Wigner Functionals and their Dynamics in Quantum-Field-Theory

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Abstract
We reformulate time evolution of systems in mixed states in terms of the classical observables of correlators using the Weyl correspondence rule. The resulting equation of motion for the Wigner functional of the density matrix is found to be of the Liouville type. To illustrate the methods developed, we explicitly consider a scalar theory with quartic self-interaction and derive the short time behaviour with the non-interacting thermal density matrix as initial condition. In the scalar case, the complete correlator hierarchy is studied and restrictions are derived for spatially homogeneous initial conditions and systems with unbroken symmetry.

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1 Introduction

The study of statistical ensembles of quantized fields out of thermal equilibrium has a number of interesting applications. Prominent examples are the study of hot QCD matter in heavy ion collisions or the behaviour of matter in the course of cosmological phase transitions. In contrast to equilibrium theory, where considerable success has been achieved in recent years [1], the theoretical framework for the description of processes far from equilibrium still lacks a systematic basis. Although some attempts have been made to derive the first few stages of a cut BBGKY-hierarchy on the basis of equal time correlators [2] and using other methods [3], a comprehensive understanding of the interrelation between observables and the abstract Schrödinger evolution for systems of quantized fields is still incomplete.

Physics of non-equilibrium processes typically involves three elements. Firstly, the description of an initial state by means of a number of – in principle measurable – observables. Secondly, time evolution defined by a dynamical equation together with the corresponding Hamiltonian operator, and third, the observation of some quantities at later times. The second and third step can be discussed on the basis of fundamental principles. In particular, time evolution of quantum mechanical systems is encoded in the von Neumann equation which determines the time evolution of the density matrix operator. Integrating time evolution to later times, it is straightforward to extract expectation values for operators. Only the first step requires a statistical assumption about the system, since complete knowledge of the initial density matrix is usually not accessible.

In this paper we focus on the dynamical aspects of statistical ensembles of quantized fields but reformulate time evolution in terms of classical quantities instead of operator evolution. This casts the theory in a form which appears more natural when one is interested in observables. Using the effective action as dynamical object generating equal time correlators, this problem has been discussed recently [4].

Based on the Weyl correspondence principle, we consider the classical counterparts for quantum mechanical operators and the density matrix. Starting with the von Neumann equation, we focus on the construction of a dynamical equation of the Liouville type for the classical counterpart of the density matrix operator. In order to illustrate the abstract result, we derive an expression for the Weyl transform of the non-interacting equilibrium density matrix and use it as an initial condition for the time evolution in an interacting system. We find that mass resummation is necessary in order to obtain a sensible physical result. Furthermore, we explicitly derive the hierarchy of equations of motion for general initial conditions for the model of a scalar field with quartic interaction. Particular conditions on field correlators for systems which exhibit spatial homogeneity and with unbroken symmetry are studied systematically.

2 Quantum-mechanics
2.1 General

In order to outline the concepts applied, we demonstrate the basic steps using a zero-dimensional quantum mechanical system as example. A harmonic one-dimensional oscillator is defined by the Hamiltonian $H = \omega a^\dagger a$ which Fock-space is spanned by the eigenstates of $H$. Systems in mixed states are described by a hermitian density matrix operator $\hat{\rho}$, normalized to unity. Expectation values of operators $\hat{A}$ are given by the trace $\langle \hat{A} \rangle = \text{tr} \hat{\rho} \hat{A}$ which is independent of the basis chosen. It can be calculated in energy-eigenstates or in position eigenstates as well,

$$\langle \hat{A} \rangle = \sum_n < n | \hat{\rho} | n > = \int dx < x | \hat{\rho} | x > .$$  \hspace{1cm} (1)

2.2 Weyl-correspondence principle

Each operator is sub-ordinated a classical observable in a state by taking the trace of the product with the density operator. An observable defined in such a way depends on the particular mixed state of the system under consideration. One may thus ask if it is possible to define the corresponding classical quantity independent of any particular density matrix, which in a more universal way permits to calculate observables in a given state. This is in fact possible by the Weyl correspondence rule \cite{5}. Suppose we can decompose an operator as

$$\hat{A} = \int d\sigma d\tau \tilde{A}(\sigma, \tau) e^{i\sigma \hat{p} + i\tau \hat{x}},$$  \hspace{1cm} (2)

where $\hat{x}$ and $\hat{p}$ are the canonical position and momentum operators resp., the corresponding classical function is defined to have the same Fourier transform,

$$A(p, x) = \int d\sigma d\tau \tilde{A}(\sigma, \tau) e^{i\sigma p + i\tau x}. \hspace{1cm} (3)$$

So far, this is only a definition of the classical counterpart. In order to justify it, we consider the quantum-mechanical expectation value of an operator in a mixed state and represent it in terms of the classical functions of the operator and the density matrix,

$$\langle \hat{A} \rangle = \int dx \int d\sigma d\tau d\sigma' d\tau' \tilde{A}(\sigma, \tau) \tilde{\rho}(\sigma', \tau') < x | e^{i\sigma \hat{p} + i\tau \hat{x}} e^{i\sigma' \hat{p} + i\tau' \hat{x}} | x > .$$  \hspace{1cm} (4)

Using $[\hat{p}, \hat{x}] = -i$, $\hat{x} | x > = x | x >$, $\exp(i\rho \hat{p}) | x > = | x - r >$, and the Campbell-Baker-Hausdorff formula,

$$e^{(\hat{A} + \hat{B})} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}[\hat{A}, \hat{B}]}, \hspace{1cm} \text{if} \hspace{1cm} [\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$$

one finds

$$\int dx \int d\sigma d\tau d\sigma' d\tau' \tilde{\rho}(\sigma, \tau) \tilde{A}(\sigma', \tau') < x + \sigma + \sigma' | x > e^{i\frac{1}{2}((\sigma - \sigma') + i(\tau + \tau')) x}, \hspace{1cm} (5)$$

and finally on account of the orthogonality of position eigenfunctions,

$$\langle \hat{A} \rangle = 2\pi \int d\sigma d\tau \tilde{\rho}(\sigma, \tau) \tilde{A}(-\sigma, -\tau). \hspace{1cm} (6)$$
That reads, in terms of the classical counterparts of $\hat{A}$ and the density matrix,

$$< \hat{A} > = \int dp \int dx \rho(p, x) A(p, x). \tag{7}$$

We conclude: A quantum-mechanical expectation value can be written in a form analogous to classical mechanics where the classical counterparts of the operator and the density matrix are given by the Weyl correspondence principle. The classical density operator $\rho(p, x)$ is commonly called Wigner function.

It should be pointed out that the correspondence rule implies a symmetric operator ordering prescription. Thus, information about ordering of operators is lost by the transformation. However, this is an intrinsic property of any correspondence rule since the classical counterparts always commute. In other words, generally, there exist distinct operators which correspond to the same classical counterpart.

### 2.3 Wigner functions

Given a density matrix, one may ask how to calculate the classical counterpart. For that purpose, we express the Wigner function in terms of the matrix element,

$$< z | \hat{\rho} | y > = \int d\sigma d\tau \hat{\rho}(\sigma, \tau) < z | e^{i\sigma \hat{p}} e^{i\tau \hat{x}} | y >, \tag{8}$$

which evaluates, using exactly the same operator relations as above, to

$$< z | \hat{\rho} | y > = \int d\tau \hat{\rho}(y - z, \tau) e^{\frac{i}{2} \tau (y + z)}. \tag{9}$$

If we let $z = x - \frac{1}{2} \sigma$, $y = x + \frac{1}{2} \sigma$, and perform a Fourier transformation, then

$$\int d\sigma e^{i\sigma p} < x - \frac{1}{2} \sigma | \hat{\rho} | x + \frac{1}{2} \sigma > = \int d\sigma d\tau e^{i\sigma p + \tau x} \hat{\rho}(\sigma, \tau) = \rho(p, x), \tag{10}$$

which is commonly used as definition of Wigner functions [6]. The offset $\pm \frac{1}{2} \sigma$ in the definition accounts for the off-diagonal matrix elements. They are interference terms which – in contrast to the diagonal ones – cannot be given a probabilistic interpretation, but nevertheless do contribute to the classical quantities.

### 3 Representation in terms of creation and annihilation operators

So far, we worked in position (momentum) representation of quantum mechanics. In order to find a link to field theory, it turns out to be useful to go over to a Fock-space representation. To further develop our theory, we will need some definitions and relations.
3.1 Definitions and Relations

We introduce \( a, a^\dagger \) related to \( \hat{p}, \hat{x} \) by \( a = \sqrt{\omega/2\hat{x}} + i\hat{p}/\sqrt{2\omega} \) from which we get
\[
\exp(i\sigma \hat{p} + i\tau \hat{x}) = \exp(\alpha a^\dagger - \alpha^* a)
\]
with \( \alpha = (i\tau - \omega \sigma)/\sqrt{2\omega} \). The displacement operator
\[
\hat{D}(\alpha) = e^{\alpha a^\dagger - \alpha^* a} = e^{\frac{i}{2}|\alpha|^2} e^{-\alpha^* a} e^{\alpha a^\dagger}
\]  \hspace{1cm} (11)
has the following properties [7].

- **Unitarity:** \( \hat{D}^\dagger(\alpha) \hat{D}(\alpha) = 1 \)

- **Shift-operator:** \( \hat{D}^{-1}(\alpha) a \hat{D}(\alpha) = a + \alpha, \quad \hat{D}^{-1}(\alpha) a^\dagger \hat{D}(\alpha) = a^\dagger + \alpha^* \)

- **The states**
\[
|\alpha > = \hat{D}(\alpha) |0 > = e^{\frac{i}{2}|\alpha|^2} \sum_n \frac{a^n}{\sqrt{n!}} |n >
\]
are over-complete.

- **Product:**
\[
< \beta | \alpha > = e^{-\frac{i}{2}(|\alpha|^2 + |\beta|^2) + \alpha \beta^*}.
\]

- **Identity:**
\[
\frac{1}{\pi} \int d^2 \alpha |\alpha > < \alpha | = 1 \).
\]

- **Trace:**
\[
tr \hat{A} = \frac{1}{\pi} \int d^2 \alpha < \alpha | \hat{A} |\alpha >.
\]

- **Multiplication property:**
\[
tr(\hat{D}(\alpha) \hat{D}(\alpha')) = \pi \delta^2(\alpha + \alpha').
\]

- **Operator Fourier-decomposition:**
\[
\hat{A} = \int d^2 \alpha \hat{A}(\alpha) e^{\alpha a^\dagger - \alpha^* a} = \int d^2 \alpha \hat{A}(\alpha) \hat{D}(\alpha).
\]

On account of this and the pre-last relation, an observable amounts to the convolution of the Fourier-components of density matrix and operator,
\[
tr(\hat{A}) = \int d^2 \alpha \int d^2 \alpha' \hat{A}(\alpha) \hat{A}(\alpha') tr(\hat{D}(\alpha) \hat{D}(\alpha')) = \int d^2 \alpha \hat{A}(\alpha) \hat{A}(\alpha).
\]  \hspace{1cm} (12)

The Fourier components are calculated using
\[
\hat{A}(\alpha) = tr \left( \hat{A} \hat{D}(-\alpha) \right).
\]  \hspace{1cm} (13)
3.2 Time evolution

Time evolution is given by the von Neumann equation, \( i\dot{\hat{\rho}} = [H, \hat{\rho}] \), i.e. for \( \hat{\rho}(\alpha) = tr (\hat{\rho}D(-\alpha)) \),

\[
\dot{\hat{\rho}}(\alpha) = i\, tr (\hat{\rho}[H, D(-\alpha)]) .
\] (14)

3.2.1 Example: Free motion

One finds

\[
[D(-\alpha), H] = \omega (\alpha a^\dagger + \alpha^* a + \alpha \alpha^*) D(\alpha).
\]

Weightened values of creation and annihilation operators in (14) can be written as partial derivatives,

\[
tr (\hat{\rho}aD(-\alpha)) = \frac{1}{2} \alpha \dot{\hat{\rho}}(\alpha), \quad tr (\dot{\hat{\rho}}a^\dagger D(-\alpha)) = -\frac{1}{2} \alpha^* \dot{\hat{\rho}}(\alpha)
\] (15)

and the equation of motion turns into a partial differential equation

\[
i \dot{\hat{\rho}} = \omega \left( \alpha^* \frac{\partial \hat{\rho}(\alpha)}{\partial \alpha} - \alpha \frac{\partial \hat{\rho}(\alpha)}{\partial \alpha} \right) .
\] (16)

Its solution is \( \hat{\rho}(\alpha e^{-i\omega t}, \alpha^* e^{i\omega t}) \) where we imposed the initial condition \( \hat{\rho}|_{t=0} = \hat{\rho}(\alpha) \).

4 Field theory

In order to generalize the setting to field theory, a Lorentz invariant formulation is called for. In that context we encounter a fundamental problem. A Lorentz invariant definition of an inner product is based on a mass-shell condition. A priori, the latter – if it exists at all – is not known in an interacting theory. However, from a perturbative point of view, it suffices to know the inner invariant product of the non-interacting theory. This product does not pre-assume any deeper dynamic property of the full theory, but merely is a necessary starting point of a well defined perturbative expansion, which simply absorbs free motion into the interaction picture representation.

4.1 Lorentz invariant product in the free case

Particles of mass \( m \) define two hyperboloids \( k_0 = \pm \omega_k \) with energy \( \omega_k = \sqrt{k^2 + m^2} \). Real on-shell functions on space-time can be Fourier decomposed as

\[
T(t, x) = \frac{1}{(2\pi)^{3/2}} \int (d\mu^+(k) + d\mu^-(k)) e^{-ikx} \tau(k)
\] (17)

where \( d\mu^\pm(k) = d^4k \delta(k^2 - m^2) \theta(\pm k_0) \) are the measure components invariant under orthochronical homogeneous Lorentz transformations \( \in L_+ \). An invariant inner product for real fields is given by

\[
(T, \Sigma) = \int (d\mu^+(k) + d\mu^-(k)) \tau^+(k) \sigma(k) = \int d\mu^+(k)(\tau^+(k)\sigma(k) + \tau(k)\sigma^+(k))
\] (18)
which reads in position space

\[(T, \Sigma) = i \int d^3 x \left( T^*(t, x) \partial_t \Sigma(t, x) - (\partial_t T^*(t, x)) \Sigma(t, x) \right). \quad (19)\]

The direction \(\partial_t\) characterizes the space-like hyper-surface on which the quantisation is performed. The inner product is constant along that direction.

The field operator in interaction picture representation

\[\Phi_I(t, x) = \frac{1}{(2\pi)^{3/2}} \int d\mu \left[ (b(k)e^{-ikx} + b^\dagger(k)e^{ikx}) \right] \quad (20)\]

decomposed into creation and annihilation operators with commutator

\[[b(k), b^\dagger(k)] = 2\omega_k \delta^3(k - k') \quad (21)\]
evolves with the free Hamiltonian

\[H_0 = \int d\mu \left[ \omega_k b^\dagger(k)b(k) \right]. \quad (22)\]

The rescaled definition of creation and annihilation operators \(a(k) = \sqrt{2\omega_k}b(k)\) used in the previous section in the zero-dimensional case, and commonly advocated to in textbooks, was introduced and discussed by Newton and Wigner \[8\]. One may regard the corresponding wave function as a Lorentz-frame dependent probability amplitude since their scalar product in position space takes the same form as in the Schrödinger theory.

The exponent of the shift operator evaluates to

\[i(\Sigma, \Pi_I) + i(T, \Phi_I) = \int d\mu (k)(\beta(k)b^\dagger(k) - \beta^*(k)b(k)), \quad \beta(k) = i\tau(k) - \omega_k\sigma(k), \quad (23)\]

where we took into account that \(\Pi_I = \dot{\Phi}_I\). For two reasons, the definition of \(\beta\) is chosen to differ by a factor \(\sqrt{2\omega_k}\) from the analog relation for \(\alpha\). The exponent formally has a Lorentz invariant form and the properties and relations derived in the previous section can be carried over to field theory straightforwardly. In particular, the coherent states chosen as basis are created by acting with the shift operator functional in interaction picture representation

\[D_I[\beta] = \exp \left\{ \int d\mu (k)(\beta(k)b^\dagger(k) - \beta^*(k)b(k)) \right\} \quad (24)\]
on the vacuum. Note that only the introduction of a Lorentz invariant product renders the exponent time independent, which will turn out crucial in what follows.

4.2 Full dynamics

It is useful to split off free (unperturbed) motion by going to the interaction picture representation of \(\hat{\rho}\) which obeys the evolution equation

\[i\dot{\hat{\rho}}_I(t) = [W_I(t), \hat{\rho}_I(t)]. \quad (25)\]
We introduce a Wigner functional decomposition

\[ \hat{\rho}_I(t) = \int D^2 \beta \rho_I[\beta](t) D_I[\beta] \]  

(26)

and its inverse, the Wigner transform of the interacting density matrix,

\[ \rho_I[\beta](t) = \text{tr}(\hat{\rho}_I(t) D_I[-\beta]), \]  

(27)

which is subject to the equation of motion

\[ \dot{\rho}_I[\beta](t) = i \text{tr}(\hat{\rho}_I(t) [W_I(t), D_I[-\beta]]). \]  

(28)

The evaluation of time dependent weightened operator expectation values,

\[ \text{tr}(\hat{\rho}(t) \hat{A}) = \text{tr}(\hat{\rho}_I(t) \hat{A}_I(t)) = \int D^2 \beta \rho_I[-\beta](t) A_I[\beta] \]  

(29)

also calls for calculating the interacting operator Fourier components \( A_I[\beta], \)

\[ A_I[\beta](t) = \text{tr}(\hat{A}_I(t) D_I[-\beta]). \]  

(30)

4.3 Equation of motion

Let us examine the commutator \([W_I(t), D[-\beta]]\) at the r.h.s. of the equation of motion more closely. We suppose that the interaction is a polynomial in the fields and momenta, to wit, also a polynomial in creation and annihilation parts. Since \( D \) acts as a shift operator, (We drop the index \( I \) in what follows.)

\[ D[-\beta]b(k) = (b(k) + \beta(k))D[-\beta], \quad D[-\beta]b^\dagger(k) = (b^\dagger(k) + \beta^*(k))D[-\beta] \]  

(31)

we get for the commutator

\[ [W[\Phi], D[-\beta]] = (W[\Phi] - W[\Phi + \Psi])D[-\beta] \]  

(32)

with

\[ \Psi(t, x) = \frac{1}{(2\pi)^{3/2}} \int d\mu^+(k)(\beta(k)e^{-ikx} + \beta^*(k)e^{ikx}). \]  

(33)

In order to draw the operator-valued commutator out of the trace in Eq. (28), it is useful to represent \( b \) and \( b^\dagger \) by suitably chosen functional derivatives acting on \( D, \)

\[ b(k)D[-\beta] = \left(2\omega_k \frac{\delta}{\delta \beta^*(k)} - \frac{1}{2} \beta(k) \right) D[-\beta], \]

\[ b^\dagger(k)D[-\beta] = \left(-2\omega_k \frac{\delta}{\delta \beta(k)} - \frac{1}{2} \beta^*(k) \right) D[-\beta]. \]  

(34)

Products of operators \( b \) and \( b^\dagger \) can be represented by replacing them with their partial derivative counterparts in inverse order. The terms with the factor \( \frac{1}{2} \) in front originate
from the fundamental commutator and are of relative order $\hbar$. The ‘classical’ field operator
\[ \Phi(t, x) = \frac{1}{(2\pi)^{3/2}} \int d\mu^+(k) 2\omega_k \left( e^{-ikx} \frac{\delta}{\delta \beta^*(k)} - e^{ikx} \frac{\delta}{\delta \beta(k)} \right) \] (35)
commutes with the displacement $\Psi(t, x)$ which permits us to write the commutator as
\[ (W[\Phi - \frac{1}{2} \Psi] - W[\Phi + \frac{1}{2} \Psi])D[-\beta]. \] (36)
The equation of motion (28) for the interacting part of the density matrix thus assumes the form of a Liouville equation
\[ \dot{\rho}[\beta](t) = iL[\beta](t)\rho[\beta](t), \quad L[\beta](t) = (W[\Phi - \frac{1}{2} \Psi] - W[\Phi + \frac{1}{2} \Psi]). \] (37)
A formal solution can be constructed by standard methods,
\[ \rho[\beta](t) = \mathcal{T} \exp \left\{ i \int_{t_0}^{t} dt' L[\beta](t') \right\} \rho[\beta](t_0) \] (38)
using the time ordering operator $\mathcal{T}$. This equation contains the full dynamical information on the Wigner transform of the density operator. The equations of motion of the c-number counterpart of $\hat{\rho}$ can be obtained by a functional integration with the classical field and momentum in the displacement operator similar to Eq. (3).

### 4.4 Equilibrium distribution

In order to illustrate the formalism derived, we consider a non-interacting system at thermal equilibrium in which interaction is switched on at some initial time. In general, canonical ensembles in thermal equilibrium with temperature $T$ are characterized by the density matrix $\hat{\rho}_{eq} = e^{-H/T}$. Due to standard arguments in perturbation theory, this density matrix can be rewritten as
\[ \hat{\rho}_{eq} = e^{-H_0/T} U_1(t_0 - i/T, t_0), \quad U_1(t_0 - i/T, t_0) = \mathcal{T} \exp \left\{ -i \int_{t_0}^{t_0-i/T} dt' W_1(t') \right\}. \] (39)
The corresponding Wigner function in interaction picture is given by
\[ \rho_{eq}[\beta](t) = \text{tr} \left( e^{-H_0/T} U_1(t_0 - i/T, t_0) D[-\beta] \right). \] (40)
Let us calculate the non-interacting equilibrium Wigner function defined by
\[ \rho^0_{eq}[\beta] = \text{tr} \left( e^{-H_0/T} D[-\beta] \right) \] (41)
which we will assume to be the initial preparation of the system. For that purpose, we consider the non-interacting part with one creation operator inserted between the statistical factor and the shift operator. Commutating $b\dagger$ to the right, using the cyclicity of the trace and the commutator with $H_0$ we find
\[ \text{tr} \left( e^{-H_0/T} b\dagger(k) D[-\beta] \right) = -\beta^*(k) \rho^0_{eq}[\beta] + e^{\omega(k)/T} \text{tr} \left( e^{-H_0/T} b\dagger(k) D[-\beta] \right). \] (42)
On the other hand one gets $b^\dagger$ in the trace by acting with the differential operator of Eq. (34) on $D$, 

$$
\left(-2\omega_k \frac{\delta}{\delta \beta(k)} - \frac{1}{2} \beta^*(k) \right) \rho^0_{eq}[\beta] = \text{tr} \left( e^{-H_0/T} b^\dagger(k) D[-\beta] \right). \tag{43}
$$

Combining this property with the previous equation and functionally integrating with respect to $\beta$, one finds, up to a normalisation constant, 

$$
\rho^0_{eq}[\beta] = \exp \left\{ \int d\mu(k) \left( \frac{1}{2} - n^-(k) \right) \beta(k) \beta^*(k) \right\} \tag{44}
$$

with $n^\pm(k) = (1 - \exp(\pm \omega_k/T))^{-1}$.

### 4.5 Non-interacting partition function as initial condition

We consider the non-interacting partition function (44) as initial condition in the time evolution (38) and expand the exponent in powers of the coupling constant. To be specific, we consider a quartic interaction term in the Hamiltonian, 

$$
W[\Phi] = \frac{\lambda}{4!} \int d^3x \Phi^4(x). \tag{45}
$$

We act with the differences of Eq. (37) on $\rho^0_{eq}[\beta]$ and obtain

$$
(\tilde{\Phi}(x) + \frac{1}{2} \Psi(x)) \rho^0_{eq}[\beta] = \Gamma(x) \rho^0_{eq}[\beta], \quad (\tilde{\Phi}(x) - \frac{1}{2} \Psi(x)) \rho^0_{eq}[\beta] = -\Gamma^*(x) \rho^0_{eq}[\beta] \tag{46}
$$

with 

$$
\Gamma(x) = \frac{1}{(2\pi)^3/2} \int d\mu^+(k) \left( \beta(k)n^+(k)e^{-ikx} + \beta^*(k)n^-(k)e^{ikx} \right). \tag{47}
$$

Green functions arise in the commutator of the differences with $\Gamma$, 

$$
\left[ \Phi(x) \pm \frac{1}{2} \Psi(x), \Gamma(y) \right] = G(x - y), \quad \left[ \Phi(x) \pm \frac{1}{2} \Psi(x), \Gamma^*(y) \right] = -G^*(x - y), \tag{48}
$$

with 

$$
G(x - y) = \frac{1}{(2\pi)^3} \int d\mu^+(k) (e^{-ik(x-y)n^-(k)} - e^{ik(x-y)n^+(k)}). \tag{49}
$$

The first order term in $\lambda$ is found to read 

$$
L[\beta](x_0) \rho^0_{eq}[\beta] = \frac{\lambda}{4!} \int d^3x W[\beta](x) \rho^0_{eq}[\beta] \tag{50}
$$

with 

$$
W(x) = 6G(0)(\Gamma^*(x)^2 - \Gamma(x)^2) + (\Gamma^*(x)^4 - \Gamma(x)^4). \tag{51}
$$

For higher orders, it turns out useful to introduce a graphical representation. We denote a factor $\Gamma$, $\Gamma^*$ by an external leg. Green functions and their complex conjugate
correspond to internal lines with an without star. Each power of the interaction term gives rise to a vertex.

In that way, the second order contribution

\[
L[\beta](x_0)L[\beta](y_0)\rho_{eq}^0[\beta] = \frac{\lambda^2}{(4!)^2} \int d^3x \int d^3y W[\beta](x, y)\rho_{eq}^0[\beta]
\]

(52)
can be represented by the graphs (2) trough (5), where legs on the l.h.s. and r.h.s. correspond to the arguments \(x\) and \(y\) of \(\Gamma\). \(W[\beta](x, y)\) involves contributions with two, four, six and eight external legs and is real.

The time dependent density matrix in \(\beta\)-presentation with the given initial condition is thus given by (We take \(t_0 = 0\).)

\[
\rho[\beta](t) = \left(1 + \frac{i\lambda}{4!} \int_0^t dx_0 \int d^3x W(x)[\beta] - \frac{\lambda^2}{(4!)^2} \int_0^t dx_0 \int_0^{x_0} dy_0 \int d^3x \int d^3y W(x, y)[\beta]\right)\rho_{eq}^0[\beta].
\]

(53)

These expressions contain all information about any operator expectation value to order \(\lambda^2\).
Figure 3: Second order with four external legs.

Figure 4: Second order with six external legs.
4.5.1 Particle density

The extraction of the particle density is achieved as follows. We act with the bilocal particle number operator $n(k_1, k_2) = b^\dagger(k_1)b(k_2)$ in $\beta$-representation on the time dependent density matrix (53) and set $\beta = 0$ afterwards. In particular, commuting

\[ n[\beta](k_1, k_2) = \left( \frac{2\omega_{k_2}}{\delta \beta^*(k_2)} - \frac{1}{2} \beta(k_2) \right) \left( -2\omega_{k_1} \frac{\delta}{\delta \beta(k_1)} - \frac{1}{2} \beta^*(k_1) \right) \quad (54) \]

to the r.h.s. using

\[ [b^\dagger[\beta](k), \Gamma(x)] = -\frac{n^+(k)}{(2\pi)^{3/2}} e^{-ikx}, \quad [b[\beta](k), \Gamma(x)] = \frac{n^-(k)}{(2\pi)^{3/2}} e^{ikx}, \]

\[ [b^\dagger[\beta](k), \Gamma^*(x)] = -\frac{n^-(k)}{(2\pi)^{3/2}} e^{-ikx}, \quad [b[\beta](k), \Gamma^*(x)] = \frac{n^+(k)}{(2\pi)^{3/2}} e^{ikx} \quad (55) \]

essentially replaces two external legs by plane waves weighted with distribution functions $n^\pm(k)$. Thus, after having set $\beta = 0$, the set of graphs that can contribute are those with two external legs only. Moreover, explicit calculation shows that the diagrams in Fig. (1) vanish and the first two graphs of Fig. (2) cancel after integration over $x$. The zeroth order term gives ($\omega_1 \equiv \omega_{k_1}$)

\[ -2\delta^3(k_1 - k_2)\omega_1 n^+(k_1) \quad (56) \]

and the third and fourth diagram in Fig. (2) contribute, after integration over $x$, $y$, and $x_0$, $y_0$

\[ \lambda^2 \delta^3(k_1 - k_2) \frac{G^2(0)}{(2\omega_1)^3} (n^+(k_1) - n^-(k_1)) \sin^2(\omega_1 t). \quad (57) \]

The sunset-diagrams in Fig. (3) are the ones far most complicated. They contribute ($\tau = x_0 - y_0$)

\[ \lambda^2 \left( \frac{\delta^3(k_1 - k_2)}{(2\pi)^9} \right) \int_0^t dx_0 \int_0^{x_0} dy_0 (e^{-i\omega_1 \tau} n^-(k_1) + e^{i\omega_1 \tau} n^+(k_1)) \int d^3xe^{i(k_1 \cdot x - \lambda^2 t^3(x, \tau) + h.c.,}

\[ l(x, \tau) = \int \frac{d^3p}{2\omega_p} (e^{-i\omega_p \tau + ip \cdot x} n^-(p) - e^{i\omega_p \tau - ip \cdot x} n^+(p)). \quad (58) \]

Let us discuss the contribution (57) in more detail. It exhibits a harmonic time dependence and does not decrease with time as one may expect for the particle number density which presumably approaches an equilibrium value. The situation is even
worse for off-diagonal operator expectation-values. One finds for the contribution from the third and fourth diagram in Fig. (2) to the operator $b(k_1)b(k_2)$

$$\lambda^2 \delta^3(k_1 + k_2) \frac{G^2(0)}{(2\omega_1)^2} \left( \sin^2 \omega_1 t + i(t \omega_1 - \sin \omega_1 t \cos \omega_1 t) \right) (n^+(k_1) - n^-(k_1)),$$

(59)

which even contains terms linear in time. This indicates a breakdown of the expansion of the time ordered exponent in the evolution (58). A crude estimate of the domain of validity of the expansion performed can be given by the requirement that the exponent remains smaller than unity, i.e. for times $\lambda t \ll 1$.

### 4.6 Resummation

As well known in equilibrium finite temperature field theory, consistency in the infrared regime requires a resummation to be carried out to reorganize the perturbative series (1). As anticipated in the example given, for non-equilibrium density distributions the necessity of resummation also arises for dynamical reasons. Here, resummation boils down to add a mass square $M^2$ to the original Hamiltonian and compensate it by a two-vertex

$$-\frac{1}{2} \int d^3 x M^2 \Phi^2(x)$$

(60)

in the interaction part. This term changes the Liouville-operator in the equations of motion, which gives rise to a number of additional diagrams. Those are such that each graph with closed loops $\propto G(0)$ gets a mass counterpart in a way that they compensate for the choice

$$M^2 = \frac{\lambda}{2} G(0),$$

(61)

as illustrated in Fig. (4).

The resummed mass $m^2 + M^2$ appears now hidden in the Lorentz-covariant volume element $d\mu^+$ and the corresponding energy eigenvalues $\sqrt{m^2 + M^2 + k^2}$ both appearing in $G(0)$. In that sense, Eq. (61) is a consistency condition for the mass counter term. It is interesting to observe that not the first order dynamical contributions to the particle number, which vanish, enforce the resummation, but the time evolution of the second order terms (57) necessitate the reorganisation of the perturbative series. The redefined theory gets its second order contributions (58) solely from the non-local sunset-graphs.
5 General initial conditions

We generalize the particular density matrix considered in the previous section by a Wigner density functional of the connected graphs expressed in a functional power series in $\beta$ (See Appendix.), i.e.

$$
\log \rho[\beta](t) = \sum_{n=1}^{\infty} \frac{1}{n!} \left( \prod_{i=1}^{n} \int d\mu^+(k_i) \right) f_n^{(\sigma)}(t; k_1, \ldots, k_n) \beta^{\sigma_1}(k_1) \ldots \beta^{\sigma_n}(k_n),
$$

(62)

where elements of the set $\{\sigma\} = \{\sigma_1, \ldots, \sigma_n\}$ can assume values $+$ and $-$ which refer to starred and unstarred $\beta$’s respectively. The correlators $f_n$ may also explicitly depend on time. For a given order in $\beta$, not all functions $f_n$ are independent. They have to be symmetric with respect to pairwise exchange of two momenta, both corresponding to starred $(\sigma = +)$ or unstarred $(\sigma = -)$ pairs of $\beta$’s. Furthermore, since physical density matrices have to be hermitian, the relation $D[\beta] = D[-\beta]^\dagger$ implies invariance of $\rho[\beta]$ with respect to simultaneous hermitian conjugation and sign flip of $\beta$. This implies for the correlators $f$

$$
f_n^{(\sigma)}(t; k_1, \ldots, k_n) = (-)^n f_n^{(\sigma^*)}(t; k_1, \ldots, k_n)
$$

(63)

The number of independent correlators is $(n + 2)/2$ for $n$ even and $(n + 1)/2$ for $n$ odd.

Let us study the r.h.s. of the equation of motion (37). Acting with the Liouville operator on $\rho[\beta] = \exp(\log \rho[\beta])$ gives

$$
L[\beta] \rho[\beta] = -\frac{\lambda}{6} \int d^3x \Psi(x) \left( 3[\dot{\Phi}(x), [\Phi(x), \log \rho]]\dot{\Phi}(x), \log \rho] + \right.
$$

$$
\left. + ([\Phi(x), \log \rho])^3 + [\dot{\Phi}(x), [\Phi(x), [\Phi(x), \log \rho]]] + \frac{1}{4} \Psi^2(x)[\dot{\Phi}(x), \log \rho] \right) \rho.
$$

(64)

The first few terms may best be studied by introducing a graphical notation. We represent $\log \rho$ by the graphs depicted in Fig. (7).

The blob in the middle denotes the correlators $f$, and each external leg a factor containing $\beta$ or $\beta^*$. We do not explicitly split the sum over $\{\sigma\}$ into their summands – each graph is understood as the sum over all independent $f_n$’s for a fixed order $n$. Acting with $\dot{\Phi}(x)$ on an external leg cuts it off and replaces it by a plane wave. We denote cut legs by a cross. The factor $\Psi$ is represented by a cut leg without blob since it corresponds to a unit cut one-point correlator. The integration over space graphically joins all crossed legs in the point $x$. The time derivative $i\partial_t$ in the equations of motion is symbolized by a dot. The motion of the system to order $\beta^4$ is depicted in Figs. (8-11).

Let us clarify the magnitude of these graphs in orders of $\hbar$. The relevant quantities have the following dimension.

| object | $L[\beta]$ | $\Phi$ | $\Psi$ | $\beta$ | $\delta\delta\beta$ | $f_n$ |
|--------|------------|--------|--------|--------|-----------------|------|
| order in $\hbar$ | 1 | 1/2 | 3/2 | $-1/2$ | $-5/2$ | $-3n/2$ |
\[ \ln \rho = + \frac{\lambda}{2} + \frac{\lambda}{3!} + \frac{\lambda}{4!} + \frac{\lambda}{5!} + \frac{\lambda}{6!} + \ldots + \frac{\lambda}{7!} \]

Figure 7: \( n \)-th order term in \( \log \rho \).

\[ \dot{\rho} = + \frac{\lambda}{2} + \frac{\lambda}{6} + \frac{\lambda}{6} = \frac{\lambda}{2} \]

Figure 8: First stage of the hierarchy of the equations of motion.

\[ \dot{\rho} = \lambda + \lambda + \lambda + \lambda \]

Figure 9: Second stage of the hierarchy of the equations of motion.
Figure 10: Third stage of the hierarchy of the equations of motion.
Figure 11: Fourth stage of the hierarchy of the equations of motion.
One can easily check that all graphs are of the same order in $\bar{h}$ except for the last in Fig. (10) and the third at the r.h.s. in Fig. (11), which are suppressed by a factor $\bar{h}^2$. In general, all those terms originate from the last summand $\propto \Psi^2$ in Eq. (64). A systematic expansion thus requires to keep all but those terms of higher order. However, the structure of the whole hierarchy is such that the time derivative of correlators of order $n$ involves correlators of order $n + 2$ and lower on the r.h.s. in the equations of motion. The $\bar{h}^2$ suppressed terms are of order $n - 2$ in $\beta$. In Fig. (12), for any $n$, all graphs are shown which involve higher or equal order correlators at the r.h.s. They are responsible for the fact that cutting the hierarchy gives a non-closed system of equations. Even worse, the hierarchy cannot be cut at some order by the condition $f_n = 0$ for $n$ greater than some fixed number, since that would contradict the equations for $\dot{f}_n$ containing nonvanishing contributions at the r.h.s coming from lower order correlators.

6 Particular configurations

Many systems of physical interest exhibit particular symmetries which imply restrictive conditions on the correlators $f_n$. 

Figure 12: n-th order stage of the equations of motion.
6.1 Spatially homogeneous systems

Spatially homogeneous systems are characterized by the invariance of operator products with respect to translation in space, to wit,
\[
\text{tr} \left( \hat{\Phi}(t, x_1) \hat{\Phi}(t, x_2) \ldots \hat{\Phi}(t, x_n) \hat{\rho} \right) = \text{tr} \left( \hat{\Phi}(t, 0) \hat{\Phi}(t, x_2 - x_1) \ldots \hat{\Phi}(x_n - x_1) \hat{\rho} \right). \quad (65)
\]
The corresponding expression in terms of Wigner transforms is found by replacing \(\Phi(t, x)\) by \(\hat{\Phi}(t, x) - \frac{1}{2} \Psi(t, x)\), the density operator by its transform and the trace by a functional integral. Let us pick that term which only contains \(\hat{\Phi}(t, x_i)\)'s, act with it on \(\rho[\beta]\) and set \(\beta = 0\) afterwards. Without loss of generality we may furthermore set \(t = 0\) since time evolution commutes with spatial translations. The condition (65) implies
\[
\left( \prod_{i=1}^{n} \int d\mu^+(k_i) e^{ik_i x_i \sigma_i} \right) f_n^{(\sigma)}(k_1, \ldots, k_n) = \\
\left( \prod_{i=1}^{n} \int d\mu^+(k_i) \right) \exp \left( i \sum_{i=2}^{n} k_i (x_i - x_1) \sigma_i \right) f_n^{(\sigma)}(k_1, \ldots, k_n). \quad (66)
\]
However, this equation can only hold for correlators which are such that the exponents at both sides are equal. That implies the particular form
\[
f_n^{(\sigma)}(k_1, \ldots, k_n) = f_n^{(\sigma), \text{hom}}(k_1, \ldots, k_n) \delta \left( \sum_{i=1}^{n} \sigma_i k_i \right) \quad (67)
\]
where the homogeneous correlator includes one redundant momentum. The delta-function of the \(\sigma\)-averaged momenta generalizes momentum conservation for spatially homogeneous systems to the correlators. Spatial homogeneity and isotropy is a constant of motion, to wit, homogeneous initial conditions evolve to homogeneous correlators.

6.2 Unbroken symmetry.

Another physically interesting particular situation are configurations with unbroken symmetry. They are characterized by vanishing expectation values of the field operator, i.e.
\[
\text{tr} \left( \hat{\Phi}(t, x) \hat{\rho} \right) = 0. \quad (68)
\]
Again, this condition implies a restriction on the Wigner transforms. The operator \(\hat{\Phi}(t, x) - \frac{1}{2} \Psi(t, x)\) decreases \(\hat{\Phi}\) resp. increases \(\Psi\) the number of \(\beta\)'s in the trace by one. Comparing all terms with equal number of \(\beta\)'s, which have to vanish separately, one easily finds that all odd correlators have to vanish,
\[
f_n^{(\sigma), \text{hom}}(k_1, \ldots, k_n) = 0, \quad n \in \mathbb{N}_{\text{odd}}. \quad (69)
\]
Closer inspection of the graphical representations given in Figs. (8-11) and their higher order counterparts reveals that the time derivative of odd correlators also vanishes if they represent a system with unbroken symmetry, which is necessary for consistency. The symmetry conservation is a consequence of the invariance of the Hamiltonian under sign flip of the field.
7 Conclusion and Outlook

In this paper we reformulated the von Neumann equation for the density matrix in terms of the classical observables of field correlators using the Weyl correspondence principle and the language of Wigner functions. We found a Liouville equation for the Weyl-transform which expands into an infinite hierarchy of equations of which we showed that they cannot be cut consistently at a finite order. Time evolution is known exactly, and can be – at least perturbatively – be integrated to later times. Further modelling of physical scenarios, however, includes additional statistical assumptions entering in realistic initial conditions on the density matrix. Based on the present work, investigations in that direction are currently under progress.

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Appendix: Proper and Improper Correlators

We call the set of correlators \( f_n(t; k_1, \ldots, k_n) \) proper correlators if they cannot be written as a product of two functions, i.e.

\[
 f_n(t; k_1, \ldots, k_n) \neq u_m(t; k_{r_1}, \ldots, k_{r_m}) v_{n-m}(t; k_{r_{m+1}}, \ldots, k_{r_n})
\]  

(70)

where \( m < n \) and \( \{r_1, \ldots, r_n\} \) denotes an arbitrary permutation of the set of indices \( \{1, \ldots, n\} \). In particular, proper correlators are not the product of correlators of lower order. Conversely, improper correlators can always be written as a product.

We now prove that the exponentiated logarithm in the definition Eq.(62) exactly produces all improper correlators which are necessary to describe a general density matrix \( \rho[\beta] \). Let us for the moment drop the plus/minus index referring to starred and unstarred components and consider all contributions to a given order \( n \). (Here order is meant to be the number of \( \beta \) and \( \beta^* \).) The possible types of improper graphs may be described by a partition of \( n \) in the following way. Be \( \{l_1, \ldots, l_n\} \) a set of natural numbers \( l_\nu \in \mathbb{N}_0 \) such that \( \sum_{\nu=1}^n l_\nu = n \), then this set describes an ensemble of proper correlators which contains \( l_\nu \) times – \( l_\nu \) may also be zero – a proper correlator of order \( \nu \), and which altogether represents one improper correlator of total order \( n \). We determine the combinatorial factor of that improper correlator. It has \( n \) momenta which can be attached in \( n! \) permutations to the \( \beta \)'s. However, in this way we over-counted indistinguishable contractions among the momenta of the proper subgraphs. For each subgraph, we have to divide by the number \( \nu! \) of permutations within a subgraph. If \( \{l\} \) contains a subgraph of order \( \nu \) more than once, \( l_\nu > 1 \), permutations of those are over-counted by a factor \( l_\nu! \). Finally, we sum over all possible partitions \( \{l\} \), which gives the \( n \)-th order summand of \( \rho[\beta] \)

\[
 \rho_n[\beta] = \sum_{\{\sigma\}} \sum_{\{l\}} n! \prod_{\nu=1}^n \int d\mu^+(k_\nu) \frac{1}{(\nu!)^{l_\nu} l_\nu!} \beta^{\sigma_\nu}(k_\nu) (f_n^{\{\sigma\}}(t; k_i))^l_\nu.
\]  

(71)

One can convince himself that restoring the \( \pm \) index contained in the sum over \( \{\sigma\} \) does not change the symmetry factors. The complete \( \beta \) transform is given by the sum

\[
 \rho[\beta] = \sum_{n=0}^{\infty} \frac{1}{n!} \rho_n[\beta],
\]  

(72)

where \( \rho_0[\beta] = 1 \) encodes unit normalisation of the density operator. The factor \( 1/n! \) has to be inserted to be consistent with the definition (62) which also involves this factor for each correlator.

In order to show that the exponentiated expression (62) equals that expression, we write the exponentiated sum in the r.h.s as a product of single exponentials. Then, the \( i \)-th summand in the expanded exponentiated \( n \)-th term in the r.h.s of (62) exactly corresponds to the term with \( l_n = i \). The correct factor \( (n!)^i i! \) in the denominator comes from the \( i \)-th power in the Taylor-expansion of the exponential function. The sum over \( \{l_1, \ldots, l_n\} \) just amounts to collect all terms in the product of the expanded exponentials which belong to order \( n \). This completes the proof.
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