Quantum-field-theoretical approach to phase-space techniques: Symmetric Wick theorem and multitime Wigner representation.

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In this work we present the formal background used to develop the methods used in earlier works to extend the truncated Wigner representation of quantum and atom optics in order to address multi-time problems. The truncated Wigner representation has proven to be of great practical use, especially in the numerical study of the quantum dynamics of Bose condensed gases. In these cases, it allows for the simulation of effects which are missed entirely by other approximations, such as the Gross-Pitaevskii equation, but does not suffer from the severe instabilities of more exact methods. The numerical treatment of interacting many-body quantum systems is an extremely difficult task, and the ability to extend the truncated Wigner beyond single-time situations adds another powerful technique to the available toolbox. This article gives the formal mathematics behind the development of our “time-Wigner ordering” which allows for the calculation of the multi-time averages which are required for such quantities as the Glauber correlation functions which are applicable to bosonic fields.

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I. INTRODUCTION

This paper is a formal corollary to the recent Ref. [1], where the truncated Wigner representation of quantum optics [2] was extended to multitime problems. (For a discussion of operator orderings, such as normal, time-normal and symmetric, we refer the reader to the classic treatise of Mandel and Wolf [3].) The goal of Ref. [1] was to develop a practical computational tool, while formal analyses were reduced to the bare necessities. In this paper we give proper justification to the formal techniques underlying Ref. [1]. The functional techniques used here are to a large extent borrowed from Vasil'ev [4]; they were first outlined in preprint [5]. However, in [5] a number of important results (notably, continuity of time-symmetrically ordered operator products) were overlooked.

Important for the putting the results of this paper in perspective is the connection between phase-space techniques and the so-called real-time quantum field theory (for details and references see [3]). According to [3], the Keldysh rotation underlying the latter is a generalisation of Weyl’s ordering to Heisenberg operators. This generalisation is nothing but the aforementioned time-symmetric ordering. This paper could thus equally be titled, “Phase space approach to real-time quantum field theory”.

For physical motivation and literature we refer the reader to the introduction to [1]. Here we only briefly touch upon the more recent developments. The truncated Wigner representation has found its main utility for the investigation and numerical modelling of Bose-Einstein condensates (BEC), where the presence of a significant third-order nonlinearity makes the exact positive-P method unstable except for very short times [7], although it is still also used in quantum optics. Over the last few years it has been used for an increasing number of investigations, with the most relevant mentioned in what follows.

The ability to include the effects of initial quantum states other than coherent was first shown numerically for trapped BEC molecular photoassociation in three papers by Olsen and Plimak [8], Olsen [9], and Olsen, Bradley, and Cavalcanti [10], using methods later published by Olsen and Bradley [11] to sample the required quantum states. Johnsson and Hope calculated the multimode quantum limits to the linewidth of an atom laser [12]. The quantum dynamics of superflows in a toroidal trapping geometry were treated by Jain et al. [13]. Ferris et al. [14] investigated dynamical instabilities of BEC at the band edge in one-dimensional optical lattices, while Hoffmann, Corney, and Drummond [15] made an attempt to combine the truncated Wigner and positive-P representations into a hybrid method for Bose fields. Corney et al. [16] used the truncated Wigner to simulate polarisation squeezing in optical fibres, a system which is mathematically analogous to BEC. The mode entanglement and Einstein-Podolsky paradox were numerically investigated in the process of degenerate four-wave mixing of BEC in an optical lattice by Olsen and Davis [17] and Ferris, Olsen, and Davis [18]. Also analysing BEC in an opti-
cal lattice, Shrestha, Javanainen, and Rusteokoski \[19\] looked at the quantum dynamics of instability-induced pulsations. Midgley et al. performed a comparison of the truncated Wigner with the exact positive-P representation and a Hartree-Fock-Bogoliubov approximate method for the simulation of molecular BEC dissociation \[20\], concluding that the truncated Wigner representation was the most useful in practical terms. This practical usefulness has been demonstrated in studies of BEC interferometry \[21\], domain formation in inhomogeneous ferromagnetic dipolar condensates \[22\], vortex unbinding following a quantum quench \[23\], a reverse Kibble-Zurek mechanism in two-dimensional superfluids \[24\], the quantum and thermal effects of dark solitons in one-dimensional Bose gases \[25\], the quantum dynamics of multi-well Bose-Hubbard models \[26\] \[27\], and analysis of a method to produce Einstein-Podolsky-Rosen states in two-well BEC \[28\]. Along with its continuing use in quantum optics, the above examples demonstrate that the truncated Wigner representation is an extremely useful approximation method, allowing for the numerical simulation of a number of processes for which nothing else is known to be as effective.

The task in \[1\] was split naturally in two. Firstly, we constructed a path-integral approach in phase space, which we called multitime Wigner representation. Within this approach, truncated Wigner equations emerged as an approximation to exact quasi-stochastic equations for paths. Secondly, we developed a way of bringing time-symmetric products of Heisenberg operators \[1\] \[2\], expressed by the path integral, to time-normal order \[3\]. The respective relations, called generalised phase-space correspondences, originate in Kubo’s formula for the linear response function \[29\] \[30\]. However, the properties of time-symmetric operator products \[1\] \[5\] were formulated without proof. Details of the limiting procedure defining the path integral were ignored as irrelevant within the truncated Wigner approximation.

The logic of the present paper is best understood by drawing an analogy with our Ref. \[31\]. In \[31\], our goal was to extend normal-ordering-based approaches of quantum stochastics beyond quartic Hamiltonians. This paper is an attempt to extend the techniques of Ref. \[31\] further, this time to the Weyl-ordering-based method of Ref. \[1\]. Particulars aside, in \[31\] we applied causal \[31\], or response \[32\] \[33\], transformation to Perel-Keldysh diagram series \[34\] \[35\] for the system in question. The result was a Wyld-type \[37\] diagram series, which we called causal series. These kind of diagram techniques are well known in the theory of classical stochastic processes \[3\] \[38\] \[39\]. It is therefore not surprising that we could reverse engineer the causal series resulting in a stochastic differential equation (SDE) for which this series was a formal solution. For quartic (collisional) interactions the result is the well-known positive-P representation of quantum optics. For other interactions, finding an SDE in the true meaning of the term is not always possible because of the Pawula theorem \[40\]. In such cases the causal series may be only approximated by a stochastic difference equation (SDE) in discretised time. Attempts to simulate emerging SDEs numerically have not been encouraging \[31\] \[41\]. This is the primary reason why in Ref. \[1\] we resorted to approximate methods.

The key point of \[31\] is a formal link existing between conventional quantum field theory (Schwinger-Perel-Keldysh’s closed-time-loop formalism) and conventional quantum optics (time-normal operator ordering and positive-P representation). The existence of such a link was first pointed out by one of the present authors in \[42\]. For the purposes of this paper, both backgrounds are inadequate or missing and have to be built from scratch. On the quantum-field-theoretical side, we develop a formal framework of “symmetric Wick theorems” expressing time-ordered operator products by symmetrically-ordered ones. Similar to Wick’s theorem proper, this allows us to construct a “symmetric” variety of Perel-Keldysh diagram series with corresponding “symmetric” propagators. On the quantum-optical side, we introduce what we called a multitime Wigner representation generalising Weyl’s ordering to multitime averages of Heisenberg operators. The necessary “flavour” of causal transformation can then be borrowed from \[5\]. The link to time-normal ordering is then based on a fundamental link between commutators of Heisenberg operators with different times and the response properties of quantum fields \[31\] \[51\] \[52\]. All our results apply to non-linear quantum systems with, to a large extent, arbitrary interaction Hamiltonians.

The existence of symmetric Wick theorems for the change of time ordering to symmetric may be of independent interest for a wider audience than that for which this paper is primarily intended. It is for this wider audience that in the appendix we present the generalisation of symmetric Wick theorems to arbitrary quantised fields.

The glue that holds the paper together is the concept of time-symmetric ordering of Heisenberg operators. Continuing the analogy with \[31\], this ordering replaces the time-normal operator ordering on which \[31\] was built. On the quantum-field-theoretical side, we express “symmetric” propagators by the retarded Greens function. The induced restructuring of “symmetric” Perel-Keldysh series automatically turns them into perturbative series for quantum averages of time-symmetrically ordered products of Heisenberg operators. On the quantum-optical side, time-symmetric ordering appears as a natural generalisation of the conventional symmetric ordering to Heisenberg operators. Quantum field theory and quantum optics are not equal here. Time-symmetric ordering emerges in quantum field theory as a fully specified formal concept. At the same time, there does not seem to be any way of guessing, save deriving, this concept from within conventional phase-space techniques without a reference to Schwinger’s closed-time-loop formalism \[43\].

The paper is organised as follows. In sections \[1\] and \[3\] two formal concepts are prepared for later use. In sec-
II. THE TIME-SYMMETRIC ORDERING

A. The oscillator basics

We introduce the common pair of bosonic creation and annihilation operators,

$$[\hat{a}, \hat{a}^\dagger] = 1,$$

and the usual free oscillator Hamiltonian,

$$\hat{H}_0 = \omega_0 \hat{a}^\dagger \hat{a}.$$  \hfill (2)

We use units where $\hbar = 1$. The symmetric (Weyl) ordering of the creation and annihilation operators is conveniently defined in terms of the operator-valued characteristic function

$$\chi(\eta, \eta^*) = e^{\eta^* \hat{a} + \eta \hat{a}^\dagger},$$

so that, by definition

$$\frac{\partial^{m+n} \chi(\eta, \eta^*)}{\partial \eta^n \partial \eta^*^m} |_{\eta=0} = W^m \hat{a}^n.$$  \hfill (4)

For simplicity, we consider a single-mode case; multimode cases are recovered formally by attaching mode index to all quantities, cf. section [V.A] and the appendix. Operator orderings act mode-wise, so that extension to many modes is straightforward.

The time-dependent creation and annihilation operators are defined as,

$$\hat{a}(t) = \hat{a} e^{-i \omega_0 t}, \quad \hat{a}^\dagger(t) = \hat{a}^\dagger(t) e^{i \omega_0 t}.$$  \hfill (5)

Formally, they are Heisenberg field operators with respect to the free Hamiltonian, e.g.,

$$i\partial_t \hat{a}(t) = [\hat{a}(t), \hat{H}_0(t)],$$

where $\hat{H}_0(t)$ is $\hat{H}_0$ in the interaction picture,

$$\hat{H}_0(t) = \omega_0 \hat{a}^\dagger(t) \hat{a}(t).$$  \hfill (7)

We shall term $\hat{a}(t), \hat{a}^\dagger(t)$ free-field, or interaction-picture, operators, because this is the role they play in real problems with interactions. Symmetric ordering is extended to free fields postulating that,

$$W \hat{a}(t_1) \cdots \hat{a}(t_m) \hat{a}^\dagger(t_{m+1}) \cdots \hat{a}^\dagger(t_{m+n}) e^{-i\omega_0(t_1+\cdots+t_m-t_{m+1}-\cdots-t_{m+n})} W^{m} \hat{a}^n.$$  \hfill (8)

Furthermore, adding an arbitrary, and, in general, time-dependent, interaction term to $\hat{H}_0$,

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$  \hfill (9)

allows us to introduce the pair of the Heisenberg fields operators proper,

$$\hat{A}(t) = U(t) \hat{a} U^\dagger(t), \quad \hat{A}^\dagger(t) = \hat{U}(t) \hat{a}^\dagger(t) U(t).$$  \hfill (10)

where the evolution operator is defined through the Schrödinger equation,

$$\frac{dU(t)}{dt} = \hat{H} U(t), \quad \lim_{t \to -\infty} \hat{U}(t) = \mathbb{1}.$$  \hfill (11)

Interaction picture is introduced in the usual way by splitting the evolution operator in two factors,

$$\hat{U}(t) = \hat{U}_0(t) \hat{U}_1(t),$$  \hfill (12)

where $\hat{U}_0(t)$ is the evolution operator with respect to $\hat{H}_0$, and $\hat{U}_1(t)$ obeys the equation,

$$\frac{d\hat{U}_1(t)}{dt} = \hat{H}_1 \hat{U}_1(t), \quad \lim_{t \to -\infty} \hat{U}_1(t) = \mathbb{1},$$  \hfill (14)

with $\hat{H}_1(t)$ being $\hat{H}_1$ in the interaction picture,

$$\hat{H}_1(t) = \hat{U}_1^\dagger(t) \hat{H}_1 \hat{U}_0(t).$$  \hfill (15)

The reader should have noticed that we adhere to certain notational conventions. Calligraphic letters are reserved for evolution and Heisenberg operators. Plain letters denote Schrödinger and interaction-picture operators, which in turn are distinguished by the absence or presence of the time argument, respectively. The Schrödinger operator $\hat{a}$ becomes $\hat{a}(t)$ in the interaction picture and $\hat{A}(t)$ in the Heisenberg picture,

$$\hat{a}(t) = U_0(t) \hat{a} \hat{U}_0(t), \quad \hat{A}(t) = U_1(t) \hat{a} U_1(t) = U_1^\dagger(t) \hat{a} U(t),$$

and similarly for other operators.

We note that, with unspecified interaction, Heisenberg operators are in essence placeholders. By specifying interaction one *ipso facto* specifies all Heisenberg operators.
B. The time-symmetric operator products

Throughout the paper we make extensive use of the concept of time-symmetric product of the Heisenberg operators \( \hat{A} \). We define it by the following recursive procedure. For a single operator the ordering is irrelevant,

\[
T^W \hat{A}(t) = \hat{A}(t), \quad T^W \hat{A}^\dagger(t) = \hat{A}^\dagger(t). \quad (17)
\]

Furthermore, if \( \hat{P}_{[>t]} \) is a time-symmetric product where all time arguments are larger than \( t \), then

\[
T^W \hat{P}_{[>t]}(t) = \frac{1}{2} [\hat{P}_{[>t]}, \hat{A}(t)]_+, \quad T^W \hat{P}_{[>t]}(t) = \frac{1}{2} [\hat{P}_{[>t]}, \hat{A}^\dagger(t)]_+ , \quad (18)
\]

where \([ \cdots ]_+\) stands for the anticommutator,

\[
[\hat{X}, \hat{Y}]_+ = \hat{X}\hat{Y} + \hat{Y}\hat{X}. \quad (19)
\]

This allows one to build a time-symmetric product of any number of factors, by applying (18) in the order of decreasing time arguments (increasing in \( \mathbb{R} \) is a typo). The result are nested anticommutators, (with

\[
T^W \hat{A}(t_1)\hat{A}(t_2)\hat{A}(t_3) = \frac{1}{4} \left[ [\hat{A}(t_1), \hat{A}(t_2)]_+, \hat{A}(t_3) \right]_+
\]

\[
= \frac{1}{4} \left[ \hat{A}(t_1)\hat{A}(t_2)\hat{A}(t_3) + \hat{A}(t_2)\hat{A}(t_1)\hat{A}(t_3) + \hat{A}(t_3)\hat{A}(t_1)\hat{A}(t_2) + \hat{A}(t_3)\hat{A}(t_2)\hat{A}(t_1) \right], \quad t_1 > t_2 > t_3, \quad (22)
\]

as opposed to

\[
T^W \hat{A}(t_1)\hat{A}(t_2)\hat{A}(t_3) = \frac{1}{4} \left[ [\hat{A}(t_1), \hat{A}(t_3)]_+, \hat{A}(t_2) \right]_+
\]

\[
= \frac{1}{4} \left[ \hat{A}(t_1)\hat{A}(t_2)\hat{A}(t_3) + \hat{A}(t_2)\hat{A}(t_1)\hat{A}(t_3) + \hat{A}(t_3)\hat{A}(t_1)\hat{A}(t_2) + \hat{A}(t_3)\hat{A}(t_2)\hat{A}(t_1) \right], \quad t_1 > t_2 > t_3. \quad (23)
\]

In these formulae, the crossed-out terms are those absent in time-symmetric operator products but occurring in symmetrised ones.

C. General properties of time-symmetric products

Equation (21) expresses a time-symmetrically ordered product of \( N \) factors as a sum of \( 2^{N-1} \) products of field operators which differ in the order of factors. In all these products the time arguments first increase then decrease (whereas in crossed-out terms in (22) and (23) the earliest operator is in the middle). This kind of time-ordered structure is characteristic of Schwinger’s closed-time-loop formalism (see Refs. [32, 13] and sections III-C and IV below, so we shall talk of Schwinger (time) sequences and of the Schwinger order of factors in Schwinger products.

It is easy to see that all possible Schwinger products appear in the sum. Indeed, the earliest time in a Schwinger sequence can only occur either on the left or on the right. That recursions (18) generate all Schwinger products can then be shown by induction, starting from pair products for which this is obvious. We may thus give an alternative definition of the time-symmetric product:

\[
\hat{X}_k = \hat{A}, \hat{A}^\dagger, k = 1, \ldots, N
\]

\[
T^W \hat{X}_1(t_1)\hat{X}_2(t_2)\cdots \hat{X}_n(t_n) = \frac{1}{2^{N-1}} \times [\cdots [\hat{X}_1(t_1), \hat{X}_2(t_2)]_+, \hat{X}_3(t_3)]_+, \cdots, \hat{X}_N(t_N)]_+, \quad t_1 > t_2 > \cdots > t_N. \quad (20)
\]

Equations (18) and (21) imply that all time arguments in a time-symmetric product are different. Extension to coinciding time arguments may be given by continuity, see below.

For two factors we find plain symmetrised combinations,

\[
T^W \hat{A}(t_1)\hat{A}(t_2) = \frac{1}{2} [\hat{A}(t_1)\hat{A}(t_2) + \hat{A}(t_2)\hat{A}(t_1)],
\]

\[
T^W \hat{A}(t_1)\hat{A}^\dagger(t_2) = \frac{1}{2} [\hat{A}(t_1)\hat{A}^\dagger(t_2) + \hat{A}^\dagger(t_2)\hat{A}(t_1)],
\]

\[
T^W \hat{A}^\dagger(t_1)\hat{A}(t_2) = \frac{1}{2} [\hat{A}^\dagger(t_1)\hat{A}(t_2) + \hat{A}(t_2)\hat{A}^\dagger(t_1)],
\]

(21)

where the order of times does not matter. For three and more factors it already does, e.g.,
The time-symmetric product of \( N \) factors is \( 1/2^{N-1} \) times the sum of all possible Schwinger products of these factors.

This definition of the time-symmetric product is illustrated in Fig. 1 where the \( 2^{N-1} \) Schwinger products comprising it are visualised as \( 2^{N-1} \) distinct ways of placing the operators on the so-called C-contour. The latter travels from \( t = -\infty \) to \( t = +\infty \) (the forward branch) and then back to \( t = -\infty \) (reverse branch). The operators are imagined as positioned on the C-contour; each operator may be either on the forward or reverse branch, cf. Fig. 1.

The order of operators on the C-contour determines the order of factors in a particular Schwinger product (from right to left, to match Eq. (58) below).

Definition of a time-symmetric product as a sum of all Schwinger products makes obvious the reality property,

\[
[T^W(\cdots)]^+ = T^W(\cdots)^t. \tag{24}
\]

This follows from the trivial fact that if a particular sequence of times is in a Schwinger order, the reverse sequence is also in a Schwinger order. Furthermore, visualisation in Fig. 1 helps us to prove the most important property of the time-symmetric products: their continuity at coinciding time arguments. Assume that a pair of times \( t, t' \) can change their mutual order but both stay either earlier or later in respect of all other times, cf. Fig. 1. Assume also that placing of all times on the C-contour except \( t, t' \) is fixed. If \( t, t' \) are not the latest times, we are left with four ways of placing them on the C-contour resulting, up to the overall coefficient, in four terms (with \( \hat{X}, \hat{Y} = \hat{A}, \hat{A}^\dagger \))

\[
\hat{Q}(t, t') = \hat{P}_t \hat{X}(t) \hat{P}_t \hat{Y}(t') \hat{P}_t + \hat{P}_t \hat{Y}(t) \hat{P}_t \hat{X}(t') \hat{P}_t + \hat{P}_t \hat{X}(t') \hat{P}_t \hat{P}_t \hat{Y}(t) \hat{P}_t, \quad t < t',
\]

\[
\hat{P}_t \hat{Y}(t') \hat{P}_t \hat{P}_t \hat{X}(t) \hat{P}_t, \quad t > t'. \tag{25}
\]

Here, the operator product \( \hat{P}_t \) comprises all operator factors with time arguments larger than \( t, t' \), \( \hat{P}_t \) comprises operators with time arguments less than \( t, t' \) placed on the forward branch of the C-contour, and \( \hat{P}_t \) comprises operators with time arguments less than \( t, t' \) placed on the reverse branch of the C-contour (see Fig. 1). Then,

\[
\lim_{t \to t'} \hat{Q}(t, t') = \hat{P}_t [\hat{X}(t), \hat{Y}(t)] \hat{P}_t - \hat{P}_t \hat{P}_t [\hat{X}(t), \hat{Y}(t)] \hat{P}_t = 0, \tag{26}
\]

because the commutator here may only be a c-number (or zero); this holds also in a multimode case. If \( t, t' \) are the latest times, then \( \hat{P}_t = 1 \) and the freedom of placing \( t, t' \) reduces to two terms,

\[
\hat{Q}(t, t') = \hat{P}_t [\hat{X}(t), \hat{Y}(t')] + \hat{Y}(t) \hat{X}(t') \hat{P}_t, \tag{27}
\]

which is independent of the order of the times \( t, t' \). Continuity of the time-symmetric products has thus been proven. Note that this spares us the necessity to specify their values at coinciding time arguments.

D. Equivalence of the time-symmetric and symmetric ordering of the free-field operators

We now prove that, when applied to free fields, the time-symmetric ordering is just a fancy way of redefining conventional symmetric ordering defined by Eqs. (4) and (3),

\[
T^W \hat{a}(t_1) \cdots \hat{a}(t_m) \hat{a}^\dagger(t_{m+1}) \cdots \hat{a}^\dagger(t_{m+n}) = W \hat{a}(t_1) \cdots \hat{a}(t_m) \hat{a}^\dagger(t_{m+1}) \cdots \hat{a}^\dagger(t_{m+n}) = e^{-i\omega(t_1 + \cdots + t_m - t_{m+1} - \cdots - t_{m+n})} W \hat{a}^{m+n} \hat{a}^{m+n}, \tag{28}
\]

so that the order of times here in fact does not matter. At first glance, equations (22) and (23) serve as counter-examples. From Eq. (22) we get,

\[
T^W \hat{a}(t_1) \hat{a}(t_2) \hat{a}^\dagger(t_3) = \frac{e^{-i\omega(t_1 + t_2 - t_3)}}{2} \times [\hat{a}^2 \hat{a}^\dagger + \hat{a}^\dagger \hat{a}^2], \quad t_1 > t_2 > t_3. \tag{29}
\]
as contrasted by the formula obtained from Eq. (23),

\[ T^W \hat{a}(t_1) \hat{a}(t_2) \hat{a}(t_3) = \frac{e^{-i\omega_0(t_1+t_2-t_3)}}{4} \times \left[ \hat{a}\hat{a} + \hat{a}^\dagger \hat{a}^\dagger + 2\hat{a}\hat{a}^\dagger \right], \quad t_1 > t_3 > t_2. \] (30)

Neither result coincides with the symmetrically-ordered product following from [4].

\[ W \hat{a}(t_1) \hat{a}(t_2) \hat{a}(t_3) = \frac{e^{-i\omega_0(t_1+t_2-t_3)}}{3} \times \left[ \hat{a}\hat{a} + \hat{a}^\dagger \hat{a}^\dagger + 2\hat{a}\hat{a}^\dagger \right]. \] (31)

However by using the commutational relation [1] it is easy to verify that

\[ \frac{1}{2} \left[ \hat{a}\hat{a} + \hat{a}^\dagger \hat{a}^\dagger + 2\hat{a}\hat{a}^\dagger \right] = \frac{1}{3} \left[ \hat{a}\hat{a} + \hat{a}^\dagger \hat{a}^\dagger + 2\hat{a}\hat{a}^\dagger \right] = W \hat{a} \hat{a}. \] (32)

To prove (23) in general we note that the recursion procedure defining the time-symmetric product may be started from the unity operator,

\[ T^W \hat{1} = \hat{1}. \] (33)

Then,

\[ T^W \hat{A}(t) = \frac{1}{2} \left[ \hat{1}, \hat{A}(t) \right]_+ = \hat{A}(t), \]
\[ T^W \hat{A}(t) = \frac{1}{2} \left[ \hat{1}, \hat{A}(t) \right]_+ = \hat{A}(t), \] (34)

in obvious agreement with [17]. Furthermore, we can replace \( \hat{1} \) in (33) by \( \chi(\eta, \eta^*) \) given by Eq. (3) and then apply the recursion [18] starting from the latest time. With the end limit \( \eta = 0 \) this replacement does not affect the resulting time-symmetric products. So, assuming that \( t' < t \),

\[ T^W \hat{a}(t) = \frac{1}{2} \left[ \chi(\eta, \eta^*), \hat{a}(t) \right]_+ |_{\eta = 0}, \]
\[ T^W \hat{a}(t) \hat{a}(t') = \frac{1}{2} \left[ \chi(\eta, \eta^*), \hat{a}(t) \hat{a}(t') \right]_+ |_{\eta = 0}. \] (35)

Similar relations hold for larger number of factors. We now transform them using the standard phase-space correspondences. Recalling that

\[ e^{i\eta \hat{a} + i\eta^* \hat{a}^\dagger} = e^{i\eta \hat{a}^\dagger} e^{i\eta^* \hat{a}} = e^{-\eta^2/2} \]

we find,

\[ \frac{\partial \chi(\eta, \eta^*)}{\partial \eta} = (\hat{a}^\dagger + \eta^*/2) \chi(\eta, \eta^*) \]
\[ = \chi(\eta, \eta^*) (\hat{a}^\dagger - \eta^*/2), \]
\[ \frac{\partial \chi(\eta, \eta^*)}{\partial \eta^*} = (\hat{a} - \eta/2) \chi(\eta, \eta^*) \]
\[ = \chi(\eta, \eta^*) (\hat{a} + \eta/2). \] (37)

Pairwise combining these relations and multiplying them by suitable time exponents we obtain

\[
\frac{1}{2} \left[ \chi(\eta, \eta^*) \hat{a}(t) \right]_+ = e^{-i\omega_0 t} \frac{\partial \chi(\eta, \eta^*)}{\partial \eta^*}, \\
\frac{1}{2} \left[ \chi(\eta, \eta^*) \hat{a}(t) \right]_+ = e^{-i\omega_0 t} \frac{\partial \chi(\eta, \eta^*)}{\partial \eta}.
\] (38)

This allows us to rewrite Eqs. (33) as

\[ T^W \hat{a}(t) = e^{-i\omega_0 t} \frac{\partial \chi(\eta, \eta^*)}{\partial \eta^*} |_{\eta = 0}, \]
\[ T^W \hat{a}(t) \hat{a}(t') = e^{-i\omega_0 (t-t')} \frac{\partial^2 \chi(\eta, \eta^*)}{\partial \eta \partial \eta^*} |_{\eta = 0}. \] (39)

For an arbitrary number of factors we have,

\[ T^W \hat{a}(t_1) \cdots \hat{a}(t_m) \hat{a}(t_{m+1}) \cdots \hat{a}(t_{m+n}) = e^{-i\omega_0 (t_1 + \cdots + t_m + \cdots + t_{m+n})} \frac{\partial^{m+n} \chi(\eta, \eta^*)}{\partial \eta \partial \eta^*} |_{\eta = 0}. \] (40)

By virtue of [1] this is another form of (23).

To conclude this paragraph we note that Eq. (28) is not as straightforward as the corresponding relation for the normal ordering:

\[ \hat{a}(t_{m+1}) \cdots \hat{a}(t_{m+n}) \hat{a}(t_1) \cdots \hat{a}(t_m): \\
= e^{-i\omega_0 (t_1 + \cdots + t_m + \cdots + t_{m+n})} \hat{a}^{t_{m+n}} \hat{a}^{t_1}. \] (41)

Here setting the free-field operators in the normal order ipso facto sets the creation and annihilation operators in the normal order, while in Eq. (28) the symmetric order is only recouped on rearranging the operators using [1]. Since the commutator contains dynamical information one may say that relation [11] is purely kinematical while equation [28] is dynamical.

E. The time-symmetric averages

The time-symmetric ordering of free-field operators delivers us “the best of both worlds.” On the one hand, it is just symmetric ordering in disguise. On the other hand, the Schwinger products of which it is build are consistent with such “big guns” as Schwinger’s closed-time-loop formalism. The time-symmetric ordering of the free-field operators correctly “guesses” certain fundamental structures underlying the interacting quantum field theory, making it an irreplaceable bridging concept when deriving perturbative relations with the symmetric ordering.

In practice, it is convenient to eliminate symmetric ordering altogether by reexpressing all information about the initial state of the system directly in terms of time-symmetric averages. We introduce the Wigner distribution in the standard way by

\[
\langle \chi(\eta, \eta^*) \rangle = \int \frac{d^2 \alpha}{\pi} W(\alpha, \alpha^*) e^{i \eta \alpha + \eta^* \alpha^*},
\] (42)
where the quantum averaging is over the initial state of the system. The symmetric averages characterising the initial state may then be written as

$$\langle W \hat{a}^n \hat{a}^*^m \rangle = \int \frac{d^2 \alpha}{\pi} W(\alpha, \alpha^*) \alpha^n \alpha^*^m. \quad (43)$$

By making use of this relation, the result of averaging Eq. (28) takes the form

$$\langle T^W \hat{a}(t_1) \cdots \hat{a}(t_m) \hat{a}^\dagger(t_{m+1}) \cdots \hat{a}^\dagger(t_{m+n}) \rangle = \int \frac{d^2 \alpha}{\pi} W(\alpha, \alpha^*) \alpha(t_1) \cdots \alpha(t_m) \times \alpha^*(t_{m+1}) \cdots \alpha^*(t_{m+n}), \quad (44)$$

where

$$\alpha(t) = e^{-i\omega_0 t}, \quad \alpha^*(t) = e^{i\omega_0 t}. \quad (45)$$

If $W(\alpha, \alpha^*) > 0$, this is nothing but stochastic moments of the random $c$-number field $\alpha(t)$, which is specified by its value at $t = 0$ (initial condition) being distributed in accordance with the probability distribution $W(\alpha, \alpha^*)$. For nonpositive $W(\alpha, \alpha^*)$ this interpretation holds by replacing probability by quasi-probability.

III. SYMMETRIC WICK THEOREMS

A. Time ordering of operators

The time ordering places operators from right to left in the order of increasing time arguments, e.g.,

$$T_+^W \hat{A}(t) \hat{A}^\dagger(t') = \theta(t - t') \hat{A}(t) \hat{A}^\dagger(t') + \theta(t' - t) \hat{A}^\dagger(t') \hat{A}(t), \quad (46)$$

and similarly for a larger number of factors. By definition, bosonic operators under the time ordering commute. The notation $T_+^W$ as distinct from $T_+$ used in 31 emphasises the fact that the $T_+^W$-ordering implies a different specification for coinciding time arguments. In 31 this specification was by normal ordering, while, not quite unexpectedly, in this paper we imply symmetric ordering. In 31 such specification was enforced by the causal regularisation which was part of the dynamical approach. A similar (but different) regularisation scheme is part of the dynamical approach in this paper, cf. section VII. Till that section we suppress all specifications related to operator orderings for coinciding time arguments. The notation $T_+^W$ should thus be regarded a placeholder for the concept full meaning of which will be made clear in section VII.

B. Symmetric Wick theorem for the time ordering

We now prove a generalisation of Wick’s theorem to the symmetric ordering. As a major simplification, results of the previous section allow us to formulate and prove the symmetric Wick theorem as a relation between the time-ordered and time-symmetrically ordered operators products:

$$A \text{ time-ordered product of interaction-picture operators equals a sum of time-symmetrically ordered products with all possible symmetric contractions, including the term without contractions.}$$

The symmetric contraction is defined, in obvious analogy to Wick’s theorem proper, as

$$-iG^W_{++}(t - t') = T_+^W \hat{a}(t) \hat{a}^\dagger(t') - T_+^W \hat{a}(t') \hat{a}^\dagger(t). \quad (47)$$

One can use here the symmetric ordering in place of the time-symmetric one, but we follow our general principle of eliminating the $W$-ordering from considerations. The cumbersome notation we use for the symmetric contraction will be explained in section VII. Below. For the oscillator,

$$-iG^W_{++}(t) = \varepsilon(t) [\hat{a}(t), \hat{a}^\dagger(0)] = \varepsilon(t) e^{-i\omega_0 t}, \quad (48)$$

where $\varepsilon(t)$ is the odd stepfunction,

$$\varepsilon(t) = \frac{1}{2} [\theta(t) - \theta(-t)]. \quad (49)$$

The symmetric Wick theorem obviously holds for one and two operators; in the latter case it coincides with Eq. (47). A general proof follows by induction. Assume the symmetric Wick theorem has been proven up to a certain number of factors and consider a time-ordered product with one “spare” factor. We choose this spare factor as the earliest one, which is thus on the right of the time-ordered product. Let it be $\hat{a}(t)$. The whole time-ordered product may then be written as

$$T_+^W \hat{a}(t_1) \cdots \hat{a}(t_m) \hat{a}(t_{m+1}) \cdots \hat{a}(t_{m+n}) \hat{a}(t) = \hat{P} \hat{a}(t), \quad (50)$$

where we have introduced a notation for the product without the “spare” factor

$$\hat{P} = T_+^W \hat{a}(t_1) \cdots \hat{a}(t_m) \hat{a}(t_{m+1}) \cdots \hat{a}(t_{m+n}). \quad (51)$$

We wish to have the spare factor symmetrically on either side of $\hat{P}$ so we write

$$\hat{P} \hat{a}(t) = \frac{1}{2} [\hat{P}, \hat{a}(t)] + \frac{1}{2} \hat{P} \hat{a}(t). \quad (52)$$

The commutator is easily calculated

$$\frac{1}{2} [\hat{P}, \hat{a}(t)] = \frac{1}{2} \sum_{k=1}^{m} \hat{P}_k \hat{a}(t_k), \hat{a}(t), \quad (53)$$

where $\hat{P}_k$ is $\hat{P}$ without the factor $\hat{a}(t_k)$; note that $\hat{P}_k$ remain time-ordered. For $t < t_k$,

$$\frac{1}{2} [\hat{a}(t_k), \hat{a}(t)] = -iG^W_{++}(t - t_k), \quad (54)$$
We now use the induction assumption and expand $\hat{P}$ and all $\mathcal{P}_k$ according to the symmetric Wick theorem. By virtue of (15), the anticommutator in (55) is then a sum of time-symmetric products. It gives us the sum of terms where contractions exclude $\hat{a}(t)$. The sum in (55) delivers the terms where $\hat{a}(t)$ is involved in a contraction. It is straightforward to verify that all terms required by the symmetric Wick theorem are recovered this way, each occurring only once.

The case when the earliest term is $\hat{a}^\dagger(t)$ is treated by simply swapping in the above $\hat{a} \leftrightarrow \hat{a}^\dagger$. Equation (52) is replaced by

$$\frac{1}{2} \left[ \hat{a}(t_k), \hat{a}^\dagger(t) \right] = -i G^W_{++}(t_k - t), \quad t < t_k$$

which indeed holds, cf. Eq. (18). The symmetric Wick theorem has thus been proven. We note that the regularisation we mentioned after Eq. (46) results, in particular, in $G^W_{++}(0) = 0$ without mathematical ambiguity. Hence the caveat of Wick’s theorem, that “no contractions should occur between operators with equal time arguments,” also applies to the symmetric Wick theorem.

C. Symmetric Wick theorem for the closed-time-loop ordering

If the initial state of the system is not vacuum, closed equations of motion cannot be written in terms of averages of the time-ordered operator products only, cf., e.g., Ref. [44]. The necessary type of ordering was introduced, rather indirectly, in Schwinger’s seminal paper [43], and later applied to developing diagram techniques for nonequilibrium nonrelativistic quantum problems by Konstantinov and Perel [35]. Extension to relativistic problems was given by Keldysh [36] under whose name the approach became known. We note that the concept of the closed time loop and the related operator ordering is much more general than the Keldysh diagram techniques commonly associated with it. As was shown in paper [31], it underlies such a phase-space concept as the time-normal ordering of Glauber and Kelly and Kleiner. In this paper we investigate the relation between the closed-time-loop and the symmetric orderings.

The closed-time-loop operator ordering is commonly defined as an ordering on the so-called C-contour which can be seen in Figs. 1 and 2. The C-contour travels from $t = -\infty$ to $t = +\infty$ (forward branch) and then back to $t = -\infty$ (reverse branch). The operators are formally assigned an additional binary argument which distinguishes operators on the forward branch from those on the reverse branch. “Earlier” and “later” are then generalised to match the travelling rule along the C-contour. All operators on the forward branch are by definition “earlier” than those on the reverse branch and go to the right. Among themselves, the operators on the forward branch are set from right to left in the order of increasing time arguments ($T^W_+$-ordered), while those on the reverse branch are set from right to left in the order of decreasing time arguments ($T^W_-$-ordered). Using that Hermitian conjugation inverts the time order of factors, the $T^W_+$-ordering may be defined as

$$T^W_+ (\cdots) = \left[ T^W_+ (\cdots) \right]^T.$$  (57)

The closed-time-loop-ordered operator product may thus be alternatively defined as a double-time-ordered product,

$$T^W_+ \hat{P}_- T^W_+ \hat{P}_+,$$  (58)

where $\hat{P}_\pm$ are two independent operator products. In terms of the C-contour, the operators in $\hat{P}_+$ are visualised as positioned on the forward branch of the C-contour, and those in $\hat{P}_-$—on the reverse branch. Factors in a double-time-ordered product are always arranged in a Schwinger sequence, cf. the opening paragraph of section II C for specifications pertaining to coinciding time arguments we refer the reader to section VII In this paper we employ Eq. (58) as a primary definition and use the concept of closed time loop only for illustration purposes.

Extension of the symmetric Wick theorem to the double time ordering employs the linear order of the C-contour. A formal generalisation of the symmetric Wick theorem to an arbitrary linearly ordered set may be found in the appendix. Hori’s form of the symmetric Wick theorem given by Eq. (67) below, of which the derivation is our goal, is in fact a particular case of the general structural relation (A.14). Nonetheless we believe that the direct proof we present here will benefit the reader.

The symmetric Wick theorem is generalised to the double-time ordering by making the symmetric contraction dependent on the positioning of the contracted pair in the double-time-ordered product (or, which is the same, on the C-contour, cf. Fig. 2). As a result we recover
four contractions:
\[-iG^W_+(t - t') = T^W_+ \hat{a}(t) \hat{a}^\dagger(t') - T^W_\mp \hat{a}(t) \hat{a}^\dagger(t'),\]
\[-iG^W_-(t - t') = T^W_\mp \hat{a}(t) \hat{a}^\dagger(t') - T^W_+ \hat{a}(t) \hat{a}^\dagger(t'),\]
\[-iG^W_+(t - t') = T^W_+ \hat{a}(t) T^W_\mp \hat{a}^\dagger(t') - T^W_\mp \hat{a}(t) \hat{a}^\dagger(t'),\]
\[-iG^W_-(t - t') = T^W_\mp \hat{a}^\dagger(t') T^W_+ \hat{a}(t) - T^W_+ \hat{a}^\dagger(t') \hat{a}(t').\]  
(59)

Unlike in Ref. [31], there are four nonzero symmetric contractions, not three. To make the genesis of the contractions clearer we retained the orderings also where they are redundant, e.g., $T^W_\mp \hat{a}(t) T^W_\mp \hat{a}^\dagger(t') = \hat{a}(t) \hat{a}^\dagger(t')$. The contraction $-iG^W_+(t)$ is exactly that defined by 417 explaining the notation. As c-number kernels, $-iG^W_+(t)$ and $-iG^W_-(t)$ are coupled by Hermitian conjugation, while $-iG^W_+(t)$ and $-iG^W_-(t)$ are Hermitian:

$-iG^W_+(t - t') = [-iG^W_+(t' - t)]^*$,

$-iG^W_-(t - t') = [-iG^W_-(t' - t)]^*$,

$-iG^W_+(t - t') = [-iG^W_+(t' - t)]^*$.

(60)

In obtaining this we used 24 as well as the similar relation for the double-time ordering,

$[T^W_- \hat{P}_- T^W_+ \hat{P}_+] = T^W_\mp \hat{P}_+ T^W_\mp \hat{P}_\mp$,

(61)

cf. Eq. 44. For the oscillator,

$-iG^W_+(t) = iG^W_-(t) = \varepsilon(t) e^{-i\omega t}$,

$-iG^W_+(t) = iG^W_-(t) = \frac{1}{2} e^{-i\omega t}$,

(62)

cf. Eq. 18.

With the contractions defined by 59 the symmetric Wick theorem reads:

A double-time-ordered product of interaction-picture operators equals a sum of time-symmetrically ordered products with all possible symmetric contractions, including the term without contractions.

This includes the time-ordered products as a special case. Importantly, the generalisation to the double-time-ordering makes the symmetric Wick theorem invariant under Hermitian conjugation. This follows from Eqs. 24 and 61, supplemented by the observation that Hermitian conjugation turns every Schwinger time sequence into a reversed sequence, so that arguments of all contractions must change sign. Equations (61) show that this is exactly the effect the complex conjugation has on the contractions, including the replacement $G^W_+ \leftrightarrow G^W_-$. It is therefore only necessary to generalise the inductive step in the above proof to the case when the "spare" operator is the earliest one under the $T^W_+$ ordering. Again, let us firstly assume that this operator is $\hat{a}(t)$. Equation (62) holds with $\hat{P}$ now being a double-time-ordered product,

$\hat{P} = T^W_- \hat{P}_- T^W_+ \hat{P}_+$.  
(63)

Equation (53) applies as well, by assuming that $\hat{P}_k$ "knows" whether $\hat{a}(t)$ originates from $\hat{P}_-$ or from $\hat{P}_+$. The critical observation is that the contractions depend in fact only on the visual order of times, so that, remembering that $t < t_k$,

$\frac{1}{2} [\hat{a}(t_k), \hat{a}(t)] = -iG^W_+(t - t_k) = -iG^W_-(t - t_k)$.

(64)

With this observation equation (50) is replaced by

$T^W_- \hat{P}_- T^W_+ \hat{P}_+ \hat{a}(t) = \frac{1}{2} [\hat{P}, \hat{a}(t)]_+$

$- i \sum_{t_k \in \hat{P}_-} \hat{P}_k^r G^W_+(t - t_k) - i \sum_{t_k \in \hat{P}_+} \hat{P}_k^r G^W_-(t - t_k)$,

(65)

where $\sum_{t_k \in \hat{P}_-}$ means summation over all $k$ such that $\hat{a}(t_k)$ originates from $\hat{P}_+$, and similarly for $\hat{P}_-$. The case when the earliest operator under the $T^W_+$ ordering is $\hat{a}(t)$ is treated similarly, the "critical observation" in this case being that, for $t_k > t$,

$\frac{1}{2} [\hat{a}(t), \hat{a}(t)] = -iG^W_+(t_k - t) = -iG^W_-(t_k - t)$.

(66)

This completes the inductive step of the proof. The symmetric Wick theorem has thus also been proven for the double time ordering.

D. Functional form of the symmetric Wick theorem

One technical tool in Ref. [31] was Hori’s form of Wick’s theorem expressing it as an application of a functional differential operator, cf. Eq. (18) in [31]. Except for the redefinition of contractions, the symmetric Wick theorem coincides with Wick’s theorem proper. This makes the functional form of Wick’s theorem equally applicable to the symmetric Wick theorem. All we need is to redefine the differential operator $\Delta_C$ given by Eq. (19) in [31] as

$\Delta^W_C \left[ \begin{array}{cccc} \delta & \delta & \delta & \delta \\ \delta a_+ & \delta a_- & \delta a_+ & \delta a_- \end{array} \right] = -i \sum_{c,c'=\pm} \int dt dt' G^W_{cc'}(t - t') \frac{\delta^2}{\delta a_c(t) \delta a_{c'}(t')}$,

(67)

where $a_\pm(t), a_{\pm}(t)$ are four independent c-number fields. Square brackets signify functionals. The symmetric contractions were defined by Eqs. (59). With these replacements we find Hori’s form of the symmetric Wick theo-
rem,
\[ T - P_+ \left[ \hat{a}, \hat{a}^\dagger \right] T + P_+ \left[ \hat{a}, \hat{a}^\dagger \right] \]
\[ = T^W \left\{ \exp \Delta_W^C \left[ \delta \hat{a}_{a+}, \delta \hat{a}_{a-}, \delta \hat{a}_{a+}, \delta \hat{a}_{a-} \right] \right\} \times P_- \left[ \hat{a}, \hat{a}^\dagger \right] P_+ \left[ \hat{a}, \hat{a}^\dagger \right] \left\{ \hat{a}, \hat{a}^\dagger \right\} . \]  
(68)

Here, \( P_+ \) and \( P_- \) are two independent functionals of time-dependent fields, and \( a \rightarrow \hat{a} \) stands for the replacement of the c-numbers by operators,
\[ a_\pm(t) \rightarrow \hat{a}(t), \quad \bar{a}_\pm(t) \rightarrow \bar{a}(t). \]  
(69)

Once again, exact meaning to Eq. (58) will be assigned by regularisations in section VII.

**IV. THE CLOSED-TIME-LOOP FORMALISM**

**A. The model**

All definitions and majority of formulae in this and the following sections do not depend on the system Hamiltonian and can be applied to any bosonic system. To be specific, and to maintain connections with our previous paper [1] we demonstrate our techniques for a one-dimensional Bose-Hubbard (1D BH) chain. This system combines simplicity of the formal model with practical relevance: starting from the seminal paper by Jakob et al. [13] the BH model evolved into a standard approach to cold atoms trapped in optical lattices. The fact that a particular relation below is specific to this model will always be stated explicitly. The simplest version of the 1D BH model describes a chain of \( N \) anharmonic oscillators with Josephson’s tunneling ("hopping") between the nearest neighbours,
\[ \hat{H} = \sum_{k=1}^{N} \left[ \omega_0 \hat{a}_{k}^\dagger \hat{a}_{k} + \frac{\kappa}{2} \hat{a}_{k}^2 \hat{a}_{k}^\dagger + \delta \left( \hat{a}_{k}^\dagger \hat{a}_{k+1} + \hat{a}_{k+1}^\dagger \hat{a}_{k} \right) \right], \]  
(70)

where \( \hat{n}_k = \hat{a}_{k}^\dagger \hat{a}_{k} \) and \( \hat{a}_{k}^\dagger, \hat{a}_{k} \) is the standard creation-annihilation pair for the \( k \)-th site, \( [\hat{a}_{k}, \hat{a}_{k'}^\dagger] = \delta_{k,k'} \). The indices are understood modulo \( N \), \( \hat{a}_{N+1} = \hat{a}_{1} \); in other words, we consider a ring rather than a chain. As usual we break Hamiltonian (70) into the “free” and “interaction” Hamiltonians,
\[ \hat{H} = \hat{H}_0 + \hat{H}_I, \quad \hat{H}_0 = \sum_{k=1}^{N} \hat{H}_{0k} = \sum_{k=1}^{N} \omega_0 \hat{n}_k. \]  
(71)

The free-field and the Heisenberg operators, \( \hat{a}_k(t), \hat{a}_k^\dagger(t) \) and \( \hat{A}_{k}(t), \hat{A}_{k}^\dagger(t) \) are defined in detailed analogy to section IIA. We exclude hopping from the free Hamiltonian making our reasoning most easily adaptable to arbitrary multi-mode bosonic systems. In particular this allows the analyses in the previous two sections to be generalised simply by applying them mode-wise.

**B. Perel-Keldysh Green functions**

We now introduce the formal framework that will serve us throughout the rest of the paper. A brief historical introduction into the Schwinger-Perel-Keldysh closed-time-loop formalism was given at the beginning of section III C. The basic quantity in this formalism is a double-time-ordered Green function
\[ \langle T^{W}_{-} \hat{A}_{k_1}^\dagger(t_1) \cdots \hat{A}_{k_m}^\dagger(t_m) \hat{A}_{k_{m+1}}^\dagger(t_{m+1}) \cdots \hat{A}_{k_{m+n}}^\dagger(t_{m+n}) \rangle \times T^{W}_{+} \hat{A}_{k'_1}^\dagger(t'_1) \cdots \hat{A}_{k'_{n+1}}^\dagger(t'_{n+1}) \cdots \hat{A}_{k'_{n}}^\dagger(t'_{n}) \rangle, \]  
(72)

where \( m, m, n, n \geq 0 \) are arbitrary integers. Specifications of Eq. (72) for equal time arguments are postponed till section VII cf. the remarks at the end of section III B. A convenient interface to the whole assemblage of functions (72) is their generating, or characteristic, functional
\[ \Xi^{W}[\bar{\zeta}_{-}, \bar{\zeta}_{+}, \bar{\zeta}_{-, \bar{\zeta}}] = \langle T^{W}_{-} \exp \left( -i \bar{\zeta}_{-} \hat{A} - i \bar{\zeta}_{+} \hat{A}^\dagger \right) \rangle \times T^{W}_{+} \exp \left( i \bar{\zeta}_{+} \hat{A} + i \bar{\zeta}_{-} \hat{A}^\dagger \right), \]  
(73)

where \( \bar{\zeta}_{\pm}(t), \bar{\zeta}_{\pm}^\dagger(t) \) are four arbitrary c-number functions per mode. Notationally we treat them, as well as the mode operators, as vectors. We follow the sign conventions of Ref. [24]. To emphasise the structural side of our analyses we employ a condensed notation,
\[ xy = \sum_{k=1}^{N} \int dt x_k(t)y_k(t), \]  
(74)
\[ xx = \sum_{k,k'=1}^{N} \int dt dt' x_k(t)X_{kk'}(t-t')y_{k'}(t'). \]  

Here, \( x_k(t) \) and \( y_k(t) \) are arbitrary functions and \( X_{kk'}(t-t') \) is an arbitrary kernel; for q-numbers the order of factors matters.

**C. Closed perturbative relations**

The main advantage of the functional framework is that the universal structural part of the perturbative calculations can be expressed as a small set of closed perturbative relations. This was demonstrated in [31] for the normal ordering, and will be demonstrated in this paper for the symmetric ordering. We wish to construct a perturbative formula the generating functional (73). By the
same means as equation (24) was found in Ref. [31] we rewrite Eq. (73) in the interaction picture as

\[
\Xi^W[\zeta_-, \bar{\zeta}_-, \zeta_+, \bar{\zeta}_+] = \left\langle \exp \left\{ -i\zeta_- \hat{a} - i\zeta_- \hat{a}^\dagger + il^W_1[\hat{a}, \hat{a}^\dagger] \right\} \right\rangle \times T^W_+ \exp \left\{ i\zeta_+ \hat{a} + i\zeta_+ \hat{a}^\dagger - il^W_1[\hat{a}, \hat{a}^\dagger] \right\}. \tag{75}
\]

Here, \(L^W_1\) is a functional of two arguments,

\[
L^W_1[\hat{a}, \hat{a}^\dagger] = \int dt H^W_1(\hat{a}(t), \hat{a}^\dagger(t)), \tag{76}
\]

where the c-number function \(H^W_1(\cdot, \cdot)\) is the symmetric form of the interaction Hamiltonian,

\[
\hat{H}_1 = WH^W_1(\hat{a}, \hat{a}^\dagger). \tag{77}
\]

The last equation is written in the Schrödinger picture. Note that

\[
\hat{U}_t = T^W_+ \exp \left\{ -il^W_1[\hat{a}, \hat{a}^\dagger] \right\} \tag{78}
\]

is the interaction-picture S-matrix. Equation (77) is general and holds for any interaction. For the Bose-Hubbard chain,

\[
\hat{H}_1 = \sum_{k=1}^{N} \left[ \frac{\kappa}{2} \delta^2_k + J (\hat{a}^\dagger_k \hat{a}_{k+1} + \hat{a}^\dagger_{k+1} \hat{a}_k) \right] = W \sum_{k=1}^{N} \left[ \frac{\kappa}{2} \delta^2_k - \kappa \delta^1_k \hat{a}_k + \frac{\kappa}{4} - J (\hat{a}^\dagger_k \hat{a}_{k+1} + \hat{a}^\dagger_{k+1} \hat{a}_k) \right] \equiv \hat{H}^W_1, \tag{79}
\]

In the above,

\[
\alpha(t) = \alpha e^{-i\omega_0 t}, \quad \alpha^*(t) = \alpha^* e^{i\omega_0 t}, \tag{84}
\]

\(W(\alpha, \alpha^*)\) is the multimode Wigner function (cf. Eq. (44)), and \(a \to \alpha\) stands for the replacement,

\[
a_\pm(t) \to \alpha(t), \quad \bar{a}_\pm(t) \to \alpha^*(t). \tag{85}
\]

Not to be confused by Eq. (83), note that the functional differential operation within the curly brackets is applied under the condition that \(a_\pm(t), \bar{a}_\pm(t)\) are four arbitrary c-number vector functions. These functions are then replaced pairwise by \(\alpha(t), \alpha^*(t)\), which depend only on the initial condition \(\alpha\). This replacement turns the functional expression in curly brackets into a function of the initial condition \(\alpha\), making averaging over the Wigner function \(W(\alpha, \alpha^*)\) meaningful.
D. Formal solution to the quantum-statistical response problem

Following Kubo, we add a source term to the Hamiltonian \( \hat{H} \),
\[
\hat{H}' = \hat{H} - \sum_{k=1}^{N} \left[ \hat{a}_k^\dagger \hat{s}_k(t) + \hat{a}_k \hat{s}_k^*(t) \right]. \tag{86}
\]

The Heisenberg operators corresponding to \( \hat{H}' \) will be denoted as \( \hat{A}'_k(t) \). Similar to \( \hat{\mathcal{A}}_k(t) \), we introduce a characteristic functional for the double-time-ordered averages of \( \hat{A}'_k(t), \hat{A}^\dagger(t) \):
\[
\Xi^W[\zeta_-, \zeta_+, \zeta_\dagger; s, s^*] = \left\langle T^W_+ \exp \left( -i\zeta_- \hat{A}' - i\zeta_+ \hat{A}^\dagger \right) \times T^W_- \exp \left( i\zeta_- \hat{A}' + i\zeta_+ \hat{A}^\dagger \right) \right\rangle. \tag{87}
\]

The condensed notation we use here was defined by \( \Xi^W \).

With a taste for the paradoxical, the message of this section may be formulated as, the quantum response problem does not exist, because the information on the response properties of the system is already present in the commutators of the field operator \( \Xi[32,33] \). Formally, this is expressed by the following relation between the characteristic functionals,
\[
\Xi^W[\zeta_-, \zeta_+, \zeta_\dagger; s, s^*] = \Xi^W[\zeta_- + s, \zeta_+ - s^*, \zeta_\dagger + s, \zeta_\dagger + s^*]. \tag{88}
\]

This formula is a trivial consequence of the closed perturbative relation \( \Xi^W \); it suffices to note that adding the source term to the Hamiltonian results in the following replacement in Eq. \( \Xi^W \):
\[
L^W_1[a, \bar{a}] \rightarrow L^W_1[a, \bar{a}] - \bar{a}s - as^*. \tag{89}
\]

Equation \( \Xi^W \) shows that all information one needs in order to predict response of a quantum system to an external source is already present in the Heisenberg field operators defined without the source. A closer inspection of Eq. \( \Xi^W \) reveals that this information is “stored” in the commutators of the Heisenberg operators. For details see Refs. \( [32,33] \).

V. THE WIGNER REPRESENTATION

A. Symmetric Wick theorem and causality in phase space

Similar to \( [31] \), the starting point of the ensuing derivation is understanding the causal structure of the symmetric contractions \( [30] \). We begin with the observation that
\[
(\omega_0 - i\frac{d}{dt}) G_{++}^W(t) = \delta(t). \tag{90}
\]
This characterises the symmetric contraction \( G_{++}^W(t) \) as a Green function of the c-number equation
\[
(\omega_0 - i\frac{d}{dt}) a_k(t) = s_k(t) + \tilde{s}_k(t). \tag{91}
\]

To spare us future redefinitions we wrote \( (91) \) as an equation for the phase-space trajectories \( a_k(t) \). We also broke the total source into the given external source \( s_k(t) \) and the self-action source \( \tilde{s}_k(t) \) accounting for the interactions. In general, \( \tilde{s}_k(t) \) is quasi-stochastic and field-dependent. Note that here we work with a quasi-stochastic equation in the classical phase space, unlike in Ref. \( [31] \) where stochastic equations in the phase space of doubled dimension were considered. As a result, here the reader encounters complex-conjugate field pairs instead of independent field pairs as in ref. \( [31] \).

While \( G_{++}^W(t) \) is obviously one of Green functions of Eq. \( (91) \), it is wrong as far as natural causality is concerned. In phase space as well as in classical mechanics physics are associated with causal response defined through the retarded Green function,
\[
G_R(t) = i\theta(t)e^{-i\omega_0t}. \tag{92}
\]

This quantity also obeys equation \( (90) \) but, unlike \( G_{++}^W(t) \), is retarded. Causal solutions of Eq. \( (91) \) are specified by replacing it by the integral equation
\[
a_k(t) = \alpha_k(t) + \int dt' G_R(t - t') [s_k(t') + \tilde{s}_k(t')], \tag{93}
\]
with the condition \( a_k(t) \to \alpha_k(t) \) as \( t \to -\infty \). By analogy with Ref. \( [31] \) we expect the in-field \( \alpha(t) \) to be defined by the multimode generalisation of Eq. \( (11) \). That is, the initial condition for Eqs. \( (91) \) is defined by the initial state of the system. Consistency of these assumptions and the way Eq. \( (91) \) is linked to quantum averages remain subject to verification.

B. The causal transformation

As in Ref. \( [31] \) we proceed by noticing that all contractions may be expressed by \( G_R(t) \). Simply by trial and error it is easy to get
\[
G_{++}^W(t) = -G_{--}^W(t) = \frac{1}{2} [G_R(t) + G_R^*(t)]; \tag{94}
\]
\[
G_{++}^W(t) = -G_{--}^W(t) = \frac{1}{2} [G_R(t) - G_R^*(t)]. \tag{94}
\]

Similar to \( [31] \), we are looking for variables which would bring \( \Delta_C^W \) given by \( (77) \) to the form
\[
\Delta_C^W = \frac{\delta}{\delta a} G_R \frac{\delta}{\delta a^*} G_R + \frac{\delta}{\delta a^*} G_R \frac{\delta}{\delta a} G_R. \tag{95}
\]
We use here condensed notation defined by Eq. (74). Equation (95) takes us to the substitution

\[ a_+(t) = a(t) - \frac{i\xi(t)}{2}, \quad \bar{a}_+(t) = a^*(t) - \frac{i\xi^*(t)}{2}, \quad a_-(t) = a(t) + \frac{i\xi(t)}{2}, \quad \bar{a}_-(t) = a^*(t) + \frac{i\xi^*(t)}{2}. \] (96)

These relations imply that

\[ a^*_+(t) = \bar{a}_-(t), \quad a^*_-(t) = \bar{a}_+(t). \] (97)

Under this condition the symmetric Wick theorem (68) remains valid. It is also consistent with the substitution (88), which in variables \( a(t), \xi(t) \) becomes,

\[ a(t) \to \alpha(t), \quad a^*(t) \to \alpha^*(t), \quad \xi(t) \to 0. \] (98)

In the below we assume that Eq. (97) holds.

C. Response in the Wigner representation

Continuing the analogy with Ref. [31], we impose the condition,

\[ -i\zeta_- a_-(t) - i\zeta_- \bar{a}_-(t) + i\zeta_+ a_+(t) + i\zeta_+ \bar{a}_+(t) = \zeta(t)a^*(t) + \zeta^*(t)a(t) + \xi(t)\sigma^*(t) + \xi^*(t)\sigma(t), \] (99)

on the linear form in Eq. (89). This results in another substitution, this time in functionals (73) and (57):

\[ \zeta_+(t) = \sigma(t) - \frac{i\zeta(t)}{2}, \quad \bar{\zeta}_+(t) = \sigma^*(t) - \frac{i\zeta^*(t)}{2}, \quad \zeta_-(t) = \sigma(t) + \frac{i\zeta(t)}{2}, \quad \bar{\zeta}_-(t) = \sigma^*(t) + \frac{i\zeta^*(t)}{2}. \] (100)

The inverse substitution reads,

\[ \zeta(t) = i[\zeta_+(t) - \zeta_-(t)], \quad \zeta^*(t) = i[\bar{\zeta}_+(t) - \bar{\zeta}_-(t)], \quad s(t) = \frac{1}{2}[\zeta_+(t) + \zeta_-(t)], \quad s^*(t) = \frac{1}{2}[\bar{\zeta}_+(t) + \bar{\zeta}_-(t)]. \] (101)

The inverse substitution reads,

\[ \zeta(t) = i[\zeta_+(t) - \zeta_-(t)], \quad \zeta^*(t) = i[\bar{\zeta}_+(t) - \bar{\zeta}_-(t)], \quad s(t) = \frac{1}{2}[\zeta_+(t) + \zeta_-(t)], \quad s^*(t) = \frac{1}{2}[\bar{\zeta}_+(t) + \bar{\zeta}_-(t)]. \] (101)

showing that (100) is a genuine change of functional variables. Similar to Eqs. (96) and (97), these relations impose conditions on the functional arguments,

\[ \zeta^*_+(t) = \bar{\zeta}_-(t), \quad \zeta^*_-(t) = \bar{\zeta}_+(t). \] (102)

These conditions do not interfere with (96) and (97) serving as characteristic functionals for the corresponding Green function, nor with (100) being a one-to-one substitution.

By definition, the generalised multitime Wigner representation emerges by applying substitution (100) to functionals (96) and (97). To start with, we note that the replacement,

\[ \zeta_{\pm}(t) \to \zeta_{\pm}(t) + s(t), \quad \bar{\zeta}_{\pm}(t) \to \bar{\zeta}_{\pm}(t) + s(t). \] (103)

cf. Eq. (88), in variables \( \zeta(t), \sigma(t) \) becomes simply,

\[ \sigma(t) \to \sigma(t) + s(t), \] (104)

with variable \( \zeta(t) \) unaffected. In variables \( \zeta(t), \sigma(t) \) functionals “with and without the sources” are naturally expressed by a single functional \( \Phi^W \),

\[ \Phi^W[\zeta, \bar{\zeta}^* | \sigma, \sigma^*] = \Xi^W[\sigma + \frac{i\zeta}{2}, \sigma^* + \frac{i\zeta^*}{2}, \sigma - \frac{i\zeta}{2}, \sigma^* - \frac{i\zeta^*}{2}], \]

\[ \Phi^W[\zeta, \bar{\zeta}^* | \sigma + s, \sigma^* + s^*] = \Xi^W[\sigma + \frac{i\zeta}{2}, \sigma^* + \frac{i\zeta^*}{2}, \sigma - \frac{i\zeta}{2}, \sigma^* - \frac{i\zeta^*}{2} | s, s^*]. \] (105)

We see that the functional variable \( \sigma(t) \) corresponds to the formal input of the system, which in turn is specified by the formal c-number source added to the Hamiltonian. We emphasise formality of both concepts. Under macroscopic conditions, an external source may become a good approximation for a laser (say). Importantly, even in this case, it remains a phenomenological model for a complex quantum device.

D. Time-symmetric operator ordering

If \( \sigma(t) \) defines an input of the system, what does the output defined by variable \( \zeta(t) \) stand for? Following [3], we postulate that, in the Wigner representation, the formal output of a system is expressed by time-symmetric averages
of the Heisenberg field operators,

\[
\langle T^W \exp \left( \zeta^* \hat{\mathcal{A}}^\dagger + \zeta \hat{\mathcal{A}} \right) \rangle \equiv \Phi^W [\zeta, \zeta^* | s, s^*] = \Xi^W \left[ \frac{i \zeta}{2}, \frac{i \zeta^*}{2}, -\frac{i \zeta}{2}, -\frac{i \zeta^*}{2} \right] |s, s^*\rangle. \tag{106}
\]

For the operator without the source,

\[
\langle T^W \exp \left( \zeta^* \hat{\mathcal{A}}^\dagger + \zeta \hat{\mathcal{A}} \right) \rangle \equiv \Phi^W [\zeta, \zeta^* | 0, 0] = \Xi^W \left[ \frac{i \zeta}{2}, \frac{i \zeta^*}{2}, -\frac{i \zeta}{2}, -\frac{i \zeta^*}{2} \right]. \tag{107}
\]

Then,

\[
\langle T^W \hat{A}_{k_1}(t_1) \cdots \hat{A}_{k_m}(t_m) \hat{A}_{k_m+1}^\dagger(t_{m+1}) \cdots \hat{A}_{k_m+m}^\dagger(t_{m+m}) \rangle
\]

\[
= \frac{\delta^{m+m} \Xi^W \left[ \frac{i \zeta}{2}, \frac{i \zeta^*}{2}, -\frac{i \zeta}{2}, -\frac{i \zeta^*}{2} \right]}{\delta \zeta_{k_1}(t_1) \cdots \delta \zeta_{k_m}(t_m) \delta \zeta_{k_{m+1}}(t_{m+1}) \cdots \delta \zeta_{k_{m+m}}(t_{m+m})} \big|_{\zeta=0}, \tag{108}
\]

and similarly for the primed operator.

It is easy to prove that Eq. (108) agrees with the recursive definition of section (111). Explicitly,

\[
\Xi^W \left[ \frac{i \zeta}{2}, \frac{i \zeta^*}{2}, -\frac{i \zeta}{2}, -\frac{i \zeta^*}{2} \right] = \langle T^W \exp \left( \frac{1}{2} \zeta^* \hat{\mathcal{A}}^\dagger + \frac{1}{2} \zeta \hat{\mathcal{A}} \right) T^W \exp \left( \frac{1}{2} \zeta^* \hat{\mathcal{A}}^\dagger + \frac{1}{2} \zeta \hat{\mathcal{A}} \right) \rangle. \tag{109}
\]

For simplicity we assume that all times on the LHS of (108) are different. We can then also assume that

\[
\zeta_k(t) = \sum_{l=1}^{m+m} \zeta_{l,k}(t) = \zeta_{1,k}(t) + \zeta_{k}(t), \tag{110}
\]

where \( \zeta_{l,k}(t) \) is nonzero only in close vicinity of \( t_l \), and that different \( \zeta_{l,k}(t) \) do not overlap. Furthermore, if \( t_1 \) is the smallest time in (108), isolating in (109) the contribution linear in \( \zeta_1 \) we can write

\[
\Xi^W \left[ \frac{i \zeta}{2}, \frac{i \zeta^*}{2}, -\frac{i \zeta}{2}, -\frac{i \zeta^*}{2} \right] \big|_{\text{linear in } \zeta_1} = \left\langle \left( \frac{1}{2} \zeta_1 \hat{\mathcal{A}} \right) \left( T^W \exp \left( \frac{1}{2} \zeta^* \hat{\mathcal{A}}^\dagger + \frac{1}{2} \zeta \hat{\mathcal{A}} \right) T^W \exp \left( \frac{1}{2} \zeta^* \hat{\mathcal{A}}^\dagger + \frac{1}{2} \zeta \hat{\mathcal{A}} \right) \right) \right\rangle
\]

\[
= \left\langle \left( \frac{1}{2} \zeta^* \hat{\mathcal{A}}^\dagger \right) \left( T^W \exp \left( \frac{1}{2} \zeta^* \hat{\mathcal{A}}^\dagger + \frac{1}{2} \zeta^* \hat{\mathcal{A}} \right) T^W \exp \left( \frac{1}{2} \zeta^* \hat{\mathcal{A}}^\dagger + \frac{1}{2} \zeta^* \hat{\mathcal{A}} \right) \right) \left( \frac{1}{2} \zeta_1 \hat{\mathcal{A}} \right) \right\rangle. \tag{111}
\]

The square brackets of the RHS of this formula delineate the range to which the remaining time orderings are applied. Clearly equation (111) is nothing but an elaborate form of the recursive definition (118). The case when the “earliest” operator is one of the \( \hat{\mathcal{A}} \)'s follows by complex conjugation of (111).

VI. DYNAMICS IN PHASE-SPACE

A. Phase-space path integral

Physically, the most natural way of looking at the system is through time-symmetric averages of the field operator in the presence of the source. Their characteristic functional \( \Phi^W [\zeta, \zeta^* | s, s^*] \) is given by Eq. (106). On the one hand, it allows one full access to quantum properties of the system expressed by Perel-Keldysh Green functions (72). On the other hand, it has an obvious phase-space interpretation found by generalising Eq. (44) to Heisenberg operators. This equation may be written as,

\[
\langle T^W \exp \left( \zeta^* \hat{a} + \zeta \hat{a}^\dagger \right) \rangle = \exp (\zeta^* \hat{\alpha} + \zeta \hat{\alpha}^\dagger), \tag{112}
\]

where, we remind,

\[
\zeta^* \hat{a} = \sum_{k=1}^{N} \int dt \zeta_k^*(t) \hat{a}_k(t), \quad \zeta \hat{a}^* = \sum_{k=1}^{N} \int dt \zeta_k(t) \hat{a}_k(t), \tag{113}
\]

and similarly for other “products.” Functions \( \alpha_k(t) = \alpha_k e^{-\omega_k t} \) depend on the initial condition \( \alpha \). The bar in
(112) symbolises quasi-averaging over the Wigner function, cf. Eq. (114). Following the pattern of Eq. (112) we postulate the path-integral representation of the functional (106),
\[
\langle T^W \exp \left( \zeta^* \mathcal{A}' + \zeta \mathcal{A}'^t \right) \rangle = \exp \left( \mathcal{S}^* + \mathcal{S} \right)_{S,S^*}. \tag{114}
\]

In this relation, \(a(t)\) is the c-number phase-space trajectory, and the bar denotes a path integral over these trajectories. We assume that trajectories obey the generic equation (93), making them dependent (conditional) on the external source \(s(t)\) and on the initial condition \(a\). The bar includes quasi-averaging over the initial condition and the own quasi-stochasticity of trajectories coming from the self-action source \(\tilde{s}_k(t)\) in (93). For comparison, in (112) the quasi-averaging is over the initial condition while the way trajectories evolve in time is non-stochastic.

B. Closed perturbative relations in the Wigner representation

Rewriting Eq. (83) in variables \(a(t), \sigma(t), \zeta(t), \) and \(\xi(t)\) defined by Eqs. (101) and (96), and replacing \(\sigma(t)\) by \(s(t)\), we obtain
\[
\langle T^W \exp \left( \zeta^* \mathcal{A}' + \zeta \mathcal{A}'^t \right) \rangle = \int \frac{d^2 \alpha_1}{\pi} \cdots \frac{d^2 \alpha_N}{\pi} W(\alpha, \alpha^*) \left\{ \exp \left( \frac{\delta}{\delta \alpha} G_R \frac{\delta}{\delta \zeta^*} + \frac{\delta}{\delta \alpha^*} G_R^* \frac{\delta}{\delta \zeta} \right) \right. \\
\times \exp \left( \zeta a^* + \zeta^* a + \zeta s^* + \zeta^* s + S^W[\zeta, \zeta^* | a, a^*] \right) \right\}_{a(t) \to \alpha(t), \zeta(t) \to 0}, \tag{115}
\]
where
\[
S^W[\zeta, \zeta^* | a, a^*] = i \int dt \left[ H^W_1 \left( a(t) + \frac{i \xi(t)}{2}, a^*(t) + \frac{i \zeta^*(t)}{2} \right) - H^W_2 \left( a(t) - \frac{i \xi(t)}{2}, a^*(t) - \frac{i \zeta^*(t)}{2} \right) \right]. \tag{116}
\]
For better understanding of Eq. (115) the reader should reread the comments following Eq. (83).

C. Multitime-Wigner equations for the Bose-Hubbard model

Equations (115), (116) are general and hold for any interaction specified by its symmetrically ordered form \(H^W_1\). For the Bose-Hubbard chain we find (omitting time arguments in the integrand)
\[
S^W[\zeta, \zeta^* | a, a^*] = - \sum_{k=1}^{N} \int dt \left\{ \kappa \left[ \left( \xi^*_{k} a^*_{k} + \xi^*_{k} a^*_{k+1} \right) \right] - \frac{\kappa}{4} \left( \xi^*_{k} a^*_{k} + \xi^*_{k} a^*_{k+1} \right) \right. \\
\left. - J \left( \xi^*_{k} a^*_{k+1} + \xi^*_{k+1} a_{k+1} + \xi^*_{k+1} a_{k+1} \right) \right\}. \tag{117}
\]
As was shown in (31), Eq. (115) may be interpreted as a solution to the generic stochastic equation in phase space formulated in section (5A). The random source in Eq. (91) is characterised by its averages conditioned on the “local field” \(a_k(t)\),
\[
\exp \sum_{k=1}^{N} \int dt \left[ \xi^*_{k}(t) \tilde{s}_k(t) + \xi_{k}(t) \tilde{s}^*_k(t) \right]_{a} = \exp S^W[\zeta, \zeta^* | a, a^*], \tag{118}
\]
so that \(S^W[\zeta, \zeta^* | a, a^*] \) is a characteristic functional for the cumulants of the random source. For the Bose-Hubbard model we have,
\[
\tilde{s}_k(t) = - \kappa a_{k}(t) ||a_{k}(t)||^2 - 1 \\
+ J [a_{k+1}(t) + a_{k-1}(t)] + \tilde{s}^{(3)}(t), \tag{119}
\]
where the actual random contribution comes from the third-order noise \(\tilde{s}^{(3)}(t)\). It is specified by the conjugate
pair of nonzero cumulants,
\[
\langle \frac{s_k^{(3)}(t)}{s_k^{(3)}(t')} \rangle_a^{(3)}(t''') = \delta_{kk'} \delta_{kk''} \delta(t-t') \delta(t''-t''') \frac{K_{kk}(t)}{2},
\]
while all other cumulants of \(s_k^{(3)}(t)\) are zero (this allowed us to specify the average in place of the cumulant). While the Wigner function responsible for the initial condition
\[
G_{R}(t) \sim \theta(t),
\]
with \(\theta(t)\) being the unit step function, one may assume, for instance, that
\[
G_{R}(t) = i\theta(t)(1-e^{-i\Lambda t})^m e^{-i\omega_0 t},
\]
where \(\Lambda \rightarrow \infty\) is implied. The regularised Green function is zero at \(t = 0\) and has \(m-1\) zero derivatives. Equation \(121\) is a toy version of the Pauli-Villars regularisation used in the quantum field theory \(48, 49\) as part of the common renormalisation procedure (cf. also \(46\)).

D. The truncated Wigner representation

Dropping the third-order noise turns the full Wigner representation into the so-called truncated Wigner representation. In more traditional phase-space techniques, the truncated Wigner is found by dropping the third-order derivatives in the generalised Fokker-Planck equation for the single-time Wigner distribution. In the absence of losses, the corresponding Langevin equation is non-stochastic. For the Hamiltonian \(70\), it coincides with Eq. \(91\), where the source is given by \(119\) without \(s_k^{(3)}\). However simple and straightforward, the conventional way of deriving the truncated Wigner leaves it unclear if it can be applied to any multitime quantum averages. In our approach here as well as in Ref. \(1\) the truncated-Wigner equations emerge as an approximation within rigorous techniques intended for calculation of the time-symmetric averages of the Heisenberg operators. The generalisation associated with extending the truncated-Wigner equations to multitime averages is thus highly nontrivial and requires a new concept: the time-symmetric ordering of the Heisenberg operators. There does not seem to be a way of guessing this concept from within the conventional phase-space techniques.

VII. THE CAUSAL REGULARISATION

Strictly speaking, all relations derived so far are leading considerations that require specifications. Two things need to be warranted: that the functional form of the symmetric Wick theorem conforms with the specification of \(T_W^+\) as symmetric ordering for coinciding time arguments, and that the stochastic integral equation \(22\) is defined mathematically. In Ref. \(31\), both problems were taken care of “in a single blow” by the causal regularisation \(31, 41, 46, 47\) of the retarded Green function \(G_R(t)\), cf. Eq. \(42\). Namely, \(G_R(t)\) should be replaced by a sufficiently smooth function while preserving its causal nature, \(G_R(t) \sim \theta(t)\). One may assume, for instance, that
\[
G_R(t) = i\theta(t)(1-e^{-\Gamma t})^m e^{-i\omega_0 t},
\]
where the limit \(\Gamma \rightarrow \infty\) is implied. The regularised Green function is zero at \(t = 0\) and has \(m-1\) zero derivatives. Equation \(121\) is a toy version of the Pauli-Villars regularisation used in the quantum field theory \(48, 49\) as part of the common renormalisation procedure (cf. also \(46\)).

In this paper as well as in \(31\), the causal regularisation of \(G_R(t)\) has a two-fold effect. Firstly, it assigns mathematical sense to equations \(61, 63\), defining them as Ito equations. In \(31\), this was in agreement with the more traditional approach based on pseudo-distributions and generalised Fokker-Planck equations \(50\). Furthermore, with \(G_R(t)\) regularised, equation \(64\) assures that the kernels \(G_W^W(t)\) are smooth functions and
\[
G_W^W(0) = 0
\]
without any mathematical ambiguity. As a result, the symmetric Wick theorem \(68\) leaves alone any product of operators with equal time arguments. Since the final expression in \(68\) is ordered symmetrically, the symmetric ordering is also enforced for any same-time product on the LHS of \(68\). Regularisation \(121\) applied to the symmetric Wick theorem \(68\) thus indeed specifies the double-time-ordered product \(53\) so that operators with equal time arguments are ordered symmetrically.

An unwanted effect of regularisation is that symmetric ordering is also enforced for same-time groups of operators split between the \(T_+^W\) and \(T_W^W\) orderings. For example, with regularisation,
\[
T_+^W \hat{a}_{kk'}(t') T_W^W \hat{a}_k(t) = W\hat{a}_k(t)\hat{a}_{kk'}^\dagger(t')
\]
\[
- \delta_{kk'} \left(1-e^{-\Gamma |t-t'|} \right)^m e^{-i\omega_0 |t-t'|}. \quad (123)
\]
This problem was also encountered in \(31\), and the solution to it remains the same: the limit \(\Gamma \rightarrow \infty\) should always precede \(t' \rightarrow t\). Then,
\[
T_+^W \hat{a}_{kk'}^\dagger(t) T_W^W \hat{a}_k(t)
\]
\[
= \lim_{\Gamma \rightarrow \infty} \lim_{t' \rightarrow t} T_+^W \hat{a}_{kk'}^\dagger(t') T_W^W \hat{a}_k(t)
\]
\[
= W\hat{a}_k(t)\hat{a}_{kk'}^\dagger(t) - \delta_{kk'} = \hat{a}_{kk'}(t)\hat{a}_k(t) \quad (124)
\]
as expected. The general recipe is to keep time arguments of operators under the \(T_+^W\) and \(T_W^W\) orderings slightly different, which is equivalent to ignoring regularisation of \(G_W^W\) and \(G_W^{W+}\). This recipe implies that the double-time-ordered averages in the limit \(\Gamma \rightarrow \infty\) are continuous functions of all time differences \(t_+ - t_-\), where \(t_+\) and \(t_-\) are time arguments of an operator pair split between the \(T_W^W\) and \(T_W^W\) orderings. This is obviously consistent with
continuity properties of the \(G_W^{(-)}\) and \(G_W^{(+)}\) kernels,

\[
\lim_{t \to 0^+} G_W^{(-)}(t) = \lim_{t \to 0^-} G_W^{(+)}(t) = G_W^{(0)},
\]

\[
\lim_{t \to 0^+} G_W^{(-)}(t) = \lim_{t \to 0^-} G_W^{(+)}(t) = G_W^{(0)},
\]  

(125)

where \(G_W^{(-)}\) and \(G_W^{(+)}\) are unregularised kernels. With this amendment all specifications enforced by regularisation only apply to operators under the time orderings. In fact, we only need to specify the \(T^W\)-ordering, defining it as time ordering for different times and symmetric ordering for equal times. The \(T^W\)-ordering remains defined by (57). We return to the problem of “unwanted effects” of regularisation in the next section.

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**VIII. THE REORDERING PROBLEM**

Assume we know a way of calculating time-symmetric averages of Heisenberg operators while the physics demand time-normal ones, or vice versa. For two-time averages this problem is solved by Kubo’s formula for the linear response function \((29, 30)\), cf. Refs. \((1, 51)\). Here we consider a general approach to reordering Heisenberg operators. Among other results we show that this always reduces to considering a response problem of sorts.

It is instructive to compare the formulae relating the time-symmetric and time-normal averages to the Perel-Keldysh Green functions \((22)\):

\[
\Phi^W [\zeta, \zeta^* | s, s^*] = 2 \mathbb{E}^{W} \left[ \frac{i \zeta}{2} + s, \frac{i \zeta^*}{2} + s^*, \frac{-i \zeta}{2} + s, \frac{-i \zeta^*}{2} + s^* \right],
\]

\[
\Phi^N [\zeta, \zeta^* | s, s^*] = \mathbb{E}^{N} [\frac{i \zeta}{2} + s, \frac{i \zeta^*}{2} + s^*, \frac{-i \zeta}{2} + s, \frac{-i \zeta^*}{2} + s*].
\]

(126)

(127)

cf. section \((\text{X})\). The functionals \(\mathbb{E}^{W}\) and \(\mathbb{E}^{N}\) are both characteristic ones for Green functions \((22)\) but imply different specifications for coinciding time arguments: \((126)\) implies symmetric ordering while \((127)\) — normal ordering. Such specifications only become of importance if Green functions (or their linear combinations) are considered for coinciding time arguments, and otherwise can be disregarded.

Mathematically, \(\mathbb{E}^{W}\) and \(\mathbb{E}^{N}\) coincide up to a singular part. Hence, up to singular parts, the functionals \(\Phi^W\) and \(\Phi^N\) differ only in a functional substitution applied to Eq. \((73)\). Time-symmetric averages appear with

\[
\begin{align*}
\eta_- &= \frac{i \zeta}{2} + s, & \eta_-^* &= \frac{i \zeta^*}{2} + s^*, \\
\eta_+ &= \frac{-i \zeta}{2} + s, & \eta_+^* &= \frac{-i \zeta^*}{2} + s^*,
\end{align*}
\]

(128)

while the time-normal ones require

\[
\begin{align*}
\eta_- &= i \zeta + s, & \eta_-^* &= s^*, \\
\eta_+ &= s, & \eta_+^* &= -i \zeta^* + s^*.
\end{align*}
\]

(129)

Both Eqs. \((128)\) and \((129)\) may be inverted, and it is straightforward to show that

\[
\Phi^W [\zeta, \zeta^* | s, s^*] = \Phi^N \left[ \frac{\zeta}{2} + s, \frac{\zeta^*}{2} + s^* \right],
\]

\[
\Phi^N [\zeta, \zeta^* | s, s^*] = \Phi^W \left[ \frac{i \zeta}{2} + s, \frac{i \zeta^*}{2} + s^* \right].
\]

(130)

In particular, for the time-normal and time-symmetric averages defined without the source we have

\[
\Phi^W [\zeta, \zeta^* | 0, 0] = \Phi^N \left[ -\frac{i \zeta}{2}, -\frac{i \zeta^*}{2} \right],
\]

\[
\Phi^N [\zeta, \zeta^* | 0, 0] = \Phi^W \left[ \frac{i \zeta}{2}, -\frac{i \zeta^*}{2} \right].
\]

(131)

These relations make it evident that the reordering problem for the Heisenberg operators is indeed equivalent to the response problem.

We remind the reader that Eqs. \((130)\) and \((131)\) hold only up to a singular part. All formulae for quantum averages following from them are only valid for different time arguments and otherwise require specifications.

We now consider an example which also illustrates how to approach coinciding time arguments. We wish to express the time-normal average

\[
\langle \hat{A}^{(1)}_k(t) \hat{A}^{(2)}_{k'}(t') \rangle = \frac{\delta^2 \Phi^N [\zeta, \zeta^* | 0, 0]}{\delta \zeta_k(t) \delta \zeta_k^*(t')} |_{\zeta = 0}
\]

(132)

by the time-symmetric ones. Combining \((132)\) with the second of Eqs. \((131)\) we have

\[
\langle \hat{A}^{(1)}_k(t) \hat{A}^{(2)}_{k'}(t') \rangle = \langle T^W \hat{A}^{(1)}_k(t) \hat{A}^{(2)}_{k'}(t') \rangle
\]

\[
+ \frac{i}{2} \left[ \frac{\delta \langle \hat{A}^{(1)}_k(t) \hat{A}^{(2)}_{k'}(t') \rangle}{\delta \zeta_k(t)} - \frac{\delta \langle \hat{A}^{(1)}_k(t) \hat{A}^{(2)}_{k'}(t') \rangle}{\delta \zeta_k^*(t')} \right] |_{s = 0}.
\]

(133)

In deriving this we used that

\[
\Phi^{W,N}(0, 0 | s, s^*) = 1,
\]

(134)

so that the derivatives purely by input arguments always disappear. In \((1)\), Eq. \((133)\) was derived by an ad hoc
method; here we show that the same relation follows from the general equations (131). For details on numerical implementation of Eq. (133) see 1.

Equation (133) is well behaved in the limit $t' \to t$. For instance, let $t' > t$. Then, by causality [32],

$$\frac{\delta \langle \hat{A}_k^{\dagger}(t) \rangle}{\delta s_k(t')} = 0. \quad (135)$$

Using (21) we rewrite (133) as

$$\frac{\delta \langle \hat{A}_k^{\dagger}(t') \rangle}{\delta s(t)} \bigg|_{s=0} = i \left\langle \left[ \hat{A}_k^{\dagger}(t'), \hat{A}_k(t) \right] \right\rangle, \quad t' > t. \quad (136)$$

We have thus rederived Kubo’s famous relation for the linear response function. Both sides here have a well-defined limit $\delta t_k k^r$ for $t \to t'$. Similarly,

$$\frac{\delta \langle \hat{A}_k^{\dagger}(t) \rangle}{\delta s_k(t')} \bigg|_{s=0} = -i \left\langle \left[ \hat{A}_k(t'), \hat{A}_k(t) \right] \right\rangle, \quad t > t'. \quad (137)$$

which is nothing but complex conjugation of (135) with the replacement $t \leftrightarrow t'$.

At the same time, Eq. (133) resists any attempt to extend it to equal time arguments. Within the causal regularisation,

$$\frac{\delta \langle \hat{A}_k^{\dagger}(t) \rangle}{\delta s_k(t)} = \frac{\delta \langle \hat{A}_k^{\dagger}(t) \rangle}{\delta s_k(t')} = 0, \quad (138)$$

giving rise to a patently wrong result,

$$\langle \hat{A}_k^{\dagger}(t) \hat{A}_k(t) \rangle = \langle T^W \hat{A}_k^{\dagger}(t) \hat{A}_k(t) \rangle. \quad (139)$$

Conversely, making the response correction in (133) nonzero for $t = t'$ inevitably causes troubles with causality under regularisation. This shows, in particular, that the “unwanted effects” of regularisation (see section VII) are unavoidable and cannot be eliminated by a better regularisation scheme. For this reason we regard it as “good conduct” to treat all quantum averages as generalised functions, making the question of their values at coinciding time arguments meaningless.

IX. CONCLUSIONS

We have developed a generalisation of the symmetric-ordered to multitime problems with nonlinear interactions. This includes generalisation of the symmetric (Weyl) ordering to time-symmetric ordering of Heisenberg operators, and of the renowned Wigner function to a path integral in phase-space. Among other results, continuity of time-symmetric operator products has been proven. A way of calculating time-normally-ordered operator products within the time-symmetric-ordering-based techniques has also been developed.

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Appendix: Structural symmetric Wick theorem for a pair of fields

In this appendix, we formulate an ultimate generalisation of the symmetric Wick theorem. It appears to cover all imaginable cases of interest and, if necessary, can be extended to fermionic fields. Firstly, let $\tau$ be a generalised time variable which belongs to some linearly ordered set with the succession symbol $\succ$. Of practical relevance are the time axis and the C-contour. Secondly, let $\hat{X}(\xi, \tau), \hat{\chi}(\xi, \tau)$ be a pair of free-field operators defined in some Fock space, (in this appendix $\hbar \neq 1$)

$$\hat{X}(\xi, \tau) = \sqrt{\hbar} \sum_{\kappa} \left[ u_{\kappa}(\xi) \hat{a}_{\kappa}(\tau) + v_{\kappa}(\xi) \hat{b}_{\kappa}(\tau) \right],$$

$$\hat{\chi}(\xi, \tau) = \sqrt{\hbar} \sum_{\kappa} \left[ \bar{u}_{\kappa}(\xi) \hat{a}^\dagger_{\kappa}(\tau) + \bar{v}_{\kappa}(\xi) \hat{b}^\dagger_{\kappa}(\tau) \right]. \quad (A.1)$$

Here, $\xi$ symbolises arguments of field operators except time; $\xi$ can contain coordinate, momentum, spin indices, and so on. The index $\kappa$ enumerates the modes of which the Fock space is built. With extensions to relativity or solid state in mind, for each mode we define two pairs of creation and annihilation operators,

$$\hat{a}_{\kappa}(\tau) = e^{-i \varphi_{\kappa}(\tau)} \hat{a}_{\kappa}, \quad \hat{a}^\dagger_{\kappa}(\tau) = e^{i \varphi_{\kappa}(\tau)} \hat{a}^\dagger_{\kappa},$$

$$\hat{b}_{\kappa}(\tau) = e^{-i \varphi_{\kappa}(\tau)} \hat{b}_{\kappa}, \quad \hat{b}^\dagger_{\kappa}(\tau) = e^{i \varphi_{\kappa}(\tau)} \hat{b}^\dagger_{\kappa}. \quad (A.2)$$

The phases $\varphi_{\kappa}(\tau)$ are c-number functions of “time;” note that Eq. (A.2) employs one phase for “particles and antiparticles” in each mode. The stationary operators obey standard commutational relations,

$$[\hat{a}_{\kappa}, \hat{a}^\dagger_{\kappa'}] = [\hat{b}_{\kappa}, \hat{b}^\dagger_{\kappa'}] = \delta_{\kappa \kappa'}. \quad (A.3)$$

Otherwise mode operators pairwise commute. The c-number functions $u_{\kappa}(\xi), \bar{u}_{\kappa}(\xi), v_{\kappa}(\xi), \bar{v}_{\kappa}(\xi)$ are replaced in particular problems by suitable solutions of a single-body equation. In nonrelativistic problems, $v_{\kappa}(\xi) = \bar{v}_{\kappa}(\xi) = 0$. For our purposes here all c-number
functions in Eqs. (A.1) and (A.2) are regarded as arbitrary.

Specification of the quantities occurring in Eqs. (A.1)–(A.3) belongs to a particular problem. It is implied that such specification should meet certain conditions of algebraic consistency. For example, summation in (A.1) should be consistent with the “Kronecker symbol” in (A.20), with \( f_\kappa \) being an arbitrary function of the mode index

\[
\sum_{\kappa'} \delta_{\kappa \kappa'} f_{\kappa'} = f_\kappa. \tag{A.4}
\]

Similar consistencies should exist between integrations and corresponding delta-functions,

\[
\int d\tau' \delta(\tau, \tau') f(\tau') = f(\tau), \quad \int d\xi' \delta(\xi, \xi') f(\xi') = f(\xi). \tag{A.5}
\]

The delta-functions and Kronecker symbols are symmetric. These consistencies extend to functional differentiations by c-number functions of \( \xi \) and \( \tau \). So, for the c-number functions \( a_\kappa(\tau), \bar{a}_\kappa(\tau) \) occurring in Eqs. (A.14), (A.15),

\[
\frac{\delta a_\kappa(\tau)}{\delta a_{\kappa'}(\tau')} = \frac{\delta a_{\kappa'}(\tau')}{\delta a_\kappa(\tau)} = \delta(\tau, \tau') \delta_{\kappa \kappa'}, \quad \frac{\delta F(a)}{\delta a_\kappa(\tau)} = \frac{\delta F(a)}{\delta \bar{a}_\kappa(\tau)} = 0, \tag{A.6}
\]

and similarly for the c-number pair \( X(\xi, \tau), \bar{X}(\xi, \tau) \) in (A.10), (A.11). Conditions (A.4)–(A.6) make all relations below algebraically defined.

Linear order of the generalised time axis allows one to define the step-function,

\[
\theta(\tau, \tau') = \begin{cases} 1, & \tau > \tau', \\ 0, & \tau < \tau' \end{cases}, \tag{A.7}
\]

and the “time” ordering,

\[
T \bar{X}(\xi, \tau) \bar{X}(\xi, \tau) = \theta(\tau, \tau') \bar{X}(\xi, \tau) \bar{X}(\xi, \tau) + \theta(\tau', \tau) \bar{X}(\xi, \tau) \bar{X}(\xi, \tau), \tag{A.8}
\]

cf. Eq. (A.14). Similar definitions apply to a larger number of factors. The time-symmetric ordering is defined replacing "larger than" by "succeed" in Eq. (20):

\[
T^W \tilde{X}_1(\tau_1) \tilde{X}_2(\tau_2) \cdots \tilde{X}_n(\tau_n) = \frac{1}{2^{N-1}} \times [\cdots [[\tilde{X}_1(\tau_1), \tilde{X}_2(\tau_2)]_+, \tilde{X}_3(\tau_3)]_+, \cdots, \tilde{X}_N(\tau_N)]_+, \\
\tau_1 > \tau_2 > \cdots > \tau_N. \tag{A.9}
\]

The proof of section III.B that for the free operators symmetric and time-symmetric orderings are the same thing generalises literally with \( t \rightarrow \tau \) and \( \omega_0 t \rightarrow \varphi_\kappa(\tau) \).

The generalised structural symmetric Wick theorem that we now wish to prove reads,

\[
TP[\bar{X}, \tilde{X}] = T^W \left\{ \exp Z_\kappa \left[ \frac{\delta}{\delta a_\kappa} \frac{\delta}{\delta \bar{a}_\kappa} \right] \right\} \times P[a, \bar{a}]_{\hat{a}_\kappa \rightarrow \hat{a}_\kappa, \tilde{a}_\kappa \rightarrow \tilde{a}_k}, \tag{A.10}
\]

where \( X(\xi, \tau), \bar{X}(\xi, \tau) \) are a pair of c-number functions and,

\[
Z_\kappa \left[ \frac{\delta}{\delta a_\kappa} \frac{\delta}{\delta \bar{a}_\kappa} \right] = -i \hbar \int d\tau' d\xi d\xi' \\
\times G^W(\xi, \tau; \xi', \tau') \delta^2(\delta X(\xi, \tau) \delta X(\xi', \tau')). \tag{A.11}
\]

Applying (A.10) to \( T \tilde{X}(\xi, \tau) \tilde{X}(\xi, \tau') \) we find that \( G^W(\xi, \tau; \xi', \tau') \) coincides with the symmetric contraction of the pair (A.11),

\[
- i \hbar G^W(\xi, \tau; \xi', \tau') = T \tilde{X}(\xi, \tau) \tilde{X}(\xi', \tau') - T^W \tilde{X}(\xi, \tau) \tilde{X}(\xi', \tau'). \tag{A.12}
\]

Since all operator reorderings occur mode-wise, it suffices to verify (A.10) for one mode; the general formula then follows by direct calculation. In the one-mode case,

\[
\tilde{X}(\xi, \tau) \rightarrow \hat{a}_\kappa(\tau), \tilde{X}(\xi, \tau) \rightarrow \hat{a}_\kappa^\dagger(\tau), \quad G^W(\xi, \tau; \xi', \tau') \rightarrow G^W_\kappa(\tau, \tau') \]

\[
= i [T \hat{a}_\kappa(\tau) \hat{a}_\kappa^\dagger(\tau') - T^W \hat{a}_\kappa(\tau) \hat{a}_\kappa^\dagger(\tau'')] \\
= i \frac{1}{2} e^{-i \varphi_\kappa(\tau') + i \varphi_\kappa(\tau')} \left[ \theta(\tau, \tau') - \theta(\tau', \tau) \right], \tag{A.13}
\]

and Eq. (A.10) becomes,

\[
TP[\hat{a}, \hat{a}^\dagger] = T^W \left\{ \exp Z_\kappa \left[ \frac{\delta}{\delta a_\kappa} \frac{\delta}{\delta \bar{a}_\kappa} \right] \right\} \times P[\hat{a}, \hat{a}^\dagger]_{\hat{a}_\kappa \rightarrow \hat{a}_\kappa, \tilde{a}_\kappa \rightarrow \tilde{a}_\kappa}, \tag{A.14}
\]

where \( a(\tau), \bar{a}(\tau) \) are a pair of arbitrary c-number functions of “time.” The “per mode” reordering exponent \( Z_\kappa \) reads,

\[
Z_\kappa \left[ \frac{\delta}{\delta a_\kappa} \frac{\delta}{\delta \bar{a}_\kappa} \right] = -i \int d\tau' d\tau' G^W_\kappa(\tau, \tau') \frac{\delta^2}{\delta a(\tau) \delta \bar{a}(\tau')}. \tag{A.15}
\]

Verification of Eq. (A.14) goes in two steps. Firstly, we note that the equivalence between the verbal and algebraic forms of Wick’s theorem proper [52] does not depend on details of the contraction and hence equally applies to the symmetric Wick theorem. Secondly, the proof of the symmetric Wick theorem for the time axis in section III.B may be literally adjusted to generalised time
replacing time $t$ by $\tau$, the symbol $>$ by $\succ$, and the contraction $G^W_{\tau' \tau}(t-t')$ by $G^W(\tau, \tau')$. We therefore regard Eq. (A.14) proven.

To verify the general relation (A.10) we note that any functional depending on the mode operators may be brought to the symmetric form by applying Eq. (A.14) mode-wise:

$$TP[\hat{X}, \hat{X}] = T^W \left\{ \exp \left\{ \sum_\kappa \left( Z_\kappa \left[ \frac{\delta}{\delta a_\kappa}, \frac{\delta}{\delta a_\kappa} \right] + Z_\kappa \left[ \frac{\delta}{\delta b_\kappa}, \frac{\delta}{\delta b_\kappa} \right] \right) \right\} P[\hat{X}, \hat{X}] |_{a \to \hat{a}} \right\}. \tag{A.16}$$

In this formula, the c-number fields $X(\xi, \tau), \hat{X}(\xi, \tau)$ are given by Eq. (A.1) without hats,

$$X(\xi, \tau) = \sqrt{\hbar} \sum_\kappa [u_\kappa(\xi)a_\kappa(\tau) + v_\kappa(\xi)b_\kappa(\tau)],$$

$$\hat{X}(\xi, \tau) = \sqrt{\hbar} \sum_\kappa [\bar{u}_\kappa(\xi)a_\kappa(\tau) + \bar{v}_\kappa(\xi)b_\kappa(\tau)], \tag{A.17}$$

where $a_\kappa(\tau), \bar{a}_\kappa(\tau), b_\kappa(\tau), \bar{b}_\kappa(\tau)$ are four independent c-number fields per mode, and $a \to \hat{a}$ is a shorthand notation for the substitution,

$$a_\kappa(\tau) \to \bar{a}_\kappa(\tau), \quad \bar{a}_\kappa(\tau) \to \hat{a}_\kappa(\tau),$$

$$b_\kappa(\tau) \to \bar{b}_\kappa(\tau), \quad \bar{b}_\kappa(\tau) \to \hat{b}_\kappa(\tau). \tag{A.18}$$

The “per mode” reordering exponents are given by (A.15). Applying the chain rule to differentiations in (A.16) we get,

$$\frac{\delta}{\delta a(\tau)} P[X, \hat{X}] = \sqrt{\hbar} \int d\xi \frac{\delta}{\delta X(\xi, \tau)} P[X, \hat{X}],$$

$$\frac{\delta}{\delta \bar{a}(\tau)} P[X, \hat{X}] = \sqrt{\hbar} \int d\xi \frac{\delta}{\delta \bar{X}(\xi, \tau)} P[X, \hat{X}],$$

$$\frac{\delta}{\delta b(\tau)} P[X, \hat{X}] = \sqrt{\hbar} \int d\xi \frac{\delta}{\delta X(\xi, \tau)} P[X, \hat{X}],$$

$$\frac{\delta}{\delta \bar{b}(\tau)} P[X, \hat{X}] = \sqrt{\hbar} \int d\xi \frac{\delta}{\delta \bar{X}(\xi, \tau)} P[X, \hat{X}]. \tag{A.19}$$

Substituting these relations into Eq. (A.16) we recover Eq. (A.10) with

$$G^W(\xi, \tau; \xi', \tau') = \sum_\kappa [u_\kappa(\xi)\bar{u}_\kappa(\xi')G^W_\kappa(\tau, \tau') + v_\kappa(\xi')\bar{v}_\kappa(\xi)G^W_\kappa(\tau', \tau)]. \tag{A.20}$$

It is readily verified that this definition of $G^W(\xi, \tau; \xi', \tau')$ agrees with (A.12). The only remaining artifact of the underlying mode expansion is then the substitution (A.18). However, with everything expressed in terms of $X(\xi, \tau), \hat{X}(\xi, \tau)$, it may be replaced by

$$X(\xi, \tau) \to \hat{X}(\xi, \tau), \quad \hat{X}(\xi, \tau) \to \hat{X}(\xi, \tau). \tag{A.21}$$

This concludes the proof of Eq. (A.10).

We conclude this appendix with a remark on scaling of fields and contractions in the classical limit $\hbar \to 0$. 

\textit{Commutators of physical quantities must scale as $\hbar$.} In this sense, quantised mode amplitudes $a_\kappa$ are not physical. The physical amplitude is $\sqrt{\hbar}a_\kappa$, which in the limit $\hbar \to 0$ becomes the classical mode amplitude [53]. For this reason the factor $\sqrt{\hbar}$ is explicitly present in the definitions of “physical fields” (A.1). The scaling $\propto \hbar$ is then removed from the contraction (A.12) by the factor $\hbar$ on the LHS. The result is that, as was demonstrated in Refs. [32, 33], Green functions (propagators) of bosonic fields are to a large extent classical quantities. In particular, they are all expressed by the \textit{response transformation} in terms of the retarded Green function of the corresponding classical field. For more details see [32, 34, 53].

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