Wick Theorem for General Initial States

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We present a compact and simplified proof of a generalized Wick theorem to calculate the Green’s function of bosonic and fermionic systems in an arbitrary initial state. It is shown that the decomposition of the non-interacting \(n\)-particle Green’s function is equivalent to solving a boundary problem for the Martin-Schwinger hierarchy; for non-correlated initial states a one-line proof of the standard Wick theorem is given. Our result leads to new self-energy diagrams and an elegant relation with those of the imaginary-time formalism is derived. The theorem is easy to use and can be combined with any ground-state numerical technique to calculate time-dependent properties.

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I. INTRODUCTION

The theory of Green’s functions is probably the most powerful and versatile formalism in physics. Due to its generality it has found widespread applications in any branch of physics dealing with many-particle systems such as in nuclear physics, condensed matter physics and atomic and molecular physics. The key of its success lies in the possibility of expanding the dressed (interacting) \(n\)-particle Green’s function \(G_n\) in terms of the bare (non-interacting) Green’s functions \(g_m, m \geq n\), which are then reduced to an (anti)symmetrized product of \(g_1\) by means of the Wick theorem.\textsuperscript{1} In his memorable talk in 1948 Feynman showed how to represent the cumbersome Wick expansion in terms of physical insightful diagrams, and since then the Feynman diagrams became an invaluable tool in many areas of physics.

The standard Green’s function formalism (GFF) is, however, applicable to non-degenerate systems initially in their ground state and cannot be straightforwardly applied to systems with more general initial states or to systems with degenerate ground states. This leaves out modern fields of research like, e.g., non-equilibrium phase transitions,\textsuperscript{2} relaxation dynamics of ultracold gases,\textsuperscript{3} response of nanoscale systems in non-equilibrium steady-states,\textsuperscript{4} optimal control theory,\textsuperscript{5} etc. The correct description of initial correlations is obviously crucial for the short-time dynamics of general quantum systems such as in transient dynamics in quantum transport\textsuperscript{4,6} or in the study of atoms and molecules in external laser fields.\textsuperscript{7,8} In the case of finite systems it is clear that initial correlations also affect the long-time dynamics due to the presence of discrete quantum numbers. However, also in extended systems initial correlations can have infinite memory when the underlying Hamiltonian is integrable. This has, for instance, recently been demonstrated for interaction quenches\textsuperscript{9-14,16} and quantum transport\textsuperscript{15} in Luttinger liquids. Another case in which the standard GFF is problematic, even for equilibrium properties, is that of systems with degenerate ground states such as in open shell atoms or molecules. These systems are ubiquitous in quantum chemistry but the standard Wick theorem can only deal with the highest spin- or angular momentum component of a multiplet.\textsuperscript{17} There is therefore a clear need to go beyond the standard GFF.

In 1975 Hall\textsuperscript{18} used the textbook expansion of time-ordered products of operators into normal-ordered products and contractions to extend the Wick theorem to arbitrary initial states. Although the general structure is outlined there, the calculations of the various prefactors is very laborious as it requires the explicit determination of the sign of all possible permutations of the \(2m\) indices of the \(g_m\)’s. Further progress was made in the classic review of Danielewicz\textsuperscript{19} in which it was shown that one can deal with arbitrary initial states by introduction of an extended Keldysh contour with an additional imaginary time track on which the initial density matrix is represented as the exponential of an, in general, \(n\)-body operator. This was worked out further in detail by Wagner\textsuperscript{20} who derived the Feynman rules for the Green’s function involving diagrams with arbitrary \(n\)-body correlators. Later the approach was used by Mozorov and Röpke\textsuperscript{21} to derive quantum kinetic equations with arbitrary initial correlations. Furthermore Bonitz and co-workers have presented alternative derivations of the equations of motion of the non-equilibrium Green’s functions with arbitrary initial correlations using functional derivative techniques and applied them to study the decay of initial correlations in an electron gas.\textsuperscript{22} Recent work has further explored how an initial density matrix on the extended Keldysh contour can be related to diagrammatic expansions on the standard Keldysh contour.\textsuperscript{23}

The aim of the present work is to extend these developments in three different ways. First of all, we recognize that the generalized Wick theorem is simply the solution of the coupled system of differential equations for the \(g_m\)’s, the so called Martin-Schwinger hierarchy (MSH),\textsuperscript{24} with proper boundary conditions. This completely avoids the introduction of normal-ordered products or contractions and therefore greatly simplifies the
mathematics. In particular the standard Wick theorem follows as a one-line proof. Secondly, our reformulation based on an initial value problem allows us to prove that the generalized Wick expansion has a form identical to that of a Laplace expansion for permanents/determinants (for bosons/fermions). Consequently, the calculation of the various prefactors is both explicit and greatly simplified. We provide a systematic way to express the $g_{mn}$ in terms of $g_1$ and of the initial $k$-particle density matrices, $k \leq m$. The latter encode all the necessary information on the initial state and are completely determined by it. When the initial state is a permanent/determinant of a single particle state the $g_{mn}$ is expressed solely in terms of the $g_1$ (standard Wick theorem). Novel terms, instead, appear for initially correlated or entangled states. Such terms have a simple diagrammatic representation and are easier to evaluate if compared to standard diagrams. Thirdly, we discuss the relation between GFF based on the generalized Wick theorem and GFF as formulated on the extended Keldysh contour. These two approaches are complementary: the former requires the knowledge of the initial state while the latter requires the knowledge of the Hamiltonian with such initial state as the ground state. Clearly the convenience of using one approach or the other depends on the information at hand. We present a straightforward proof of the existence of a Dyson equation for general initial states and derive an exact mathematical relation between its self-energy and the self-energy of GFF on the extended Keldysh contour.

II. THE STANDARD GREEN’S FUNCTION FORMALISM

Let us briefly review under which circumstances the Wick theorem can be used to calculate the $n$-particle Green’s function $G_n$. Consider a system in the state $|\Psi\rangle$ at time $t_0$ and evolving according to the time-dependent Schrödinger equation with Hamiltonian $H(t)$. At this stage the state $|\Psi\rangle$ is a general many-body state and does not have to be the ground state of $H(t_0)$. We write

$$\hat{H}(t) = \hat{H}_0(t) + \hat{W}(t),$$

(1)

where

$$\hat{H}_0(t) = \int dx \hat{\psi}^\dagger(x)h(x,t)\hat{\psi}(x)$$

(2)

is quadratic in the field operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$ (here $x$ is a one-body quantum number like, e.g., the position-spin coordinate); this decomposition is arbitrary as $\hat{H}_0(t)$ can be any one-body operator. The remaining term $\hat{W}(t)$ will often be a two-body operator describing interactions between the particles, but can in fact be a general $n$-body operator with any time-dependence. The basic quantities of the GFF are the $n$-th particle Green’s functions

$$G_n(1\ldots n; 1'\ldots n') = \frac{1}{i^n}\langle \psi| T \left\{ \hat{\psi}_H(1)\ldots \hat{\psi}_H(n)\hat{\psi}_H^\dagger(n')\ldots \hat{\psi}_H^\dagger(1') \right\} |\psi\rangle,$$

(3)

where $T$ is the time-ordering operator, the subscript “$H$” denotes the Heisenberg picture and the short-hand notation $1 = (x_1, t_1)$, $1' = (x_1', t_1')$ etc. has been introduced. The $n$-body Green’s function gives a complete description of $n$-body correlations in a many-particle system. If we write the evolution operator as $\hat{U}(t, t_0) = \hat{U}_0(t, t_0)\hat{F}(t, t_0)$, where $\hat{U}_0$ is the non-interacting evolution operator, then $\hat{F}$ is the evolution operator in the interaction picture and fulfills

$$\frac{d}{dt}\hat{F}(t, t') = \hat{W}_I(t)\hat{F}(t, t')$$

(4)

with boundary condition $\hat{F}(t, t) = 1$ (the subscript “$I$” denotes the interaction picture). Consequently, we can rewrite $G_n$ (omitting its arguments) as

$$G_n = \frac{1}{i^n}\langle \psi| \hat{F}(t_0, \infty) T \left\{ e^{i\int_{t_0}^{\infty} dt'\hat{W}_I(t')}\hat{\psi}_I(1)\ldots \hat{\psi}_I(n) \times \hat{\psi}_I^\dagger(n')\ldots \hat{\psi}_I^\dagger(1') \right\} \hat{F}(-\infty, t_0)|\psi\rangle$$

(5)

The Wick theorem applies to the $g_{mn}$’s, i.e., the time-ordered product of field operators in the interaction picture averaged over a non-interacting state $|\Phi_0\rangle$. Thus to express $G_n$ in terms of the $g_{mn}$’s Eq. (5) needs to be further manipulated. Let us choose $|\Phi_0\rangle$ as the ground state of $\hat{H}_0 = \hat{H}_0(t_0)$ and construct the Hamiltonian

$$\hat{H}^M = \hat{H}_0 + \hat{W}^M$$

(6)

with ground state $|\Psi\rangle$. According to the Gell-Mann and Low theorem\textsuperscript{26,27} the state $|\Psi\rangle$ (for a more mathematical discussion on the precise conditions see Refs. 28, 29) can be reached from $|\Phi_0\rangle$ by adiabatically turning on the interaction $W^M$. Then,

$$|\Psi\rangle = e^{i\eta}\hat{F}^M(t_0, -\infty)|\Phi_0\rangle,$$

(7)

where $\hat{F}^M$ fulfills equation (4) with $\hat{W} \rightarrow \hat{W}^M e^{-\eta(t-t_0)}$ and $\eta$ an infinitesimal positive constant. Equation (7) also implies that we can reach the state $|\Psi\rangle$ (up to a phase factor\textsuperscript{26,27}) with a backward propagation in time and hence

$$|\Psi\rangle = e^{i\eta}\hat{F}^M(t_0, \infty)|\Phi_0\rangle,$$

(8)

Exploiting these results the Green’s function $G_n$ in equation (5) takes the form

$$G_n = \frac{e^{-i\eta}}{i^n}\langle \Phi_0^+| T \left\{ e^{-i\int_{t_0}^{\infty} dt'\hat{W}_I(t')}\hat{\psi}_I(1)\ldots \hat{\psi}_I(n) \times \hat{\psi}_I^\dagger(n')\ldots \hat{\psi}_I^\dagger(1') \right\} |\Phi_0^-\rangle,$$

(9)
In most textbooks the interaction $\hat{W}(t) = \hat{W}$ is time-independent and $|\Psi\rangle = |\Psi_0\rangle$ is the ground state of $\hat{H} = \hat{H}(t_0)$; then $|\Phi_H^+\rangle = |\Phi_0\rangle$ since $\hat{W}^M = \hat{W}$. In this case we can expand the exponent in equation (9) in powers of $\hat{W}_I$, express $G_n$ in terms of the noninteracting $m$-particle Green’s functions $g_m$’s with $m \geq n$ and turn the $g_m$’s in terms of $g_1$ using the Wick theorem. To the contrary if the interaction is time-dependent and/or $|\Psi\rangle \neq |\Psi_0\rangle$, the standard Wick theorem is of no use to calculate $G_n$. Our aim is therefore to lift these restrictions in a generalized version of Wick’s theorem which can be applied to general initial states for both equilibrium and non-equilibrium systems.

III. GENERALIZED WICK THEOREM

Reading the time-arguments in equation (5) from right to left it is natural to design the Keldysh contour$^{31}$ $\gamma$ of Fig. 1 and define the generalized Green’s function

$$G_n = \frac{1}{i^n} \langle \Psi | T \{ e^{-\int_{t_f}^{t_i} d\tau \hat{W}_I(\tau) \hat{\psi}(1) \cdots \hat{\psi}(n) \} \hat{\psi}^\dagger(n') \cdots \hat{\psi}^\dagger(1') \} | \Psi \rangle,$$

(11)

with $T_c$ the contour-ordering operator and $1 = (x_1, z_1)$, $1' = (x_1', z_1')$ etc. collective indices with times $z$’s on the contour. The new $G_n$ coincides with the time-ordered one of Eq. (5) when all contour-times lie on the upper branch. Expanding the exponent in powers of $\hat{W}_I$, the Keldysh $G_n$ can be written as the sum of integrals over non-interacting Keldysh Green’s functions

$$g_m(1 \ldots m; 1' \ldots m')$$

$$= \frac{1}{i^m} \langle \Psi | T \{ \hat{\psi}(1) \cdots \hat{\psi}(m) \hat{\psi}^\dagger(1') \cdots \hat{\psi}^\dagger(m') \} | \Psi \rangle,$$

(12)

where $m > n$. For these functions a generalized Wick theorem will now be derived.

From the equations of motion of the field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$ it follows immediately that the $g_m$ in Eq. (12) fulfill the non-interacting MSH$^{24}$

$$[i\partial_{z_k} - h(k)] g_m = \sum_{j=1}^{m} (\pm)^{k+j} \delta(k, j') g_{m-1}(\bar{k}, \bar{j'}),$$

$$[i\partial_{z_j} - h(j')] g_m = \sum_{k=1}^{m} (\pm)^{k+j} \delta(k, j') g_{m-1}(\bar{k}, \bar{j'}),$$

(13)

where $\delta(k, j') = \delta(x_k, x'_j)(\delta(z_k, z'_j)$, $h$ is the one-body Hamiltonian of Eq. (2) and the upper/lower sign refers to bosons/fermions. Here and in the following the symbol $\cdots$ over the indices specifies the missing indices of $g_m$. Thus for instance $g_3(1; 2) = g_3(23; 1')$. It is worth noting that Eqs. (13) constitute a system of recursive relations since $g_m$ can be calculated from the sole knowledge of $g_{m-1}$. The solution for $g_m$ depends, of course, on the boundary conditions that we impose. The boundary conditions for $g_m$ follow directly from its definition (12)

$$\Gamma_m(x_1 \ldots x_m; x'_1 \ldots x'_m) = (\pm i)^m \lim_{z_k, z'_j \to t_i} g_m(1, \ldots m; 1', \ldots m')$$

(14)

with $z_1 < \ldots < z_m < z'_m < \ldots < z'_1$ (from now on $\lim_{z_k, z'_j \to t_i}$ will always be taken in such order) where $t_i$ is the initial time of Fig. 1 and

$$\Gamma_m(x_1 \ldots x_m; x'_1 \ldots x'_m)$$

$$= \langle \Psi | \hat{\psi}(1') \cdots \hat{\psi}(m') \hat{\psi}(x_m) \cdots \hat{\psi}(x_1) | \Psi \rangle$$

(15)

is the initial $m$-body density matrix describing the initial $m$-body correlations. One can readily verify by expanding along a row or a column that the permanent/determinant

$$g_m(1 \ldots m; 1' \ldots m') = \begin{vmatrix} g(1; 1') & \ldots & g(1; m') \\ \vdots & \ddots & \vdots \\ g(m; 1') & \ldots & g(m; m') \end{vmatrix}_{\pm}$$

$$= |g|_m$$

(16)

de of one-particle Green’s functions $g \equiv g_1$ is a solution of Eq. (13). However, in general the solution (16) will not satisfy the boundary conditions (14). This will only happen when the $m$-particle density matrix $\Gamma_m$ of equation (15) is averaged over a non-interacting state $|\Psi\rangle = |\Phi_0\rangle$. Note that this result constitutes a one-line proof of the standard Wick theorem which, in our formulation, amounts to solving a boundary problem for the MSH.

For arbitrary initial states $|\Psi\rangle$ the particular solution (16) must be supplied with the additional solution $g_m$ of the homogeneous equations

$$[i\partial_{z_k} - h(k)] g_m = 0$$

(17)

and its adjoint to satisfy the boundary conditions. For illustrative purposes we first consider the examples of $g_2$
and \( g_3 \). The most general solution of Eqs. (13) for \( m = 2 \) reads

\[
g_2 = |g|_2 + \tilde{g}_2. \tag{18}
\]

Being a homogeneous solution, \( \tilde{g}_2 = g_2 - |g|_2 \) is not discontinuous when a contour-time \( z_k \) passes through \( z'_1 \), which implies that the discontinuity of \( g_2 \) is compensated by an identical discontinuity in \( |g|_2 \). The initial value of \( \tilde{g}_2 \) is fixed by the boundary conditions (14) for \( g_2 \) and \( g \) and reads

\[
\lim_{z_k, z'_1 \to t_i} \tilde{g}_2(12; 1'2') = (\mp i)^2 C_2(x_1x_2; x'_1x'_2) \tag{19}
\]

with the correlation function

\[
C_2 \equiv \Gamma_2 - |\Gamma|_2 \tag{20}
\]

and \( \Gamma \equiv \Gamma_1 \) the one-particle density matrix. The limit in Eq. (19) is now independent of the time-ordering in which the limit is taken. The same applies to all functions \( \tilde{g}_m \) defined by Eq. (17), i.e., their limit is defined independent of the time-ordering taken. We can express \( \tilde{g}_2 \) in terms of \( g \) and \( C_2 \) as follows. The spectral function on the contour

\[
A(1; 1') \equiv i \left[ g^c(1; 1') - g^c(1; 1) \right] = (\Psi|\hat{\psi}_1(1)\hat{\psi}_1(1')|\psi) \tag{21}
\]

satisfies the homogeneous equations

\[
[i\partial_{z_1} - h(1)]A(1; 1') = [-i\partial_{z_1} - h(1')]A(1; 1') = 0, \tag{22}
\]

(hence it has no discontinuity when \( z_1 \) passes through \( z'_1 \)) and equals \( \delta(x_1, x_2) \) for \( z_1 = z'_1 \). If we define

\[
\delta_-(z) \equiv \delta(z, t_i) - \delta(z, t_f), \tag{23}
\]

where \( t_i \) and \( t_f \) are the end-points of the Keldysh contour of Fig. 1, we can write

\[
A(1, x'_1 t_i) = i \left[ g(1, x'_1 t_i) - g(1, x'_2 t_f) \right] = i \int_d \delta g(1, x'_1 \delta z) \delta_-(\delta) \tag{24}
\]

and similarly \(^3\)

\[
A(x_1 t_i, 1') = -i \int_d \delta g(x_1 \delta \bar{z}) \delta_-(\bar{z}) \tag{25}
\]

Therefore, introducing the time-local correlation function on the contour

\[
C_2(12; 1'2') \equiv \delta_-(z_1)\delta_-(z_2) \times C_2(x_1x_2; x'_1x'_2)\delta_-(z'_1)\delta_-(z'_2) \tag{26}
\]

it is immediate to realize that

\[
\tilde{g}_2(12; 1'2') = (\mp i)^2 \int d\bar{t}d\bar{z}d\bar{y}d\bar{z} g(1; \bar{1}) g(2; \bar{2}) \times C_2(\bar{1}2; \bar{1'}\bar{2'}) g(\bar{1'}; 1') g(\bar{2'}; 2') \tag{27}
\]

provides an explicit solution to the initial value problem for \( g_2 \), i.e., it satisfies Eqs. (17) and (19). Here and in the following \( \int_\gamma d\bar{t} = \int dx_1 \int dz_1 \). The diagrammatic representation of the generalized Wick theorem for \( g_2 \) is displayed in Fig. 2(a); it is worth noting that for a noninteracting initial state \( C_2 = 0 \) and the standard Wick theorem is recovered.

Inserting \( g_2 = |g|_2 + \tilde{g}_2 \) into Eq. (13) we find in a similar way that the general solution for \( g_3 \) is

\[
g_3 = |g|_3 + \sum_{k,j=1}^3 (\pm)^k+j \langle k; j' \rangle \tilde{g}_2(k; j') + \tilde{g}_3. \tag{28}
\]

where the homogeneous solution \( \tilde{g}_3 \) is fixed by the boundary conditions for \( g_3, g_2 \) and \( g \):

\[
\lim_{z_k, z'_1 \to t_i} \tilde{g}_3(123; 1'2'3') = (\mp i)^3 C_3(x_1x_2x_3; x'_1x'_2x'_3), \tag{29}
\]

with

\[
C_3 = \Gamma_3 - \sum_{k,j=1}^3 (\pm)^k+j \Gamma(x_k; x'_j)C_2(\bar{x}_k; \bar{x}'_j) - |\Gamma|_3. \tag{30}
\]

Using the (anti)-symmetry of \( \tilde{g}_2 \) and \( \tilde{g}_3 \) one can readily check that \( g_3 \) in Eq. (28) is properly (anti)-symmetric in the primed and the unprimed variables. The second term in Eq. (28) has exactly the same structure of a generalized Laplace expansion for permanents/determinants. As we shall see this is a general feature of all terms of the
expansion of \( g_m \). Similarly to the two-particle case we can define the time-local density matrix function on the contour and write

\[
\tilde{g}_3(123;1'2'3') = (\mp i)^3 \int \prod_{k=1}^{3} dk \, g(k; \bar{k}) \times C_3(123;1'2'3') \prod_{j=1}^{3} dj \, g(j'; j').
\]

The diagrammatic representation of the generalized Wick theorem for \( g_3 \) is displayed in Fig. 2(b). For instance, the second diagram of the last line in Fig. 2(b) gives the contribution \((\pm)^{3+2} g(3,2')\tilde{g}_3(12;1'3')\) to Eq. (28). Note that the sign of a diagram is given by \((\pm)^{n_c}\) where \(n_c\) is the number of crossings of Green’s function lines. Alternatively it is given by \((\pm)^{n_c}\) where \(n_c\) is the number of transpositions needed to reorder the labels \(k\bar{k}\) and \(j'j''\) in Eq. (28) to 123 and 1'2'3', as is readily checked for our example.

At this point it is not difficult to guess the solution for \( g_m \). Let us introduce the collective ordered indices \( K = (k_1 \ldots k_l) \), with \( k_1 < \ldots < k_l \) and \( X_K = (x_{k_1} \ldots x_{k_l}) \), and define

\[
C_l(K; J') = \left( \prod_{\alpha=1}^{l} \delta_-(z_{\alpha_k}) \right) C_l(X_K; X'_j) \left( \prod_{\beta=1}^{l} \delta_-(z'_{\beta_j}) \right)
\]

where \( C_l(X_K; X'_j) \) is defined by the recursive relations

\[
C_l(X_K; X'_j) = \Gamma_l(X_K; X'_j) - \sum_{n=1}^{l-2} \sum_{PQ} (\pm)^{|P+Q|} \times |\Gamma|_n(X_P; X'_Q) C_{n-l}(\bar{X}_P; \bar{X}'_Q) - |\Gamma|_1(X_K; X'_j)
\]

(32)

with \( C_2 \equiv \Gamma_2 - |\Gamma|_2 \). In equation (32) the sum runs over all ordered sequences \( Q = (q_1 \ldots q_n) \), \( P = (p_1 \ldots p_n) \) with indices between 1 and \( l \), and the sign is determined by

\[
|P+Q| = \sum_{\alpha=1}^{n} (q_\alpha + p_\alpha).
\]

(33)

For example, let \( l = 5 \) and \( n = 2 \) with \( P = (1,4) \) and \( Q = (2,4) \) and hence \( \bar{P} = (2,1) \) and \( \bar{Q} = (1,3) \). We then have \( X_P = (x_1, x_4) \), \( X'_Q = (x'_2, x'_4) \) and the complementary collective coordinates \( \bar{X}_P = (x_2, x_3, x_5) \), \( \bar{X}'_Q = (x'_1, x'_3, x'_5) \). The corresponding term for \( C_5 \) under the summation sign in (32) is given by

\[
(\pm)^{1+4+2+4} |\Gamma|_2(x_1x_4; x'_2x'_4) C_3(x_2x_3x_5; x'_1x'_3x'_5)
\]

\[
= \pm \frac{\Gamma(x_1; x'_2)}{\Gamma(x_4; x'_2)} \frac{\Gamma(x_1; x'_4)}{\Gamma(x_4; x'_4)} C_3(x_2x_3x_5; x'_1x'_3x'_5).
\]

We will now prove the generalized Wick theorem:

**Theorem:** The solution of the MSH of Eqs. (13) with the boundary conditions (14) is

\[
g_m = |g|_m + \sum_{l=1}^{m-2} g_m^{(l)} + \tilde{g}_m
\]

(35)

where we defined

\[
g_m^{(l)}(K; J') \equiv \sum_{PQ} (\pm)^{|P+Q|} |g|_l(P; Q') \tilde{g}_{m-l}(\bar{P}; \bar{Q}')
\]

(36)

and, in complete analogy with \( \tilde{g}_2 \) and \( \tilde{g}_3 \),

\[
\tilde{g}_l(K; J') = (\mp i)^l \int \prod_{\gamma=1}^{l} dk \, g(k; \bar{k}) \times C_l(K; J') \prod_{\beta=1}^{l} dj \, g(j'; j').
\]

(37)

Equations (35)-(37) give a complete solution of the initial value problem for the MSH for both equilibrium and nonequilibrium systems. The only input is the initial m-body correlations incorporated in \( \Gamma_m \). Let us make some additional remarks. The function \( \tilde{g}_m^{(l)} \) is the sum of all possible diagrams with a single correlation block \( C_{m-l} \) in which \( m-l \) Green’s function lines enter and leave, multiplied by \( l \) separate Green’s function lines. For instance, for \( m = 5 \) and \( l = 2 \) the term of the sum in Eq. (35) with \( P = (1,4) \) and \( Q = (2,4) \) has the diagrammatic representation in Fig. 3 and corresponds to Eq. (34). The sign of the diagrams is \((\pm)^{n_c}\) where \( n_c \) equals the number of crossings (in Fig. 3 \( n_c = 3 \) for the first diagram and \( n_c = 6 \) for the second diagram). Although the general structure of \( g_m \) was outlined in Refs. 18,19 our theorem contains a precise statement on how to construct it. When \( \Psi \) is a non-interacting product state the recursive relations in Eq. (32) yield \( C_l = 0 \), hence \( \tilde{g}_l = 0 \) and consequently \( g_m = |g|_m \), i.e., we recover the standard Wick theorem, in agreement with the previous discussion. The generalized Wick theorem superseeds all common limitations of the standard GFF, i.e., the non-degeneracy of the ground state, the assumptions of the Gell-Mann and Low theorem and the requirement of a time-independent Hamiltonian for times \( t \to \pm \infty \). Finally we would like to point out that Eq. (35) has the structure of the permanant/determinant of the sum of
two matrices $A$ and $B$. Indeed according to the Laplace formula

$$|A + B|_m = |A|_m + \sum_{l=1}^{m-1} \sum_{PQ} |\pm|^{P+Q} |A_{ij}(P; Q)|B_{m-l}(\bar{P}; \bar{Q}) + |B|_m$$

(38)

where $|A|_m(P; Q)$ is the permanent/determinant of the $l \times l$ matrix obtained with the rows $P$ and the columns $Q$ of the matrix $A$. In the special case $l = m$ we have $P = Q = (1 \ldots m)$ and hence $|A|_m(P; Q) = |A|_m$. The same notation has been used for the matrix $B$. With the identification $A_{jk} = g(k; j')$ and $B_{m-l}(\bar{P}; \bar{Q}) = \bar{g}_{m-l}(\bar{P}; \bar{Q})$ for $l = 1 \ldots m - 2$ and the definition $g_1 \equiv 0$ Eqs. (35) and (38) become identical. We can thus symbolically write the generalized Wick theorem as

$$g_m = |g + \bar{g}|_m$$

(39)

whose precise meaning is given by Eq. (35).

- Proof: The proof consists of two steps. We first prove that $g_m$ satisfies the MSH. For this purpose it is enough to prove the MSH for each $g^{(l)}_m$ since, as already noticed, the MSH is obviously satisfied by $|g|_m$. We will consider only the first of equations (13) as the same reasoning applies to the second. If we act with $(i\delta_{zk} - h(k))$ on a particular diagram of $g^{(l)}_m$ the result is zero if $k$ is an ingoing line to a $C_l$-block. This follows immediately from the definition (37) and Eq. (22). To the contrary, if the diagram contains a free line $g(k; j')$ the result is $(\pm)^{k+j} \delta(k, j') \times [\text{a diagram for } \bar{g}_{m-1}(k; j')]$. Thus, $(i\delta_{zk} - h(k)) \sum [\text{all diagrams in } g^{(l)}_m] \text{ containing } g(k; j')] = (\pm)^{k+j} \delta(k, j') \bar{g}^{(l)}_{m-1}(k; j')$. The MSH for $g^{(l)}_m$ follows from this relation when summing over all $j$. Taking into account that $(i\delta_{zk} - h(k)) \bar{g}_m = 0$ we conclude that $g_m$ satisfies the MSH.

Next we prove that $g_m$ has the correct boundary conditions (14). In Eq. (35) we take the limit $z_k \to t_i$. Since $|g|_l \to (\mp) |\Gamma|_l$ and $\bar{g}_{m-l} \to (\mp)^{m-l} |C_m-t|_l$ we find

$$\lim_{z_k \to t_i} (\pm)^m g_m = |\Gamma|_m + \sum_{l=1}^{m-2} \sum_{PQ} (\pm)^{P+Q} |\Gamma|_l |C_m-t+C_m.$$  

(40)

Writing the last term $C_m$ as in equation (32) we see by inspection that all terms of the sum cancel out and the r.h.s. reduces to $\Gamma_m$. We therefore exactly satisfy the boundary condition (14). This concludes the proof.}

IV. GENERALIZED GREEN’S FUNCTION FORMALISM

With our generalized Wick theorem we can now directly expand the one-particle Green’s function $G \equiv G_1$ in powers of the interaction $W_I$, see Eq. (11). In what follows we restrict the analysis to interactions which are represented by two-body operators like, e.g., the Coulomb interaction. From Eq. (11) the interacting Green’s function is then given by

$$G(a, b) = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{i}{2} \int_{\gamma} w(1, 1') \ldots w(k, k')$$

(41)

$$\times g_{2k+1}(a, 1, 1' \ldots k, k'; b, 1^+, 1^+ \ldots k^+, k^+)$$

in which $w(j, j')$ is the two-body interaction and we integrate over all space-time coordinates $j$ and $j'$ for $j = 1 \ldots k$. By inserting Eq. (35) into Eq. (41) we obtain a diagrammatic expansion of the interacting Green’s function. For example, to first order in the interaction we only need the $g_3$ of Fig. 2. If we then take into account that the disconnected pieces vanish we find that to first order in the interaction the Green’s function is given by the connected diagrams displayed in Fig. 4. In general the expansion of $G$ in powers of $W_I$ leads to a diagrammatic series which starts end ends with a $g$-line. The kernel of this expansion is therefore the reducible self-energy which we denote by $\Sigma^{(r)}$. In the case of general initial states the $\Sigma^{(r)}$-diagrams contain at most one correlation block and either begin and end with an interaction line (we call their sum $\Sigma^{(r)}$) or begin/end with an interaction line and end/begin with a correlation block (we call their sum left/right reducible self-energy $\Sigma^{(r)}_{L,R}$).19 This means that the general structure of the diagrammatic expansion is

$$G(1; 2) = g(1; 2) + \int_{\gamma} g(1; \bar{1}) \Sigma^{(r)}_{L}(1; 2) g(2; 2)$$

(42)

where $\Sigma^{(r)}_{tot} = \Sigma^{(r)} + \Sigma^{(r)}_{L} + \Sigma^{(r)}_{R}$ and34

$$\Sigma^{(r)}_{L}(1; 2) = \Sigma^{(r)}_{L}(1; x_2) \delta_-(z_2),$$

(43)

$$\Sigma^{(r)}_{R}(1; 2) = \delta_-(z_1) \Sigma^{(r)}_{R}(x_1; 2).$$

(44)

Thus the self-energy is modified by the addition of a left/right reducible self-energy which is non-zero only if its right/left time-parameter is one of the end-points of

\[ G = \begin{pmatrix} C_1 & \pm & \ldots & \pm & C_1 \\ \pm & C_1 & \pm & \ldots & \pm \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \pm & \pm & \ldots & C_1 & \pm \end{pmatrix} \]

FIG. 4: First-order expansion of $G$ for a two-body interaction. The last three diagrams vanish since both lines enter a $C_l$ block and hence the internal time-integration can be reduced to a point. This is a completely general feature.
V. RELATION TO THE IMAGINARY TIME
FORMALISM AND EXISTENCE OF A DYSON
EQUATION

We next discuss the relation between the above results and the imaginary-time formalism, and in doing so will also generalize some recent work by Garny and Müller. The average over the state $|\Psi\rangle$ can also be computed by tracing the field operators with $\tilde{\rho}(\beta) = e^{-\beta \hat{H}^M}/\text{Tr}[e^{-\beta \hat{H}^M}]$ where $\beta$ is a real positive number (inverse temperature) and then letting $\beta \to \infty$. We remind the reader that $\hat{H}^M$ is the Hamiltonian with $|\Psi\rangle$ as ground state, see Eq. (6), and can be a general $n$-body operator. This is discussed in more detail in Refs. 19–21. Then,

\[
G_n(1\ldots n; 1'\ldots n') = \frac{1}{i^n} \text{Tr}[e^{-\beta \hat{H}_0} T_{\gamma_e} \{e^{-i \int_{\gamma_e} dx \hat{W}_e(z)} \hat{\psi}_I(1) \ldots \hat{\psi}_I(n) \hat{\psi}_I^\dagger(n') \ldots \hat{\psi}_I^\dagger(1') \}] \text{Tr}[e^{-\beta \hat{H}^M}]
\]

(45)

where $\gamma_e$ is the extended Keldysh contour of Fig. 5 and $\hat{W}(z) = \hat{W}^M$ for $z$ on the imaginary track of the extended contour. These new Green’s functions coincide with the old ones when all contour-times lie on the original Keldysh contour $\gamma_e$. The advantage of this formulation is that the corresponding new non-interacting Green’s functions can be expanded using the standard Wick theorem, $g_{0,m} = |g_0|_m$, since both $g_{0,m}$ and $g_0$ obey the Kubo-Martin-Schwinger boundary conditions, i.e., they are periodic/antiperiodic in the contour-time arguments. Note that $g_{0,m} \neq g_m$: the former is averaged with $\rho_0(\beta) = e^{-\beta \hat{H}_0}/\text{Tr}[e^{-\beta \hat{H}_0}]$ while the latter with $\tilde{\rho}(\beta)$. The new Green’s function with both arguments on $\gamma$ obeys the equations of motion (integral over barred variables is understood)

\[
[i\partial_{z_1} - h(1)]G(1, 2) = \delta(1, 2) + \int_\gamma \Sigma_e(1, \bar{1})G(\bar{1}; 2)
\]

\[+ i \int_\beta \Sigma_e^\dagger(1, \bar{1})G'(\bar{1}; 2),
\]

(46)

and its adjoint, where $\Sigma_e$ is the standard self-energy, i.e., the same as in Wagner work, with internal integrals over all space and contour-times on $\gamma_e$. In Eq. (46) the symbol $\hat{\Sigma}$ specifies that the first contour argument lies on $\gamma$ and the second on the imaginary track; the opposite is specified by $\hat{\Sigma}$. We will now derive an elegant relation between $\Sigma_e$ and the reducible self-energy $\Sigma_{\text{tot}}$, relation which will be used to prove the existence of a Dyson equation on $\gamma$ for general initial states. From the Langreth rules on $\gamma_e$ we have

\[
G^\dagger(1, 2) = -i \int d\bar{x} G^M(1, \bar{x}t_0)G^A(\bar{x}t_0, 2)
\]

\[+ [G^M \ast \Sigma^\dagger, G^A](1, 2).
\]

(47)

In this equation $G^{R/A}(1, 2) = \pm \theta(\pm t_1 - t_2)[G^R(1, 2) - G^A(1, 2)]$ is the retarded/advanced Green’s function, $G^M$ is the Matsubara Green’s function with both arguments on the imaginary track, and we used the short-hand notation “*” for convolutions between $t_0$ and $t_0 - i\beta$ and “.” for convolutions between $t_0$ and $\infty$. Inserting this result into the last term of Eq. (46) and taking into account that for any function $f(x, t) = f(xt)$ it holds

\[
\int_\gamma f(\bar{1})G(\bar{1}; 2) = \int_{t_0}^{\infty} d\bar{x} d\bar{t} f(\bar{x}\bar{t})G^A(\bar{x}\bar{t}, 2),
\]

(48)

we find

\[
[i\partial_{z_1} - h(1)]G(1, 2) = \delta(1, 2)
\]

\[+ \left[\Sigma_e + \Sigma_e^\dagger \ast G^M \ast \Sigma_e^\dagger + \Sigma_e, L\right] \cdot G(1, 2),
\]

(49)

where

\[
\Sigma_e, L(1, 2) = -i[\Sigma_e^\dagger \ast G^M](1, x_2t_0)\delta_-(z_2).
\]

(50)

Similarly for the adjoint equation we have

\[
[-i\partial_{z_2} - h(2)]G(1, 2) = \delta(1, 2)
\]

\[+ \left[G \cdot \left(\Sigma_e + \Sigma_e^\dagger \ast G^M \ast \Sigma_e^\dagger + \Sigma_e, R\right)\right] (1, 2),
\]

(51)

the Keldysh contour. The diagrammatic expansion of these new self-energies is very similar to that of the standard GFF, as it is exemplified in Fig. 4. The only extra ingredient is the appearance of the $C_n$-blocks which describe the initial $m$-body correlations.
with
\[ \Sigma_{c,R}(1;2) = \delta_-(z_1) i [G^M \star \Sigma_1^L](x_1 t_0;2). \] (52)

Given the self-energy and the Green’s function with arguments on the imaginary track we can regard Eqs. (49) and (51) as the equations of motion for \( G \) with arguments on \( \gamma \). To integrate these equations we cannot use the non-interacting Green’s function \( g_0 \) which satisfies the Kubo-Martin-Schwinger relations as the point \( t_0 - i \beta \) does not belong to \( \gamma \). However we can use the non-interacting Green’s function \( g \) of Eq. (12) since it satisfies
\[ \lim_{z, z \to t^-} g(1;2) = \lim_{z, z \to t^-} G(1;2) = \Gamma(x_1;x_2). \] (53)

Thus if we define the total self-energy as
\[ \Sigma_{\text{tot}} = \Sigma_e + \Sigma_e \star G^M \star \Sigma_e + \Sigma_{e,L} + \Sigma_{e,R} \] (54)
we can write the following Dyson equation on \( \gamma \) (integral over barred variables is understood)
\[ G(1;2) = g(1;2) + \int_{\gamma} g(1;\bar{1}) \Sigma_{\text{tot}}(\bar{1};2) G(\bar{2},2). \] (55)

Comparing now this equation with (42) we deduce an important relation between the reducible self-energy \( \Sigma_{\text{tot}}^{(r)} \) written in terms of correlation blocks and the irreducible self-energy \( \Sigma_{\text{tot}} \) written in terms of integral over the imaginary track
\[ \Sigma_{\text{tot}}^{(r)} = \Sigma_{\text{tot}} + \Sigma_{\text{tot}} g \Sigma_{\text{tot}} + \Sigma_{\text{tot}} g \Sigma_{\text{tot}} g \Sigma_{\text{tot}} + \ldots \] (56)
This relation constitute a bridge between two different and complementary approaches [each built to optimize the nature (density matrix or Hamiltonian) of the initial information] and give a deep insight in the physics of initial correlations. Indeed we can now express \( \Sigma_{\text{tot}} \) in terms of \( \Sigma_{\text{tot}}^{(r)} \) to obtain an irreducible self-energy in terms of correlation blocks. From Eq. (56) we have
\[ \Sigma_{\text{tot}}^{(r)} = \Sigma_{\text{tot}} \frac{1}{1 - g \Sigma_{\text{tot}}} \] (57)
and hence
\[ \Sigma_{\text{tot}} = \Sigma_{\text{tot}}^{(r)} (1 - g \Sigma_{\text{tot}}) \]
\[ = \Sigma_{\text{tot}}^{(r)} - \Sigma_{\text{tot}}^{(r)} g \Sigma_{\text{tot}}^{(r)} + \Sigma_{\text{tot}}^{(r)} g \Sigma_{\text{tot}}^{(r)} g \Sigma_{\text{tot}}^{(r)} - \ldots \] (58)

Inserting this expansion into Eq. (55) we obtain a Dyson equation in which the irreducible self-energy depends only on \( g \) and correlation blocks.

VI. SOME APPLICATIONS AND CONCLUSIONS

The rules to expand the Green’s function around any initial state constitute a powerful theoretical tool and the range of applicability can be faster than we can imagine at present. Possible applications are in quantum chemistry where spin-degenerate ground-states are ubiquitous while the standard Wick theorem can only cope with the highest spin component. The generalized Wick theorem is not limited to determinantal states thereby permitting to resolve the spin-multiplet properties. This versatility can be used in the context of quantum entanglement as well. Another application is in the formalism of the rate equations which gives rise to negative time-dependent probabilities when the standard Wick theorem is applied to initially correlated states. Corrections with the \( C_i \)-blocks should result in an improved theory. The generalized Wick theorem also allows us to address the effect of integrability-breaking perturbations using the exact Green’s function of the integrable model. More generally the generalized Wick theorem can be combined with any ground-state numerical technique to calculate time-dependent properties. Indeed from the ground-state density matrix we can calculate the non-equilibrium Green’s function to any order in the interaction strength.

The practical implementation of the generalized Wick theorem is no more difficult than the standard Wick theorem. We expect that the generalized Wick theorem will be useful in a broad range of physical problems both in and out of equilibrium. We wish to conclude by observing that even though all derivations in this work pertain to Green’s functions defined as averages over an initial state the generalization to Green’s function defined as ensemble averages is straightforward and no extra complications arise.

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