

The structure of Green functions in quantum field theory with a general state

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Abstract. In quantum field theory, the Green function is usually calculated as the expectation value of the time-ordered product of fields over the vacuum. In some cases, especially in degenerate systems, expectation values over general states are required. The corresponding Green functions are essentially more complex than in the vacuum, because they cannot be written in terms of standard Feynman diagrams. Here, a method is proposed to determine the structure of these Green functions and to derive nonperturbative equations for them. The main idea is to transform the cumulants describing correlations into interaction terms.

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1. Introduction

High-energy physics uses quantum field theory mainly to describe scattering experiments through the S-matrix. In solid-state or molecular physics, we are rather interested in the value of physical observables, such as the charge and current densities inside the sample or the response to an external perturbation. At the quantum field theory (QFT) level, these quantities are calculated as expectation values of Heisenberg operators. For example, the current density for a system in a state $|\Phi\rangle$ is $\langle\Phi|\mathbf{J}(x)|\Phi\rangle$, where $|\Phi\rangle$ and $\mathbf{J}(x)$ are written in the Heisenberg picture.

The first QFT calculation of Heisenberg operators was made by Dyson in two difficult papers [1, 2] that were completely ignored. At about the same time, Gell-Mann and Low discovered that, when the initial state of the system is non-degenerate, the expectation value of a Heisenberg operators can be obtained by a relatively simple formula [3]. The Gell-Mann and Low formula has been immensely successful and is a key element of the many-body theory of condensed matter [4, 5].

Its main advantage over the formalism developed by Dyson is that all the standard tools of QFT can be used without change.

However, it was soon realized that the assumption of a nondegenerate initial state is not always valid. As a matter of fact, the problem of what happens when the initial state is not trivial is so natural that it was discussed in many fields of physics: statistical physics [6], many-body physics [7], solid-state physics [8], atomic physics [9], quantum field theory and nuclear physics [10, 11]. As a consequence, the theory developed to solve this problem received several names such as nonequilibrium quantum field theory (or quantum statistical mechanics) with initial correlations (or with cumulants, or for open shells, or for degenerate systems). It is also called the closed-time path or the (Schwinger-)Keldysh approach for an arbitrary initial density matrix.

It should be stressed that the problem of the quantum field theory of a degenerate system is not only of academic interest. For instance, many strongly-correlated systems contain open-shell transition metal ions which are degenerate by symmetry. This degeneracy makes the system very sensitive to external perturbation and, therefore, quite useful for the design of functional materials.

The elaboration of a QFT for degenerate systems took a long time. It started with Symanzik [12] and Schwinger [13] and made slow progress because the combinatorial complexity is much higher than with standard QFT. To illustrate this crucial point, it is important to consider an example. According to Wick's theorem, the time-ordered product of free fields can be written in terms of normal order products:

$$\begin{aligned} T\varphi(x_1)\dots\varphi(x_4) &= :\varphi(x_1)\dots\varphi(x_4): + \sum_{ijkl} :\varphi(x_i)\varphi(x_j): G_0(x_k, x_l) \\ &\quad + \sum_{ijkl} :\varphi(x_k)\varphi(x_l): G_0(x_i, x_j) + \sum_{ijkl} G_0(x_i, x_j)G_0(x_k, x_l), \end{aligned}$$

where the quadruplet of indices (i, j, k, l) runs over $(1, 2, 3, 4)$, $(1, 3, 2, 4)$ and $(1, 4, 2, 3)$. The expectation value of this expression over the vacuum gives the familiar result $\sum_{ijkl} G_0(x_i, x_j)G_0(x_k, x_l)$. However, when the initial state $|\psi\rangle$ is not the vacuum (as in solid-state physics), we obtain

$$\begin{aligned} \langle\psi|T\varphi(x_1)\dots\varphi(x_4)|\psi\rangle &= \langle\psi|:\varphi(x_1)\dots\varphi(x_4):|\psi\rangle + \sum_{ijkl} \rho_2(x_i, x_j)G_0(x_k, x_l) \\ &\quad + \sum_{ijkl} \rho_2(x_k, x_l)G_0(x_i, x_j) + \sum_{ijkl} G_0(x_i, x_j)G_0(x_k, x_l), \end{aligned}$$

where $\rho_2(x, y) = \langle\psi|:\varphi(x)\varphi(y):|\psi\rangle$. If we assume, for notational convenience, that the expectation value of the normal product of an odd number of field operators is zero, the fourth cumulant $\rho_4(x_1, \dots, x_4)$ is defined by the equation

$$\langle\psi|:\varphi(x_1)\dots\varphi(x_4):|\psi\rangle = \rho_4(x_1, \dots, x_4) + \sum_{ijkl} \rho_2(x_k, x_l)\rho_2(x_i, x_j).$$

If we put $g = G_0 + \rho_2$, the free four-point Green function becomes

$$\langle \psi | T \varphi(x_1) \dots \varphi(x_4) | \psi \rangle = \rho_4(x_1, \dots, x_4) + \sum_{ijkl} g(x_i, x_j) g(x_k, x_l).$$

When $\rho_4 = 0$, the expression is the same as over the vacuum, except for the fact that the free Feynman propagator G_0 is replaced by g . When this substitution is valid, standard QFT can be applied without major change and the structure of the interacting Green functions is not modified. For fermionic systems described by a quadratic Hamiltonian H_0 , this happens when the ground state is nondegenerate, so that $|\psi\rangle$ is a Slater determinant. When $\rho_4 \neq 0$, the expression becomes essentially different because the cumulant ρ_4 appears as a sort of free Feynman propagator with four legs. In general, the expectation value of a time-ordered product of n free fields involves ρ_k with $k \leq n$.

In other words, the perturbative expansion of the Green functions can no longer be written as a sum of standard Feynman diagrams. Generalized Feynman diagrams have to be used, involving free Feynman propagators with any number of legs [6, 7, 14].

Because of this additional complexity, the structure of the Green functions for degenerate systems is almost completely unknown. The only result available is the equivalent of the Dyson equation for the one-body Green function $G(x, y)$ [7]

$$G = (1 - A)^{-1}(G_0 + C)(1 - B)^{-1}(1 + \Sigma G),$$

where A , B , C and Σ are sums of one-particle irreducible diagrams. When the initial state is nondegenerate, $A = B = C = 0$ and the Dyson equation $G = G_0 + G_0 \Sigma G$ is recovered.

In the present paper, a formal method is presented to determine the structure of Green functions for degenerate systems. The main idea is to use external sources that transform the additional propagators ρ_n into *interaction terms*. This brings the problem back into the standard QFT scheme, where many structural results are available.

2. Expectation value of Heisenberg operators

Let us consider a physical observable $A(t)$, for instance the charge density or the local magnetic field. In the Heisenberg picture, this observable is represented by the operator $A_H(t)$ and the value of its observable when the system is in the state $|\Phi_H\rangle$ is given by the expectation value $\langle A(t) \rangle = \langle \Phi_H | A_H(t) | \Phi_H \rangle$.

Going over to the interaction picture, we write the Hamiltonian of the system as the sum of a free and an interaction parts: $H(t) = H_0 + H_I(t)$, we define the evolution operator $U(t, t') = T(\exp(-i \int_{t'}^t H_I(t) dt))$ and we assume that the state $|\Phi_H\rangle$ can be obtained as the adiabatic evolution of an eigenstate $|\Phi_0\rangle$ of H_0 . The expectation value of A becomes

$$\langle A(t) \rangle = \langle \Phi_0 | U(-\infty, t) A(t) U(t, -\infty) | \Phi_0 \rangle,$$

where $A(t)$ on the right hand side is the operator representing the observable in the interaction picture. The identity $1 = U(t, \infty)U(\infty, t)$ and the definition $S = U(\infty, -\infty)$ enable us to derive the basic expression for the expectation value of an observable in the interaction picture:

$$\langle A(t) \rangle = \langle \Phi_0 | S^\dagger T(A(t)S) | \Phi_0 \rangle. \quad (2.1)$$

When $|\Phi_0\rangle$ is nondegenerate, this expression can be further simplified into the Gell-Mann and Low formula

$$\langle \Phi | A(t) | \Phi \rangle = \frac{\langle \Phi_0 | T(A(t)S) | \Phi_0 \rangle}{\langle \Phi_0 | S | \Phi_0 \rangle}.$$

If the system is in a mixed state, as is the case for a degenerate system by Lüders' principle, the expectation value becomes

$$\langle A(t) \rangle = \sum_n p_n \langle \Phi_n | S^\dagger T(A(t)S) | \Phi_n \rangle,$$

where p_n is the probability to find the system in the eigenstate $|\Phi_n\rangle$. It will be convenient to use more general mixed states $\sum_{mn} \omega_{mn} |\Phi_m\rangle \langle \Phi_n|$, where ω_{mn} is a density matrix (i.e. a nonnegative Hermitian matrix with unit trace). Such a mixed state corresponds to a linear form ω defined by its value over an operator O :

$$\omega(O) = \sum_{mn} \omega_{mn} \langle \Phi_n | O | \Phi_m \rangle.$$

Then, the expectation value of $A(t)$ becomes

$$\langle A(t) \rangle = \omega(S^\dagger T(A(t)S)). \quad (2.2)$$

3. QFT with a general state

In all practical cases, the operator representing the observable $A(t)$ in the interaction picture is a polynomial in φ and its derivatives. Its expectation value (2.2) can be expressed in terms of Green functions that are conveniently calculated by a formal trick due to Symanzik [12] and Schwinger [13], and reinterpreted by Keldysh [15].

The first step is to define an S-matrix in the presence of an external current j as $S(j) = T(e^{-i \int H^{\text{int}}(t) dt + i \int j(x)\varphi(x) dx})$, where H^{int} is the interaction Hamiltonian in the interaction picture. The interaction Hamiltonian is then written in terms of a Hamiltonian density $V(x)$, so that $\int H^{\text{int}}(t) dt = \int V(x) dx$ and the generating function of the interacting Green functions is defined by $Z(j_+, j_-) = \omega(S^\dagger(j_-)S(j_+))$. The interacting Green functions can then be obtained as functional derivatives of Z with respect to the external currents j_+ and j_- . For example

$$\langle T(\varphi(x)\varphi(y)) \rangle = -\frac{\delta^2 Z(j_+, j_-)}{\delta j_+(x)\delta j_+(y)}, \quad \text{and} \quad \langle \varphi(x)\varphi(y) \rangle = \frac{\delta^2 Z(j_+, j_-)}{\delta j_-(x)\delta j_+(y)}.$$

As in standard QFT, the connected Green functions are generated by $\log Z$.

In the functional method [16, 17], the generating function Z of the interacting system is written as $Z = e^{-iD} Z_0$, where D is the interaction in terms of functional derivatives

$$D = \int V\left(\frac{-i\delta}{\delta j_+(x)}\right) - V\left(\frac{i\delta}{\delta j_-(x)}\right) dx,$$

and where $Z_0(j_+, j_-) = \omega(S_0^\dagger(j_-)S_0(j_+))$, with $S_0(j) = T(e^{i \int j(x)\varphi(x)dx})$. Note that $Z_0(j_+, j_-)$ is the generating function of the free Green functions.

A straightforward calculation [17] leads to

$$Z^0(j_+, j_-) = e^{-1/2 \int \mathbf{j}(x) G'_0(x, y) \mathbf{j}(y) dx dy} e^{\rho'(j_+ - j_-)},$$

where $\mathbf{j} = (j_+, j_-)$ is the source vector,

$$G'_0(x, y) = \begin{pmatrix} \langle 0|T(\phi(x)\phi(y))|0\rangle & -\langle 0|\phi(y)\phi(x)|0\rangle \\ -\langle 0|\phi(x)\phi(y)|0\rangle & \langle 0|\bar{T}(\phi(x)\phi(y))|0\rangle \end{pmatrix}, \quad (3.1)$$

is a free Green function (with \bar{T} the anti-time ordering operator) and

$$e^{\rho'(j)} = \omega(:e^{i \int j(x)\varphi(x)dx}:) \quad (3.2)$$

defines the generating function $\rho'(j)$ of the cumulants of the initial state ω .

The free Green function G'_0 describes the dynamics generated by the free Hamiltonian H_0 . It can also be written in terms of advanced and retarded Green functions [13].

The idea of describing a state by its cumulants was introduced in QFT by Fujita [6] and Hall [7]. It was recently rediscovered in nuclear physics [10, 11] and in quantum chemistry [18].

The next step is to modify the definition of the free Green function. The cumulant function is Taylor expanded

$$\rho'(j) = \sum_{n=2}^{\infty} \frac{1}{n!} \int dx_1 \dots dx_n \rho_n(x_1, \dots, x_n) j(x_1) \dots j(x_n).$$

The expansion starts at $n = 2$ because $\omega(1) = 1$ and the linear term can be removed by shifting the field φ . The bilinear term $\rho_2(x, y)$ is included into the free Green function by defining

$$G_0(x, y) = G'_0(x, y) + \rho_2(x, y) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix},$$

and the corresponding cumulant function becomes

$$\begin{aligned} \rho(j) &= \rho'(j) - (1/2) \int dx dy j(x) \rho_2(x, y) j(y) \\ &= \sum_{n=3}^{\infty} \frac{1}{n!} \int dx_1 \dots dx_n \rho_n(x_1, \dots, x_n) j(x_1) \dots j(x_n). \end{aligned}$$

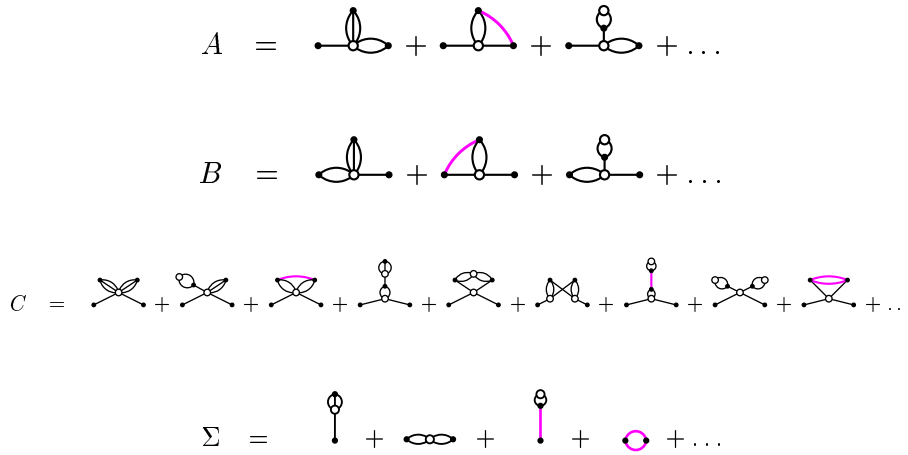
In standard QFT, only the first and last diagrams of the right hand side are present. In the general case when all $\rho_n \neq 0$, the number of diagrams is still much larger.

4.1. Generalized Dyson equation

As mentioned in the introduction, the only known result concerning the structure of Green functions with a general state was derived by Hall for the one-body Green function $G(x, y)$ [7]

$$G = (1 - A)^{-1}(G_0 + C)(1 - B)^{-1}(1 + \Sigma G).$$

In diagrammatic terms the quantities A , B , C and Σ are sums of one-particle irreducible diagrams. If we take our example of the Green function of φ^3 theory up to second order, we find



In standard QFT, we have $A = B = C = 0$ and the diagrammatic representation of Σ contains much less terms. However, the difference with standard QFT is not only limited to the number of diagrams. The definition (3.2) of the cumulant function, and the fact that the free field φ is a solution of the Klein-Gordon equation imply that ρ_n is a solution of the Klein-Gordon equation in each of its variables. Thus, $A(x, y)$, $B(x, y)$ and $C(x, y)$ are solutions of the Klein-Gordon equation for x and y . As a consequence, applying the Klein-Gordon operator to the Green function gives us $(\square + m^2)G = (1 - B)^{-1}(1 + \Sigma G)$. In other words, applying the Klein-Gordon operator kills a large number of terms of G . This is in stark contrast with standard QFT, where $(\square + m^2)G = 1 + \Sigma G$ and amputating a Green function does not modify its structure. This important difference makes some tools of standard QFT (e.g. amputated diagrams or Legendre transformation) invalid in the presence of a general state.

All those difficulties explain the scarcity of results available in non-perturbative QFT with a general state. Apart from Hall's work [7], the only non-perturbative

results are Tikhodeev's cancellation theorems [23, 24] and the equation of motion for the Green functions [25].

In the next section, we present a simple trick to derive the structure of Green functions with a general state.

4.2. Quadrupling the sources

We first determine the main formal difference between standard QFT and QFT with a general state. In both cases, the generating function of the Green functions can be written $Z = e^{-iD} Z_0$, where D describes the interaction and Z_0 the initial state. In the presence of a general state, the interaction D is simple but Z_0 is made non standard by the cumulant factor e^ρ . The idea of the solution is to transfer the cumulant function ρ from Z_0 to D , because powerful functional methods were developed to deal with general interactions D . These methods were first proposed by Dominicis and Englert [26] and greatly expanded by the Soviet school [27, 28, 29, 30, 31, 32, 33, 34, 35].

This transfer from the initial state to the interaction can be done easily by introducing two additional external sources k_+ and k_- and using the identity

$$e^{\rho(j_+ - j_-)} = e^{\rho(-i\frac{\delta}{\delta k_+} - i\frac{\delta}{\delta k_-})} e^{i \int (j_+(x)k_+(x) - j_-(x)k_-(x)) dx} \Big|_{k_+ = k_- = 0}.$$

The term involving ρ can now be transferred from Z_0 to D by defining the new generating function

$$\bar{Z}(j_\pm, k_\pm) = e^{-i\bar{D}} \bar{Z}_0(j_\pm, k_\pm),$$

where the modified interaction is

$$\bar{D} = \int V\left(\frac{-i\delta}{\delta j_+(x)}\right) - V\left(\frac{i\delta}{\delta j_-(x)}\right) dx - i\rho\left(-i\frac{\delta}{\delta k_+} - i\frac{\delta}{\delta k_-}\right),$$

and the modified free generating function is

$$\bar{Z}_0(j_\pm, k_\pm) = e^{-1/2 \int \mathbf{J}(x) \bar{G}_0(x, y) \mathbf{J}(y) dx dy},$$

with $\mathbf{J} = (j_+, j_-, k_+, k_-)$. The modified free Green function \bar{G}_0 is now a 4x4 matrix that can be written as a 2x2 matrix of 2x2 matrices

$$\bar{G}_0 = \begin{pmatrix} G_0 & -i\mathbf{1} \\ -i\mathbf{1} & 0 \end{pmatrix}.$$

In contrast to the standard case, the free Green function \bar{G}_0 is invertible

$$\bar{G}_0^{-1} = \begin{pmatrix} 0 & i\mathbf{1} \\ i\mathbf{1} & G_0 \end{pmatrix},$$

and it is again possible to use amputated diagrams and Legendre transformations. The free generating function \bar{Z}_0 is the exponential of a function that is bilinear in the sources, and all the standard structural tools of QFT are available again. We illustrate this by recovering Hall's analogue of the Dyson equation.

4.3. An algebraic proof of Hall's equation

The free generating function \bar{Z}_0 has a standard form and the Dyson equation holds again: $\bar{G} = \bar{G}_0 + \bar{G}_0 \bar{\Sigma} \bar{G}$, where \bar{G} is the 4x4 one-body Green function obtained from the generating function \bar{Z} and $\bar{\Sigma}$ is the corresponding self-energy. Each 4x4 matrix is written as a 2x2 matrix of 2x2 matrices. For example

$$\bar{G} = \begin{pmatrix} \bar{G}_{11} & \bar{G}_{12} \\ \bar{G}_{21} & \bar{G}_{22} \end{pmatrix}.$$

We want to determine the structure of the 2x2 Green function G , which is equal to \bar{G}_{11} when $k_+ = k_- = 0$.

The upper-left component of the Dyson equation for \bar{G} is

$$\bar{G}_{11} = G_0 + (G_0 \bar{\Sigma}_{11} - i \bar{\Sigma}_{21}) \bar{G}_{11} + (G_0 \bar{\Sigma}_{12} - i \bar{\Sigma}_{22}) \bar{G}_{21}. \quad (4.1)$$

The lower-left component gives us $\bar{G}_{21} = -i(1 + i \bar{\Sigma}_{12})^{-1}(1 + \bar{\Sigma}_{11} \bar{G}_{11})$. If we introduce this expression for \bar{G}_{21} into equation (4.1), rearrange a bit and use the operator identity $1 + O(1 - O)^{-1} = (1 - O)^{-1}$, we obtain

$$(1 + i \bar{\Sigma}_{21}) \bar{G}_{11} = (G_0 - \bar{\Sigma}_{22})(1 + i \bar{\Sigma}_{12})^{-1}(1 + \bar{\Sigma}_{11} \bar{G}_{11}).$$

Hall's equation is recovered by identifying $A = -i \bar{\Sigma}_{21}$, $B = -i \bar{\Sigma}_{12}$ and $C = -\bar{\Sigma}_{22}$, where the right hand side is taken at $k_+ = k_- = 0$. Note that Hall's equation is now obtained after a few lines of algebra instead of a subtle analysis of the graphical structure of the diagrams.

With the same approach, all the nonperturbative methods used in solid-state physics, such as the GW approximation [36] and the Bethe-Salpeter equation [37, 38], can be transposed to the case of a general initial state. This will be presented in a forthcoming publication.

5. Determination of the ground state

QFT with a general state was studied because the initial eigenstate of a quantum system is sometimes degenerate. However, it remains to determine which density matrix ω_{mn} of the free Hamiltonian leads to the ground state of the interacting system.

A solution to this problem was inspired by quantum chemistry methods [39]. A number of eigenstates $|\Phi_n\rangle$ of H_0 are chosen, for example the complete list of degenerate eigenstates corresponding to a given energy. These eigenstates span the so-called *model space* and the ground state of the interacting system is assumed to belong to the adiabatic evolution of the model space. This model space generates, for each density matrix, a linear form ω as described in equation (2.2). The problem boils down to the determination of the density matrix ω_{mn} that minimizes the energy of the interacting system.

This minimization leads to an effective Hamiltonian and the proper density matrix is obtained by diagonalizing the effective Hamiltonian. This type of method is typical of atomic and molecular physics [40]. However, the effective Hamiltonian

can now be determined by powerful non-perturbative Green function methods. Therefore, the present approach leads to a sort of unification of quantum chemistry and QFT: it contains standard QFT when the dimension of the model space is one, it contains standard quantum chemistry (more precisely many-body perturbation theory) when the Green functions are expanded perturbatively.

Therefore, the present approach might help developing some new nonperturbative methods in quantum chemistry. On the other hand, quantum chemistry has accumulated an impressive body of results. The physics Nobel-prize winner Kenneth Wilson stated that [41] “Ab initio quantum chemistry is an emerging computational area that is fifty years ahead of lattice gauge theory.” Therefore, the experience gained in quantum chemistry can be used to solve some of the remaining problems of the present approach, such as the removal of the secular terms[14] to all order.

6. Conclusion

The present paper sketched a new method to determine the Green functions of quantum field theory with a general state. The main idea is to transform the cumulant function describing the initial state into an interaction term. As a consequence, the cumulants become dressed by the interaction, providing a much better description of the correlation in the system.

An alternative method would be to work at the operator level, as was done recently by Dütsch and Fredenhagen [42], and to take the expectation value at the end of the calculation. This would have the obvious advantage of dealing with a fully rigorous theory. However, we would lose the non-perturbative aspects of the present approach.

Although this approach seems promising, much remains to be done before it can be applied to realistic systems: (i) our description is purely formal; (ii) the degenerate initial eigenstates lead to secular terms that must be removed [14]; (iii) renormalization must be included, although this will probably not be very different from the standard case, because all the singularities of the free system are restricted to G_0 .

Interesting connections can be made with other problems. For example, the cancellation theorem [23] seems to be interpretable as a consequence of the unitarity of the S-matrix. It would extend Veltman’s largest time equation [43] to the case of spacetime points with equal time. Another exciting track would be a connection with noncommutative geometry. Keldysh[15] noticed that the doubling of sources could be replaced by a doubling of spacetime points. In other words, $j_{\pm}(x)$ becomes $j(x_{\pm})$, where x_{\pm} are two copies of the spacetime point x : time travels from the past to the future for x_+ and in the other direction for x_- . Sivasubramanian and coll. [44] have proposed to interpret this doubling of spacetime points in terms of noncommutative geometry. It would be interesting to follow this track for our quadrupling of spacetime points.

From the practical point of view, the main applications of our scheme will be for the calculation of strongly-correlated systems, in particular for the optical response of some materials, such as gemstones, that remain beyond the reach of the standard tools of contemporary solid-state physics.

After the completion of this work, we came across a little known article by Sergey Fanchenko, where the cumulants are used to define an effective action [45]. His paper is also interesting because it gives a path integral formulation of quantum field theory with a general state. His approach and the one of the present paper provide complementary tools to attack nonperturbative problems of quantum field theory with a general state.

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