The $\gamma$-operator method and Feynman graphs in quantum optics

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Abstract. It is shown that in quantum optics of extended media, when constructing the Feynman graphs, a specific unitary transformation can be used to avoid the questionable procedure of transition to the thermodynamic limit. Thereby, the calculations can be made considerably more precise, and there occurs the possibility of discovering new optical phenomena.

1. Introduction
The method of the Green quantum functions is the most efficient and convenient method for studying the time evolution of quantized electromagnetic field in extended media. The advantage of this method is the possibility of exceeding the limits of the perturbation theory by means of performing the partial summation of the perturbation theory terms of series represented in the form of a series of the Feynman graphs. The construction of the graph technique is based on the Wick theorem [1]. Although the Wick theorem is exact, using it to construct a closed equation with respect to the quantum Green function requires certain approximations associated with the thermodynamic limit [2, 3]. The punctuality of such approximations cannot be precisely estimated, and it can be very small. The construction of the theory of superconductivity is an example of such a situation. In this case, the standard methods for solving the Schrödinger equation are insufficient. It took several decades to develop the proper mathematical apparatus. In the present work, it is explained how to avoid involving the above approximations. The proposed method for solving the quantum electrodynamics equations is illustrated by an example of interaction of the quantized transverse electromagnetic field with the atomic Maxwellian gas. It is shown that as a result of the transition to the new representation ($\gamma$-representation), the perturbation theory terms of series that are inconvenient for further mathematical manipulations automatically disappear. We assume that in the representation of the secondary quantization, the wave function $\Psi(t)$ of the system under consideration satisfies the Schrödinger equation

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = \left[ \hat{H}_a + \hat{H}_{ph} + e \int \psi^+ (r,R) (r-R)^\nu \hat{E}^{\nu} (r) \psi (r,R) dr dR \right] \Psi(t), \quad e < 0.$$
We also assume that the gas consists of atoms with one valence electron. In the rationalized Gaussian system of units, the operator of the electric field vector of the electromagnetic field has the following form:

\[
\hat{E}_k^\nu(r) = i \sqrt{\frac{\hbar c k}{2\nu}} e_k^\nu (\hat{a}_{kl} e^{jkr} - \hat{a}_{kl}^+ e^{-jkr}),
\]

where \( \hat{a}_{kl} \) and \( \hat{a}_{kl}^+ \) are the photon annihilation and creation operators in the state described by the wave vector \( k \) and the index of linear polarization \( \lambda = 1, 2 \). It will be convenient for us to consider that

\[
\hat{a}_{kl} = \frac{1}{\sqrt{2}} \left( \zeta_{kl} + \frac{\partial}{\partial \zeta_{kl}} \right), \quad \hat{a}_{kl}^+ = \frac{1}{\sqrt{2}} \left( \zeta_{kl} - \frac{\partial}{\partial \zeta_{kl}} \right), \quad \text{and} \quad \left[ \hat{a}_{kl}, \hat{a}_{kl'}^+ \right] = \delta_{\lambda l} \delta_{kk'}.
\]

We will not specify the physical meaning of the \( \zeta_{kl} \) arguments. Next, \( V \) is the quantization volume, and the photon linear polarization vectors \( e_k^\nu \) are perpendicular to the \( k \) vector. We also assume that the operator

\[
\hat{\psi}(r,R) = \sum_{jp} \psi_j(r-R) \exp(i p R / \hbar) \hat{b}_{jp} / \sqrt{V}.
\]

corresponds to the atoms of the Maxwellian gas. Here, \( R \) is the center of gravity of an individual atom, \( r \) is the valence electron coordinate in that atom, and \( p \) is the atom momentum. The wave function \( \psi_j(r-R) \) describes the electron state with energy \( \epsilon_j \) in the atom. We can assume that the Maxwellian gas consists of atoms obeying the Bose-Einstein statistics and therefore, their annihilation \( \hat{b}_{jp} \) and creation \( \hat{b}_{jp}^+ \) operators satisfy the commutation relation

\[
\left[ \hat{b}_{jp}, \hat{b}_{jp'}^+ \right] = \delta_{jj'} \delta_{pp'}.
\]

Next, we may write that

\[
\hat{H}_a = \sum_{jp} \epsilon_j(p) \hat{b}_{jp}^+ \hat{b}_{jp}, \quad \epsilon_j(p) = \epsilon_j + \frac{p^2}{2M}, \quad \text{and} \quad \hat{H}_{ph} = \sum_{k\lambda} \hbar c k \hat{a}_{kl} \hat{a}_{kl}^+.
\]

Here, \( M \) is the mass of an individual atom in the gas, and in all equations, the summation over the \( V \) indices is implied.

2. Research method

We will study the evolution of the photon system using the method of the quantum Green functions within the formalism introduced by L. V. Keldysh [4]. We define the quantum Green function in the standard way:

\[
D_{\nu\nu'}^{\nu\nu'}(r; t; r', t') = \frac{1}{i\hbar} \left\langle \hat{T} E_{\nu}^\nu(r, t) E_{\nu'}^\nu'(r', t') \right\rangle_0.
\]

Here, \( E_{\nu}^\nu(r, t) \) is the electromagnetic field strength operator in the Heisenberg representation, \( \hat{T} \) is the chronological operator [4] along the time loop extending from the point \( t \to -\infty \) \((l = 1)\) to the point \( t \to +\infty \), and then returning back to the point \( t \to -\infty \) \((l = 2)\). The angle brackets \( \left\langle \right\rangle_0 \) mean
the averaging over the system wave functions in the absence of interaction between photons and atomic gas.

We recall that when calculating the \( D^{(\nu)}_{\nu} (r,t; r', t') \) function, we are faced with the need to calculate the expressions such as

\[
\sum_{k_1\nu_1 k_2\nu_2} \cdots \left\{ \hat{T} \hat{a}_{k_1\lambda_1} (t_1) \hat{a}_{k_2\lambda_2} (t_2) \cdots \hat{a}_{k_1\lambda_1} (t'_1) \hat{a}_{k_2\lambda_2} (t'_2) \cdots \right\}_0 ,
\]

in which the photon creation \( \hat{a}_{k\lambda} (t) \) and annihilation \( \hat{a}_{k\lambda} (t) \) operators are defined in the interaction representation and depend on time. Expression (2) has a peculiarity. It can include operators with equal indices \( (k\lambda) \). For example,

\[
\sum_{k_1\nu_1 k_2\nu_2} \cdots \left\{ \hat{T} \hat{a}_{k_1\lambda_1} (t_1) \hat{a}_{k_2\lambda_2} (t_2) \hat{a}_{k_1\lambda_1} (t_3) \cdots \hat{a}_{k_2\lambda_2} (t'_1) \hat{a}_{k_1\lambda_1} (t'_2) \hat{a}_{k_2\lambda_2} (t'_3) \cdots \right\}_0.
\]

If we neglect all terms that are similar to expression (3), the remaining terms of expression (2) can be written as different products of functions of the following type:

\[
\sum_{k_1} \left\{ \hat{T} \hat{a}_{k\lambda} (t) \hat{a}_{k\lambda} (t') \right\}_0.
\]

This observation is very important, since it makes it possible to present the original expression (2) as a product of only this kind of functions, and to develop a technique for calculating the arising series. As for the terms similar to expression (3), they are usually omitted [2, 3], since by mistake, they are considered to be small. Obviously, the errors of such approach are large enough. It is fundamentally impossible to exclude such approximation from this formalism because in the quantum optics, the high order correlators can never be accurately expressed through the correlators of the lower orders.

For example, the equality

\[
\left\{ \hat{a}_{k_1\lambda_1} \hat{a}_{k_2\lambda_2} \hat{a}_{k_1\lambda_1} \hat{a}_{k_2\lambda_2} (t_1) \hat{a}_{k_1\lambda_1} (t'_1) \right\} = \left\{ \hat{a}_{k_1\lambda_1} \hat{a}_{k_2\lambda_2} \hat{a}_{k_1\lambda_1} \hat{a}_{k_2\lambda_2} (t'_2) \right\}
\]

is fatally broken at \( (k_1, \lambda_1) = (k_2, \lambda_2) \). Thus, fundamentally, the quantum Green function (1) cannot be expressed only through the correlators of the second order.

If we consider the theory, in which the higher-order correlators simply do not arise, the mentioned difficulty disappears. The proposed \( \Gamma \)-operator method [5] discards this problem.

The \( \Gamma \)-representation is constructed as follows. Let us introduce the convenient notations. To exclude the high powers of the \( \hat{a}_{k\lambda} \) and \( \hat{a}_{k\lambda} \) operators from the formulas, in the representation of the secondary quantization, we write the wave function of the free field (conglomerate) of photons determined by the occupation numbers \( N_{k\lambda} \) in the following form:

\[
\Phi_N (\xi) = \Pi_{k\lambda} \varphi_{N_{k\lambda}} (\xi_{k\lambda}).
\]

Here, \( \varphi_{N_{k\lambda}} (\xi_{k\lambda}) \) are the wave functions of the quantum oscillator. The multidimensional vectors \( N = \ldots, N_{k_2} \ldots \) and \( \xi = \ldots, \xi_{k_2} \ldots \) determine the parameters of the \( \varphi_{N_{k\lambda}} (\xi_{k\lambda}) \) functions. Using the \( N_{k\lambda} \) axes, we will construct the infinite-dimensional space (\( \Gamma \)-space), in which the state of the system of free photons is described by a point.

Let us introduce new notations. Now we will write the wave function of the photon conglomerate \( \Phi_N (\xi) \) using the wave functions of the quantum oscillator in the following form:

\[
\Phi_N (\xi) = \Pi_{\nu=0} \varphi_0 (\xi_N) \cdots \varphi_0 (\xi_N^\nu).
\]

If photons forming the conglomerate are entirely absent, the wave function of such vacuum state is \( \varphi_0 (\xi_0) \Pi_{\nu=0} \varphi_0 (\xi_N^\nu) \). The photon conglomerate can be either empty, or filled. Therefore, we need only the \( \varphi_0 (\xi_N^\nu) \) functions at \( \nu = 0, 1 \). Let us introduce [5] the operators of creation \( \hat{\nu} (N) = (\xi_N - \partial / \partial \xi_N) / \sqrt{2} \) and annihilation \( \hat{\mu} (N) = (\xi_N + \partial / \partial \xi_N) / \sqrt{2} \) of the photon
conglomerate \( N \). It is evident that 
\[
\hat{\mathcal{U}}(N) \hat{\mathcal{U}}^+(N') = \delta_{NN'} , \quad \hat{\mathcal{U}}^+(N) \phi_0(N) = \phi_1(N) \quad \text{and} \quad \hat{\mathcal{U}}(N) \phi_1(N) = \phi_0(N).
\]
Let us introduce the notation \( \hat{\mathcal{V}}_N = \prod_{N=1}^N \phi_0(N) \). The wave functions of all possible photon conglomerates 
\[
\hat{\mathcal{V}}^+(N) \hat{\mathcal{V}}^+(N') = \phi_1(N) \prod_{N=1}^N \phi_0(N') \quad \text{form the complete basis of the wave functions determined by the Schrödinger equation. Therefore, any solution of the Schrödinger equation \( \hat{\mathcal{V}} \) can be expanded in series of these functions:}
\]
\[
\langle \hat{\mathcal{V}} \rangle = \sum N C(N,t) \hat{\mathcal{V}}^+(N) \langle \hat{\mathcal{V}} \rangle.
\]
It is important to note that the constructions like 
\[
\hat{\mathcal{V}}^+(N) \hat{\mathcal{V}}^+(N') \hat{\mathcal{V}}^+(N') \quad \text{that are mathematically possible have no physical meaning and so, they are absent among the basic functions.}
\]
So far, it is only a question of different notations, and the \( \Phi_N(\xi) \) and \( \hat{\mathcal{V}}^+(N) \langle \hat{\mathcal{V}} \rangle \) wave functions describe the same field of free photons, but in different representations. However, the \( \Gamma \) -presentation has an important advantage following from the formulas
\[
\hat{\mathcal{V}}(N) \hat{\mathcal{V}}^+(N) = \phi_1(N) \prod_{N=1}^N \phi_0(N') \quad \text{and} \quad \hat{\mathcal{V}}(N) \hat{\mathcal{V}}^+(N') = \phi_0(N) \prod_{N=1}^N \phi_0(N').
\]
Just these properties determine the appropriateness of using the \( \Gamma \) -representation, and considerably simplify the calculation results obtained using the Wick theorem.

The possibility of using the \( \Gamma \) -representation in calculations occurs due to its unitary connection with the representation of secondary quantization. In fact, the \( \Phi_N(\xi) \) functions forming the complied basis set in the theory of secondary quantization and the \( \hat{\mathcal{V}}^+(N) \langle \hat{\mathcal{V}} \rangle \) functions used in the \( \Gamma \) -representation are connected by the unitary transformation determined by the following operator:
\[
\hat{O}(\xi) = \hat{\mathcal{V}}^+(\xi) \langle \hat{\mathcal{V}} \rangle, \quad \text{where} \quad \hat{O}(\xi) = \sum \hat{\mathcal{V}}(N) \Phi_N(\xi).
\]
It is easy to verify that
\[
\hat{O}(\xi) \Phi_N(\xi) = \int \sum \hat{\mathcal{V}}^+(N') \Phi_N(\xi)d\xi = \hat{\mathcal{V}}^+(N) \langle \hat{\mathcal{V}} \rangle, \quad d\xi = \prod_{k,l} d\xi_{k,l},
\]
\[
\hat{O}(\xi) \hat{\mathcal{V}}^+(N) = \sum \hat{\mathcal{V}}^+(N') \Phi_N(\xi) \hat{\mathcal{V}}^+(N) \langle \hat{\mathcal{V}} \rangle = \Phi_N(\xi).
\]
If \( \hat{K}(\xi,\xi') \) is some operator in the representation of secondary quantization, then in the \( \Gamma \) -representation, the quantum average of this operator will be calculated in accordance with the following formula:
\[
\langle \hat{K} \rangle = \int \langle \hat{\mathcal{V}}^+(\xi') \hat{K}(\xi',\xi) \hat{\mathcal{V}}(\xi) \rangle \langle \hat{\mathcal{V}} \rangle d\xi d\xi'.
\]
In the \( \Gamma \) -representation, instead of function (1) we have to deal with the quantum Green function
\[
G_\theta = \frac{1}{i\hbar} \int \langle \hat{\mathcal{V}}^+(\xi,t) \hat{\mathcal{V}}^+(\xi',t') \rangle \langle \hat{\mathcal{V}} \rangle d\xi d\xi'.
\]
The $\Phi_t(\xi,t)$ operators are the $\hat{\Phi}_t(\xi)$ operators written in the Heisenberg representation, within which they become the time-dependent operators. Symbol $\langle \phi_{t_0} \rangle$ denotes the wave function of non-interacting systems. Instead of expressions (2), we will now deal with the following structures:

$$
\sum_{N_1} \sum_{N_2} \ldots \langle \hat{\Phi}_{t_1}(N_1,t_1)\hat{\Phi}^*(N_2,t_2) \ldots \hat{\Phi}(N_1,t_1')\hat{\Phi}^*(N_2,t_2') \ldots \rangle_{t_0} = A + B
$$

The summation over the $N_{1,2}$ vectors implies the summation over all possible conglomerates. According to the Wick theorem, such correlators can be represented in the form of two series $A$ and $B$ of different structure. The series $A$ consists exclusively of products of correlators of the $\hat{\Phi}(N,t)$ and $\hat{\Phi}^*(N,t)$ operators. However, according to (4), due to specific properties of the $\langle \phi_{t_0} \rangle$ functions, of all the normal products of the operators, there remain only those containing the only one annihilation operator. The construction $B$ is greatly simplified. Now each its summand consists of the $i\hbar \Delta$-type correlators and one correlator of the $\Gamma$-representation, without using any approximations (in particular, transitions to the thermodynamic limit), the quantum Green functions (5) can be expressed only in terms of the bilinear correlators of two types: $i\hbar \Delta = \langle (\hat{T} - \hat{N})\hat{\Phi}(N,t)\hat{\Phi}^*(N,t) \rangle$ and

$$
\rho = \langle \hat{\Phi}^*(N,t')\hat{\Phi}(N,t) \rangle_{t_0}
$$

Next, the polarization operators can be introduced in the standard way, and the Feynman graph summation technique can be developed. When using such method for calculations, the absence of any forced approximations makes it possible to discover the correlation effects previously unknown. A particular example of using the specific properties of the $\Gamma$-representation is considered in [6], where the possibility is indicated of the coupled photon pair formations in quantum optics of gases.

3. Conclusions

In the extended optical media, the accepted form of the procedure for transition to the thermodynamic limit in the framework of the quantum Green functions’ technique can cause the errors that are hard to be estimated. The $\Gamma$-presentation, solving this problem, actually means the replacement of the multi-particle problem by the one-particle one in the multidimensional space. Instead of the creation and annihilation operators for single photon, such a replacement requires the introduction of the creation and annihilation operators for their conglomerates. Within the quantum Green function technique, after the introduction of the polarization operators, the explicit summation can be applied to a series of normal products of such operators. In this case, no approximations are required. This approach makes the known results more precise and predicts the existence of the optical effects previously unknown.

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