Boundary Conditions and Correlations in Path Integrals for Quantum Field Theory of Thermal and Non-Equilibrium States

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Abstract

For thermal equilibrium systems it is shown, how the Kubo-Martin-Schwinger boundary condition may be used to factorize the generating functional of Green functions at least on the level of the full two-point function. Genuine non-equilibrium system exhibit correlations that one may also incorporate in the path integral. One one hand this provides a natural tool for a perturbative expansion including these correlations. On the other hand it allows to prove that in general non-equilibrium systems the generating functional does not factorize.

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I. INTRODUCTION

To a great extent, modern physics has turned its attention to non-equilibrium systems. Relativistic heavy-ion collisions [1] and the early universe [2] are two very complementary examples for such systems. They have in common however, that their theoretical description to some extent follows guidelines of relativistic quantum field theory.

Among these guidelines is the feature that causal propagation of particles requires empty (particle) states to propagate forward in time, whereas occupied states propagate backward in time. For the vacuum this guideline leads to the Feynman boundary condition of the two-point Green function (propagator), for thermal equilibrium states it leads to the Kubo-Martin-Schwinger (KMS) boundary condition [3]. For non-equilibrium states however, this guideline requires to double the Hilbert space for the theoretical description: Since the occupation of states may change with time, one has to carry time-forward as well as time-backward boundary condition along throughout a computation.

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Causality therefore imposes an additional $2 \times 2$ matrix structure on field theoretical descriptions of non-equilibrium states. This holds also in the path integral formulation of quantum field theory, which we consider of particular importance for some physical problems: It is the basis of correlation expansion schemes [1] as well as of derivations of finite temperature diagram rules [3,4]. Furthermore, it is used in lattice gauge theory, and may be found as the principal object in the recent discussion of the equivalence of different thermal equilibrium limits of quantum field theory [7,8].

With the present paper we wish to demonstrate, that one may greatly reduce the calculational effort required to take the Hilbert space doubling into account in path integrals. This is possible due to a diagonalization scheme for the $2 \times 2$ matrix structure [3,4]. Apart from this more technical improvement (which might be considered conceptual as well), we also address the question of boundary conditions in general. We present a recipe, how to introduce initial correlations (which are a genuine non-equilibrium effect) into the path integral formalism [11,12].

The doubling of the Hilbert space exists in several different flavors, the two most common are the Schwinger-Keldysh or closed time path method (CTP) [13] and thermo field dynamics (TFD) [14]. Since one may show, that apart from conceptual differences they lead to identical results, we will use them as equivalent in the present paper: Computations are carried out in the CTP formalism, but we will make use of results obtained in TFD.

The paper is organized as follows: In the next section, we introduce our technical improvement into the path integral representation of a free quantum field. In section 3, the considerations are extended to the interacting case. Section 4 is devoted to the problem of initial correlations in terms of Wightman functions. In section 5 we replace the Wightman functions of the correlations by a cumulant expansion, and close the argumentation of this paper by relating this expansion to a classical integral equation including temporal boundary conditions.

II. BOUNDARY CONDITIONS IN THE PATH INTEGRAL

The first step in our discussion is to introduce the concept of diagonalization in the Schwinger-Keldysh or TFD method. To this end we study the physically trivial example of a free scalar quantum field. Throughout the paper we will use (in a somewhat sloppy fashion) two different notations for space-time arguments of fields, $\phi_x \equiv \phi(x)$. The Lagrangian for the free scalar field is

$$L_0(\phi) = -\frac{1}{2} \phi_x \left( \Box + m^2 \right) \phi_x.$$  \hspace{1cm} (1)

The action integral extends over the whole three-dimensional coordinate space, but in time direction has a more complicated structure. Due to the fact, that our system has a presumably irreversible time evolution, the time component of the action integral follows the contour depicted in fig. 1: Forward in time as well as backward in time, separated by an infinitesimal amount above and below the real time axis (For brevity, we do not discuss the foundation for this action integral, but rather refer to a review article on the doubling of the Hilbert space [15]). In terms of the time contour, the generating functional for Green functions is
\[ Z_0 [J] = \int \mathcal{D}[\phi] \exp \left[ i \int d^4 x \left( \mathcal{L}_0(\phi) + \phi_x J_x \right) \right], \quad (2) \]

and Green functions are \textit{contour} ordered along \( C \). Thus, in taking functional derivatives with respect to \( J \) it will make a difference whether the space-time arguments of \( J \) are on the upper or lower part of the contour \( C \).

Since under the contour ordering symbol the fields on the upper and lower branch of the contour commute at any time, we may treat them as two completely different fields. This is also mathematically more correct, because in thermal states the KMS condition induces a doubling of the Hilbert space \([13]\). Indeed, with this step one recovers the concept of thermo field dynamics \([14]\). The two fields will be distinguished by a lower index, \( \phi_{1,x} \) is the field on the upper branch of the time contour.

The generating functional for the Green functions of these two free fields is obtained as

\[ Z_0 [J_1, J_2] = \int \mathcal{D}[\phi_1, \phi_2] \exp \left[ i \int d^4 x \left( \tilde{\mathcal{L}}_0(\phi_1, \phi_2) + \phi_{1,x} J_{1,x} - \phi_{2,x} J_{2,x} \right) \right], \quad (3) \]

with the free Lagrangian

\[ \tilde{\mathcal{L}}_0(\phi_1, \phi_2) = -\frac{1}{2} \phi_{1,x} (\Box + m^2) \phi_{1,x} + \frac{1}{2} \phi_{2,x} (\Box + m^2) \phi_{2,x} \quad (4) \]

and two independent classical source currents \( J_1 \) and \( J_2 \).

Since we are dealing with free fields, the generating functional may be obtained in closed form,

\[ Z_0 [J_1, J_2] = \exp \left[ -\frac{i}{2} \int d^4 x d^4 y \left( J_{1,x} D_J(x - y) J_{1,y} - J_{2,x} \overline{D_J(x - y)} J_{2,y} \right) \right]. \quad (5) \]

The question now arises, which boundary conditions to choose for the two propagators \( D_J(x - y) \) and \( \overline{D_J}(x - y) \). Both are resolvents to the free Klein-Gordon equation, e.g.

\[ (\Box + m^2) D_J(x - y) = -\delta^4(x-y). \quad (6) \]

We may use Occam’s razor as a guideline at this point: The simplest choice clearly are retarded and advanced boundary conditions, since they are free of any influence of the occupation of states. Due to the introduction of the path integral as running along a contour \textit{forward} and \textit{backward} in time, we therefore chose \( D_J(x - y) \) to be the free retarded propagator

\[ D_J(x - y) = D^R_0(x - y) = -i \Theta(x^0 - y^0) \left[ \phi(x), \phi(y) \right]. \quad (7) \]

The other propagator concurrently is chosen to have an advanced boundary condition in time,

\[ \overline{D_J}(x - y) = D^A_0(x - y) = -i \Theta(y^0 - x^0) \left[ \phi(x), \phi(y) \right]. \quad (8) \]
With this ansatz we have completely decoupled the two fields on the upper and lower time branch of the time-path depicted in fig. 1. In particular it is obvious, that mixed functional derivatives of this generating functional are zero when the sources are set to zero:

\[
\left( \frac{\delta^2}{\delta J_1(x) \delta J_2(y)} Z_0 [J_1, J_2] \right)_{J_1 = J_2 = 0} = 0 .
\] (9)

One may now introduce an interaction, and expand the theory perturbatively in terms of the propagators \( D_J \) and \( \overline{D}_J \). The perturbation expansion is incredibly simple, since it is free of any occupation number factors, like e.g., Bose-Einstein distribution functions. Moreover, several types of diagrams in such a perturbative expansion are trivially zero, like e.g. a loop integral over two retarded propagators.

However, it is also obvious that the sources \( J_1 \) and \( J_2 \) introduced in the path integral are not the causal sources necessary to calculate physically meaningful quantities. Instead we need to define physical external sources \( j_1 \) and \( j_2 \), which are obtained by a linear functional from the diagonal sources \( J_1 \) and \( J_2 \). The linearity assures, that the condition \( J_1 = J_2 = 0 \) simply translates into \( j_1 = j_2 = 0 \).

We obtain them by demanding that the mixed second functional derivatives of the generating functional fulfill the Kubo–Martin-Schwinger (KMS) boundary condition [3]

\[
\left( \frac{\delta^2}{\delta j_1(x) \delta j_2(y)} Z_0 [j_1, j_2] \right)_{j_1 = j_2 = 0} = 0 .
\] (10)

This is equivalent to a periodicity condition of the fields in the imaginary time direction.

To obtain the linear functional relating the \( j \)-sources to the \( J \)-sources, it is convenient to switch to a Fourier representation

\[
j_i(x) = \int_0^\infty \frac{dE}{2\pi} \int \frac{d^3k}{(2\pi)^3} e^{i k x} \left( e^{-i E x^0} j_i^{(+)}(E, k) + e^{i E x^0} j_i^{(-)}(E, k) \right)
\] (11)

for \( i = 1, 2 \), and similarly for the sources \( J_i \). The shift in the imaginary time direction then simply translates into a multiplication with a Boltzmann factor. One possible way to express the KMS condition amounts to a linear relationship between the two types of sources, obtained from the Boltzmann factor as

\[
\begin{pmatrix}
J_1^{(+)}(E, k) \\
J_2^{(+)}(E, k)
\end{pmatrix}
= \mathcal{B}(n_B(E))^{-1}
\begin{pmatrix}
J_1^{(+)}(E, k) \\
J_2^{(+)}(E, k)
\end{pmatrix}
\]

\[
\begin{pmatrix}
J_1^{(-)}(E, k) \\
J_2^{(-)}(E, k)
\end{pmatrix}
^T
\begin{pmatrix}
J_1^{(-)}(E, k) \\
J_2^{(-)}(E, k)
\end{pmatrix}
^T
\tau_3 \mathcal{B}(n_B(E)) \tau_3 ,
\] (12)

with a matrix

\[
\mathcal{B}(n_B(E)) = \begin{pmatrix}
1 + n_B(E) & -n_B(E) \\
-1 & 1
\end{pmatrix}
\] (13)
depending on the Bose-Einstein distribution function
\[ n_B(E) = \frac{1}{e^{\beta E} - 1}. \] (14)

It is well known, that this matrix constitutes a *thermal Bogoliubov transformation*, which combines particle and hole states in a way that guarantees a causal propagation in a thermal system \[ \text{[9,10].} \]

Historically, this transformation was discovered in the attempt to simplify perturbative calculations at finite temperature \[ \text{[9].} \] Hence, in the present section we are progressing in the reverse direction: We started from a simple perturbation expansion for the doubled fields, and then recover a causal description in terms of a Bogoliubov transformation of these fields.

By comparison with standard results of thermo field dynamics, we obtain the Bogoliubov symmetry as \[ \text{[10].} \]

\[ j_1^{(-)}(E, \mathbf{k}) j_1^{(+)}(E, \mathbf{k}) - j_2^{(-)}(E, \mathbf{k}) j_2^{(+)}(E, \mathbf{k}) = 
J_1^{(-)}(E, \mathbf{k}) J_1^{(+)}(E, \mathbf{k}) - J_2^{(-)}(E, \mathbf{k}) J_2^{(+)}(E, \mathbf{k}). \] (15)

Of course, this relation admits many solutions for the Bogoliubov transformation matrix; it may be any element from the symplectic group in two dimensions \( \text{Sp}(2) \). Even the requirement of the KMS relation \[ \text{[10]} \] leaves us with some freedom for the transformation matrix. However, it may be shown that for equilibrium states this freedom in the choice of the Bogoliubov matrix is irrelevant since it is a kind of gauge fixing \[ \text{[10]} \] – whereas for non-equilibrium states (where the parameter \( n \) is no longer an equilibrium distribution function) the choice of eq. \[ \text{[13]} \] is the simplest possibility.

The final step in our treatment of the generating functional for the free thermal Green functions is to obtain it in closed form for the causal sources \( j_1 \) and \( j_2 \). Obviously the result is
\[ Z_0[j_1,j_2] = \exp \left[ -\frac{i}{2} \int d^4 x d^4 y \ j_{a,x} D^{ab}_0(x-y) j_{b,y} \right]. \] (16)

The matrix-valued propagator in the exponent is conveniently expressed in momentum space, it has matrix elements
\[ D_0^{11}(k) = \Delta_F(k) - 2\pi i n_B(\omega_k) \delta(k_0^2 - \omega_k^2) \]
\[ D_0^{12}(k) = -2\pi i \delta(k_0^2 - \omega_k^2) \text{sign}(k_0) n_B(k_0) \]
\[ D_0^{21}(k) = -2\pi i \delta(k_0^2 - \omega_k^2) \text{sign}(k_0) (1 + n_B(k_0)) \]
\[ D_0^{22}(k) = -\Delta_F^*(k) - 2\pi i n_B(\omega_k) \delta(k_0^2 - \omega_k^2), \] (17)

where \( \Delta_F \) is the Feynman propagator
\[ \Delta_F(k) = (k_0^2 - \omega_k^2 + i\epsilon)^{-1} \] (18)
and \( \Delta_F^* \) its complex conjugate. The matrix elements are the four well known thermal Green functions: \( D^{11} \) is the causal propagator, \( D^{12} \equiv D^< \) and \( D^{21} \equiv D^> \) are the thermal Wightman functions and \( D^{22} \) is the anti-causal propagator.

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III. INTERACTING FIELDS IN EQUILIBRIUM STATES

In the previous section we have shown, how a technically simple description in terms of retarded and advanced propagators may be translated into a causal description through the use of a thermal Bogoliubov transformation. In the present section we extend this formalism to systems of interacting particles. For simplicity we assume, that other fields have been integrated out, i.e., the interaction appears in the form of a non-local self interaction. In general, also polynomial self-interactions like e.g. a $\phi^4$-theory fall under our description.

The interaction is given by an arbitrary interaction Hamiltonian, which we express in terms of a field operator in the interaction picture labeled $\hat{\phi}_x$. In this Hamiltonian, the field operators are replaced by field amplitudes belonging to the two representations of the doubled Hilbert space:

$$ H_{\text{int}}[\phi', \phi'] = H_{\text{int}}[\hat{\phi} \to \phi'_1] - H_{\text{int}}[\hat{\phi} \to \phi'_2]. $$

The primes in this equation indicate the fact, that so far we have not stated the temporal boundary conditions for the fields entering here. These follow from the almost trivial fact that also the interacting Green functions have to obey the KMS condition, i.e., the primed fields must be replaced by differential operators, according to

$$ \phi'_i(x) \to -\frac{i\delta}{\delta j_i(x)} Z_0[j_1, j_2]. $$

Consequently, the generating functional for Green functions in a thermal equilibrium state and containing the proper boundary conditions is given by

$$ Z[j_1, j_2] = \exp \left( -i \int d^4x H_{\text{int}} \left[ \frac{-i\delta}{\delta j_1}, \frac{-i\delta}{\delta j_2} \right] \right) Z_0[j_1, j_2], $$

where we have to use the final expression for $Z_0$ of eq. (16). This generating functional is well known, and has been used very often in the existing literature. It gives the correct Schwinger-Keldysh structure of the perturbation series.

However, the virtue of the path integral representation is that it goes beyond perturbation theory. Thus, we think it useful to apply the diagonalization concept of the previous section also to the interacting case presented here. Naturally this task is much more tedious than for the case of free fields. We therefore restrict the discussion to the level which is most important for any application, i.e., to the level of the full two-point Green function of the system.

To this end we first define the generating functional for irreducible vertex functions in the usual way, cf. ref. [16, p.476]:

$$ \Gamma[\phi_1, \phi_2] = \log[Z[j_1, j_2]] - i \int d^4x \left( j_1(x)\phi_1(x) - j_2(x)\phi_2(x) \right). \quad (22) $$

$\Gamma$ is the effective action functional for the interacting fields; for these we introduce a doublet to simplify the notation:

$$ \Phi_x = \left( \phi_1(x) \atop \phi_2(x) \right). \quad (23) $$
A power series expansion for the effective action functional then yields

$$\Gamma = \frac{1}{2} \partial_t \Phi^T \tau_3 \partial_t \Phi - \frac{1}{2} \Phi^T \tau_3 \left(-\Delta + m^2\right) \Phi - \frac{1}{2} \Phi^T \int d^4y \Pi(x - y) \Phi_y + \mathcal{O}(\Phi^3).$$

(24)

Here, $\Pi(x - y)$ is the $2 \times 2$ matrix valued one-particle irreducible self energy function of the system, and $\tau_3 = \text{diag}(1, -1)$. In principle one may also obtain the higher order terms of such an expansion, but for the purpose of the present paper we restrict ourselves to the first nontrivial piece involving the self energy function $\Pi$.

Since we deal with an equilibrium system, we may assume the self energy function to depend only on the difference of the space-time arguments. Consequently, one may perform the Fourier transform into

$$\tilde{\Gamma}(E, k) = \frac{1}{2} \Phi(E, k)^T \left(\tau_3 (E^2 - \omega_k^2) - \Pi(E, k)\right) \Phi(E, k).$$

(25)

In accordance with the previous sections, the doublet is related to another field $\Xi$ by a Bogoliubov transformation

$$\Phi(E, k) = (\mathcal{B}(n_B(E)))^{-1} \Xi(E, k),$$

$$\Phi(E, k)^T \tau_3 = \Xi(E, k)^T \tau_3 \mathcal{B}(n_B(E)).$$

(26)

The fields $\Xi$ are therefore those which diagonalize the effective action functional up to second order.

$$\tilde{\Gamma}(E, k) =$$

$$\frac{1}{2} \Xi(E, k)^T \tau_3 \left(\frac{E^2 - \omega_k^2 - \Pi^R(E, k)}{E^2 - \omega_k^2 - \Pi^A(E, k)}\right) \Xi(E, k).$$

(27)

$\Pi^R$ and $\Pi^A$ are the retarded and advanced self energy functions in momentum space, they are mutually complex conjugate and analytical functions of the energy parameter in at least one half plane:

$$\Pi^{R,A}(E, k) = \text{Re}\Pi(E, k) \mp i\pi\sigma(E, k)$$

$$= \int dE' \sigma(E', k) \frac{\sigma(E', k)}{E - E' \pm i\epsilon}.$$

(28)

They are also related to the components of the matrix-valued self energy function by the simple relations

$$\Pi^R(E, k) = \Pi^{11}(E, k) + \Pi^{12}(E, k),$$

$$\Pi^A(E, k) = \Pi^{11}(E, k) + \Pi^{21}(E, k).$$

(29)

More details of the diagonalization procedure, which (at least to the level of two-point functions, as considered here) may be formulated also for non-equilibrium states, can be found in refs. [9,10].
We proceed by reversing the Legendre transform, i.e., we want to establish how the interaction affects the diagonalization of the generating functional for Green functions. This reversal is straightforward, and one obtains for the generating functional in terms of the decoupled currents $J_1$ and $J_2$

$$Z[J_1, J_2] = \exp \left[ -\frac{i}{2} \int d^4x \, d^4y \left( J_{1,x} D^R(x-y) J_{1,y} - J_{2,x} D^A(x-y) J_{2,y} \right) + \mathcal{O}(J^3) \right].$$

(30)

The retarded and advanced propagator occurring here are, of course, not the free propagators. Instead they are obtained from a spectral function $A(E, k)$

$$D^{R,A}(E, k) = \text{Re} D(E, k) \mp i\pi A(E, k) = \int dE' \frac{A(E', k)}{E - E' \pm i\varepsilon}$$

(31)

which in turn is related to the self energy function components by

$$A(E, k) = \frac{\sigma(E, k)}{(E^2 - \omega_k^2 - \text{Re} \Pi(E, k))^2 + \pi^2 \sigma^2(E, k)}.$$

(32)

The final step of the diagonalization procedure for the interacting case then is to perform the Bogoliubov transformation to the physical source currents conforming to the KMS condition. Quite similar to eq. (16) we obtain

$$Z[j_1, j_2] = \exp \left[ -\frac{i}{2} \int d^4x \, d^4y \, j_{a,x} D^{ab}(x-y) j_{b,y} + \mathcal{O}(j^3) \right],$$

(33)

but the matrix valued propagator here is (in momentum space)

$$D^{(ab)}(E, k) = \int_{-\infty}^{\infty} dE' A(E', k) \times$$

$$\left( B(n_B(E')) \right)^{-1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \left( \begin{pmatrix} 1 \\ E - E' + i\varepsilon \end{pmatrix} \right)^{-1} \left( \begin{pmatrix} 1 \\ E - E' - i\varepsilon \end{pmatrix} \right) \frac{1}{E - E'} \tau_3.$$

(34)

Consequently, the thermal Bogoliubov transformation (12) diagonalizes the effective action functional up to the level of the full two-point function also for the interacting case. One may easily check, that in the limit of a free spectral function the full matrix valued propagator (34) reduces to the free one, eq. (17). For the generating functional of Green functions, this diagonalization implies a factorization into upper and lower contour, see fig. 1.
IV. GENERATING FUNCTIONAL WITH INITIAL CORRELATIONS

The next question to be addressed is how the above formulation has to be modified in the non-equilibrium case, i.e., how to treat particle propagation on a non-equilibrium background. To answer it we recall the principal feature of a non-equilibrium system: The occupation numbers of single particle states are not fixed a priori. For a perturbative treatment this implies some difficulty, since one may not be able to find operators which "annihilate" the non-equilibrium state.

Consequently one may not use the "standard" Wick theorem to obtain the perturbative propagators. Necessary is a more advanced formulation of this important tool of perturbation theory. It has been shown some time ago that such a re-formulation amounts to the inclusion of initial correlations \[17,18,11,12\], which basically arise when a non-equilibrium "density matrix" is not a Gaussian in the full fields.

The initial correlations appear in a perturbative expansion as additional vertex functions, coupling one, three, four, five, six or more fields, but not two fields. To explain this in more detail, we leave the path integral formulation for the moment, and resort to a Fock space picture with free field operators. To distinguish them from the C-number valued field amplitudes of the path integral formulation, we denote Fock space operators by a hat symbol, i.e., \( \hat{\phi}_x \). The expectation value \( \langle \cdot \rangle \) denotes the trace over this Fock space with some non-equilibrium density matrix.

In this picture we then apply Wicks theorem to a time-ordered product of \( L \) field operators; resulting in a sum of products of normal ordered pieces and C-number valued contractions. By normal ordering we will henceforth understand to shift all free-field annihilation operators to the rightmost side, i.e., a normal ordering with respect to the vacuum. However, our results also hold for more general normal ordering prescriptions with respect to an arbitrary equilibrium state: The argumentation is based on the undeniable fact that normal ordering is not possible with respect to a state that has unknown occupation numbers.

Consequently, in a non-equilibrium state the expectation value of a time-ordered product of \( L \) free field operators is

\[
\langle T[\hat{\phi}_x^L] \rangle = \sum_{\text{perm}} \sum_{n=0}^{[L/2]} C^{(L-2n)} (i D_{ne0}^{11})^n
\]

\[
= \sum_{n=0}^{[L/2]} \frac{L!}{(L-2n)! n! 2^n} C^{(L-2n)} (i D_{ne0}^{11})^n , \tag{35}
\]

where \( \sum_{\text{perm}} \) indicates the sum over all possible permutations of the \( L \) space-time coordinates, giving rise to the numerical factor in case of symmetrized space-time arguments (second line of eq. (35)).

\( D_{ne0}^{11} \) is the free causal propagator for the non-equilibrium state and the functions \( C^{(n)} \) are called correlation kernels \[11\]. They may be expressed as a sum over expectation values of "vacuum-normal ordered" products.

The advantage of the correlation kernels is that each of them appears only once in a specific order of the perturbative expansion. Note, that the only correlation kernel not present in a general non-equilibrium state is the two-point correlation: It is absorbed in the
propagator of the perturbative expansion. The odd correlation kernels only appear when the expectation values of the field under consideration are nonzero. In this respect, the inclusion of initial correlations is a convenient way to obtain a perturbative expansion also for such fields without previous subtraction of the expectation value.

\[ D_{n0}^{ab}(x, y) = -i \left( \begin{array}{c} \langle T \left[ \hat{\phi}_x, \hat{\phi}_y \right] \rangle \\ \langle \hat{\phi}_x \hat{\phi}_y \rangle \\ \langle A \left[ \hat{\phi}_x, \hat{\phi}_y \right] \rangle \end{array} \right). \]  

(36)

A[·] denotes the anti time-ordered product. In equilibrium states this reduces to the matrix of eq. (17).

It is obvious, that the other matrix elements of this propagator occur in the Wick expansion of totally anti-time ordered, or mixed products (see ref. [11] for a complete discussion). It is therefore important to realize that the initial correlations do not distinguish between the two types of indices, i.e., they are not contour-ordered functions in the Schwinger-Keldysh formalism.

We now drop the advantage of having a simple perturbative expansion, and replace the correlation kernels by their expansion into expectation values of simple field operator products. It has been shown in ref. [11], that this is also possible in terms of the Wightman functions rather than in terms of normal ordered products. This has the advantage that our result becomes independent of the type of normal ordering prescription we chose. Indeed, using for the unordered (Wightman) functions the abbreviation

\[ P_{1\ldots L}^{(L)} = \langle \hat{\phi}_1 \ldots \hat{\phi}_L \rangle \]  

(37)

we may write

\[ C_{1\ldots K}^{(K)} = \sum_{n=0}^{[L/2]} \frac{L!}{(L-2n)! n! (-2)^n} P_{1\ldots L-2n}^{(L-2n)} \langle \hat{\phi} \rangle^n. \]  

(38)

Again, the numerical factor is due to the sum over all permutations of the space-time arguments, i.e., we understand the above expression to be symmetrized in these.

The reason for this rewriting is, that one may easily obtain the generating functional for the correlation kernels in terms of the initial state Wightman functions,

\[ W[\eta] = \exp \left( \frac{1}{2} \int d^4x d^4y \eta_x \langle \hat{\phi}_x \hat{\phi}_y \rangle \eta_y \right) \langle \exp \left( i \int d^4z \eta_z \hat{\phi}_z \right) \rangle. \]  

(39)

The correlation kernels are obtained from this by subsequent derivatives, i.e.,

\[ C_{1\ldots K}^{(K)} = \left( \frac{(-i)^K \delta^K}{\delta \eta_1 \ldots \delta \eta_K} W[\eta] \right)_{\eta=0}. \]  

(40)

The generating functional of the time-ordered functions therefore is
\[ Z^{11}[\eta] = \left\langle T \left[ \exp \left( i \int d^4 z \eta_z \hat{\phi}_z \right) \right] \right\rangle \]
\[ = \exp \left( -\frac{1}{2} \int d^4 x d^4 y \eta_x \left( iD^{11}_{\text{ne}0}(x, y) - \left\langle \hat{\phi}_x \hat{\phi}_y \right\rangle \right) \eta_y \right) \]
\[ \times \left\langle \exp \left( i \int d^4 z \eta_z \hat{\phi}_z \right) \right\rangle \]
\[ = \exp \left[ -\frac{1}{2} \int d^4 x d^4 y \eta_x iD^{11}_{\text{ne}0}(x, y) \eta_y \right] \times W[\eta] . \]

(41)

From these expressions it is obvious how the equilibrium nature of a state is connected to the vanishing of the correlation kernels \( C \): It is a gaussian of the fields \( \hat{\phi} \), and therefore the generating functional \( W \) is identical to 1.

Finally, we extend this formula to the matrix valued formulation. As we have indicated above, this brings into play the other matrix elements of eq. (36). Furthermore the correlation kernels are identical for both types of indices, thus one has to replace the current \( \eta \) in the functional \( W[\eta] \) by the sum of \( j_1 \) and \( j_2 \). The interaction is introduced in a perturbative way as in eq. (21). The generating functional for non-equilibrium Green functions therefore is

\[ Z_{\text{ne}}[j_1, j_2] = \exp \left( -i \int d^4 u \mathcal{H}_{\text{int}} \left[ \frac{-i \delta}{\delta j_{1,u}} \frac{-i \delta}{\delta j_{2,u}} \right] \right) \times \]
\[ \exp \left[ -\frac{1}{2} \int d^4 x d^4 y j_{a,x} \left( iD^{ab}_{\text{ne}0}(x, y) - \left\langle \hat{\phi}_x \hat{\phi}_y \right\rangle \right) j_{b,y} \right] \times \]
\[ \left\langle \exp \left[ i \int d^4 z \left( j_{1,z} + j_{2,z} \right) \hat{\phi}_z \right] \right\rangle . \]

(42)

This allows to recover the full perturbation expansion for non-equilibrium Green functions in an arbitrary state. States with nonzero field expectation value as well as states with complicated correlations are handled correctly by this expression.

However, missing in this framework is the connection to the preceding sections, i.e., to the question of temporal boundary conditions. This gap will be closed in the following section.

V. CUMULANT EXPANSION AND PATH INTEGRALS

The expression for generating functional of free non-equilibrium Green functions in an arbitrary system is given in Eq. (2). We now proceed along the line of thought underlying the path integral formulation: Fields are expanded around their classical value, i.e., we set \( \phi_x = \phi_x^c + \phi_x^q \). The classical field \( \phi_x^c \) is the solution of the field equation with an external current as source

\[ (\Box_x + m^2) \phi_x^c = J_x . \]

(43)

Inserting this equation into (2) allows to rewrite the generating functional as
\begin{align}
Z_0 [J] &= \int \mathcal{D}[\phi^n] \exp \left[ \frac{i}{2} \int d^4 x \left( \frac{\hat{\phi}^n}{(\square_x + m^2) \phi^n} \right) \right] \\
&\quad \times \exp \left[ \frac{i}{2} \int d^4 x \left( \phi_x^{cl} J_x \right) \right].
\end{align}

The first factor is a trivial Gaussian integral, i.e., it amounts to a phase of the whole expression and will be set to 1 henceforth. For \( \phi^{cl} \) in the second factor the classical solution obeying the correct boundary conditions must be substituted. In the case of equilibrium systems we may split up the fields and currents due to their location on the contour \( \mathcal{C} \) depicted in fig. 1:

\[ \phi_x^{cl} = -\int d^4 y \begin{cases} 
D^R(x - y)J_{1,y} & \text{if } x \text{ on upper contour} \\
D^A(x - y)J_{2,y} & \text{if } x \text{ on lower contour.}
\end{cases} \]

This reproduces the generating functional from eq. (43). Another possibility for this splitting is the causal boundary condition

\[ \phi_x^{cl} = -\int d^4 y \begin{cases} 
D^{1a}(x - y)j_{a,y} & \text{if } x \text{ on upper contour} \\
D^{2a}(x - y)j_{a,y} & \text{if } x \text{ on lower contour},
\end{cases} \]

which results in the expression (46) for the generating functional.

Here therefore is the place, where the temporal boundary condition enters the calculation of \( Z[J] \). We now ask the question, how this classical equation has to be modified for non-equilibrium states.

To this end, we introduce the irreducible cumulants by relating them to the generating functional of the correlation kernels [19]:

\[ W[\eta] = i \int d^4 x \left\langle \hat{\phi}_x \right\rangle \eta_x + \sum_{n=3}^{\infty} \int d^4 \eta_1 \ldots d^4 \eta_n \frac{i^n}{n!} C^{(n)} \eta_1 \ldots \eta_n \]

\[ = \exp \left[ i \int d^4 x \left\langle \hat{\phi}_x \right\rangle \eta_x + \sum_{n=3}^{\infty} \int d^4 \eta_1 \ldots d^4 \eta_n \frac{i^n}{n!} \kappa(1, \ldots, n) \eta_1 \ldots \eta_n \right]. \]

In other words, the logarithm of the generating functional for cumulants equals the generating functional for the correlation kernels.

These cumulants \( \kappa(1, \ldots, n) \) appear more than once in a given order of perturbation theory, whereas the correlation kernels appear only once. The use of cumulants therefore allows a resummation of the perturbation series similar to the Dyson equation; as well as the simple formulation of a linked cluster theorem [19].

For completeness we quote the expectation value of a time-ordered product in terms of these cumulants, i.e., the equivalent of eq. (35):

\[ \left\langle T[\hat{\phi}^L] \right\rangle = \sum_{\text{perm}} \sum_{n=0}^{\left\lfloor \frac{L}{2} \right\rfloor} \sum_{j=0}^{L - 2n} \kappa\{\hat{\phi}^{L-2n}\}_j \left( i D_{11} - \left\langle \hat{\phi} \right\rangle \left\langle \phi \right\rangle \right)^n, \]
where $\kappa\{\hat{\phi}^T\}_j$ denotes a product of $j$ cumulants not containing 2-point cumulants whose arguments are a partition of the $L$ arguments into $j$ disjoint sets.

Inserting these definitions in eq. (41), we obtain for the causal generating functional in terms of the cumulants

\[
Z_{\omega_0}[j_1, j_2] = \exp \left[ -\frac{1}{2} \int d^4x d^4y \, j^a_2 \imath D^{ab}_{\omega_0}(x, y) j^b_2 \right. \\
+ i \int d^4x \langle \hat{\phi}_x \rangle (j_{1,x} + j_{2,x}) \\
+ \sum_{n=3}^{\infty} \int d^41 \ldots d^4n \frac{i^n}{n!} \kappa(1, \ldots n) \prod_{i}(j_{1,i} + j_{1,i}) \right],
\]

(49)

where $j_{1,i} \equiv j_1(x_i), i = 1 \ldots n$. Note, that one may subtract the cumulant $\kappa(x, y) = \langle \hat{\phi}_x \hat{\phi}_y \rangle$ from the propagator and then obtains a complete series over all values of $n$ for the last term. Also, the introduction of an interaction may be carried out as presented in section 3.

We now use the results of section 2 to make the transformation into the retarded/advanced picture involving the currents $J_x$. Although in section 2 we deal with an equilibrium state, it is clear that there exists a similar diagonalization transformation for the non-equilibrium case. To see this more clearly, we perform the Fourier transform of eq. (36) with respect to $(x - y) \to P$, and write it in terms of the two arguments $P$ and $X = (x + y)/2$. It follows that

\[
\mathcal{B}(N_{XP}) \left( D^{(ab)} \right) \tau_3 \left( \mathcal{B}(N_{XP}) \right)^{-1} = \\
\left( \begin{array}{cc}
D_{XP}^R & (N_{XP} D_{XP}^{21} - (1 + N_{XP}) D_{XP}^{12}) \\
0 & D_{XP}^A 
\end{array} \right),
\]

(50)

where we may chose $N_{XP}$ in such a way that also the upper right corner of the propagator matrix is zero. In ref. [10] is is shown, that the corresponding $N_{XP}$ fulfills a transport equation and in the equilibrium limit approaches a Bose-Einstein distribution function. It is therefore indeed the generalized non-equilibrium distribution function.

However, at the level of the external sources $j$, $J$ this transformation has the disadvantage to be more complicated than eq. (12). It mixes various momentum components of the $j_i$ to obtain the $J_i$ and vice versa [10]:

\[
\int d^4x d^4y \, j_{a,x} D^{(ab)}(x, y) j_{b,y} \\
= \int \frac{d^4q}{(2\pi)^4} \frac{d^4p}{(2\pi)^4} d^4X \, e^{-i(q-p)X} \left( \begin{array}{c}
\hat{j}_{1,q} \\
\hat{j}_{2,q}
\end{array} \right)^T \tau_3 \left( \mathcal{B}(X, (p + q)/2) \right)^{-1} \tau_3 \\
\times \left( \begin{array}{c}
D_{XP}^R(X, (p + q)/2) \\
0
\end{array} \right) \mathcal{B}(X, (p + q)/2) \left( \begin{array}{c}
\hat{j}_{1,q} \\
\hat{j}_{2,q}
\end{array} \right).
\]

The “new” currents are marked by the horizontal braces. Let us note at this point, that the momentum mixing Bogoliubov transformation naturally couples the system to gradients in
the generalized distribution function. This allows to calculate transport coefficients \[10\] as well as non-equilibrium effects in two-particle interferometry \[20\].

This separation however fails when taking into account the higher order terms, i.e., those with correlations built in. Consequently, for a general non-equilibrium state the generating functional for Green functions does not factorize into a part of the upper branch and one on the lower branch of fig.1. This may also be seen from the equation that is fulfilled by the classical field $\phi^c$:

$$
\phi^c_x = -i \frac{\delta}{\delta J_{1,x}} Z[j_1, j_2] = \sum_{n=1}^{\infty} \frac{1^{n-1}}{(n-1)!} \int \mathcal{D}J_1 \ldots \mathcal{D}J_n \langle \text{Tr} \left[ \hat{\phi}_1 \ldots \hat{\phi}_n \hat{\phi}_x \right] \rangle 
$$

$$
= \langle \hat{\phi}_x \rangle - \int d^4 y \, D^{1a}(x,y) j_{a,y} + \sum_{n=3}^{\infty} \frac{i^n}{n!} \int d^4 y_1 \ldots d^4 y_n \, \prod_{i} (j_{1,i} + j_{2,i}) \kappa(1, \ldots, n, x) . \quad (52)
$$

This equation contains the boundary condition for the classical field $\phi^c$. Its is also obtained by application of a linked cluster theorem to the perturbation expansion, i.e., when evaluating the perturbation series for the classical field amplitude by hand considering only contributions from connected diagrams.

Furthermore, it is obvious that it also approaches the Kubo-Martin-Schwinger (KMS) boundary condition (periodicity in the imaginary time direction) in the limit of zero cumulants, because it is then equivalent to eq. (46).

**VI. CONCLUSION**

With the present paper we achieved two goals. First of all we have extended the concept of diagonalized matrix valued propagators into the path integral formulation of quantum field theory. We were able to show, how to construct a simple perturbative expansion involving only retarded and advanced Green functions. This diagonalization procedure exploits a thermal Bogoliubov symmetry of the system \[9\]. The presence of this symmetry allows even simpler thermal Feynman rules when switching to a lower dimensional representation of the symplectic group \[10\].

The diagonalization of the action integral amounts to a factorization of the generating functional for Green functions. Our result therefore includes the one of ref. \[7\], but is more general since we have achieved the factorization also for the full two-point function.

The second major goal we have achieved with the present paper is the inclusion of initial correlations into the path integral framework. This might be a future asset for two very different reasons. On one hand it allows to obtain a perturbative expansion also for truly non-equilibrium systems, where the boundary conditions for particle propagation are fuzzy at best. To this end one may use the results of section 4, where the correlations were introduced via the initial state Wightman functions. In particular, one may think of a practical application to transport theory, where the perturbative treatment only works for
some time. Thereafter one has to requantize the system with new degrees of freedom, e.g.,
with new quasi-particles. For the next time step then the correlations of the initial state
play the role of additional vertices [11].

On the other hand, the correlations were related to a cumulant expansion of the action
integral [19]. In this formulation, as presented in the last section of this paper, we were able
to write down the integral equation fulfilled by the classical field amplitude. It is this integral
equation which proves the close relationship between initial correlations and the boundary
condition in time that one has to implement in quantum field theory for non-equilibrium
states.

We have furthermore proven, that the path integral for quantum fields in non-equilibrium
states does not factorize into pieces on the upper and lower Keldysh contour.
REFERENCES

[1] Quark Matter 95 Proceedings, Nucl. Phys. A590, 3c (1995); Quark Matter 93 Proceedings, Nucl. Phys. A566, 1c (1994)
[2] D. Boyanovsky, H. J. de Vega and R. Holman, in Advances in Astrofundamental Physics, Erice Chalonge Course, N. Sánchez and A. Zichichi Editors, World Scientific, 1995.
[3] R. Kubo, J.Phys.Soc. Japan 12 (1957) 570;
   C.Martin and J.Schwinger, Phys.Rev. 115 (1959) 1342
[4] E.Calzetta and B.L.Hu, Phys.Rev. D37 (1988) 2878
[5] R.L.Kobes and G.W.Semenoff, Nucl.Phys. B260 (1985) 714 and
   Nucl.Phys. B272 (1986) 329
[6] P.Aurenche and T.Becherrawy, Nucl.Phys. B379 (1992) 259
[7] T.S.Evans and D.A.Steer, Wick’s Theorem at Finite Temperature,
   Imperial/TP/95-96/18; hep-ph/9601268
[8] T.S.Evans, Nucl.Phys. B374 (1992) 340
[9] P.A.Henning and H.Umezawa, Nucl.Phys. B417 (1994) 463 and
   Phys.Lett. B303 (1993) 209
[10] P.A.Henning, Phys.Rep. 253 (1995) 235 – 380
[11] P.A.Henning, Nucl.Phys. B337 (1990) 547
[12] R.Fauser and H.H.Wolter, Nucl.Phys. A584 (1995) 604
[13] J.Schwinger, J.Math.Phys. 2 (1961) 407;
   L.V.Keldysh, Zh.Exsp.Teor.Fiz. 47 (1964) 1515 and JETP 20 (1965) 1018
[14] H.Umezawa,
   Advanced Field Theory: Micro, Macro and Thermal Physics
   (American Institute of Physics, 1993)
[15] N.P.Landsman and Ch.G.van Weert, Phys.Rep. 145 (1987) 141
[16] C.Itzykson and J.B.Zuber,
   Quantum Field Theory (McGraw-Hill, New York 1980)
[17] S.Fujita, J.Phys.Soc. Japan 26 (1969) 585 and
   J.Phys.Soc. Japan 27 (1969) 1096;
   A.G.Hall, J.Phys. A8 (1975) 214 and Physica A 80 (1975) 369
[18] P.Danielewicz, Ann.Phys. 152 (1984) 239 and 305
[19] R.Fauser and H.H.Wolter, Nucl.Phys. A (1996) in press
[20] P.A.Henning, C.Höbling, M.Blasone and L.Razumov,
   Act.Phys. Hungarica, New Series “Heavy Ion Physics”
   Vol. 1 In memoriam of E.Wigner (1995) 249
FIG. 1. Time path for the action integral entering the generating functional.