On the evaluation of the correlation functions in quantum statistical physics

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1. Evaluation of the time-dependent (dynamic) or equilibrium (static) correlation functions is one of the most important problems in quantum statistical physics. There are a number of methods used to solve this problem, the simplest and most convenient of which is the method of two-time retarded and advanced Green's functions, which were introduced in 1959 by Bogolyubov and Tyablikov¹ (see also the review²). This method can be used to solve in a unified way many problems in both equilibrium and non-equilibrium statistical mechanics,³⁻⁷ including the evaluation of the thermodynamic characteristics of a system, the kinetic coefficients, and also the generalized susceptibility.

The main difficulty arising in the use of this Green's function method consists in the necessity of choosing a method of breaking off (decoupling) the infinite chain of equations of motion for the increasingly complicated Green's functions. Such a procedure is, of course, nonunique except in those cases when the problem has an explicit small parameter (e.g., in the hydrodynamic or high-frequency region), in which case the decoupling procedure is completely equivalent to the procedure of selecting the important diagrams in the diagram expansion method.⁸

A great deal of interest in statistical physics centers on problems in which the system undergoes a phase transition (e.g., a ferromagnet in the Ising or Heisenberg models). For constructing the solution in the entire temperature region there is no single small parameter, and the decoupling is done in a heuristic way (as, e.g., in the Tyablikov approximation¹⁻⁴ in the problem of a Heisenberg ferromagnet). The only justification for such a decoupling or any of its numerous modifications (see, e.g., the Supplement to Refs. 4 and 6) is that it yields reasonable approximations throughout the entire range of temperatures and fields, that the sum rules are satisfied to sufficient accuracy, or, possibly, other additional physical conditions. These last include, e.g., the presence of gapless Goldstone modes, finite values of the critical temperature for systems with a phase transition, fulfillment of symmetry requirements for the correlation functions, etc.

Unfortunately, at the present time there are no methods for choosing *a priori* a specific form of decoupling, nor is there a mathematically rigorous justification for such a choice (or even an precise estimate of its accuracy). Nevertheless, there are a number of rather well developed approximate methods that enable one to take into account in a systematic and unambiguous way the contribution of the higher approximation in evaluating the Green's functions. In all these methods it is necessary to break at some step the chain of equations for the Green's functions, but now it

is not the original chain, as in the early papers (see Refs. 1 and 2), but a suitably reconfigured chain that is broken. In the present paper we successfully use for this purpose various different versions of projection operations that permit reconfiguration of the chain of equations for the Green's functions in such a way that each equation of the chain in the succeeding step describes the evolution in a space which is orthogonal to the dynamical variables appearing in preceding step. Then the equations of the reconfigured chain couple Green's functions that are irreducible with respect to the previous functions of lower order. This substantially simplifies the construction of the approximations for the two-time retarded and advanced Green's functions and in practice replaces the diagram method that has been successfully applied, e.g., to the causal Green's functions at T=0 or the Matsubara Green's functions at $T\neq 0$ (see Ref. 8).

2. One of the most frequently employed methods based on the introduction of projection operators is the Mori method,^{9,10} which was applied directly to the two-time Green's functions in Refs. 11 and 12. A characteristic feature of these methods is the time dependence of the correlation functions in terms of the projected, or reduced, evolution operators, which becomes increasingly complicated with each step. Although this dependence remains undeciphered in the Mori method, it is clear that it necessitates making additional approximations. In the papers by Tserkovnikov¹³⁻¹⁵ an alternative method of constructing the chain of equations for the Green's functions was developed, based on differentiation with respect to the two times and being on the whole equivalent to the Mori method, but making explicit the action of the reduced evolution operators. The Tserkovnikov method has been developed in two completely equivalent versions: for the energy (E)representation, 13,14 and for the time (t) representation 15 (see Ref. 17 for examples of the application of this method); the details of the derivation and examples of the application of the E representation, which is more convenient in practice, can be found in Refs. 14 and 16, respectively.

The main result of the projection method in the Tserkovnikov formulation for the *E* representation is as follows. Suppose a physical system is described by a Hamiltonian *H* and the so-called basis operators A_1 and B_1 (each of which for a specific physical problem can be represented by a row or column). For the majority of systems considered in quantum statistical mechanics there is an infinite system of operator equations of motion (\hbar =1), which determines the sequence of operators of increasing complexity A_n and B_n (n=1,2,...),

$$i\dot{A}_{n} = [A_{n},\mathcal{H}]_{-}$$

$$= \omega(n,n)A_{n} + U(n,n+1)A_{n+1}, \quad -i\dot{B}_{n}^{+} \qquad (1)$$

$$= \mathcal{H}, B_{n}]_{-}$$

$$= B_{n}^{+}v^{+}(n,n) + B_{n+1}^{+}V^{+}(n+1,n).$$

The matrix $\omega(n,n)$ [and, respectively, $v^+(n,n)$] relates the operator $i\dot{A}_n$ with the operator A_n (respectively, $-i\dot{B}_n^+$ with B_n^+) and describes the "free evolution" of the system; the matrix U(n,n+1) [respectively, $V^+(n+1,n)$] which relates the operator $i\dot{A}_n$ to the operator A_{n+1} (respectively, $i\dot{B}_n^+$ to B_{n+1}^+), takes the influence of the "interaction" into account.

The main objects of study in quantum statistical mechanics are the time correlation functions $\langle A(t) | B^+(t') \rangle$ or the closely related Green's functions

$$\langle \langle A(t) | B^{+}(t') \rangle \rangle = -\frac{i}{\hbar} \theta(t-t') \langle A(t) | B^{+}(t') \rangle$$

(see, e.g., Refs. 1-8), where $\langle ... \rangle$ denotes an average over the Gibbs canonical (or grand canonical) ensemble, $\theta(t-t')=1$ for t > t', $\theta(t-t')=0$ for t < t', and $\langle A(t) | B^+(t') \rangle$ is taken to mean one of the bilinear combinations constructured from the operators A(t), $B^+(t')$:

$$\langle A(t) | B^{+}(t') \rangle^{K} = \frac{i}{\hbar} \int_{t}^{\infty} \langle [A(t_{1}), B^{+}(t')]_{-} \rangle dt_{1},$$

$$\langle A(t) | B^{+}(t') \rangle^{T} = \int_{0}^{\beta} \langle A(t) B^{+}(t'+i\hbar\tau) \rangle d\tau,$$

$$\langle A(t) | B^{+}(t') \rangle = \frac{1}{i\hbar} \langle [A(t), B^{+}(t')]_{\eta} \rangle,$$

(2)

$$\langle A(t) | B^+(t') \rangle = \langle A(t) B^+(t') \rangle$$
 or $\langle B^+(t') A(t) \rangle$.

The Green's functions corresponding to the different ways of choosing $\langle A(t) | B^+(t') \rangle$ in (2) are, respectively, the Kubo relaxation function, the scalar product determining the isothermal susceptibility at t' = t, the retarded or advanced (anti) commutator ($\eta = \pm 1$) Green's function, and the causal Green's function. The equations of motion for all these Green's functions are based on Eq. (1) and are identical in form (the only difference is the form of the initial condition $\langle A | B^+ \rangle$). Since in the equilibrium case all the average quantities $\langle A(t) | B^+(t') \rangle$ depend only on the time difference t-t', it is convenient to go over the E representation and obtain according to Ref. 13 the Dyson equation for the Fourier transform $\langle \langle A_1 | B_1^+ \rangle \rangle_E$ of the Green's function constructed from the basis operators A_1 , B_1^+ (see Ref. 14 for the generalization to the case of the Green's function $\langle \langle A_n | B_n^+ \rangle \rangle_E$ for n > 1):

$$(E-\omega(1,1) - U(1,2)\langle A_2 | B_1^+ \rangle \langle A_1 | B_1^+ \rangle^{-1} - U(1,2)$$

$$\times \langle \langle A_2 | B_2^+ \rangle \rangle_E^{(1)} V^+ (2,1) \langle A_1 | B_1^+ \rangle^{-1})$$

$$\times \langle \langle A_1 | B_1^+ \rangle \rangle_E = \langle A_1 | B_1^+ \rangle.$$
(3)

The mass operator on the left-hand side of (3) is expressed in terms of the irreducible (with respect to the initial Green's function) part of $\langle \langle A_1 | B_1^+ \rangle \rangle_E$, which has the form

$$\langle \langle A | B^+ \rangle \rangle_E^{(1)} \equiv \langle \langle A | B^+ \rangle \rangle_E$$

- $\langle \langle A | B_1^+ \rangle \rangle_E \langle \langle A_1 | B_1^+ \rangle \rangle_E^{-1}$
 $\times \langle \langle A_1 | B^+ \rangle \rangle_E;$
(4)

it is clear that any operator A or B^+ that can be expressed linearly in terms of the operators A_1 and B_1^+ , respectively, will not contribute to (4) i.e.,

$$\langle\langle A_1 | B^+ \rangle\rangle_E^{(1)} = \langle\langle A | B_1^+ \rangle\rangle_E^{(1)} = 0$$
(5)

for any A and B^+ . Thus relation (4) does in fact perform a projection or, what is the same, a separation of the irreducible part with respect to the basis operators A_1 , B_1^+ , which is another way of saying that a transition has occurred into a subspace orthogonal to the initial basis operators.

3. It is clear from Eqs. (3)-(5) that the maximum possible contribution to the mass operator in the case when the equations of motion (2) are linearized with respect to the operator A_1 or B_1^+ (independently of the specific way that the linearization is carried out and of the choice of coefficients in it) is given by so-called generalized Hartree-Fock approximation (GHFA), which, according to Eq. (3), has the form

$$\langle \langle A_1 | B_1^+ \rangle \rangle_E \approx \langle A_1 | B_1^+ \rangle [E - (\omega(1,1) + U(1,2)) \\ \times \langle A_2 | B_1^+ \rangle \langle A_1 | B_1^+ \rangle^{-1})]^{-1}.$$
 (6)

In other words, Eqs. (3)–(5) imply that any attempt to go beyond the framework of the GHFA with the help of linearized equations of motion for the basis operators A_1 , B_1^+ will give a manifestly zero result.

One can construct approximations different from the GHFA only by constructing some nontrivial approximation for the Green's function $\langle \langle A_2 | B_2^+ \rangle \rangle_E^{(1)}$, which determines the mass operator and which is clearly of a higher order than the initial function $\langle \langle A_1 | B_1^+ \rangle \rangle_E$. A systematic procedure for constructing the corresponding infinite chain of equations for the irreducible Green's functions of arbitrary orders, with an increasing degree of irreducibility, was set forth in Refs. 13 and 14, and examples of its application are given in Ref. 16.

We note that the approximation expressions for the Green's function $\langle \langle A_1 | B_1^+ \rangle \rangle_E$ (or, correspondingly, for the spectrum of elementary excitations) of the form (6) in the scalar case have been proposed previously by many authors, including Roth,¹⁸ Plakida,¹⁹ Kalashnikov and Fradkin,²⁰ Tahir-Kheli and Jarrett,²¹ and also Wallace.²² The authors of Refs. 18–22 used different physical approaches: in Refs. 18 and 19 the Green's function method was used; in Refs. 20 and 21, the spectral intensity method with accuracy up to allowing the lower moments; and, in Ref. 22, an effective linearization of equations of motion of

the form (2). A common finding of these and a number of other papers is that the GHFA expressions of the form (6) are the maximum possible within the framework of the idea of a "single-particle" linearization without expansion of the initial operator basis. In these expressions the effect of the mean field of the system on the effective spectrum of the (noninteracting and undamped) quasiparticles used to model the given system is taken into account.

(As we know, the ordinary mean field approximation presupposes that the localization procedure is carried out back at the stage of the initial Hamiltonian and not at the state of the first equation of motion, as in the GHFA.)

Later Sawada²³ confirmed the hypothesis made in Ref. 24 that the GHFA spectrum is optimal in a variational sense and yields the minimum free energy functional in the given class of solutions (this was shown in reference to a Heisenberg ferromagnet in Ref. 25; one should, however, pay heed to the discussion in Refs. 26, 27 as to the applicability of the "exact" GHFA near the Curie point).

4. In connection with the results presented above, it was dismaying to read in *Uspekhi* the recent article by Sarry,²⁸ which we think is seriously deficient from the standpoint of both methodology and results. For evaluating correlation functions, Sarry formulates a so-called (in his terminology) "direct algebraic method," which is ostensibly free of any ambiguities and "volitional solutions," admits 'exact self-consistency" and "nonlinear linearization" of the initial equations of motion, and is, moreover (in the words of the author) mathematically rigorous "from beginning to end."

Perhaps this paper, which abounds in arbitrary and fallacious assertions, should not be taken seriously but left to the conscience of its author and the referees. However, it was published in our esteemed journal and contains pointed and completely unproven criticism of the Green's function method, whose development and current level of refinement are clearly not adequately understood by its author.

(For example, he cites the lack of "convincing" justification for the decoupling method, even though such methods can be justified *a priori* only in the context of perturbation theory in the case when the problem contains an explicit small parameter, and, in the absence of such, only by the self-consistency of the results.)

For these reasons we think it would be helpful to prevent any possible misunderstandings on the part of readers who are just becoming acquainted the Green's function method, since the scientific look, abundance of formulas, and verbosity of that $paper^{28}$ might temporarily obscure the fundamental errors of its author.

First of all, the "direct algebraic method" and its results are essentially not original but are completely equivalent to the well-known GHFA, which was derived not only by Roth,¹⁸ who is cited in Ref. 28, but also, independently, in a number of other papers¹⁹⁻²⁷ (see Sec. 3). This approximation is sometimes sufficient for an adequate description of a system at the level of the so-called first-order theories (a detailed comparative analysis of which for the example of a Heisenberg ferromagnet is reviewed by Rudoĭ in Ref. 6). However, even in this approximation there is a significant degree of ambiguity in the evaluation of the right-hand side of Eq. (6), especially in systems with nontrivial kinematic properties of the operators (e.g., spin operators; see Ref. 17 and the Supplement to Ref. 4). Moreover, it is wrong to try to claim ultimate truth for the GHFA, as is done in Ref. 28. The author of that paper naively assumes that by means of some technical contrivances (e.g., the Jacobi identity of the commutators) he can force practically all the essential dynamical and kinematical information about any system having a strong interaction into a "procrustean bed" of some effective frequencies (or of the K matrix in the notation of Ref. 28). This, of course, is far from being the case, as the author of Ref. 28 could have seen if he had taken the trouble to acquaint himself with the literature;⁴⁻¹⁷ in particular, in Ref. 17 it is shown for the example of a Heisenberg ferromagnet that it is fundamentally necessary to take into account along with the GHFA the contribution of the mass operator from Eq. (3). True, he does mention casually the necessity of expanding the operator basis even in his scheme, but nowhere does he attempt to implement this idea.

5. In conclusion, we wish to point out one egregiously bad mistake that clearly demonstrates the level of "mathematical culture" of Ref. 28. In the framework of the standard BCS model, for which it has been rigorously proven⁷ that an asymptotically exact solution exists, the author of Ref. 28 manages to obtain some new equation for the critical point, the physical meaning of which, in his words, is not clear. According to this equation, superconductivity is ostensibly possible in the BCS model not only for an attractive potential but also for a repulsive potential in a certain range of electron density. It is easy to see, however, that this "result" stems simply from errors in evaluating the commutators appearing in the GHFA, specifically, from ignoring the role of taking the thermodynamic limit, $N \to \infty$, $V \to \infty$, N/V = const, while at the same time keeping in Eq. (3.5.25) of Ref. 28 terms of different orders in the parameter 1/N. Of course, the correct result is given only by Eq. (3.5.26) of that paper, which agrees with the long-known and well-known formula (see, e.g., Ref. 8). The "new" equation (3.5.27) [and the equations (3.5.28)and (3.5.29) that follow from it] is simply the result of the aforementioned misunderstanding [which the author of Ref. 28 for some reason calls an "interesting physical property" of Eq. (3.5.25)] and also the completely incorrect discussions that come between Eqs. (3.5.26) and (3.5.27), on the grounds of which the author drops terms $\sim N^2$ in comparison with $\sim N$.

In the other examples given in Ref. 28, the results, although not wrong, are largely "rehashes" of the well known results of the GHFA. This only points up the fallaciousness of the claim of its author to have created a new method of evaluating correlation functions in quantum statistical physics. *Deceased.

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