\frac{1}{2} \beta \epsilon_{\mathbf{k}} \right) = 3.$$

3.2. Ising model

The familiar Ising model in the spin deviation operators is conveniently reduced to an expression in the creation and annihilation operators of fictitious fermions at the lattice sites^{18,20}

$$H = \bar{B} \sum_f \hat{n}_f - \frac{J}{2} \sum_{f,j} \hat{n}_f \hat{n}_j, \quad \bar{B} \equiv \lambda B + \frac{zJ}{2}. \quad (3.2.1)$$

Further, it is convenient to introduce the operator \hat{O}_k ($k = 0, 1, 2, \dots, z$), which is the sum of the C_z^k products of operators \hat{n}_j taken k at a time from among the z occupation-number operators of the sites j ($j = 1, 2, \dots, z$) nearest to the investigated site f . The use of \hat{O}_k allows one to reduce considerably the number of unknown correlation functions and, hence, the number of equations for them, except for the case of the one-dimensional model (e.g., 8 instead of 10 for a square lattice and 12 instead of 18 for a close-packed lattice), since here there can only be correlation functions of the form $\langle \hat{O}_k \rangle$ and $\langle \hat{n}_f \hat{O}_k \rangle$.

The first equation of motion for (3.2.1) is

$$[\hat{a}_f, H]_- = \bar{B} \hat{a}_f - J \hat{O}_1 \hat{a}_f \equiv \bar{B} \hat{a}_f - J \hat{d}_f^{(1)}. \quad (3.2.2)$$

Therefore, the commutator of order k is of the form

$$[\hat{d}_f^{(k)}, H]_- = (\bar{B} - k + 1) \hat{d}_f^{(k-1)} - k J \hat{d}_f^{(k)}.$$

Thus in the basis $\hat{a}_f, \hat{O}_k \equiv \hat{d}_f^{(k)}$ it is easy to calculate the exact K matrix. However, it does not permit one to calculate correlation functions of the form $\langle \hat{O}_k \rangle$, and therefore the system of equations obtained for the correlation functions $\langle \hat{n}_f \hat{O}_k \rangle$ will not be closed.

Returning to the equation of motion (3.2.2),

$$[\hat{a}_f, H]_- = K_{11} \hat{a}_f + K_{12} \hat{d}_f, \quad (3.2.3)$$

we write the second equation of motion as

$$[\hat{d}_f, H]_- = K_{21} \hat{a}_f + K_{22} \hat{d}_f, \quad (3.2.4)$$

and find the coefficients K_{21} and K_{22} from formulas (2.1.16) and (2.1.17), for which purpose we must calculate the matrices N and \bar{N} in the basis \hat{a}_f, \hat{d}_f :

$$\begin{aligned} N_{11} &\equiv \langle [\hat{a}_f, \hat{a}_f^+]_+ \rangle = 1, \\ N_{12} &\equiv \langle [\hat{a}_f, \hat{d}_f^+]_+ \rangle = \langle \hat{O}_1 \rangle = N_{21}, \\ N_{22} &\equiv \langle [\hat{d}_f, \hat{d}_f^+]_+ \rangle = \langle \hat{O}_1^2 \rangle, \\ \bar{N}_{11} &\equiv \langle \hat{a}_f \hat{a}_f^+ \rangle = 1 - \langle \hat{n}_f \rangle, \\ \bar{N}_{12} &\equiv \langle \hat{a}_f \hat{d}_f^+ \rangle = \langle (1 - \hat{n}_f) \hat{O}_1 \rangle = \bar{N}_{21}, \\ \bar{N}_{22} &\equiv \langle \hat{d}_f \hat{d}_f^+ \rangle = \langle (1 - \hat{n}_f) \hat{O}_1^2 \rangle. \end{aligned} \quad (3.2.5)$$

It can be seen that these second-order matrices are the corresponding upper left-hand corners of the same matrices in the basis $\hat{d}_f^{(k)}$, i.e., of the matrices

$$\begin{aligned} N_{nm} &\equiv \langle [\hat{O}_{n-1} \hat{a}_f, \hat{O}_{m-1} \hat{a}_f^+]_+ \rangle = \langle \hat{O}_{n-1} \hat{O}_{m-1} \rangle, \\ \bar{N}_{nm} &\equiv \langle \hat{O}_{n-1} \hat{O}_{m-1} \hat{a}_f \hat{a}_f^+ \rangle = \langle (1 - \hat{n}_f) \hat{O}_{n-1} \hat{O}_{m-1} \rangle, \end{aligned}$$

whereas the K matrix (3.2.3), (3.2.4), as will be seen from the following formulas (3.2.6), (3.2.7), is not the upper left-

hand corner for the K matrix in the same basis.

Substituting matrix elements (3.2.5) into formulas (2.1.16) and (2.1.17), we can obtain

$$K_{21} = 2J \frac{\langle \hat{n}_f \hat{O}_2 \rangle \langle \hat{O}_1 \rangle - \langle \hat{n}_f \hat{O}_1 \rangle \langle \hat{O}_2 \rangle}{\langle \hat{n}_f \hat{O}_1 \rangle - \langle \hat{n}_f \rangle \langle \hat{O}_1 \rangle}, \quad (3.2.6)$$

$$K_{22} = \bar{B} - J - 2J \frac{\langle \hat{n}_f \hat{O}_2 \rangle - \langle \hat{n}_f \rangle \langle \hat{O}_2 \rangle}{\langle \hat{n}_f \hat{O}_1 \rangle - \langle \hat{n}_f \rangle \langle \hat{O}_1 \rangle}. \quad (3.2.7)$$

These expressions contain four correlation functions of different types:

$$\langle \hat{O}_1 \rangle, \langle \hat{O}_2 \rangle, \langle \hat{n}_f \hat{O}_1 \rangle, \langle \hat{n}_f \hat{O}_2 \rangle.$$

These correlation functions can be calculated by considering the following correlation functions in the dressing-undressing method:

$$\langle \hat{n}_f \rangle, \langle \hat{a}_f \hat{d}_f \rangle, \langle \hat{d}_f \hat{a}_f^+ \rangle.$$

The second of these three correlation functions gives two independent equations, since it contains two different basis operators.

Thus the first correlation function gives the equation

$$\begin{aligned} \langle \hat{n}_f \rangle &\equiv \langle \hat{a}_f^+ \hat{a}_f \rangle = \langle \hat{a}_f | \beta | \hat{a}_f^+ \rangle = F_{11} \langle \hat{a}_f \hat{a}_f^+ \rangle + F_{12} \langle \hat{d}_f \hat{a}_f^+ \rangle; \\ \langle \hat{a}_f^+ \hat{d}_f \rangle &= \langle \hat{d}_f | \beta | \hat{a}_f^+ \rangle = F_{21} \langle \hat{a}_f \hat{a}_f^+ \rangle + F_{22} \langle \hat{d}_f \hat{a}_f^+ \rangle. \end{aligned}$$

From which we find the two correlation functions

$$\begin{aligned} \langle \hat{n}_f \rangle &= \frac{F_{11} + \langle \hat{O}_1 \rangle F_{12} + \det F}{1 + \text{sp } F + \det F}, \\ \langle \hat{a}_f^+ \hat{d}_f \rangle &\equiv \langle \hat{n}_f \hat{O}_1 \rangle = \frac{(1 + F_{11}) \langle \hat{O}_1 \rangle - F_{21}}{1 + \text{sp } F + \det F}. \end{aligned}$$

Similarly, for the other correlation functions

$$\begin{aligned} \langle \hat{a}_f^+ \hat{d}_f \rangle &= \langle \hat{a}_f | \beta | \hat{a}_f^+ \hat{O}_1 \rangle = F_{11} \langle \hat{a}_f \hat{a}_f^+ \hat{O}_1 \rangle \\ &\quad + F_{12} \langle \hat{d}_f \hat{a}_f^+ \hat{O}_1 \rangle = F_{11} \langle \hat{a}_f \hat{a}_f^+ \rangle + F_{12} \langle \hat{d}_f \hat{a}_f^+ \rangle, \\ \langle \hat{d}_f^+ \hat{d}_f \rangle &\equiv \langle \hat{n}_f \hat{O}_1^2 \rangle = \langle \hat{d}_f | \beta | \hat{d}_f^+ \rangle = F_{21} \langle \hat{a}_f \hat{a}_f^+ \rangle + F_{22} \langle \hat{d}_f \hat{a}_f^+ \rangle. \end{aligned}$$

These equations lead to the expressions

$$\begin{aligned} \langle \hat{n}_f \hat{O}_1 \rangle &= \frac{(F_{11} + \det F) \langle \hat{O}_1 \rangle + F_{12} \langle \hat{O}_1^2 \rangle}{1 + \text{Sp } F + \det F}, \\ \langle \hat{d}_f \hat{a}_f^+ \rangle &\equiv \langle (1 - \hat{n}_f) \hat{O}_1^2 \rangle = \frac{(1 + F_{11}) \langle \hat{O}_1^2 \rangle - F_{21} \langle \hat{O}_1 \rangle}{1 + \text{Sp } F + \det F}. \end{aligned}$$

3.3. Heisenberg model

The EOM method applied to the Heisenberg model with the widely known Tyablikov decoupling of the equations of motion³⁵ enables one to calculate the magnetization of the system quite simply, but great difficulties are encountered when one attempts to calculate the specific heat.⁴⁵ This is because the Tyablikov scheme permits calculation of only the transverse correlation function, but in order to calculate the internal energy in this method one also needs to know the longitudinal correlation function. It turns out that this difficulty can be overcome by appealing to the so-called longitudinal Hartree-Fock approximation to the Heisenberg Hamiltonian.⁴⁶ It has been shown⁴⁶ that this approxi-

mation corresponds exactly to the Tyablikov approximation in the case of a ferromagnetic version of the Heisenberg model and to the Ginzburg–Fain approximation⁴⁷ for an antiferromagnetic version.

The ferromagnetic version of the Heisenberg model is³⁵

$$H = -\lambda B \sum_f \hat{S}_f^z - \frac{1}{2} \sum_{f,f'} J_{ff'} (\hat{S}_f^+ \hat{S}_{f'}^- + \hat{S}_f^z \hat{S}_{f'}^z), \quad J_{ff'} > 0.$$

The longitudinal Hartree–Fock approximation is of the form⁴⁶

$$H''_{\text{HF}} = -\alpha \sum_f \hat{S}_f^z - \frac{1}{2} \sum_{f,f'} J_{ff'} \hat{S}_f^+ \hat{S}_{f'}^- = -\alpha \hat{S}_0^z - \frac{1}{2} \sum_{\mathbf{k}} J_{\mathbf{k}} \hat{S}_{\mathbf{k}}^+ \hat{S}_{-\mathbf{k}}^-; \quad (3.3.1)$$

here we have introduced the notation

$$\alpha \equiv \lambda B + J_0 \langle \hat{S}_f^z \rangle, \quad J_0 \equiv \sum_{f-f'} J_{f-f'}$$

It can be seen immediately from (3.3.1) that for calculating the internal energy of this system it is sufficient to know only the transverse correlation function and the magnetization. For calculating the transverse correlation function one needs the commutator

$$[\hat{S}_f^\pm, H''_{\text{HF}}]_- = \pm \alpha \hat{S}_f^\pm \mp \hat{S}_f^z \sum_{f'} J_{f-f'} \hat{S}_{f'}^\pm. \quad (3.3.2)$$

On the next application of the longitudinal Hartree–Fock approximation the operator of the longitudinal component in (3.3.2) should be replaced by its average value, i.e., one must use the commutator

$$[\hat{S}_{\mathbf{k}}^\pm, H''_{\chi\Phi}]_- = \pm (\alpha - \langle \hat{S}_f^z \rangle J_{\mathbf{k}}) \hat{S}_{\mathbf{k}}^\pm \equiv \pm \xi_{\mathbf{k}} \hat{S}_{\mathbf{k}}^\pm, \quad (3.3.3)$$

where we have used the notation

$$\xi_{\mathbf{k}} \equiv \lambda B + J_0 (1 - \gamma_{\mathbf{k}}) \langle \hat{S}_f^z \rangle, \quad \gamma_{-\mathbf{k}} = \gamma_{\mathbf{k}} \equiv J_{\mathbf{k}} J_0^{-1}.$$

Using (3.3.3) together with formula (2.1.8'), we immediately find the transverse correlation function

$$\langle \hat{S}_{\mathbf{k}}^\pm \hat{S}_{\mathbf{k}'}^\pm \rangle = \pm N^{1/2} \frac{2 \langle \hat{S}_f^z \rangle \delta_{-\mathbf{k}\mathbf{k}'}}{1 - \exp(\mp \beta \xi_{\mathbf{k}})}.$$

Since the commutator (3.3.3) vanishes to the right of the transition point, the longitudinal Hartree–Fock approximation can be used to study the problem only to the left of this point. This also pertains to the antiferromagnetic version of the Heisenberg model. If we now use the relation

$$\hat{S}_f^z = \hat{S}_f^+ \hat{S}_f^- - \frac{1}{2} \rightarrow \langle \hat{S}_f^z \rangle = \frac{1}{N} \sum_{\mathbf{k}} \langle \hat{S}_{\mathbf{k}}^+ \hat{S}_{\mathbf{k}}^- \rangle - \frac{1}{2}, \quad (3.3.4)$$

we can construct the entire thermodynamics of the Heisenberg ferromagnet in this approximation (which coincides completely with the Tyablikov approximation).

The antiferromagnetic version of the Heisenberg model is conveniently taken in the form³⁴

$$H = -\lambda B \left(\sum_{f_1} \hat{S}_{f_1}^z + \sum_{f_2} \hat{S}_{f_2}^z \right) - \frac{1}{2} \sum_{f_1, f_2} J_{f_1 f_2} (2 \hat{S}_{f_1}^z \hat{S}_{f_2}^z + \hat{S}_{f_1}^+ \hat{S}_{f_2}^- + \hat{S}_{f_2}^+ \hat{S}_{f_1}^-), \quad J_{f_1 f_2} < 0.$$

The longitudinal Hartree–Fock approximation for this Hamiltonian has the form⁴⁶

$$H''_{\text{HF}} = -\alpha_1 \sum_{f_2} \hat{S}_{f_2}^z - \alpha_2 \sum_{f_1} \hat{S}_{f_1}^z - \frac{1}{2} \sum_{f_1, f_2} J_{f_1 f_2} (\hat{S}_{f_1}^+ \hat{S}_{f_2}^- + \hat{S}_{f_2}^+ \hat{S}_{f_1}^-), \quad (3.3.5)$$

where we have introduced the notation

$$\alpha_i \equiv \lambda B + J_0 \langle \hat{S}_{f_i}^z \rangle, \quad i = 1, 2.$$

The Hamiltonian (3.3.5) gives the commutators

$$[\hat{S}_1^\pm(\mathbf{k}), H''_{\text{HF}}]_- = \mp \alpha_2 \hat{S}_1^\pm(\mathbf{k}) \mp J_{\mathbf{k}} \langle \hat{S}_{f_1}^z \rangle \hat{S}_2^\pm(\mathbf{k}), \quad (3.3.6)$$

$$[\hat{S}_2^\pm(\mathbf{k}), H''_{\text{HF}}]_- = \mp \alpha_1 \hat{S}_2^\pm(\mathbf{k}) \mp J_{\mathbf{k}} \langle \hat{S}_{f_2}^z \rangle \hat{S}_1^\pm(\mathbf{k}).$$

Here the second equation of motion is obtained from the first by the replacement $1 \leftrightarrow 2$. Making use of the commutators

$$[\hat{S}_{\mathbf{k}}^\pm, \hat{S}_{\mathbf{k}'}^\pm]_- = \pm \hat{S}_{\mathbf{k}+\mathbf{k}'}^\pm, \quad [\hat{S}_{\mathbf{k}}^\pm, \hat{S}_{\mathbf{k}'}^\mp]_- = \pm 2 \hat{S}_{\mathbf{k}+\mathbf{k}'}^z,$$

and the lattice transforms

$$\hat{S}_f^z = \frac{1}{N^{1/2}} \sum_{\mathbf{k}} \hat{S}_{\mathbf{k}}^z e^{-i\mathbf{k}f}, \quad \hat{S}_f^\pm = \frac{1}{N^{1/2}} \sum_{\mathbf{k}} \hat{S}_{\mathbf{k}}^\pm e^{\mp i\mathbf{k}f},$$

we can easily calculate the transverse correlation functions from the equations of motion (3.3.6) by the dressing-undressing method. Relation (3.3.4) can then be used to calculate the sublattice magnetizations. The internal energy of the antiferromagnet can be calculated from (3.3.5) after a lattice Fourier transform is taken. This approximation coincides completely with the Ginzburg–Fain theory.⁴⁷

3.4. Hubbard model

Here we will consider a generalized (degenerate) Hubbard model, which differs from the ordinary (nondegenerate) Hubbard model only in the possible values of the spin index of the operators—it can now take on more than two values. The most important application of this model is in the theory of transition metals, where it allows one to take into account rather simply the degeneracy of the 3d levels of the atoms of these metals.⁴⁸ In this case the spin index will take on ten values, i.e., the 3d electrons are treated as fermions with spin 9/2, and so their energy in the band will be degenerate not only with respect to the true spin but also with respect to the magnetic quantum number.

Thus we are considering the model

$$H = \sum_{i,j,\nu} t_{ij\nu} \hat{C}_{i\nu}^+ \hat{C}_{j\nu} + \frac{1}{2} \sum_j \hat{N}_j (\hat{N}_j - 1), \quad (3.4.1)$$

where we have used the notation

$$\hat{N}_j \equiv \sum_{\nu} \hat{n}_{j\nu} = \sum_{\nu} \hat{C}_{j\nu}^+ \hat{C}_{j\nu}.$$

Expression (3.4.1) will of course go over to the ordinary (nondegenerate) Hubbard model if the index ν takes on only two values. The physical justification of this version (3.4.1) of the Hubbard model lies in the fact that the “distance” between bands corresponding to atoms with different numbers of 3d electrons is in general much larger (these “distances” are of the order of tens of eV) than the widths of

these bands themselves (which are generally not more than ten eV; Ref. 4).

1) From the one-electron commutator

$$[\hat{C}_{j\nu}, H]_- = \sum_j t_{jj'} \hat{C}_{j'\nu} + i\bar{N} \hat{C}_{j\nu} \equiv \sum_j t_{jj'} \hat{C}_{j'\nu} + i\hat{d}_{j\nu}$$

we see that it is convenient to deal with the lattice Fourier transforms of the operators

$$\hat{C}_{\mathbf{k}\nu} \equiv \frac{1}{N^{1/2}} \sum_j e^{ikj} \hat{C}_{j\nu},$$

i.e., with the commutator

$$[\hat{C}_{\mathbf{k}\nu}, H]_- = t_{\mathbf{k}} \hat{C}_{\mathbf{k}\nu} + i\hat{d}_{\mathbf{k}\nu} \equiv K_{11} \hat{C}_{\mathbf{k}\nu} + K_{12} \hat{d}_{\mathbf{k}\nu}. \quad (3.4.2)$$

Then the second, three-electron commutator must be expanded in this basis:

$$[\hat{d}_{\mathbf{k}\nu}, H]_- = K_{21} \hat{C}_{\mathbf{k}\nu} + K_{22} \hat{d}_{\mathbf{k}\nu}, \quad (3.4.3)$$

and the coefficients of the expansion must be calculated according to formulas (2.1.16) and (2.1.17), since the K matrix is real-valued. Now it remains to calculate the matrices N and \bar{N} , in order to have the possibility of using formulas (2.1.16) and (2.1.17). Straightforward calculations give

$$[\hat{C}_{\mathbf{k}\nu}^\pm, \hat{d}_{\mathbf{k}\nu}^\mp]_+ = \frac{1}{N} \sum_j (\hat{N}_j - \hat{n}_{j\nu}) \equiv \hat{\gamma}_\nu, \quad (3.4.4)$$

$$[\hat{d}_{\mathbf{k}\nu}, \hat{d}_{\mathbf{k}\nu}^\dagger]_+ = \frac{1}{N} \sum_j (\hat{N}_j - \hat{n}_{j\nu})^2 \equiv \kappa_\nu$$

under the obvious condition

$$[\hat{C}_{\mathbf{k}\nu}, \hat{C}_{\mathbf{k}'\nu}^\dagger]_+ = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\nu\nu'},$$

which follows from the condition that such anticommutator relations hold in coordinate space. Here it is noteworthy that the anticommutators (3.4.4) turn out to be independent of the quasi-momentum. The averaged values of these operators are

$$\begin{aligned} \gamma_\nu &= \langle \hat{N}_j - \hat{n}_{j\nu} \rangle = n - n_\nu, \\ \kappa_\nu &= \langle (\hat{N}_j - \hat{n}_{j\nu})^2 \rangle, \\ \langle \hat{N}_j \rangle &= \sum_\nu \langle \hat{n}_{j\nu} \rangle = \sum_\nu n_\nu = n. \end{aligned} \quad (3.4.5)$$

Thus the N matrix of this version of the Hubbard model has the form

$$\begin{aligned} N_{11} &\equiv \langle [\hat{C}_{\mathbf{k}\nu}, \hat{C}_{\mathbf{k}\nu}^\dagger]_+ \rangle = 1, \\ N_{12} &\equiv \langle [\hat{C}_{\mathbf{k}\nu}, \hat{d}_{\mathbf{k}\nu}^\dagger]_+ \rangle = \gamma_\nu = N_{21}, \\ N_{22} &\equiv \langle [\hat{d}_{\mathbf{k}\nu}, \hat{d}_{\mathbf{k}\nu}^\dagger]_+ \rangle = \kappa_\nu. \end{aligned} \quad (3.4.6)$$

The \bar{N} matrix is also easily calculated by the dressing-undressing method. It is more convenient to calculate \bar{N}_{11} and \bar{N}_{21} first. To do this we must consider the system

$$\begin{aligned} \langle \hat{n}_{\mathbf{k}\nu} \rangle &= \langle \hat{C}_{\mathbf{k}\nu} [\beta] \hat{C}_{\mathbf{k}\nu}^\dagger \rangle = F_{11} (1 - \hat{n}_{\mathbf{k}\nu}) + F_{12} \langle \hat{d}_{\mathbf{k}\nu} \hat{C}_{\mathbf{k}\nu}^\dagger \rangle, \\ \langle \hat{C}_{\mathbf{k}\nu}^\dagger \hat{d}_{\mathbf{k}\nu} \rangle &= \langle \hat{d}_{\mathbf{k}\nu} [\beta] \hat{C}_{\mathbf{k}\nu}^\dagger \rangle = F_{21} (1 - \hat{n}_{\mathbf{k}\nu}) + F_{22} \langle \hat{d}_{\mathbf{k}\nu} \hat{C}_{\mathbf{k}\nu}^\dagger \rangle. \end{aligned}$$

Solving these equations with allowance for the second anticommutator (3.4.6), we obtain

$$\begin{aligned} \langle \hat{n}_{\mathbf{k}\nu} \rangle &= (F_{11} + \gamma_\nu F_{12} + \det F)(1 + \text{Sp } F + \det F)^{-1}, \\ \langle \hat{d}_{\mathbf{k}\nu} \hat{C}_{\mathbf{k}\nu}^\dagger \rangle &\equiv \bar{N}_{21} = [(1 + F_{11})\gamma_\nu - F_{21}](1 + \text{Sp } F + \det F)^{-1}, \end{aligned} \quad (3.4.7)$$

$$1 - \langle \hat{n}_{\mathbf{k}\nu} \rangle = (1 + F_{22} - \gamma_\nu F_{12})(1 + \text{Sp } F + \det F)^{-1}.$$

Now it remains to calculate \bar{N}_{12} and \bar{N}_{22} from the equations

$$\begin{aligned} \langle \hat{d}_{\mathbf{k}\nu}^\dagger \hat{d}_{\mathbf{k}\nu} \rangle &= \langle \hat{d}_{\mathbf{k}\nu} [\beta] \hat{d}_{\mathbf{k}\nu}^\dagger \rangle = F_{21} \langle \hat{C}_{\mathbf{k}\nu} \hat{d}_{\mathbf{k}\nu}^\dagger \rangle + F_{22} \langle \hat{d}_{\mathbf{k}\nu} \hat{d}_{\mathbf{k}\nu}^\dagger \rangle, \\ \langle \hat{C}_{\mathbf{k}\nu}^\dagger \hat{C}_{\mathbf{k}\nu} \rangle &= \langle \hat{C}_{\mathbf{k}\nu} [\beta] \hat{C}_{\mathbf{k}\nu}^\dagger \rangle = F_{11} \langle \hat{C}_{\mathbf{k}\nu} \hat{d}_{\mathbf{k}\nu}^\dagger \rangle + F_{12} \langle \hat{d}_{\mathbf{k}\nu} \hat{d}_{\mathbf{k}\nu}^\dagger \rangle. \end{aligned}$$

These equations, with allowance for the third anticommutator (3.4.6), give

$$\begin{aligned} \langle \hat{C}_{\mathbf{k}\nu} \hat{d}_{\mathbf{k}\nu}^\dagger \rangle &\equiv \bar{N}_{12} = [(1 + F_{22})\gamma_\nu - \kappa_\nu F_{12}](1 + \text{Sp } F + \det F)^{-1}, \\ \langle \hat{d}_{\mathbf{k}\nu} \hat{d}_{\mathbf{k}\nu}^\dagger \rangle &\equiv \bar{N}_{22} = [(1 + F_{11})\kappa_\nu - \gamma_\nu F_{21}](1 + \text{Sp } F + \det F)^{-1}. \end{aligned}$$

From the first of relations (3.4.7) it is easy to obtain the principal two-site correlation function

$$\begin{aligned} \langle \hat{C}_{j\nu} \hat{C}_{j'\nu} \rangle &= \frac{1}{N} \sum_{\mathbf{k}} e^{ik(j-j')} \langle \hat{n}_{\mathbf{k}\nu} \rangle \\ &= \frac{1}{N} \sum_{\mathbf{k}} e^{ik(j-j')} \frac{F_{11} + \gamma_\nu F_{12} + \det F}{1 + \text{Sp } F + \det F}, \end{aligned} \quad (3.4.9)$$

since in the presence of translational invariance the correlation functions are diagonal with respect to the quasi-momentum:

$$\begin{aligned} \langle \hat{A}_{\mathbf{k}} \hat{B}_{\mathbf{k}'} \rangle &= \frac{1}{N} \sum_{j,j'} e^{i(\mathbf{k}j - \mathbf{k}'j')} \langle \hat{A}_j \hat{B}_{j'} \rangle \\ &= \frac{1}{N} \sum_j e^{i(\mathbf{k} - \mathbf{k}')j} \sum_{j'} e^{i\mathbf{k}(j-j')} \langle \hat{A}_j \hat{B}_{j'} \rangle \\ &= \frac{1}{N} \sum_j e^{i(\mathbf{k} - \mathbf{k}')j} \langle \hat{A}_j \hat{B}_{j'} \rangle_{\mathbf{k}} = \langle \hat{A}_j \hat{B}_{j'} \rangle_{\mathbf{k}} \delta_{\mathbf{k}\mathbf{k}'}. \end{aligned}$$

The two-site correlation function of higher order $\langle \hat{C}_{j\nu} \hat{d}_{j'\nu}^\dagger \rangle$ is obtained in an analogous way using the first of expressions (3.4.8). Further, since

$$\begin{aligned} \langle \hat{C}_{j\nu} \hat{d}_{j'\nu}^\dagger \rangle &\equiv \langle \hat{C}_{j\nu} \hat{C}_{j'\nu}^\dagger \hat{N}_j \rangle = n - \langle \hat{N}_j \hat{n}_{j\nu} \rangle, \\ \langle \hat{N}_j^2 \rangle &= \sum_\nu \langle \hat{N}_j \hat{n}_{j\nu} \rangle, \end{aligned}$$

we can also calculate the principal single-site correlation function

$$\langle \hat{N}_j (\hat{N}_j - 1) \rangle = 9n - \frac{1}{N} \sum_{\mathbf{k},\nu} \frac{(1 + F_{22})\gamma_\nu - \kappa_\nu F_{12}}{1 + \text{Sp } F + \det F}. \quad (3.4.10)$$

Now, using the second formula in (3.4.5), we can easily calculate the quantity

$$\kappa_\nu = n_\nu + 8n - \sum_{\nu'} \frac{1}{N} \sum_{\mathbf{k}} \left[\frac{(1 + F_{22})\gamma_{\nu'} - \kappa_{\nu'} F_{12}}{1 + \text{Sp } F + \det F} \right]_{\nu'} (1 - 2\delta_{\nu\nu'}). \quad (3.4.11)$$

Finally, it is useful to give the relation

$$N_{11} K_{21} + N_{12} (K_{22} - K_{11}) - N_{22} K_{12} = 0, \quad (3.4.12)$$

(where as the N matrix one can take either of the two matrices N and \bar{N}), to which the matrix relations (2.1.10) and

(2.1.13) reduce in the case when the matrices in them are real; explicitly:

a) for the N matrix Eq. (3.4.12) takes the form

$$K_{21} = \alpha_v K_{12} + \gamma_v (K_{11} - K_{22}); \quad (3.4.13)$$

b) for the \bar{N} matrix Eq. (3.4.12) becomes

$$(1 + F_{22})K_{21} = (1 + F_{11})\alpha_v K_{12} + [(1 + F_{22})\gamma_v - \alpha_v F_{12}](K_{11} - K_{22}). \quad (3.4.14)$$

The determinant of system (3.4.13), (3.4.14) does not coincide with the determinant $\bar{N}_{11}N_{12} - N_{11}\bar{N}_{12}$, since in Eq. (3.4.14) a term $\gamma_v F_{12}K_{21} = \gamma_v F_{21}K_{12}$ has canceled out. Incidentally, it was from formula (3.4.12) that we obtained formulas (2.1.16) and (2.1.17). The expressions for $\bar{N}_{12} = \bar{N}_{21}$ have a different appearance but are actually identical.

2) For model (3.4.1) we can examine the atomic limit

$$H = t_0 \sum_{j'} \hat{n}_j + \frac{I}{2} \sum_j \hat{N}_j (\hat{N}_j - 1), \quad (3.4.15)$$

which is obtained by letting $t_{jj'} \rightarrow t_0 \delta_{jj'}$, where

$$t_0 \equiv \frac{1}{N} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \equiv \bar{\epsilon}_{\mathbf{k}}$$

is the average value of $\epsilon_{\mathbf{k}}$ in the band. For model (3.4.15), as for the Ising model, we can find the exact form of the K matrix if we take as the basis the operators $\hat{N}_j^k \hat{C}_{jv}$, $k = 0, 1, 2, \dots, 10$:

$$[\hat{N}_j^k \hat{C}_{jv}, H]_- = t_0 \hat{N}_j^{k-1} \hat{C}_{jv} + I \hat{N}_j^k \hat{C}_{jv}. \quad (3.4.16)$$

In the case when the spin index assumes only two values, the system of equations of motion (3.4.16) is closed already in the second step:

$$[\hat{C}_{jv}, H]_- = t_0 \hat{C}_{jv} + I \hat{d}_{jv}, \quad \hat{d}_{jv} \equiv \hat{n}_{j-\sigma} \hat{C}_{jv}, \\ [\hat{d}_{jv}, H]_- = (t_0 + I) \hat{d}_{jv}$$

Here this K matrix can also be obtained easily from the general formulas (2.1.16) and (2.1.17) with the help of the matrices N and \bar{N} .

3) In this paragraph the K matrix

$$K = \begin{pmatrix} t_k & I \\ K_{21} & K_{22} \end{pmatrix} = I \begin{pmatrix} t_k/I & 1 \\ K_{21}/I & K_{22}/I \end{pmatrix},$$

corresponding to expansions (3.4.2) and (3.4.3), where

$$t_k \equiv \sum_{j-j'} t_{jj'} \exp[i\mathbf{k}(j-j')]$$

and $t_{jj'}$ is the energy of transition of an electron from site j to site j' , will be replaced by the limiting expression for $I \rightarrow \infty$, i.e., by the matrix

$$K_{\text{lim}} = I \begin{pmatrix} 0 & 1 \\ K_{21}/I & K_{22}/I \end{pmatrix}. \quad (3.4.17)$$

Here it is assumed that the remaining ratios stay finite in this limit, while the first ratio goes to zero. The solutions obtained using (3.4.17) will be local, since the dependence on

the quasimomentum has completely dropped out because of the assumption $K_{11} = 0$. Physically this case corresponds to replacing the band by a level (the atomic limit), and mathematically it corresponds to replacing the operator $[(1/N)\Sigma_k]$ by unity. The first analytical consequence of the purely local approximation is the equality

$$\langle \hat{n}_{\mathbf{k}\nu} \rangle = \langle \hat{n}_{\nu} \rangle = n_{\nu}.$$

The main benefit of this approximation is that it affords the possibility, and again only for certain particular cases, of carrying out analytical manipulations to the end, and this in turn makes it extremely easy to see the role of degeneracy of nonspin origin in the onset of magnetic order. This requires comparing the solutions of the nondegenerate and degenerate versions, where the first is obtained from the second by the simple substitution

$$n_{\nu} \rightarrow n_{\sigma}, \quad \gamma_{\nu}, \alpha_{\nu} \rightarrow n_{-\sigma}. \quad (3.4.18)$$

The F matrix (2.4.5) corresponding to the investigated limit (3.4.17) is of the form

$$F(\beta; K) = \begin{pmatrix} \frac{1}{2} \left(1 + \frac{K_{22}}{R} \right) & -\frac{I}{R} \\ -\frac{K_{21}}{R} & \frac{1}{2} \left(1 - \frac{K_{22}}{R} \right) \end{pmatrix} e^{1/2\beta(R-K_{22})}. \quad (3.4.19)$$

At the same time, relation (3.4.13) also simplifies:

$$K_{21} = K_{12}\alpha_{\nu} - K_{22}\gamma_{\nu}, \quad K_{12} = I.$$

The matrix (3.4.19) has only two nontrivial forms: the first corresponds to the condition

$$R \equiv I \left[\left(\frac{K_{22}}{I} \right)^2 + 4 \left(\frac{K_{21}}{I} \right)^2 \right]^{1/2} = K_{22} \equiv \frac{\alpha_{\nu}}{\gamma_{\nu}} I \neq 0,$$

and the second to the condition

$$R \pm K_{22} > 0.$$

Here we will consider only the first and a particular case of the second, when $K_{22} = 0$.

Thus if we adopt the first condition, the K matrix will have the form

$$K_{\nu} = I \begin{pmatrix} 0 & 1 \\ 0 & \alpha_{\nu}/\gamma_{\nu} \end{pmatrix}, \quad K_{\sigma} = I \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix},$$

and therefore

$$F_{\nu}(\pm\beta) = \begin{pmatrix} 1 \mp \gamma_{\nu}/\alpha_{\nu} & \\ 0 & 0 \end{pmatrix}, \quad F_{\sigma}(\pm\beta) = \begin{pmatrix} 1 & +1 \\ 0 & 0 \end{pmatrix}.$$

For this F matrix formula (3.4.11) leads to the curious equality $\alpha_{\nu} = \gamma_{\nu}$, and formula (3.4.9) for the average values gives

$$2n_{\sigma} = 1 - n_{-\sigma}, \quad 2n_{\nu} = 1 - \gamma_{\nu}.$$

These equations have only symmetric solutions $n_{-\sigma} = n_{\sigma} = 1/3$ and $n^{-} = n^{+} = 5/11$, respectively, and these solutions are possible only for one value $n = n_{-\sigma} + n_{\sigma} = 2/3$ and $n = n^{-} + n^{+} = 10/11$, respectively (here $n^{\pm} \equiv \Sigma_{\nu}^{\pm} n_{\nu}$).

If we adopt the second condition, then the K matrix

assumes the form

$$K_v = I \begin{pmatrix} 0 & 1 \\ \kappa_v & 0 \end{pmatrix}, \quad K_\sigma = I \begin{pmatrix} 0 & 1 \\ n_\sigma & 0 \end{pmatrix},$$

and therefore

$$F_v(\pm \beta) = \begin{pmatrix} F_{11} & F_{12} \\ \kappa_v F_{12} & F_{11} \end{pmatrix}.$$

Now formula (3.4.9) gives the equation

$$\langle \hat{n}_v \rangle = n_v = \frac{1}{2} \left(1 - \frac{\gamma_v}{\kappa_v^{1/2}} \right). \quad (3.4.20)$$

For the nondegenerate case it becomes

$$2n_\sigma = 1 - n_\sigma^{1/2}$$

and has only the symmetric solution $n_{-\sigma} = n_\sigma = 1/4$ for $n = 1/2$. For the degenerate case Eq. (3.4.20) contains two unknown quantities, n_v and κ_v , and we must solve the system

$$2n_v = 1 - \frac{\gamma_v}{\kappa_v^{1/2}},$$

$$2\kappa_v = 2\gamma_v + \sum_{v'} (\gamma_{v'} - \kappa_{v'}^{1/2})(1 - 2\delta_{vv'}).$$

The second equation of this system is obtained from (3.4.11) after it is rewritten in the more symmetric form

$$\kappa_v = \gamma_v + \frac{1}{N} \sum_k \sum_{v'} \left(\frac{\gamma F_{11} + \kappa F_{12} + \gamma \det F}{1 + \text{Sp } F + \det F} \right)_{vv'} (1 - 2\delta_{vv'}). \quad (3.4.21)$$

The second equation of this system can be simplified to

$$\kappa_v = \kappa_v^{1/2} + \frac{1}{2} \sum_{v'} (\gamma_{v'} - \kappa_{v'}^{1/2}) = \kappa_v^{1/2} - \sum_{v'} \gamma_{v'} n_{v'} (1 - 2n_{v'})^{-1}, \quad (3.4.22)$$

by using the expression for κ_v from the first equation:

$$\kappa_v^{1/2} = \gamma_v (1 - 2n_v)^{-1}.$$

Now (3.4.22) can be rewritten as

$$(1 - n_v) n_v + (1 - 2n_v)^2 \sum_{v'} \frac{\gamma_{v'} n_{v'}}{1 - 2n_{v'}} = (1 - n) n,$$

or as

$$(1 - 2n_v)^2 = (1 - 2n)^2 (1 - 4q)^{-1} \equiv Q, \quad (3.4.23)$$

$$q \equiv \sum_{v'} \gamma_{v'} n_{v'} (1 - 2n_{v'})^{-1}.$$

The quadratic (in n_v) equation (3.4.23) has the solution

$$n_v^{I,II} = \frac{1}{2} (1 \pm Q^{1/2}). \quad (3.4.24)$$

The most interesting case physically is when these roots are nonnegative and different, i.e., when $0 < Q < 1$. The quantity Q can be calculated from the equation

$$(1 - 2n)^2 Q^{-1} = 1 - 4q \\ = 1 - 4 \left[\frac{(n - n_v^I) n_v^I}{1 - 2n_v^I} p + \frac{(n - n_v^{II}) n_v^{II}}{1 - 2n_v^{II}} (10 - p) \right],$$

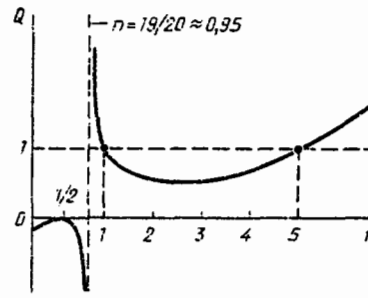


FIG. 1.

which is the definition of Q according to (3.4.23). By substituting roots (3.4.24) into this equation we can obtain an equation for Q :

$$Q^2(20n - 19)^2 - 2Q(1 - 2n)^2(20n - 19) + (1 - 2n)^4 \\ = [(1 - 2n)^2 + Q^2 + 2Q(1 - 2n)](10 - 2p)^2 Q, \quad (3.4.25)$$

which in the general case is a cubic equation. It goes over to a quadratic equation in two cases, which we will examine here. The first case corresponds to $n = 1/2$, and here (3.4.25) becomes

$$Q^{1/2} = 9(10 - 2p)^{-1} \rightarrow Q = 81(10 - 2p)^{-2}, \quad 1 \leq p < 5.$$

This value of Q for $1 < p < 5$ gives only one non-negative root according to (3.4.24). The second case corresponds to the condition $p = 5$. Then the right-hand side of (3.4.25) goes to zero, and we obtain a quadratic equation for Q that has one multiple root:

$$Q = (1 - 2n)^2(20n - 19)^{-1}.$$

The function $Q(n)$ is shown schematically in Fig. 1. Thus the condition $0 < Q < 1$ is satisfied for values $(19/20) < n < 5$. Since we are still considering the case $p_2 = p_1 = 5$, the following condition should also hold:

$$p_1 n_v^I + p_2 n_v^{II} = n \rightarrow 5(n_v^I + n_v^{II}) = n,$$

which implies that $n = 5$ and therefore $Q = 1$. Here the roots (3.4.24) are $n_v^I = 1$; $n_v^{II} = 0$. The filling schemes of the single-electron states are shown in Fig. 2 (only the schemes which are physically different in regard to the magnetic moment are given). The three other possible schemes are obtained by mirror reflection of the left- and right-hand parts of these schemes with respect to the plus/minus line separating them, followed by an interchange of the sign $+ \leftrightarrow -$. Finally, it should be noted that in this case the principal single-site correlation function (3.4.10) is equal to

$$\langle \hat{N}_j (\hat{N}_j - 1) \rangle = \frac{1}{2} \sum_v (\gamma_v - \kappa_v).$$

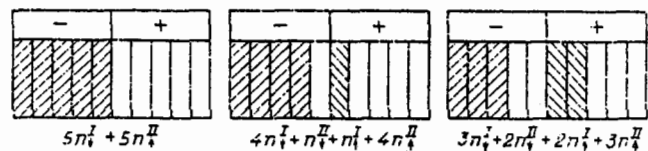


FIG. 2.

3.5. Bardeen-Cooper-Schrieffer (BCS) theory

Here the DA method is applied to the BCS model Hamiltonian. To avoid excessive complication of the already complex procedure of actually carrying out an exact "linearization," here we will from the start consider only the case of a local interaction of electrons (in coordinate space the potential is proportional to a delta function—a contact interaction). What is extremely important here is that such a potential permits carrying out exact self-consistency to the end, and therefore the local BCS model is exceptionally important for demonstrating the DA method. Moreover, the final analytical results of the BCS problem for the gap, critical temperature, etc. are ordinarily given for a potential of just this form.

The BCS model Hamiltonian is of the form³¹

$$\bar{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} (\hat{n}_{\mathbf{k}} + \hat{n}_{-\mathbf{k}}) + \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}'}. \quad (3.5.1)$$

The operators $\hat{b}_{\mathbf{k}}^{\pm}$ obey rather complicated commutation relations

$$\begin{aligned} [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}]_{-} &= 0, \quad \hat{b}_{\mathbf{k}}^2 = 0, \\ [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}^{\dagger}]_{-} &= (1 - \hat{n}_{\mathbf{k}} - \hat{n}_{-\mathbf{k}}) \delta_{\mathbf{k}\mathbf{k}'}, \\ [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}^{\dagger}]_{+} &= 1 - (\hat{n}_{\mathbf{k}} - \hat{n}_{-\mathbf{k}})^2. \end{aligned}$$

We see from the last anticommutator that these operators can, if desired, obey mixed Bose-Fermi commutation relations if discussion is limited to configurations of the electronic system which are such that any two paired one-electron states are simultaneously either filled or empty. This restriction actually would make sense, since (3.5.1) does not mix such configurations with configurations that also contain half-filled paired one-electron states. Here, however, we will not impose this condition.

In the contact approximation Eq. (3.5.1) becomes

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} (\hat{n}_{\mathbf{k}} + \hat{n}_{-\mathbf{k}}) + \frac{V}{N} \hat{\Delta}^{\dagger} \hat{\Delta}, \quad (3.5.2)$$

and it is this Hamiltonian that we will use everywhere below. It is obtained from (3.5.1) by the substitutions

$$\sum_{\mathbf{k}} \hat{b}_{\mathbf{k}} \equiv \sum_{\mathbf{k}} \hat{C}_{-\mathbf{k}} \hat{C}_{\mathbf{k}} = \sum_{\mathbf{k}} \hat{C}_{-\mathbf{k}\downarrow} \hat{C}_{\mathbf{k}\uparrow} \equiv \hat{\Delta}, \quad V_{\mathbf{k}\mathbf{k}'} \rightarrow \frac{V}{N}, \quad V^* = V,$$

where N is the number of cells in the sample.

It turns out^{30,31,34} that the results of the original BCS theory can be obtained very simply if the the exact equations of motion

$$[\hat{C}_{\mathbf{k}}, H]_{-} = \varepsilon_{\mathbf{k}} \hat{C}_{\mathbf{k}} + \frac{V}{N} \hat{C}_{-\mathbf{k}}^{\dagger} \hat{\Delta} = (\varepsilon_{\mathbf{k}} + \frac{V}{N}) \hat{C}_{\mathbf{k}} + \frac{V}{N} \hat{\Delta} \hat{C}_{-\mathbf{k}}^{\dagger}, \quad (3.5.3)$$

$$[\hat{C}_{-\mathbf{k}}^{\dagger}, H]_{-} = \frac{V}{N} \hat{\Delta}^{\dagger} \hat{C}_{\mathbf{k}} - \varepsilon_{\mathbf{k}} \hat{C}_{-\mathbf{k}}^{\dagger}$$

are linearized by the Valatin scheme

$$[\hat{C}_{\mathbf{k}}, H]_{-} \approx \varepsilon_{\mathbf{k}} \hat{C}_{\mathbf{k}} + \frac{V}{N} (\hat{\Delta}) \hat{C}_{-\mathbf{k}} \equiv K_{11} \hat{C}_{\mathbf{k}} + K_{12} \hat{C}_{-\mathbf{k}}^{\dagger}, \quad (3.5.4)$$

$$[\hat{C}_{-\mathbf{k}}^{\dagger}, H]_{-} \approx \frac{V}{N} (\hat{\Delta}^{\dagger}) \hat{C}_{\mathbf{k}} - \varepsilon_{\mathbf{k}} \hat{C}_{-\mathbf{k}}^{\dagger} \equiv K_{21} \hat{C}_{\mathbf{k}} + K_{22} \hat{C}_{-\mathbf{k}}^{\dagger}.$$

To this system of equations of motion it is helpful to add two more:

$$\begin{aligned} [\hat{C}_{-\mathbf{k}}, H]_{-} &\approx \varepsilon_{\mathbf{k}} \hat{C}_{-\mathbf{k}} - \frac{V}{N} \hat{\Delta} \hat{C}_{\mathbf{k}}^{\dagger} \equiv K_{11}(-\mathbf{k}) \hat{C}_{-\mathbf{k}} + K_{12}(-\mathbf{k}) \hat{C}_{\mathbf{k}}^{\dagger} \\ &= K_{11} \hat{C}_{-\mathbf{k}} - K_{12} \hat{C}_{\mathbf{k}}^{\dagger}, \end{aligned} \quad (3.5.5)$$

$$\begin{aligned} [\hat{C}_{\mathbf{k}}^{\dagger}, H]_{-} &\approx -\frac{V}{N} \hat{\Delta}^{\dagger} \hat{C}_{-\mathbf{k}} - \varepsilon_{\mathbf{k}} \hat{C}_{\mathbf{k}}^{\dagger} \\ &\equiv K_{21}(-\mathbf{k}) \hat{C}_{-\mathbf{k}} + K_{22}(-\mathbf{k}) \hat{C}_{\mathbf{k}}^{\dagger} = -K_{21} \hat{C}_{-\mathbf{k}} + K_{22} \hat{C}_{\mathbf{k}}^{\dagger}, \end{aligned}$$

the exact expressions for which are

$$[\hat{C}_{-\mathbf{k}}, H]_{-} = \varepsilon_{\mathbf{k}} \hat{C}_{-\mathbf{k}} - K_{12} \hat{C}_{\mathbf{k}}^{\dagger} \hat{\Delta} = \frac{K_{11} \hat{C}_{-\mathbf{k}} - K_{12} \hat{D}_{-\mathbf{k}}}{(K_{11} + K_{12}) \hat{C}_{-\mathbf{k}} - K_{12} \hat{\Delta} \hat{C}_{\mathbf{k}}^{\dagger}}, \quad (3.5.6)$$

$$\begin{aligned} [\hat{C}_{\mathbf{k}}^{\dagger}, H]_{-} &= -\varepsilon_{\mathbf{k}} \hat{C}_{\mathbf{k}}^{\dagger} - \frac{V}{N} \hat{\Delta}^{\dagger} \hat{C}_{-\mathbf{k}} \\ &= \frac{-K_{11} \hat{C}_{\mathbf{k}}^{\dagger} - K_{12} \hat{D}_{\mathbf{k}}^{\dagger}}{(K_{11} + K_{12}) \hat{C}_{\mathbf{k}}^{\dagger} + K_{12} \hat{C}_{-\mathbf{k}} \hat{\Delta}^{\dagger}}. \end{aligned}$$

From a comparison of (3.5.3) with (3.5.6), we see that this problem has the symmetry properties

$$\begin{aligned} K_{11}(-\mathbf{k}) &= K_{11}(\mathbf{k}) \equiv K_{11}, \quad K_{12}(-\mathbf{k}) = -K_{12}, \\ K_{21}(-\mathbf{k}) &= -K_{21}, \quad K_{22}(-\mathbf{k}) = K_{22}. \end{aligned} \quad (3.5.7)$$

Thus for Hamiltonian (3.5.2), the K matrix linearized by the Valatin scheme is

$$K = \begin{pmatrix} \varepsilon_{\mathbf{k}} & \frac{V}{N} \Delta \\ K_{12}^* & -K_{11} \end{pmatrix}. \quad (3.5.8)$$

The eigenvalues of this matrix give the energy spectra of the possible elementary excitations. For excitations with positive energy this spectrum is of the form

$$E_{\mathbf{k}} = \left[\varepsilon_{\mathbf{k}}^2 + \left(\frac{V}{N} \right)^2 |\Delta|^2 \right]^{1/2}. \quad (3.5.9)$$

Now it is easy to obtain the basic equation of the BCS theory for the gap $|\Delta|^2$ by the "dressing-undressing" method. For this it is necessary to calculate the correlation function $\langle \hat{b}_{\mathbf{k}} \rangle$. Using (3.5.4) and (3.5.5), we can write successively

$$\langle \hat{b}_{\mathbf{k}} \rangle = \langle \hat{C}_{-\mathbf{k}} \hat{C}_{\mathbf{k}} \rangle = \langle \hat{C}_{\mathbf{k}} [\beta] \hat{C}_{-\mathbf{k}} \rangle = F_{11} \langle \hat{C}_{\mathbf{k}} \hat{C}_{-\mathbf{k}} \rangle + F_{12} \langle \hat{C}_{-\mathbf{k}}^{\dagger} \hat{C}_{-\mathbf{k}} \rangle, \quad (3.5.10)$$

$$\langle \hat{C}_{-\mathbf{k}} \hat{C}_{-\mathbf{k}}^{\dagger} \rangle = \langle \hat{C}_{-\mathbf{k}}^{\dagger} [\beta] \hat{C}_{-\mathbf{k}} \rangle = F_{21} \langle \hat{C}_{\mathbf{k}} \hat{C}_{-\mathbf{k}} \rangle + F_{22} \langle \hat{C}_{-\mathbf{k}}^{\dagger} \hat{C}_{-\mathbf{k}} \rangle.$$

The solution of this system gives

$$\begin{aligned} \langle \hat{n}_{\pm \mathbf{k}} \rangle &= \frac{1 + F_{11}}{1 + \text{Sp } F + \det F} = \frac{1 + F_{11}}{2 + \text{Sp } F} \\ &= \frac{1}{2} \left[1 - \frac{K_{11}}{E_{\mathbf{k}}} \text{th} \left(\frac{1}{2} \beta E_{\mathbf{k}} \right) \right], \end{aligned} \quad (3.5.11)$$

$$\langle \hat{b}_{\mathbf{k}} \rangle = F_{12} (2 + \text{Sp } F)^{-1}. \quad (3.5.12)$$

Equation (3.5.12) directly yields an equation for the gap

$$1 = -\frac{V}{N} \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} \text{th} \left(\frac{1}{2} \beta E_{\mathbf{k}} \right) \quad (3.5.13)$$

and an equation for the critical temperature

$$1 = -\frac{V}{N} \sum_{\mathbf{k}} \frac{1}{2\varepsilon_{\mathbf{k}}} \text{th} \left(\frac{1}{2} \beta \varepsilon_{\mathbf{k}} \right). \quad (3.5.14)$$

These equations agree completely with the equations of the BCS theory. The "dressing-undressing" method can also be used to calculate very simply the other correlation functions, such as

$$\langle \hat{\Delta}^+ \hat{\Delta} \rangle = |\Delta|^2 + \sum_{\mathbf{k}} n_{\mathbf{k}}^2 \approx |\Delta|^2, \quad (3.5.15)$$

$$\langle \hat{n}_{\mathbf{k}} \hat{n}_{-\mathbf{k}} \rangle - \langle \hat{n}_{\mathbf{k}} \rangle \langle \hat{n}_{-\mathbf{k}} \rangle = \frac{F_{12}}{2 + \text{Sp } F} \frac{F_{21}}{2 + \text{Sp } F} = b_{\mathbf{k}} b_{\mathbf{k}}^* = |b_{\mathbf{k}}|^2.$$

In the exactly self-consistent approach the first equation of the exact system (3.5.3) remains unchanged:

$$[\hat{C}_{\mathbf{k}}, H]_- = \varepsilon_{\mathbf{k}} \hat{C}_{\mathbf{k}} + \frac{V}{N} \hat{C}_{-\mathbf{k}}^+ \hat{\Delta} \equiv \varepsilon_{\mathbf{k}} \hat{C}_{\mathbf{k}} + \frac{V}{N} \hat{D}_{\mathbf{k}} \equiv K_{11} \hat{C}_{\mathbf{k}} + K_{12} \hat{D}_{\mathbf{k}}, \quad (3.5.16)$$

and the expansion coefficients of the three-electron commutator

$$[\hat{D}_{\mathbf{k}}, H]_- = K_{21} \hat{C}_{\mathbf{k}} + K_{22} \hat{D}_{\mathbf{k}} \quad (3.5.17)$$

in the exact basis of the first commutator are found with the help of the Jacobi identity (2.1.2).

The symmetry properties (3.5.7) of the K matrix, which in the Valatin scheme are taken directly from the expansions (3.5.4) and (3.5.5), are determined here from general analytical arguments, since the expansion (3.5.17) is now unknown. The first line of (3.5.5) is, of course, valid here too.

If we use the triple $1 = \hat{C}_{-\mathbf{k}}, 2 = \hat{D}_{\mathbf{k}}, 3 = H$, then (2.1.2) yields

$$[\hat{\Delta}, H]_- = K_{12} (\hat{n}_{\mathbf{k}} - \hat{n}_{-\mathbf{k}}) \hat{\Delta} + T \hat{\Delta},$$

while the triple $1 = \hat{C}_{\mathbf{k}}, 2 = \hat{D}_{-\mathbf{k}}, 3 = H$ leads to a different result:

$$[\hat{\Delta}, H]_- = -K_{12} (\hat{n}_{\mathbf{k}} - \hat{n}_{-\mathbf{k}}) \hat{\Delta} + T \hat{\Delta}.$$

From these two equations we get two new equations:

$$(\hat{n}_{\mathbf{k}} - \hat{n}_{-\mathbf{k}}) \hat{\Delta} = 0 \rightarrow K_{21}(-\mathbf{k}) = -K_{21},$$

$$[\hat{\Delta}, H]_- = T \hat{\Delta} \rightarrow T = 0 \rightarrow K_{22} = -K_{11},$$

i.e., the K matrix, as in the Valatin scheme, is again traceless.

Thus to complete the exact self-consistency procedure it remains only to find the form of the element K_{21} of the desired K matrix. This is most simply done by introducing the N matrix

$$N_{11} \equiv \langle [\hat{C}_{\mathbf{k}}, \hat{C}_{\mathbf{k}}^+]_+ \rangle = 1,$$

$$N_{12} \equiv \langle [\hat{C}_{\mathbf{k}}, \hat{D}_{\mathbf{k}}^+]_+ \rangle = n_{-\mathbf{k}} = N_{21},$$

$$N_{22} \equiv \langle [\hat{D}_{\mathbf{k}}, \hat{D}_{\mathbf{k}}^+]_+ \rangle = \langle \hat{\Delta}^+ \hat{\Delta} \rangle + \langle \hat{n}_{-\mathbf{k}} \sum_{\mathbf{k}'} (1 - \hat{n}_{\mathbf{k}'} - \hat{n}_{-\mathbf{k}'}) \rangle + n_{-\mathbf{k}}$$

and using formula (3.4.12). This gives

$$K_{21} = K_{12} \langle \hat{\Delta}^+ \hat{\Delta} \rangle + (2K_{11} + K_{12}) n_{-\mathbf{k}} + \langle \hat{n}_{-\mathbf{k}} \sum_{\mathbf{k}'} (1 - \hat{n}_{\mathbf{k}'} - \hat{n}_{-\mathbf{k}'}) \rangle K_{12}. \quad (3.5.18)$$

Here it should be noted that if the Jacobi identity (2.1.2) is written for the triple $1 = \hat{C}_{\mathbf{k}}, 2 = \hat{D}_{\mathbf{k}}^+, 3 = H$, then by comparing the result with (3.5.18) one can obtain the interesting relation

$$\langle [\hat{n}_{-\mathbf{k}}, H]_- \rangle = 0.$$

If instead the Jacobi identity is written for the triple $1 = \hat{C}_{-\mathbf{k}}, 2 = \hat{D}_{-\mathbf{k}}^+, 3 = H$ and the result is compared with a relation analogous to (3.5.18) but obtained for the \bar{N} matrix in which the substitution $\mathbf{k} \rightarrow -\mathbf{k}$ has been made, we can then obtain

$$\langle [\hat{n}_{\mathbf{k}}, H]_- \rangle = 0,$$

which, by the way, follows directly from the previous relation, since (3.5.2) is invariant with respect to the substitution $\mathbf{k} \rightarrow -\mathbf{k}$ if $\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}$, as we are assuming. The last two relations imply that the correlation function is real:

$$\langle \hat{\Delta}^+ \hat{\Delta} \rangle = \langle \hat{\Delta}^+ \hat{\Delta} \rangle \equiv \langle \hat{\Delta}^+ \hat{\Delta} \rangle^*.$$

Thus the final form of the K matrix in the exactly self-consistent scheme is

$$K = \begin{pmatrix} \varepsilon_{\mathbf{k}} & \frac{V}{N} \\ (3.5.18) & -K_{11} \end{pmatrix}. \quad (3.5.19)$$

Now instead of (3.5.9) we obtain a spectrum

$$E_{\mathbf{k}} = \left[\varepsilon_{\mathbf{k}}^2 + \left(\frac{V}{N} \right)^2 \langle \hat{\Delta}^+ \hat{\Delta} \rangle \right]^{1/2}, \quad (3.5.20)$$

and the gap correlation function is calculated from the two equations

$$\langle \hat{D}_{\mathbf{k}}^+ \hat{C}_{\mathbf{k}} \rangle = \langle \hat{C}_{\mathbf{k}} [\beta] \hat{D}_{\mathbf{k}}^+ \rangle = F_{11} \langle \hat{C}_{\mathbf{k}} \hat{D}_{\mathbf{k}}^+ \rangle + F_{12} \langle \hat{D}_{\mathbf{k}} \hat{D}_{\mathbf{k}}^+ \rangle,$$

$$\langle \hat{D}_{\mathbf{k}}^+ \hat{D}_{\mathbf{k}} \rangle = \langle \hat{D}_{\mathbf{k}} [\beta] \hat{D}_{\mathbf{k}}^+ \rangle = F_{21} \langle \hat{C}_{\mathbf{k}} \hat{D}_{\mathbf{k}}^+ \rangle + F_{22} \langle \hat{D}_{\mathbf{k}} \hat{D}_{\mathbf{k}}^+ \rangle.$$

It turns out to be

$$\langle \hat{\Delta}^+ \hat{\Delta} \rangle \equiv \sum_{\mathbf{k}} \langle \hat{\Delta}^+ \hat{\Delta}_{\mathbf{k}} \rangle = \sum_{\mathbf{k}} [n_{\mathbf{k}}^2 + A_{\mathbf{k}} F_{12} (2 + \text{Sp } F)^{-1}], \quad (3.5.21)$$

$$A_{\mathbf{k}} \equiv \langle \hat{n}_{-\mathbf{k}} [1 - \sum_{\mathbf{k}'} (\hat{n}_{\mathbf{k}'} - \hat{n}_{-\mathbf{k}'})] \rangle + \langle \hat{\Delta}^+ \hat{\Delta} \rangle. \quad (3.5.22)$$

Formula (3.5.11) actually remains unchanged in its outward form:

$$\langle \hat{n}_{\pm \mathbf{k}} \rangle = \frac{1 + F_{11} + n_{\mp \mathbf{k}} F_{12}}{2 + \text{Sp } F} \approx \frac{1 + F_{11}}{2 + \text{Sp } F},$$

but here $E_{\mathbf{k}}$ is taken according to (3.5.20). Expression (3.5.22) can be reduced to the form

$$A_{\mathbf{k}} = \langle \hat{\Delta}^+ \hat{\Delta} \rangle + (1 - n) N n_{\mathbf{k}}, \quad (3.5.23)$$

where N is the number of sites in the sample, and n is the electron density

$$n = \frac{1}{N} \sum_{\mathbf{k}} (\langle \hat{n}_{\mathbf{k}} \rangle + \langle \hat{n}_{\mathbf{k}'} \rangle) = n_{\uparrow} + n_{\downarrow}, \quad (3.5.24)$$

the physical values of which for the model under study (the s band) lie on the segment $0 \leq n \leq 2$. In obtaining (3.5.23) we have used the correlation functions

$$\langle \hat{n}_{\mathbf{k}'} \hat{n}_{-\mathbf{k}} \rangle = n_{\mathbf{k}'} n_{-\mathbf{k}} + \frac{F_{12} F_{21}}{(2 + \text{Sp } F)^2} \delta_{\mathbf{k}\mathbf{k}'},$$

$$\langle \hat{n}_{-\mathbf{k}'} \hat{n}_{-\mathbf{k}} \rangle = n_{-\mathbf{k}'} n_{-\mathbf{k}} + (1 - n_{-\mathbf{k}}) n_{-\mathbf{k}} \delta_{\mathbf{k}\mathbf{k}'},$$

$$\langle \hat{n}_{\mathbf{k}} \hat{n}_{-\mathbf{k}} \rangle = F_{11} (2 + \text{Sp } F)^{-1}.$$

The second of formulas (3.5.15) remains valid here, but now $F_{21} \neq F_{12}^*$, since $K_{21} \neq K_{12}^*$, and therefore this correlation function is no longer equal to $|b_k|^2$.

Thus the basic equation (3.5.21) for the gap now has the form

$$\begin{aligned} & \langle \hat{\Delta} + \hat{\Delta} \rangle [1 - \sum_{\mathbf{k}} F_{12}(2 + \text{Sp } F)^{-1}] \\ & = \sum_{\mathbf{k}} [n_k^2 + (1 - n)Nn_k F_{12}(2 + \text{Sp } F)^{-1}]. \end{aligned} \quad (3.5.25)$$

The structure of this equation is radically different from that of the Valatin equation (3.5.12), which can be rewritten as

$$\Delta [1 - \sum_{\mathbf{k}} \bar{F}_{12}(2 + \text{Sp } F)^{-1}] = 0, \quad F_{12} = \Delta \bar{F}_{12}. \quad (3.5.26)$$

In fact, in this equation one cannot directly set $\Delta = 0$ in order to calculate the transition temperature: here one must first move to the left from the neighborhood of the transition point and then divide both sides of this equation by the now supposedly nonzero Δ , and only then obtain an equation for the behavior of the gap as a function of temperature, tacitly assuming that this equation still applies in the immediate vicinity of the transition point and therefore, ultimately, can be used to determine the transition temperature itself by formally setting $\Delta = 0$. That this may not be so is indicated by the aforementioned impossibility of directly setting to zero the gap in the truly original equation for it, i.e., in Eq. (3.5.26), both sides of which contain this parameter Δ as a factor. In contrast, Eq. (3.5.25) fully admits a simple setting of the gap $\langle \hat{\Delta} + \hat{\Delta} \rangle$ to zero for directly obtaining the transition temperature itself, since its structure is such that it does not require first making a leftward excursion from the neighborhood of the transition point. In addition, this equation yields in a natural way two relations for the behavior of the gap as a function of temperature: one for the immediate neighborhood of the transition point, and another for the rest of the temperature interval to the left of this neighborhood. This is a consequence of an interesting analytical property of Eq. (3.5.25): its left-hand side is proportional to N^2 and its right-hand side is proportional to N . Therefore, to the left of the transition point but outside its immediate neighborhood (where $\langle \hat{\Delta} + \hat{\Delta} \rangle \neq 0$) only the left-hand side of (3.5.25) remains, while in the immediate vicinity of the transition point, including the transition point itself, only the right-hand side remains. The left-hand side of (3.5.25), after a factor $\langle \hat{\Delta} + \hat{\Delta} \rangle \neq 0$ is divided out, leads to a BCS temperature dependence of the gap $\langle \hat{\Delta} + \hat{\Delta} \rangle$. In contrast, the right-hand side of (3.5.25)

$$\sum_{\mathbf{k}} [n_k^2 + (1 - n)Nn_k F_{12}(2 + \text{Sp } F)^{-1}] = 0 \quad (3.5.27)$$

gives a new temperature dependence of the gap $\langle \hat{\Delta} + \hat{\Delta} \rangle$ in the neighborhood of the transition point. This dependence can be rewritten as

$$1 = -\frac{V}{N} \sum_{\mathbf{k}} \frac{2}{n} \left[\frac{\epsilon_{\mathbf{k}}^2}{V E_{\mathbf{k}}} \text{th} \left(\frac{1}{2} \beta E_{\mathbf{k}} \right) + n - 1 \right] \frac{\text{th}(\beta E_{\mathbf{k}}/2)}{2 E_{\mathbf{k}}}. \quad (3.5.28)$$

By directly setting the gap to zero in this equation (since it is valid precisely in the immediate neighborhood of the transi-

tion point) we obtain an equation determining the transition point:

$$1 = -\frac{\bar{V}}{N} \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}} \text{th} \left(\frac{1}{2} \beta \epsilon_{\mathbf{k}} \right), \quad \bar{V} \equiv 2V \frac{n-1}{n+1}, \quad (3.5.29)$$

which outwardly agrees in form with the equation (3.5.14) of the Valatin scheme. However, in (3.5.29) the potential is different.

The left-hand side of (3.5.25), which determines the temperature dependence $\langle \hat{\Delta} + \hat{\Delta} \rangle(T)$ outside the neighborhood of the transition point has a solution only for $V < 0$ and $0 < n < 2$. Equation (3.5.29), on the other hand, which is valid only in the neighborhood of the transition point, has a solution in the case $V < 0$ for $1 < n < 2$; for $n < 1$ there is no solution in this case, but for $n < 1$ and $V > 0$ there is a solution, although the physical meaning of this case is not clear.

Since Eq. (3.5.14) has the solution⁴⁹

$$t_c = 1.44W \exp \frac{1}{\rho V}, \quad (3.5.30)$$

where W is the half-width of the s band, solution (3.5.29) can be written (where $|V| \equiv U$):

$$T_c = 1.44W \exp \left(\frac{1}{2} \frac{1}{\rho V} \frac{n+1}{n-1} \right) = t_c \exp \left(\frac{1}{2} \frac{1}{\rho U} \frac{n-3}{n-1} \right), \quad n > 1. \quad (3.5.31)$$

The dependence of the transition temperature on n is shown in Fig. 3. For the case $n = 1$ there is nevertheless a completely determinate value of the transition temperature—it is zero for any sign of V . This is a well-known result for the s band in the Hubbard and Heisenberg models,⁵¹ but for the BCS problem it is apparently obtained here for the first time. We see from the plot of the dependence of the transition point on n that high transition temperatures can be associated with cases $n > 3$, as is possible, for example, if the s states are replaced by $3d$ states and it is assumed that the structure of formula (3.5.31) is basically preserved, as is in fact the case in the nondiagonal Hartree–Fock approximation for the nondegenerate ($0 < n < 2$) and degenerate ($0 < n < 10$) Hubbard models.⁴⁹ Incidentally, the nondegenerate Hubbard model

$$H = \sum_{j,j',\sigma} t_{jj'} \hat{C}_{j\sigma}^+ \hat{C}_{j'\sigma} + \frac{U}{2} \sum_{j,\sigma} \hat{n}_{j\sigma} \hat{n}_{j-\sigma} \quad (3.5.32)$$

which is obtained from (3.4.1) if the index ν takes on only two values, has become widely employed of late in connection with high-temperature superconductivity, and the opinion exists that it is the coordinate representation of the BCS model (3.5.2). This is not the case. These models are related

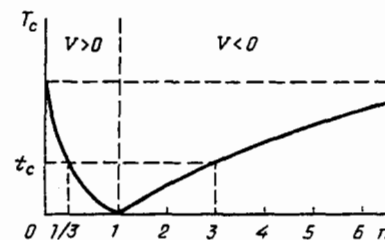


FIG. 3.

in the same way as are the Brillouin–Wigner and Rayleigh–Schrödinger expansions: in the solution of problem (3.5.2), for example, by ordinary perturbation theory the contributions from the perturbation vanish in all orders in the thermodynamic limit, whereas in problem (3.5.32) they remain finite. Indeed, in the quasimomentum representation the Hubbard Hamiltonian (3.5.32) has the form

$$H = \sum_{\mathbf{k}, \sigma} t_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma} + \frac{U}{2N} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{Q}, \sigma} \hat{C}_{\mathbf{k}, \sigma}^+ \hat{C}_{\mathbf{k}_2, \sigma} \hat{C}_{\mathbf{Q}-\mathbf{k}_1, -\sigma}^+ \hat{C}_{\mathbf{Q}-\mathbf{k}_2, -\sigma}$$

One can extract the BCS Hamiltonian (3.5.2) from this expression, but only one value (zero) of the quasimomentum transfer ($\mathbf{Q} = 0$) must be taken into account:

$$H = \sum_{\mathbf{k}, \sigma} t_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k}_1, \mathbf{k}_2} \hat{b}_{\mathbf{k}_1}^+ \hat{b}_{\mathbf{k}_2}$$

The inverse transition into the coordinate representation here gives (3.5.32) but with a factor of $1/N$ in front of the single-site part (in making this transition one must remember that in the Hubbard model it has been assumed that $U_{j'j} = U\delta_{j'j}$).

At this point in the discussion it is appropriate to point out that at the present time no one has yet proposed a mathematically correct means of describing a transition from a “normal” state to an “abnormal” (magnetic, superconducting, superfluid) state. Therefore, by proceeding from the solution of a problem formulated for a “normal” state no one has yet managed to obtain a solution that would describe the transition to an “abnormal” state and the properties of the “abnormal” state itself. For now one can only try to turn a necessity into a virtue by reversing the direction of study. The BCS Hamiltonian was written with precisely this circumstance in mind—it originates in an “abnormal” state. Therefore, its solution should be analyzed starting from the lowest temperatures and moving to the right, toward higher temperatures. Only such an analysis is admitted by Eq. (3.5.26) of the original BCS theory. Therefore in this theory the transition point can only be taken as the temperature at which the gap *vanishes*, i.e., this temperature describes the transition only from the “abnormal” to the “normal” state. The distinctive property of (3.5.25) is that it can work in both directions, i.e., it also works for describing the transition proper from the “normal” to the “abnormal” state, even though this equation was obtained from a formulation of the problem in the “abnormal” state. Therefore it also permits the introduction of the concept of the temperature at which the gap *appears*, and in the present case this temperature agrees with the temperature at which the gap vanishes, since in moving from right to left in Eq. (3.5.25) first only the right-hand side exists (since here by assumption $\langle \hat{\Delta} + \hat{\Delta} \rangle \equiv 0$). In Eq. (3.5.26), however, moving from right to left is not possible at all, since in this case it has the form $0 = 0$. In principle the temperatures T_c^- and T_c^+ can be different, as could be the case if one recognizes the possible existence of a supercooled “normal” and a superheated “abnormal” state, and the true T_c would lie somewhere in between them.

Finally, let us say a few words concerning the result of the analysis of the BCS problem by the exactly self-consistent method. It would be simplest, of course, to reject this result if only because it differs from the original BCS result,

which is commonly regarded even as being exact (in the thermodynamic limit). But in the present case I do not believe that it can be dismissed so simply on such grounds, for at least two reasons. First, in this approach there are no ambiguities and/or arbitrary actions—a novel, mathematically exact procedure is carried out from start to finish. Second, the problems of statistical physics can admit several exact solutions: the simplest and best-known example of this is the Hartree–Fock problem. Therefore it seems to me that it is not only rightful but also even expedient to publish this result.

APPENDIX

1. In theoretical calculations of the properties of many-body systems it is often necessary to do a Fourier time transform as an intermediate step, since this ordinarily leads to algebraic equations of the form

$$\Phi(E)\varphi(E) = F(E) \quad (\text{A1})$$

for the unknown function $\Phi(E)$. A formal solution of such equations is simple to find:

$$\Phi(E) = \frac{F(E)}{\varphi(E)} \quad (\text{A2})$$

However, this solution is generally not complete, since Eq. (A1) will be just as well satisfied by a solution of a different form:

$$F(E) = \frac{F}{\varphi} + A(E)\delta(\varphi(E)), \quad (\text{A3})$$

in view of the identity

$$\varphi(E)(\delta\varphi(E)) \equiv 0, \quad (\text{A4})$$

which applies on the assumption that $\varphi(E)$ has zeros at several values $E = E_j, j = 1, 2, \dots$. Thus the most complete solution of (A1) should be a solution of the form (A3), and that is what should always be used. This solution contains an unknown function $A(E)$, the specific form of which can ordinarily be established on the basis of the analytical properties of the function $\Phi(E)$ in the complex energy plane. The functions of the energy representation are ordinarily intermediate and are used in obtaining the final results in the integrand. Incidentally, relations containing the delta function, i.e., relations of the type (A3), necessarily presuppose a subsequent integration over the independent variable of its argument.

Integration of relations of the type (A3) are most conveniently done in the complex energy plane with the help of the residue theorem. Since in practice $\varphi(E)$ most often has only simple zeros, in this case, as is well known,²⁵ the delta function can be represented concretely as

$$\delta(\varphi) = \sum_{j=1}^n \delta(E - E_j) |\varphi'(E_j)|^{-1}, \quad \varphi(E_j) \equiv \varphi_j = 0. \quad (\text{A5})$$

Using this expression and analytically continuing all the functions of relation (A3) into the complex energy plane (for this it is sufficient to make the substitution $E \rightarrow z$ everywhere, since a function of the complex variable $z = x + iy$ is analytic if it depends on x and y only in this combination, i.e., if it is a function of only one independent variable z), we can do the integration by the residue theorem. The singularities

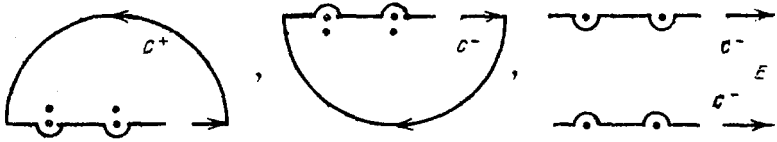


FIG. 4.

of the integrands will consist of the zeros of $\varphi(E_j)$, which lie on the real energy axis at the points $E = E_j$ and have residues F_j/φ'_j , and singularities of the delta function $\delta(E - E_j)$, which lie in the complex energy plane at points $z_j = E_j \pm i\varepsilon$ [see formula (1.1.12) for the delta function]. Now one ordinarily makes two additional assumptions which almost always are justified in practice. First, if the functions F/φ and $A\delta(\varphi)$ taken as a whole have singularities in addition to those mentioned, they will be of a pole type. Second, the contour of integration along the real energy axis can actually be closed in either the upper or the lower half of the complex energy plane, i.e., so that the contribution from these semi-circles should vanish for $|z| \rightarrow \infty$. The contours used in the integration are shown in Fig. 4.

Thus, the integral of relation (A3) is given by

$$\int_{C^\pm} \Phi(z) dz = \int_{C^\pm} \left(\frac{F(z)}{\varphi(z)} + A(z)\delta(\varphi(z)) \right) dz$$

$$= \pm 2\pi i \sum_j \left(\frac{F_j}{\varphi'_j} \pm \frac{1}{2\pi i} \frac{A_j}{|\varphi'_j|} \right) = \sum_j \frac{1}{\varphi'_j} \left(\pm 2\pi i F_j + \frac{\varphi'_j}{|\varphi'_j|} A_j \right). \quad (\text{A6})$$

On the other hand, by taking the integrals only along the E axis $\equiv \bar{C}^\pm$ one can obtain

$$\int_{\bar{C}^\pm} \frac{F(z)}{\varphi(z)} dz = \text{v.p.} \int_{-\infty}^{\infty} \frac{F(E)}{\varphi(E)} dE \pm \pi i \sum_j \frac{F_j}{\varphi'_j}, \quad (\text{A7})$$

and this result must be equal to the previous result if the contribution from the large arcs vanish. Equating the two results gives the value of the integral along the E axis in the Cauchy principal value sense:

$$\text{v.p.} \int_{-\infty}^{\infty} \left[\frac{F(E)}{\varphi(E)} \right] dE = \sum_j \frac{1}{\varphi'_j} \left(\pm \pi i F_j + \frac{\varphi'_j}{|\varphi'_j|} A_j \right). \quad (\text{A8})$$

In concluding this paragraph of the Appendix it is useful to note the following fact. In the literature one encounters (separately) two expressions for the derivative of the delta function,

$$x\delta'(x) = -\delta(x), \quad \frac{\delta(x)}{x} = -\delta'(x), \quad (\text{A9})$$

which, were it not for the previous material in this Appendix, could be shown to be identical. However, in view of identity (A4), the first formula of (A9) does not imply the second formula but rather the more general formula

$$\delta'(x) = -\frac{\delta(x)}{x} + \text{const} \cdot \delta(x) \quad (\text{A10})$$

because of the identity $x\delta(x) \equiv 0$. Therefore, it is important to ascertain which of the two formulas in (A9) is the original; if it is the first, then the second formula is incorrect, and if it is the second, then the first is correct also. Direct differentiation of the generally accepted expression²⁵

$$\delta(x) \equiv \lim_{\varepsilon \rightarrow +0} \frac{1}{\pi} \frac{\varepsilon}{x^2 + \varepsilon^2} \quad (\text{A11})$$

unexpectedly leads to two different expressions:

$$\delta'(x) = -\frac{1}{\pi} \lim_{\varepsilon \rightarrow +0} \frac{2x\varepsilon}{(x^2 + \varepsilon^2)^2}$$

$$= -\frac{1}{\pi} \lim_{\varepsilon \rightarrow +0} \left\{ \frac{2x\varepsilon}{x^4 + 2x^2\varepsilon^2} \frac{2x\varepsilon}{(x^2 + 2ix\varepsilon)(x^2 - 2ix\varepsilon)} \right\} = -\frac{1}{x} \times \left\{ \frac{\sqrt{2}\delta(x)}{\delta(x)} \right\},$$

where in the first case we have dropped the ε^4 term and in the second we have dropped the ε^2 term in each of the cofactors. Since this result *uniquely* implies the formulas

$$x\delta'(x) = -\sqrt{2}\delta(x), \quad = -\delta(x), \quad (\text{A12})$$

it is easy to verify which of these two formulas corresponds to the basic meaning of the relations containing the delta function and its derivatives: the integral of the two sides of any such relation should give the same result. This condition is satisfied by the second formula in (A12). Thus the second formula in (A2) is the original, and so (A10) should be rejected. Finally, it should be noted that of the two formulas in (A9) the second is important in practice, since it enables one to replace the hard-to-integrate function $\delta(x)/x$ by the easily integrable (by parts) function $\delta'(x)$, and formulas (A9) are more correctly written

$$\frac{\delta(x)}{x} = -\delta'(x) \rightarrow x\delta'(x) = -\delta(x). \quad (\text{A13})$$

2. The operator $\hat{B} \equiv f(\hat{A})$ is considered to be a function of the operator \hat{A} if their eigenvalues are related by the same functional dependence as the operators themselves, i.e.,

$$\hat{B}\Psi_n = B_n\Psi_n = f(A_n)\Psi_n, \quad (\text{A14})$$

where Ψ_n is the common eigenfunction of these operators. A function $f(\hat{A})$ of operator argument \hat{A} has meaning (is defined) only for those eigenvalues A_n of the operator \hat{A} for which the function $f(A_n)$ of the nonoperator argument A_n has meaning (is defined).

The derivative of an operator with respect to a nonoperator argument on which it depends explicitly is defined in the usual way:

$$\frac{\partial \hat{A}}{\partial p} \equiv \lim_{p' \rightarrow p} \frac{\hat{A}(p') - \hat{A}(p)}{p' - p}. \quad (\text{A15})$$

According to this definition the product of operators is differentiated according to the same rule as for the product of nonoperator quantities, but with the original order of the operators in their product preserved in the differentiation.

In quantum theoretical physics all the functional dependences on operators (even among those which are formally admissible) are encountered by no means equally of-

ten. The most important and frequently used is the exponential dependence on an operator. For example, the statistical operator—the basic operator of quantum statistical physics—is just such an operator. It therefore makes sense to obtain a formula for the derivative

$$\frac{\partial f(\hat{A}(\lambda))}{\partial \lambda} \equiv \frac{\partial \hat{B}(\lambda)}{\partial \lambda} \quad (\text{A16})$$

of such an operator with respect to a parameter when $f(\hat{A})$ is the exponential function:

$$\hat{B}(\lambda) \equiv \exp(\beta \hat{A}(\lambda)). \quad (\text{A17})$$

It is for this case (and for handbook purposes) that the inconvenient and asymmetric expressions in the form of “left” and “right” derivatives are presented in the literature [cf. Ref. 52, (p. 329 in Russian original)].

By direct calculation one can verify the auxiliary formula

$$\frac{\partial \hat{A}^n(\lambda)}{\partial \lambda} = \sum_{m=1}^n \hat{A}^{m-1} \frac{\partial \hat{A}}{\partial \lambda} \hat{A}^{n-m}, \quad (\text{A18})$$

which gives a rule for differentiating a power-law function of operator argument, which, in turn, is a function of a non-operator argument λ . Now, using (A18), we can easily obtain the desired formula for differentiating an exponential function:

$$\frac{\partial}{\partial \lambda} \exp(\beta \hat{A}(\lambda)) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{m=1}^n \hat{A}^{m-1} \frac{\partial \hat{A}}{\partial \lambda} \hat{A}^{n-m}. \quad (\text{A19})$$

If $\partial \hat{A} / \partial \lambda$ commutes with \hat{A} , this leads directly to the usual formula

$$\frac{\partial}{\partial \lambda} \exp(\beta \hat{A}) = \beta e^{\beta \hat{A}} \frac{\partial \hat{A}}{\partial \lambda} = \beta \frac{\partial \hat{A}}{\partial \lambda} e^{\beta \hat{A}}. \quad (\text{A20})$$

In quantum statistics it is very often necessary to differentiate not the statistical operator itself but only its trace. Since the trace of a product of operators does not change upon cyclic permutations of those operators, here, generally speaking, we do not need to pay attention to the noncommutative property of an operator and its derivative, and we can write the derivative (A19) immediately in the form (A20). As an example that is of interest from the standpoint of applications one can obtain an analog of the Feynman theorem for the thermodynamic potential. In quantum mechanics the Feynman theorem has the form⁵²

$$\frac{\partial U}{\partial \lambda} \equiv \frac{\partial}{\partial \lambda} \int \Psi^* H \Psi dv = \int \Psi^* \frac{\partial H}{\partial \lambda} \Psi dv. \quad (\text{A21})$$

The thermodynamic potential is⁵²

$$\beta \Omega = -\ln \text{Sp}\{\exp[-\beta(H + \mu \hat{N})]\}, \quad (\text{A22})$$

and then in quantum statistics the Feynman theorem becomes

$$\frac{\partial \Omega}{\partial \lambda} = \langle \frac{\partial H}{\partial \lambda} \rangle, \quad (\text{A23})$$

where $\langle \dots \rangle$ denotes statistical averaging.

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