# Once again about analytical methods of calculating correlation functions in quantum statistical physics 

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#### Abstract

About two years ago I published a paper in this journal under the title "Analytical methods of calculating correlation functions in quantum statistical physics"'[1]. Recently a methodological note 'On the evaluation of the correlation functions in quantum statistical physics" was published by D N Zubarev and Yu G Rudoi [2]. In the words of its authors, my paper "abounds in arbitrary or erroneous statements', and they were impelled to write only because of the "strong and completely unsubstantiated criticism'' of the Green function method. Leaving to the authors' conscience the style they chose in their printed defence of the Green function method, I shall try to provide a brief and, whenever possible, quite complete answers to all their critical comments. However, I must first briefly recall the principal features of the method I proposed in that paper. They can be summarised as follows.


(1) It is assumed that in the case of the investigated system it is possible to construct a basis of operators $\left\{\hat{A}_{j}\right\}$, which is usually incomplete but nevertheless closed (in a nonoperator manner) with respect to the operation of commutation with the Hamiltonian of the system:

$$
\begin{equation*}
\left[\hat{A}_{j}, H\right]_{-}=\sum_{j^{\prime}=1}^{n} K_{j j^{\prime}} \hat{A}_{j^{\prime}}, \quad j=1,2,3, \ldots, n \tag{1}
\end{equation*}
$$

Here all the basis operators generally have different orders. If all the operators are of the same order, then on this basis the initial problem becomes completely linear in the most direct sense and, therefore, its solution is then exact and the operator basis is complete.
(2) An incomplete set of operators can be closed 'by force' if the values of the coefficients $K_{n j^{\prime}}$ in the expansion described by Eqn (1) are selected with the aid of the Jacobi operator identity, which has to be satisfied exactly. In the case of a two-operator basis, this identity is

$$
\begin{equation*}
\left[\hat{A_{1}},\left[\hat{A_{2}}, H\right]_{-}\right]_{-}-\left[\hat{A_{2}},\left[\hat{A_{1}}, H\right]_{-}\right]_{-}-\left[\left[\hat{A_{1}}, \hat{A_{2}}\right]_{-}, H\right]_{-}=0 \tag{2}
\end{equation*}
$$

Substituting here the expansions of the appropriate commutators

$$
\begin{aligned}
& {\left[\hat{A_{1}}, H\right]_{-}=K_{11} \hat{A_{1}}+K_{12} \hat{A_{2}},} \\
& {\left[\hat{A_{2}}, H\right]_{-}=K_{21} \hat{A_{1}}+K_{22} \hat{A_{2}},}
\end{aligned}
$$

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and the value of the mutual commutator $\left[\hat{A_{1}}, \hat{A_{2}}\right]_{-}$, we can find the required values of $K_{2 j^{\prime}}$. In this way, the whole approximation of the solution of the initial problem 'resides', here in its $K$ matrix and then only in its elements $K_{n j^{\prime}}$, because the expansion of just one last ( $n$ th) commutator is always inexact. The expansion of all the preceding commutators is always exact because of the method used to construct them.
(3) The basis $\left\{\hat{A}_{j}\right\}$ is established in such a way that any correlation function of the investigated system necessarily contains at least one of these operators. This circumstance, together with the cyclic invariance of the value of the trace relative to the operator product (the correlation functions contain precisely such traces) and the exact 'undressing' formula

$$
\begin{equation*}
\hat{A_{j}}[\beta]=\sum_{j^{\prime}=1}^{n}[\exp (-\beta K)]_{j j^{\prime}} \hat{A}_{j^{\prime}} \tag{3}
\end{equation*}
$$

for the 'dressed' basis operator

$$
\hat{A_{j}}[\beta] \equiv \exp (\beta H) \hat{A_{j}} \exp (-\beta H)
$$

makes it possible to derive directly the required closed system of $n$ algebraic equations for the required correlation functions:

$$
\begin{align*}
& \left\langle\hat{B} \hat{A}_{j}\right\rangle=\left\langle\hat{A}_{j}[\beta] \hat{B}\right\rangle=\sum_{j^{\prime}=1}^{n}[\exp (-\beta K)]_{j j^{\prime}}\left\langle\hat{A}_{j^{\prime}} \hat{B}\right\rangle \\
& j=1,2, \ldots, n \tag{4}
\end{align*}
$$

$$
\langle\ldots\rangle \equiv \operatorname{Tr}[\exp (-\beta H) \ldots][\operatorname{sp}(-\beta H)]^{-1}
$$

If a given correlation function includes initially several basis operators, it can be used to write down the same number of independent equations.
(4) Eqn (4)-which is the main formula in the 'dressing-undressing' method-applies to the case of non-temporal correlation functions, which are the usual statistical averages representing the equilibrium states of a system (in this case the Hamiltonian of the system does not depend explicitly on time). However, if there is a time dependence, the required correlation functions can be found without any major changes in the system of equations (4), with the exception of the transformation $\beta \rightarrow \beta=\beta+\mathrm{i} t$, because the temporal correlation function of an equilibrium state of a system is

$$
\left\langle\hat{B}\left[t_{2}\right] \hat{A}_{j}\left[t_{1}\right]\right\rangle=\left\langle\hat{B} \hat{A}_{j}[t]\right\rangle=\left\langle\hat{A}_{j}[\beta+\mathrm{i} t] \hat{B}\right\rangle, \quad t \equiv t_{1}-t_{2}
$$

The temporal correlation functions may be used, at least in the linear approximation, to study also transient
processes in physical systems (when the Hamiltonian of the system is an explicit function of time) because all the kinetic coefficients of nonequilibrium systems considered in the linear approximation can be expressed in terms of their equilibrium temporal correlation functions that correspond to equilibrium states of these systems.

We can now analyse the critical comments made in Ref. [2] about my paper [1].
(I) I shall deal with the statement that my opponents were forced (at least in their own opinion) to write in order to "prevent possible misunderstandings in the case of those readers who are approaching the Green function method for the first time".

In my paper [1] I simply noted the long-known principal calculation shortcoming of the Green function method, which is the absence of a regular procedure for termination of the usually infinite chain of equations of motion for the Green functions. For my own part I added just two comments: first, the anticommutator and commutator Green functions cannot be regarded as (technically!) equivalent; second, the spectral theorem of the Green function method is in practice frequently used incorrectly and this may be due to the fact that Zubarev [3] gives examples of how this theorem should be used in specific calculations, but in fact he applies it in its generally incorrect form in such examples, as demonstrated by Eqns (3.28) and (5.11) in Ref. [3]. However, these two comments from me can hardly be regarded as a criticism of the Green function method and particularly as a strong criticism.

I shall now expand these comments. As far as the termination method is concerned, this does not come from me: it has long been known; moreover, it is in fact acknowledged by my opponents (third paragraph on the first page of their paper). The next two comments do in fact come from me. Their meaning is as follows. The technical inequivalence of the use of the anticommutator and commutator Green functions in specific calculations is related particularly to the correct application of the spectral theorem in the Green function method. This theorem has the following form, which is given by Eqn (3.25) in Ref. [3]:

$$
\begin{equation*}
G(\omega+\mathrm{i} \varepsilon)-G(\omega-\mathrm{i} \varepsilon)=-\mathrm{i}\left[\exp \left(\omega \theta^{-1}\right)-\eta\right] J(\omega) \tag{5}
\end{equation*}
$$

A mathematically correct solution of Eqn (5), which gives the spectral intensity $J(\omega)$ of the required correlation functions for $\eta=1$, is [1, 4]

$$
\begin{align*}
J(\omega)= & \{\mathrm{i}[G(\omega+\mathrm{i} \varepsilon)-G(\omega-\mathrm{i} \varepsilon)]  \tag{6}\\
& \left.\times\left[\exp \left(\omega \theta^{-1}\right)-1\right]^{-1}\right\}+f \delta(\omega)
\end{align*}
$$

i.e. there is a singular term because of the condition

$$
\begin{equation*}
\left[\exp \left( \pm \omega \theta^{-1}\right)-1\right] \delta(\omega) \equiv 0 \tag{7}
\end{equation*}
$$

which ensures that the initial equation (5) is satisfied when solution (6) is substituted in it. It is shown in Ref. [5] that the exact anticommutator and commutator functions respectively admit and do not admit a pole at the point $\omega=0$, and that the residue of the exact anticommutator Green function at this point does indeed determine the unknown function $f$ which occurs in solution (6). This very important (in practice) analytical property of the exact Green functions has not been discussed by $\mathrm{N} N$

Bogolyubov and S V Tyablikov [6, 7] or by D N Zubarev [3]. It is important because the anticommutator or the commutator Green functions calculated approximately (in practice only approximate calculations are possible) may admit a pole at the point $\omega=0$. The pole of an approximately calculated commutator Green function can then be removed by specifying the necessary conditions and the residue at this pole of the anticommutator Green function yields an approximate expression for the unknown function $f$ in solution (6) (the function $f$ is independent of $\omega$ ). Therefore, if we wish to know a priori how to write correctly solution (6) - with or without a singular term - we must always begin with calculation of an anticommutator Green function in the approximation adopted for the task in hand. Then, if it is found that there is no such pole, there should be no singular term in solution (6). In other words, only the commutator Green functions do not generally close the Green function method.
(II) I shall now consider the criticism of D N Zubarev and Yu G Rudoi of the 'direct algebraic method' (DAM) that I propose for calculating correlation functions in quantum statistical physics. The essence of their criticism of the DAM itself can in fact be reduced to the statement that this method is, first, not original but essentially equivalent to the familiar Roth method [8]; second, it does not - in principle-permit going beyond the generalised Hartree-Fock approximation; third, and in spite of all this, I propose the DAM as the method that makes it possible to obtain results pertaining to the 'truth in the final instance'. None of these statements of my opponents corresponds to reality. First, as far as the 'truth in the final instance' is concerned, there is no such statement or even such an expression anywhere in my paper.

Second, the fact that the DAM is not equivalent to the Roth scheme should be obvious even to a nonspecialist. The Roth scheme is intended solely to unify the decoupling of an infinite chain of equations of motion for the Green functions: it does not yield the actual equations of motion for the Green functions and it just supplements the method of equations of motion by a universal decoupling procedure. Only the combination of the Green function method with the Roth scheme proves a completely closed method for the calculation of correlation functions; without a universal decoupling procedure the Green function remains internally unclosed and is essentially an incomplete method for calculating correlation functions in quantum statistical physics.

The DAM however yields both the equations of motion (and this is done directly for the required correlation functions and not for some intermediate functions of the Green type in the Green function method), as well as a universal method for decoupling them, i.e. the DAM is an internally closed method for calculating the correlation functions. The DAM differs from the Green function method because it is internally closed, but also because of its exceptional mathematical and technical simplicity: there are no differential equations, no spectral transformations and the associated spectra theorem in the Green function method, and there is no need to calculate jumps across the real axis of the functions of complex variables; finally, there is no need to calculate any Fourier integrals: the algebraic equations can be written down immediately for the required correlation functions.

The procedure of decoupling by the DAM is based on a rigorous mathematical relationship, which is the Jacobi operator identity and, moreover, it differs from the Roth scheme which is essentially arbitrary although universal: in the Roth scheme a commutator or an anticommutator is taken from both parts of the expansion described by Eqn (1) with operators which are Hermitian conjugates of the operators $\left\{\hat{A}_{j}\right\}$. This is followed by averaging of the resultant relationships:

$$
\begin{align*}
\left.\left\langle\left[\hat{A}_{j}, H\right]_{-}, \hat{A}_{j^{\prime}}^{+}\right]_{\mp}\right\rangle \equiv E_{j j^{\prime}}= & \sum_{j^{\prime \prime}} K_{j j^{\prime \prime}}\left\langle\left[\hat{A}_{j^{\prime \prime}}, \hat{A}_{j^{\prime}}^{+}\right]_{\mp}\right.  \tag{8}\\
& \equiv \sum_{j^{\prime \prime}} K_{j j^{\prime \prime}} N_{j^{\prime \prime} j^{\prime}}
\end{align*}
$$

If the $N$ matrix has an inverse, Eqn (8) can be used to find the required $K$ matrix $E=K N \rightarrow K=E N^{-1}$ from the 'known' $E$ and $N$ matrices. It should be pointed out that Roth does not propose a procedure for constructing the basis system of the operators $\left\{\hat{A}_{j}\right\}$.
(III) I shall now consider the actual physical approximation. In the DAM it depends on three factors: the decoupling method (whether one should use the Roth scheme, the Jacobi identity, or something else); the operators selected as the operator basis for the solution of the problem; third, the dimensionality of the adopted basis: an increase in this dimensionality by just unity has the effect of going beyond the framework of the preceding approximation. Therefore, the statement of $\mathrm{D} N$ Zubarev and Yu G Rudoi that the DAM does not allow us to go beyond the generalised Hartree-Fock approximation is at least strange.
(IV) Finally, let us consider the error which I have been alleged to have made in discussing the Bardeen - Cooper Schrieffer (BCS) model. First, the criticism by $D \mathrm{~N}$ Zubarev and $\mathrm{Yu} G$ Rudoi of my result does not contain anything new on the topic compared with my own opinion given at the end of the discussion of this model. Second, they say that I deliberately left in the gap equation two terms of different orders in $N$, which is the number in any part of matter. There is no error there: as is well known to all those that calculate the properties of large systems from first principles, it is not permissible to limit the answer to just the leading terms because of, in the final analysis, unavoidable transition to the statistical limit. Here is a simple example. In the Brillouin - Wigner expansion for the energy of a large system only one (first) term of the expansion is proportional to $N$ and all the other terms are of the order of unity. What should one do then: retain just this term? Moreover, there are also such cases when the term of a higher order in any range of values of the physical parameters of the system vanishes and then, naturally, it is necessary to include the contribution of the nonvanishing term which is of the next lower order of magnitude. This is precisely the case in the equation I derived for the gap in the BCS model. Allowance for this circumstance leads to the conclusion that the BCS theory is valid only outside the vicinity of the transition point, always to the left of it, whereas at the transition point itself a different equation applies. This conclusion is obtained naturally within the framework of some decoupling, which is specifically that which exactly satisfies the Jacobi identity. In the formal mathematical sense it is more rigorous than the Valatin decoupling, although only the
latter exactly reproduces the BCS result. In a calculation of the properties of many interacting bodies there are naturally such cases when a more rigorous (from the formal mathematical point of view) refinement does not improve the physical result, but makes it worse. In such cases one can speak of the physical unacceptability of the more refined result and not of a 'scandalous mathematical error'.

In conclusion, I would like to state firmly that - in spite of, or maybe because of, the fact that the comments have been signed by D N Zubarev (who is undoubtedly a very authoritative specialist in these matters, whom I know personally, and with whom I have discussed various problems including the DAM)-a reader interested in the essence of the problem of analytical methods for calculating correlation functions should be capable of recognising the true position. As far as my paper is concerned, it is sufficient to read carefully the introduction and the first two paragraphs as well as the last paragraph in the second section.

Now for the final comment. In my opinion an interesting method for calculating correlation functions has been developed by R R Nigmatullin at the Theoretical Physics Department of the Kazan State University [9, 10]. Unfortunately, although this method was included in the first draft of my paper [1], it was somehow omitted from its text in the subsequent revisions.

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