Transport equations including many-particle correlations for an arbitrary quantum system. General formalism

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Abstract

We present a new method to derive transport equations for non-relativistic quantum many-particle systems. This method uses an equation-of-motion technique and is applicable to interacting fermions and (or) bosons in arbitrary time-dependent external fields. Using a cluster expansion of the r-particle density matrices the infinite hierarchy of equations of motion for many-particle expectation values is transposed into an equivalent one in terms of correlations. This new hierarchy permits a systematic breaking of the hierarchy at any order. Diagrams are derived for these transport equations. In a second paper the method is tested for exactly soluble electron-phonon models in one dimension.

I. INTRODUCTION

In this work, the first one in a series of two papers on transport equations, we present a new formalism for the time evolution of one-particle distribution functions which allows the inclusion of many-body correlations. In the second paper we derive the transport equations for an electron-phonon system and compare the numerical results with the exact solutions of one-dimensional models (polaron model, Tomonaga-Luttinger model).

Very often non-equilibrium phenomena in quantum many-particle systems are studied by the use of real-time Green's function techniques (Martin and Schwinger [2,3], Kadanoff and Baym [4], Keldysh [5], Langreth and Wilkins [6,7]). For a review see Ref. [1]. In the Keldysh formalism the perturbative expansion uses a time integration over a path in the complex plane. If only interested in the one-particle distribution function, one usually applies the generalized Kadanoff-Baym ansatz [8,9,4], which was justified by Schoeller [10] as a partial resummation in the diagrammatic expansion. The transport equation obtained in the Born approximation is of the form of a non-Markovian Boltzmann equation with renormalized one-particle propagators, usually taken the same as in equilibrium. In Ref. [10] initial correlations are also discussed, but it does not seem to be possible to apply the same resummation method including the initial correlations. This stems from the fact that the correlations are not taken into account as time-dependent quantities.
Motivated by the work of Schoeller, we present a method which enables the inclusion of the correlations as dynamical quantities. Only single-time expectation values of operators are considered in contrast to Green’s function techniques. In the course of this work (cf. part II) it will become clear that the transport equations with correlations already include the renormalization of one-particle propagators in the dynamics. There is no need to calculate retarded and advanced Green’s functions independently of the distribution functions.

As the dynamics of all quantities is just given by the Hamiltonian in the form of an equation of motion (EOM) (Schrödinger or von-Neumann equation), it seems to be more natural to consider only single-time quantities. The problem to be solved is how to cut off the infinite hierarchy of equations of motion in a consistent way. It will be shown that the expansion of the expectation values of many-body operators in terms of correlations (or, diagrammatically speaking, “connected parts”) allows a systematic decoupling of the hierarchy at any given order. The lowest order (almost) agrees with the usual decoupling procedure to obtain the Born approximation.

II. EQUATIONS OF MOTION AND CORRELATIONS

In this section the method will be explained for a fermionic system with two-particle interaction in time-dependent external fields described by the Hamiltonian

\[
H = \sum_i \epsilon_i \psi_i^\dagger \psi_i + \sum_{i,j} h_{ij}^{ext}(t) \psi_i^\dagger \psi_j + \frac{1}{2!} \sum_{i_1,i_2,j_1,j_2} v_{i_1,j_1,i_2,j_2} \psi_{i_1}^\dagger \psi_{j_1} \psi_{i_2} \psi_{j_2} = H_0^t + V .
\]

(1)

The fermionic annihilation and creation operators are denoted by \( \psi_i \) and \( \psi_i^\dagger \), the index \( i \) referring to the one-particle states. In the interaction term \( V \) the matrix elements \( v_{i_1,j_1,i_2,j_2} \) are supposed to be anti-symmetric in the first and second pair of indices \( (v_{i_2,j_1,i_1,j_2} = v_{i_1,j_2,i_2,j_1}) \). The external fields are described by the time-dependent hermitian matrix \( h_{ij}^{ext}(t) \). Sometimes we use the notation \( h_{ij}(t) = \delta_{ij} \epsilon_i + h_{ij}^{ext}(t) \) for the one-particle Hamiltonian matrix.

The method is not restricted to this type of systems. It may as well be applied to systems with bosons, even with “anomalous” (i.e. not conserving the particle number) expectation values like \( \langle bb \rangle \). The necessary small alterations are mentioned from time to time in this presentation and in part II the method is applied to an electron-phonon system.

Throughout this work we use the Heisenberg representation, so that the following equation of motion for operators holds:

\[
\frac{d}{dt} A(t) + i [A, H^t_0](t) = -i [A, V](t) .
\]

(2)

For the case of an operator \( A = \psi_{k_1} \cdots \psi_{k_n} \psi_{k_n'}^\dagger \cdots \psi_{k_1'}^\dagger \) and the Hamiltonian of Eq. (1) the equation of motion reads

\[
\frac{d}{dt} \left( \psi_{k_1} \cdots \psi_{k_n} \psi_{k_n'}^\dagger \cdots \psi_{k_1'}^\dagger \right)(t)
+ i \sum_j \left\{ h_{k_1,j}(t) \left( \psi_j \psi_{k_2} \cdots \psi_{k_n} \psi_{k_n'}^\dagger \cdots \psi_{k_1'}^\dagger \right)(t) + \cdots \right\}
\]

(3)
\[-i \sum_i \{ h_{ik_1}(t) \left( \psi_{k_1} \cdots \psi_{k_n} \psi_{k'_n}^\dagger \cdots \psi_{k'_2} \psi_{k'_1}^\dagger \right)(t) + \cdots \} \]
\[= -\frac{1}{4} \sum_{i_{11},i_{22}} u_{i_{11},j_{12}} \left[ \psi_{k_1} \cdots \psi_{k_n} \psi_{k'_n}^\dagger \cdots \psi_{k'_2} \psi_{k'_1}^\dagger, \psi_{i_{11}}^\dagger \psi_{i_{21}} \psi_{j_{12}} \psi_{j_{11}} \right](t) , \]

or more specifically for the case without external fields
\[
\begin{bmatrix}
\frac{d}{dt} + i (\epsilon_{k_1} + \cdots + \epsilon_{k_n} - \epsilon_{k'_1} - \cdots - \epsilon_{k'_n})
\end{bmatrix}
\left( \psi_{k_1} \cdots \psi_{k_n} \psi_{k'_n}^\dagger \cdots \psi_{k'_2} \psi_{k'_1}^\dagger \right)(t)
\[= -\frac{1}{4} \sum_{i_{11},i_{22}} u_{i_{11},j_{12}} \left[ \psi_{k_1} \cdots \psi_{k_n} \psi_{k'_n}^\dagger \cdots \psi_{k'_2} \psi_{k'_1}^\dagger, \psi_{i_{11}}^\dagger \psi_{i_{21}} \psi_{j_{12}} \psi_{j_{11}} \right](t) . \quad (4)
\]

The same equations of motion hold for the expectation values of these multi-particle operators taken with an initial statistical operator \( \rho_0 \) at time \( t_0 \), \( \langle A \rangle_t = \text{Tr} [\rho_0 A(t)] \). (The Heisenberg representation of an operator is supposed to be such that \( A(t_0) = A \).) For our method to work \( \rho_0 \) does not have to be of any special form. As the case of a non-diagonal one-particle matrix \( h_{ij}(t) \) is notationally cumbersome, but does not pose any additional problems in the derivation of the kinetic equations, we will carry out the derivation for the case of a diagonal one-particle Hamiltonian, adding the necessary alterations for non-vanishing external fields in the end.

Thus, given the initial state \( \rho_0 \) (mixed or pure) at time \( t_0 \), we have to solve an infinite hierarchy of ordinary differential equations (ODE). Of course, this is usually not feasible and some kind of decoupling procedure is needed. Starting with one-particle expectation values \( \langle \psi_{k'}^\dagger \psi_{k} \rangle_t \) the EOM involve expectation values of two-particle operators. In the equation of these quantities the “collision term” (the right hand side (rhs) of Eq. (4)) is often approximated by factorizing all expectation values into products of one-particle expectation values as if the Wick theorem holds for an arbitrary state of the system. In this way a non-Markovian Boltzmann equation in Born approximation is obtained.

In this work we present a method to extend this procedure beyond the Born approximation. It yields again an infinite hierarchy of EOM, which is still exact, but now in terms of correlations. In contrast to the usual hierarchy of EOM mentioned above, this hierarchy allows the decoupling at any given order without any ambiguities. The essential ingredient is the following cluster expansion \([10]\) of products of field operators, i.e. creation and annihilation operators, denoted by \( B_i \):
\[
\langle B_1 \rangle_t = \langle B_1 \rangle_t^c ,
\]
\[
\langle B_1 B_2 \rangle_t = \langle B_1 B_2 \rangle_t^c + \langle B_1 \rangle_t^c \cdot \langle B_2 \rangle_t^c ,
\]
\[
\langle B_1 B_2 B_3 \rangle_t = \langle B_1 B_2 B_3 \rangle_t^c + \langle B_1 B_2 \rangle_t^c \cdot \langle B_3 \rangle_t^c + \langle B_2 \rangle_t^c \cdot \langle B_1 B_3 \rangle_t^c + \langle B_1 \rangle_t^c \cdot \langle B_2 B_3 \rangle_t^c + \langle B_1 \rangle_t^c \cdot \langle B_2 \rangle_t^c \cdot \langle B_3 \rangle_t^c ,
\]
\[
\vdots
\]

The \( n \)-th order correlations \( \langle B_1 B_2 \cdots B_n \rangle_t^c \) are defined recursively. The operators need not be normal-ordered. Every expectation value \( \langle B_1 B_2 \cdots B_n \rangle_t \) is decomposed into sums over products of correlations in the following way: The sum extends over all disjoint partitions of the set \( \{1, \ldots, n\} \). The product is taken over the correlations corresponding to each subset
in the partition. Inside each correlation the order of the field operators is retained. The overall sign of the product is determined by the sign of the permutation of fermionic field operators necessary to disentangle overlapping correlations. As we assume that the initial statistical operator as well as the Hamiltonian conserve the total number of fermions, only correlations with an equal number of fermionic creation and annihilation operators occur. Because of this property the sign of each decomposition into correlations is well defined.

So far, the cluster expansion has been written down for both, fermionic and bosonic operators. For fermionic systems the particle number must be conserved and the usual rules for permutations of fermionic operators apply. The one-particle correlations coincide with the corresponding distribution functions

\[
\langle \psi_i \psi^\dagger_j \rangle_t = \langle \psi_i \psi^\dagger_j \rangle^c_t, \\
\langle \psi^\dagger_j \psi_i \rangle_t = \langle \psi^\dagger_j \psi_i \rangle^c_t,
\]

and the two-particle correlations \( \langle \psi_{i_1} \psi_{j_2}^\dagger \psi_{j_1}^\dagger \psi_{j_2} \rangle_t^c \), for example, are defined by

\[
\langle \psi_{i_1} \psi_{i_2}^\dagger \psi_{j_2}^\dagger \psi_{j_1}^\dagger \psi_{j_2} \rangle_t = \langle \psi_{i_1} \psi_{i_2}^\dagger \psi_{j_2}^\dagger \psi_{j_1}^\dagger \psi_{j_2} \rangle^c_t + \langle \psi_{i_1} \psi_{j_2}^\dagger \psi_{j_1}^\dagger \psi_{j_2} \rangle^c_t - \langle \psi_{i_1} \psi_{j_2}^\dagger \psi_{j_1}^\dagger \psi_{j_2} \rangle^c_t. 
\]

From the canonical anti-commutation rules it follows immediately that

\[
\langle \psi_i \psi^\dagger_j \rangle^c_t = \delta_{ij} - \langle \psi^\dagger_j \psi_i \rangle^c_t.
\]

In all higher-order correlations the fermionic operators anti-commute, i.e.

\[
\langle \ldots \psi_i \psi_j^\dagger \ldots \rangle^c_t = -\langle \ldots \psi_j^\dagger \psi_i \ldots \rangle^c_t, \\
\langle \ldots \psi_i \psi_j \ldots \rangle^c_t = -\langle \ldots \psi_j \psi_i \ldots \rangle^c_t,
\]

which can be easily proved by induction. Therefore, it is sufficient to consider the following anti-normal ordered correlations:

\[
\langle \psi_{k_1} \ldots \psi_{k_n} \psi_{k_1}^\dagger \ldots \psi_{k_n}^\dagger \rangle^c_t, \quad n \geq 1 .
\]

We will call the one-particle correlations \((n = 1)\) contractions.

Any expectation value of the form \( \langle \psi_{k_1} \ldots \psi_{k_n} \psi_{k_1}^\dagger \ldots \psi_{k_n}^\dagger \rangle_t \) can be expressed in terms of correlations as can be seen directly from the definition of the correlations in Eq. (5). This enables us to transform the infinite hierarchy of EOM into an equivalent one in terms of correlations. So far, nothing seems to be gained. But we will see that the EOM for the correlations allow an easy and unambiguous breaking of the hierarchy at any desired order, in contrast to the usual EOM. The lowest order is usually of the type of a non-Markovian Boltzmann equation in Born approximation.

In the next section we derive diagrams for the correlations which are as convenient as usual Feynman graphs for organizing the calculations. It turns out that the temporal evolution of correlations is determined by “connected” diagrams only.

We start with the EOM for the one-particle distribution function
\[
\left[ \frac{d}{dt} + i(\epsilon_{k_1} - \epsilon_{k'_1}) \right] \langle \psi_{k_1} \psi_{k'_1}^\dagger \rangle_t^c
= -i \sum_{i_1,i_2,j_1,j_2} \left\{ \langle \psi_{k_1} \psi_{k'_1}^\dagger \psi_{i_1} \psi_{i_2}^\dagger \psi_{j_1} \psi_{j_2}^\dagger \rangle_t - \langle \psi_{i_1} \psi_{i_2}^\dagger \psi_{j_1} \psi_{j_2}^\dagger \psi_{k_1} \psi_{k'_1}^\dagger \rangle_t \right\}
\]
\[
= -i \sum_{j_1,j_2} \left\{ -\frac{1}{2} \left( \langle \psi_{k_1} \psi_{k'_1}^\dagger \rangle_t^c + \langle \psi_{k'_1} \psi_{k_1}^\dagger \rangle_t^c \right) \cdot \langle \psi_{j_1} \psi_{j_2} \psi_{i_2}^\dagger \psi_{i_1}^\dagger \rangle_t^c
+ \frac{1}{2} \left( \langle \psi_{k_1} \psi_{k'_1}^\dagger \psi_{j_1} \psi_{j_2}^\dagger \rangle_t^c + \langle \psi_{k'_1} \psi_{k_1} \psi_{j_2} \psi_{j_1}^\dagger \rangle_t^c \right) \cdot \langle \psi_{i_1} \psi_{i_2} \psi_{k_1} \psi_{k'_1}^\dagger \rangle_t^c
+ \left( -\langle \psi_{k_1} \psi_{k'_1}^\dagger \psi_{j_1} \psi_{j_2}^\dagger \rangle_t^c \langle \psi_{k'_1} \psi_{k_1} \psi_{j_2} \psi_{j_1}^\dagger \rangle_t^c + \langle \psi_{k'_1} \psi_{k_1} \psi_{j_2} \psi_{j_1}^\dagger \rangle_t^c \langle \psi_{k_1} \psi_{k'_1} \psi_{j_1} \psi_{j_2}^\dagger \rangle_t^c \right) \cdot \langle \psi_{i_2} \psi_{i_1} \psi_{k_1} \psi_{k'_1}^\dagger \rangle_t^c \right\}.
\]

The reader might wonder why in the first step we did not calculate explicitly the commutator leaving only terms with four instead of six fermionic operators. It turns out that the cluster expansion and the derivation of diagrammatic rules is easier when one leaves the commutator as it is. Of course, after the cluster expansion of the commutator the correlations with six field operators cancel because of the rule Eq. (10). Only terms with at least one contraction remain because the non-trivial part of the fermionic anti-commutation rules shows up only in the contractions. In addition, we simplified the result by combining terms differing only in the exchange of the two annihilation or creation operators of the interaction term. This is possible as we use anti-symmetrized interaction matrix elements. In this way the prefactor of \(1/4 = 1/2!\cdot 1/2!\) is sometimes replaced by \(1/2!\) or 1. Later, we will give a simple diagrammatic rule to determine this so-called symmetry factor. For pedagogical reasons we have not simplified \(\langle \psi_{i_1}^\dagger \psi_{j_1} \rangle_t^c + \langle \psi_{j_1}^\dagger \psi_{i_1} \rangle_t^c = \delta_{ij}\) as we will do from now on.

In the next step, the EOM for the newly encountered correlations \(\langle \psi_{k_1} \psi_{k'_2} \psi_{k_2}^\dagger \psi_{k'_1}^\dagger \rangle_t^c\) is needed. It can be calculated in the following way: By definition
\[
\langle \psi_{k_1} \psi_{k'_2} \psi_{k_2}^\dagger \psi_{k'_1}^\dagger \rangle_t^c = \langle \psi_{k_1} \psi_{k_2} \psi_{k_2}^\dagger \psi_{k'_1}^\dagger \rangle_t - \langle \psi_{k_1} \psi_{k'_2} \psi_{k_2}^\dagger \psi_{k'_1}^\dagger \rangle_t + \langle \psi_{k_1} \psi_{k_2}^\dagger \psi_{k'_2} \psi_{k'_1}^\dagger \rangle_t,
\]
so that the EOM for \(\langle \psi_{k_1} \psi_{k'_2} \psi_{k_2}^\dagger \psi_{k'_1}^\dagger \rangle_t^c\) is needed. It reads
\[
\left[ \frac{d}{dt} + i(\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k'_1} - \epsilon_{k'_2}) \right] \langle \psi_{k_1} \psi_{k_2}^\dagger \psi_{k'_2}^\dagger \psi_{k'_1}^\dagger \rangle_t^c
\]
\[
= -i \sum_{j_1,j_2} \left\{ -\frac{1}{2} \delta_{i_1,k_1} \langle \psi_{k_2} \psi_{j_2} \psi_{j_1} \psi_{k'_1}^\dagger \psi_{i_2}^\dagger \psi_{i_1}^\dagger \rangle_t^c + (k_1 \leftrightarrow k_2)
\right.
\]
\[
+ \frac{1}{2} \delta_{j_1,k_1} \langle \psi_{k_2} \psi_{j_2} \psi_{k'_1}^\dagger \psi_{i_2}^\dagger \psi_{i_1}^\dagger \psi_{k'_2}^\dagger \rangle_t^c - (k'_1 \leftrightarrow k'_2)
\right.
\]
\[
+ \frac{1}{2} \left( \langle \psi_{k_1} \psi_{i_1}^\dagger \psi_{i_2}^\dagger \psi_{k'_2}^\dagger \psi_{k'_1}^\dagger \rangle_t^c - \langle \psi_{i_1} \psi_{i_2}^\dagger \psi_{k_1} \psi_{k'_2}^\dagger \psi_{k'_1}^\dagger \rangle_t^c \right) \cdot \langle \psi_{j_1} \psi_{j_2} \psi_{i_2}^\dagger \psi_{i_1}^\dagger \rangle_t^c
\]
\[
+ \frac{1}{2} \left( \langle \psi_{k'_1} \psi_{i_1}^\dagger \psi_{i_2}^\dagger \psi_{k'_2}^\dagger \psi_{k_1} \rangle_t^c - \langle \psi_{i_1} \psi_{i_2}^\dagger \psi_{k'_1} \psi_{k'_2}^\dagger \psi_{k_1} \rangle_t^c \right) \cdot \langle \psi_{j_1} \psi_{j_2} \psi_{i_2}^\dagger \psi_{i_1}^\dagger \rangle_t^c
\]
\[
\left. + \left[ \langle \psi_{k_1} \psi_{k'_2} \psi_{i_1}^\dagger \psi_{i_2}^\dagger \psi_{k'_1}^\dagger \psi_{k'_2}^\dagger \rangle_t^c - \langle \psi_{i_1} \psi_{i_2}^\dagger \psi_{k_1} \psi_{k'_1} \psi_{k'_2}^\dagger \psi_{k'_2}^\dagger \rangle_t^c \right) \cdot \langle \psi_{j_1} \psi_{j_2} \psi_{i_2}^\dagger \psi_{i_1}^\dagger \rangle_t^c
\right]
\]
\[
- \frac{1}{2} \delta_{i_1,k_1} \langle \psi_{k_2} \psi_{k'_2} \psi_{k'_1}^\dagger \psi_{k'_2}^\dagger \psi_{i_2}^\dagger \psi_{i_1}^\dagger \rangle_t^c + \frac{1}{2} \delta_{j_1,k'_1} \langle \psi_{k_2} \psi_{k'_2} \psi_{k'_1}^\dagger \psi_{k'_2}^\dagger \psi_{i_2}^\dagger \psi_{i_1}^\dagger \rangle_t^c.
\]
We obtain the following EOM for \( \langle \psi_{k_1} \psi_{k_2} \psi_{k_1'} \psi_{k_2'} \rangle_t \):

\[
\frac{d}{dt} + i \left( \epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_1'} - \epsilon_{k_2'} \right) \psi_{k_1} \psi_{k_2} \psi_{k_1'} \psi_{k_2'}
\]

\[
= \left[ \frac{d}{dt} + i (\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_1'} - \epsilon_{k_2'}) \right] \langle \psi_{k_1} \psi_{k_2} \psi_{k_1'} \psi_{k_2'} \rangle_t
\]

\[
- \{ \langle \psi_{k_1} \psi_{k_1'} \rangle_t \left[ \frac{d}{dt} + i (\epsilon_{k_1} - \epsilon_{k_1'}) \right] \langle \psi_{k_2} \psi_{k_2'} \rangle_t \}
\]

\[
+ \{ \langle \psi_{k_2} \psi_{k_2'} \rangle_t \left[ \frac{d}{dt} + i (\epsilon_{k_1} - \epsilon_{k_1'}) \right] \langle \psi_{k_1} \psi_{k_1'} \rangle_t \}
\]

\[
+ \{ \langle \psi_{k_1} \psi_{k_1'} \rangle_t \left[ \frac{d}{dt} + i (\epsilon_{k_2} - \epsilon_{k_2'}) \right] \langle \psi_{k_2} \psi_{k_2'} \rangle_t \}
\]

\[
+ \{ \langle \psi_{k_2} \psi_{k_2'} \rangle_t \left[ \frac{d}{dt} + i (\epsilon_{k_2} - \epsilon_{k_2'}) \right] \langle \psi_{k_1} \psi_{k_1'} \rangle_t \}
\]

\[
- \frac{i}{2} \sum_{j_1, j_2} \delta_{j_1, k_1} \langle \psi_{k_2} \psi_{j_2} \psi_{j_1} \psi_{k_1'} \psi_{k_2'} \rangle_t + (k_1 \leftrightarrow k_2)
\]

\[
+ \frac{1}{2} \delta_{j_1, k_1'} \langle \psi_{k_2} \psi_{j_2} \psi_{j_1} \psi_{k_1} \psi_{k_2'} \rangle_t - (k_1' \leftrightarrow k_2')
\]

\[
+ \frac{1}{2} \left( \langle \psi_{k_1} \psi_{k_1'} \rangle_t \langle \psi_{k_2} \psi_{k_2'} \rangle_t \right) - \langle \psi_{k_1} \psi_{k_1'} \rangle_t \langle \psi_{k_2} \psi_{k_2'} \rangle_t
\]

\[
+ \frac{1}{2} \left( \langle \psi_{k_1} \psi_{k_1'} \rangle_t \langle \psi_{k_2} \psi_{k_2'} \rangle_t \right) - \langle \psi_{k_1} \psi_{k_1'} \rangle_t \langle \psi_{k_2} \psi_{k_2'} \rangle_t
\]

\[
- \langle \psi_{k_2} \psi_{k_2'} \rangle_t \langle \psi_{k_1} \psi_{k_1'} \rangle_t - \langle \psi_{k_2} \psi_{k_2'} \rangle_t \langle \psi_{k_1} \psi_{k_1'} \rangle_t
\]

\[
+ \frac{1}{2} \delta_{j_1, k_1} \langle \psi_{k_2} \psi_{j_2} \psi_{j_1} \psi_{k_1'} \psi_{k_2'} \rangle_t - (k_1 \leftrightarrow k_2)
\]

\[
+ \frac{1}{2} \delta_{j_1, k_1'} \langle \psi_{k_2} \psi_{j_2} \psi_{j_1} \psi_{k_1} \psi_{k_2'} \rangle_t - (k_1' \leftrightarrow k_2')
\]

We would like to mention that the diagrams presented in the next section facilitate the
determination of the EOM in quite the same way as Feynman graphs do in equilibrium theory. Note that the EOM for the correlation is the same as the EOM for the corresponding $n$-point function with just some terms missing. Diagrammatically these terms correspond to unconnected graphs.

Now we want to describe the procedure for the breaking of the hierarchy of EOM. With the two-particle interaction the EOM for a given correlation of order $n$ contains correlations of order $l \leq n + 1$. If a calculation up to order $n$ is desired, we just neglect the correlations of order $n + 1$ in the EOM for the correlations of order $n$ and get a closed system of ODE for the correlations of order $l \leq n$. This procedure has the advantage of working without ambiguities at every given order. In addition, the transport equations are already of the form in which they are usually solved, i.e. as a system of ODE. This system allows for the inclusion of initial correlations up to order $n$, that means that additional information about the initial state $\rho_0$ can be included compared with the usual approaches. It should be clear that our approximation method is in some sense an expansion in powers of $V \cdot \Delta t$, where $V$ is the typical interaction strength and $\Delta t = t - t_0$ is the time passed since the initial time. But at the given order it is the best possible approximation for the one-particle distribution function. No resummation as in ordinary perturbation theory [10] is needed.

The same procedure does not work for the usual hierarchy of EOM because the EOM for the $2n$-point function $\langle \psi_k \cdots \psi_{k_1} \psi_{k_1}^\dagger \cdots \psi_{k_1}^\dagger \rangle_t$ essentially involves only $2(n + 1)$-point functions. Therefore, these functions cannot just be neglected. Some kind of decoupling mechanism is needed. This was done e.g. by Zimmermann and Wauer [11] in one order higher than Born approximation for a Jaynes-Cummings model. But as the only consistent way of doing it is in terms of a cluster expansion, it is best to start with correlations from the beginning.

Another noteworthy feature of our method is the fact that the derivatives $\left( \frac{d}{dt} \right)^l \langle \psi_{k_1} \cdots \psi_{k_n} \psi_{k_1}^\dagger \cdots \psi_{k_1}^\dagger \rangle_t$ at the initial time $t = t_0$ are correctly described for $0 \leq l \leq n - 1$ when the cut-off is at order $n$. A further advantage of using correlations is the fact that they vanish for all orders $n \geq 2$ in the case of a non-interacting system in a grand-canonical ensemble (Wick’s theorem [12]), in contrast to $n$-point functions. For this reason the EOM for correlations yield better results for systems with weak interaction showing relaxation into thermal equilibrium (cf. part II). The most convincing argument in favor of this method are the very promising results in comparison with the exact model calculations presented in II for one-dimensional electron-phonon systems. In three dimensions the order of the system of ODE is already huge at the level of the Born approximation so that it seems not feasible to go even one order higher. Even in a homogeneous system with momentum conservation, for example, the $n$-th order correlation has $2n - 1$ free momentum indices, i.e. the number of ODE is of the order $N^{(2n-1)d}$, where $N^d$ is the number of one-electron states. Because of this fact numerical calculations in three dimensions are often performed assuming an isotropic distribution in $\vec{k}$-space, thus reducing the effective dimension. With electron-phonon instead of electron-electron interaction, the situation is slightly better, because the usual electron-phonon interaction term contains only products of three instead of four field operators.

Before turning to diagrams, we discuss the kinetic equations in the lowest approximations. Neglecting all correlations of order $n \geq 2$ we obtain
\[
\frac{d}{dt} \langle \psi_k^\dagger \psi_{k'}^\dagger \rangle_t^c + i \sum_j \bar{\epsilon}_{k,j} (t) \langle \psi_j \psi_{k'}^\dagger \rangle_t^c - i \sum_i \langle \psi_k^\dagger \psi_i^\dagger \rangle_t^c \bar{\epsilon}_{ik'} (t) = 0 , \tag{16}
\]

which is just the propagation in the external fields with the one-particle energies corrected by the time-dependent Hartree-Fock energies \( v_{ij}^{HF} (t) := \sum_i \bar{v}_{ii,j} \langle \psi_j \psi_{j'} \rangle_t^c + \bar{\epsilon}_{jj} (t) := \delta_{ij} \epsilon_i + \hbar \epsilon_{ij}^{\text{ext}} (t) + v_{ij}^{HF} (t) \). Note that we have added the contribution of the external fields again. This equation does not contain a "collision term". At least the next order has to be retained. We obtain the following closed system of ODE:

\[
\frac{d}{dt} \langle \psi_k^\dagger \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t + i \sum_j \left\{ \epsilon_{k,j} (t) \langle \psi_j \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t - \bar{\epsilon}_{k,j} (t) \langle \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \psi_{k'}^\dagger \rangle_t \right\} 
- i \sum_i \left\{ \langle \psi_k^\dagger \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t \epsilon_{ik'} (t) + \langle \psi_{k'}^\dagger \psi_{k'}^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t \epsilon_{ik'} (t) \right\} 
+ i \left( \sum_{j j'} V_{k,k',j,j'} (t) \langle \psi_j \psi_{j'} \psi_{j'} \psi_{j'} \rangle_t - \sum_{i i'} (V_{i',i,i',i'} (t))^* \langle \psi_{i'} \psi_{i'} \psi_{i'} \psi_{i'} \rangle_t \right) 
+ i \sum_{i j' j''} W_{i,j',j''} (t) \langle \psi_{j'} \psi_{j''} \psi_{j''} \psi_{j''} \rangle_t - \langle \psi_{i'} \psi_{i'} \psi_{i'} \psi_{i'} \rangle_t \right\} 
- i \sum_{i j' j''} V_{i,j',j''} (t) \langle \psi_{i'} \psi_{i'} \psi_{j'} \psi_{j''} \rangle_t 
- \langle \psi_{i'} \psi_{i'} \psi_{i'} \psi_{i'} \rangle_t \right\} \right) , \tag{17}
\]

\[
\frac{d}{dt} \langle \psi_k^\dagger \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t + i \sum_j \left\{ \epsilon_{k,j} (t) \langle \psi_j \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t - \bar{\epsilon}_{k,j} (t) \langle \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \psi_{k'}^\dagger \rangle_t \right\} 
- i \sum_i \left\{ \langle \psi_k^\dagger \psi_k^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t \epsilon_{ik'} (t) + \langle \psi_{k'}^\dagger \psi_{k'}^\dagger \psi_k^\dagger \psi_{k'}^\dagger \rangle_t \epsilon_{ik'} (t) \right\} 
+ i \left( \sum_{j j'} V_{k,k',j,j'} (t) \langle \psi_j \psi_{j'} \psi_{j'} \psi_{j'} \rangle_t - \sum_{i i'} (V_{i',i,i',i'} (t))^* \langle \psi_{i'} \psi_{i'} \psi_{i'} \psi_{i'} \rangle_t \right) 
+ i \sum_{i j' j''} W_{i,j',j''} (t) \langle \psi_{j'} \psi_{j''} \psi_{j''} \psi_{j''} \rangle_t - \langle \psi_{i'} \psi_{i'} \psi_{i'} \psi_{i'} \rangle_t \right\} 
- i \sum_{i j' j''} V_{i,j',j''} (t) \langle \psi_{i'} \psi_{i'} \psi_{j'} \psi_{j''} \rangle_t 
- \langle \psi_{i'} \psi_{i'} \psi_{i'} \psi_{i'} \rangle_t \right\} \right) \right) \right) , \tag{18}
\]

The time-dependent Hartree-Fock corrections of the one-particle energies as well as the terms with

\[
V_{k,k,j,j'} (t) = \sum_{i,i'} \langle \psi_{i'}^\dagger \psi_k^\dagger \psi_{i'}^\dagger \psi_k^\dagger \rangle_t - \langle \psi_{i'}^\dagger \psi_k^\dagger \psi_{i'}^\dagger \psi_k^\dagger \rangle_t \tag{19}
\]

and

\[
W_{k,k',j,j'} (t) = \sum_{i,i'} \langle \psi_{i'}^\dagger \psi_{k'}^\dagger \psi_{i'}^\dagger \psi_{k'}^\dagger \rangle_t - \langle \psi_{i'}^\dagger \psi_k^\dagger \psi_{i'}^\dagger \psi_k^\dagger \rangle_t \tag{20}
\]

which correct the correlated propagation of two particles, are not obtained by a naive decoupling procedure for the two-particle expectation values.

For the special case of a homogeneous, spin-independent initial state \( \rho_0 \) and a momentum and spin conserving Hamiltonian without external fields, the EOM simplify considerably. We denote the one-particle distribution function by \( n_k (t) := \langle \psi_k^\dagger \psi_k \rangle_t^c \) with \( k = (\vec{k}, \sigma) \).
\[
\frac{d}{dt} n_k(t) = -\frac{i}{2} \left\{ \sum_{k_1k_2,k_1'k_2'} v_{kk_2,k_1'k_2'} \langle \psi_{k_1'} \psi_{k_2'}^\dagger \psi_{k_2}^\dagger \psi_k \rangle_t^c - \text{c.c.} \right\}, \tag{21}
\]

\[
\left[ \frac{d}{dt} + i(\epsilon_{k_1}(t) + \epsilon_{k_2}(t) - \epsilon_{k_1'}(t) - \epsilon_{k_2'}(t)) \right] \langle \psi_{k_1'} \psi_{k_2'}^\dagger \psi_{k_2}^\dagger \psi_k \rangle_t^c 
+ \frac{i}{2} \sum_{j_1j_2} v_{k_1j_2,k_2j_2}(1 - n_{k_1}(t) - n_{k_2}(t)) \langle \psi_{j_1} \psi_{j_2}^\dagger \psi_{k_2}^\dagger \psi_{k_1} \rangle_t^c 
- \frac{i}{2} \sum_{i_1i_2} v_{i_1i_2,k_1'i_2'(k_1')(1 - n_{k_1}(t) - n_{k_1'}(t)) \langle \psi_{k_1} \psi_{k_2} \psi_{i_2} \psi_{i_1} \rangle_t^c 
+ \frac{i}{2} \sum_{i_1i_2} v_{i_1i_2,k_1'i_2'(k_1')(1 - n_{k_1}(t) - n_{k_1'}(t)) \langle \psi_{k_1} \psi_{k_2} \psi_{i_2} \psi_{i_1} \rangle_t^c 
- (k_1 \leftrightarrow k_2) - (k_1' \leftrightarrow k_2') + (k_1 \leftrightarrow k_2, k_1' \leftrightarrow k_2') 
= -iv_{k_1,k_2,k_1'k_2'} \left( (1 - n_{k_1})(1 - n_{k_2})n_{k_1'}(1 - n_{k_2'})(1 - n_{k_2})(1 - n_{k_2'}) \right). \tag{22}
\]

In this form, the ODEs are solved numerically. Neglecting the Hartree-Fock contribution and the other corrections on the lhs of the second equation, this EOM can easily be integrated:

\[
\langle \psi_{k_1} \psi_{k_2} \psi_{k_2'} \psi_{k_1'}^\dagger \rangle_t^c = \langle \psi_{k_1} \psi_{k_2} \psi_{k_2'} \psi_{k_1'}^\dagger \rangle_0 e^{-i(\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_1'} - \epsilon_{k_2'})(t - t_0)} 
- iv_{k_1,k_2,k_1'k_2'} \int_{t_0}^{t} dt' e^{-i(\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_1'} - \epsilon_{k_2'})(t - t')} \times \left( (1 - n_{k_1})(1 - n_{k_2})\langle n_{k_1'}n_{k_2'} - n_{k_1}n_{k_2} - n_{k_1'}n_{k_2} (1 - n_{k_1'})(1 - n_{k_2}) \right)(t') \right). \tag{23}
\]

In the case of no initial correlations, the transport equation for the one-particle distribution function can then be written as an integro-differential equation:

\[
\frac{d}{dt} n_k(t) = -\sum_{k_1k_2,k_1'k_2'} |v_{kk_2,k_1'k_2'}|^2 \int_{t_0}^{t} dt' \cos((\epsilon_{k_1'} + \epsilon_{k_2'} - \epsilon_k - \epsilon_{k_2})(t - t')) \times \left( n_{k_1}n_{k_2}(1 - n_{k_1'})(1 - n_{k_2'}) - (1 - n_{k_1})(1 - n_{k_2})\langle n_{k_1'}n_{k_2'} \rangle(t') \right). \tag{24}
\]

For a local two-particle interaction \((k_1 = (k_1', \sigma_1), \text{etc.})\)

\[
v_{k_1,k_2,k_1'k_2'} = \left\{ \tilde{v}_{k_1'-k_1} \delta_{\sigma_1\sigma_1'} \delta_{\sigma_2\sigma_2'} - \tilde{v}_{k_2'-k_2} \delta_{\sigma_1\sigma_1'} \delta_{\sigma_2\sigma_2'} \right\} \delta_{k_1+k_2,k_1'+k_2'} \tag{25}
\]

and for an initially spin-independent distribution \((n_{k}(t) := n_{k',\sigma}(t))\) we obtain

\[
\frac{d}{dt} n_k(t) = -2 \sum_{k_1k_2,k_1'k_2'} \delta_{k_1+k_2,k_1'+k_2'} \left\{ 2(\tilde{v}_{k_1-k_1})^2 - \tilde{v}_{k_1-k_1} \tilde{v}_{k_1-k_2} \right\} 
\times \int_{t_0}^{t} dt' \cos((\epsilon_{k_1'} + \epsilon_{k_2'} - \epsilon_k - \epsilon_{k_2})(t - t')) \times \left( n_{k_1}n_{k_2}(1 - n_{k_1'})(1 - n_{k_2'}) - (1 - n_{k_1})(1 - n_{k_2})\langle n_{k_1'}n_{k_2'} \rangle \right) \tag{26}
\]

which is the usual non-Markovian Boltzmann equation with a collision term for the electron-electron interaction in Born approximation.
III. DIAGRAMS

The diagrams described in this section represent the differential equations for the correlations. Therefore they contain only one interaction vertex in contrast to ordinary Feynman graphs. In addition there are graphic elements for the correlations, the so-called correlation bubbles [10], which in our context stand for time-dependent quantities and not for initial correlations. Note that there is no time or energy integration associated with a diagram as it characterizes the temporal evolution of the correlation at time \( t \).

The diagrams are derived for our example, but they are easily extended for systems with bosons and fermions, for systems with three-particle interactions etc. The main elements of the diagrams are the following:

1. The vertex: An internal vertex (Fig. 1) represents the interaction. The matrix element \( v_{i_1 i_2, j_1 j_2} \) is associated with it. Incoming (outgoing) lines characterize annihilation (creation) operators. In order to simplify the determination of the correct sign, we sometimes use another diagrammatic element in which the creation operator \( \psi_{j_n}^{\dagger} \) is paired with the annihilation operator \( \psi_{i_n} \) (Fig. 2).

An external vertex (Fig. 3) represents a single creation or annihilation operator.

2. The contraction: A contraction (Fig. 4) connects two vertices and refers either to the one-particle expectation value \( \langle \psi_{k_1} \psi_{k_1}^{\dagger} \rangle_t \) or \( \langle -\langle \psi_{k_1}^{\dagger} \psi_{k_1} \rangle_c \rangle_t \). This will be explained later.

3. The correlation bubble: A correlation bubble possesses incoming and outgoing lines. The total number of lines must be different from two, otherwise it is a contraction. For the case of a fermionic system only the following correlations occur:

\[
\langle \psi_{k_1} \cdots \psi_{k_n} \psi_{k_1}^{\dagger} \cdots \psi_{k_1}^{\dagger} \rangle_t, \quad n \geq 2 .
\]

The corresponding correlation bubble is shown in Fig. 5. In order to determine the sign, it is better to pair the fermionic creation and annihilation operators in such a way that \( \psi_{k_i} \) and \( \psi_{k_i}^{\dagger} \) constitute a pair \( (i = 1, \ldots, n) \), which is graphically expressed as shown in Fig. 6.

We begin by describing the diagrammatic rules for the part of the time derivative due to the interaction of the \( n \)-particle expectation values \( \langle \psi_{k_1} \cdots \psi_{k_n} \psi_{k_1}^{\dagger} \cdots \psi_{k_1}^{\dagger} \rangle_t \). The corresponding diagram consists of \( 2n \) external vertices and one interaction vertex. These vertices are connected in all possible ways by contractions and correlation bubbles. This corresponds to the cluster expansion of the commutator \( \langle [\psi_{k_1} \cdots \psi_{k_n} \psi_{k_1}^{\dagger} \cdots \psi_{k_1}^{\dagger}, V] \rangle_t \). The following rules apply for the prefactor and the sign:

1. The prefactor: Usually the factor \( \frac{1}{2!} \cdot \frac{1}{2!} \) can be omitted due to the symmetry properties of the interaction matrix elements \( v \) because the graph which is obtained by a permutation of the creation and annihilation operators in the interaction term yields the same contribution. For this class of graphs only one “unlabeled” graph is written down. There is only one exception if the interaction vertex is connected with a correlation bubble by two lines in the same direction, a so-called pair of equivalent lines. In this case a factor of \( \frac{1}{2!} \) remains as the corresponding permutation yields the same “labeled” graph. In addition, there is always the factor \( (-i) \) of Eq. (2).
2. The sign: In addition to the pairing of creation and annihilation operators in the interaction vertex and in the correlation bubbles, the external vertices are grouped into pairs of a creation and an annihilation operator in the same way as for the correlations, i.e. \( \psi_{k_i} \) and \( \psi_{k'_i}^\dagger \) \((i = 1, \ldots, n)\) form a pair. Then, the overall sign is given by

\[
(-1)^n (-1)^L ,
\]

where \( L \) is the number of fermionic loops in the deformed diagrams in which the paired external vertices coincide and \((-1)^n\) is the sign of the permutation normal-ordering the external pairs. This sign rule can be proved in the same way as for usual Green’s function methods [13].

The description of the resulting differential equation

\[
\left[ \frac{d}{dt} + i \left( \epsilon_{k_1} + \cdots + \epsilon_{k_n} - \epsilon_{k'_1} - \cdots - \epsilon_{k'_n} \right) \right] \langle \psi_{k_1} \cdots \psi_{k_n} \psi_{k'_n}^\dagger \cdots \psi_{k'_1}^\dagger \rangle_t \\
= -i \sum_{\text{diagr.}} (-1)^{n+L} \frac{1}{2n_e} \sum_{i_1j_1,i_2j_2} v_{i_1j_1,i_2j_2} X_{\text{diagr.}} ,
\]

(\( n_e = \text{number of pairs of equivalent lines, } L \) is introduced above), is thus complete except for the “collision term” \( X_{\text{diagr.}} \), which is composed of the contractions and the correlations. In the cluster expansion every partition of \( \langle \psi_{k_1} \cdots \psi_{k_n} \psi_{k'_n}^\dagger \cdots \psi_{k'_1}^\dagger \cdot V \rangle_t \) corresponds to a partition of \( \langle V \cdot \psi_{k_1} \cdots \psi_{k_n} \psi_{k'_n}^\dagger \cdots \psi_{k'_1}^\dagger \rangle_t \). Since the correlations are (except for the sign) independent of the relative order of the creation and annihilation operators, the two terms differ only in the contributions of the contractions. Therefore the collision term \( X_{\text{diagr.}} \) is the product of the following contributions:

1. all correlations;

2. all contractions which start and end at the interaction vertex in the normal-ordered form \((-\langle \psi_i^\dagger \psi_j \rangle_c^t)\) as the interaction term was supposed to be normal-ordered;

3. the contractions between external vertices in anti-normal order \( \langle \psi_{k_i} \psi_{k'_j}^\dagger \rangle_c^t \) as they appear in this order on the lhs of the differential equation;

4. the following contribution of the remaining contractions between the interaction vertex and the external vertices, when these lines are labeled as in Fig. [7]

\[
\left( \langle \psi_{k_1} \psi_{k'_1}^\dagger \rangle_c^t \cdots \langle \psi_{k_s} \psi_{k'_s}^\dagger \rangle_c^t \right) \left( -\langle \psi_{k'_1}^\dagger \psi_{j_1} \rangle_c^t \right) \cdots \left( -\langle \psi_{k'_r}^\dagger \psi_{j_r} \rangle_c^t \right)
\]

\[
= -\left( -\langle \psi_{k'_1}^\dagger \psi_{j_1} \rangle_c^t \right) \cdots \left( -\langle \psi_{k'_r}^\dagger \psi_{j_r} \rangle_c^t \right) \left( \psi_{k_1} \psi_{k'_1}^\dagger \right) \cdots \left( \psi_{k_s} \psi_{k'_s}^\dagger \right)
\]

At least one contraction between the interaction vertex and an external vertex is necessary for the graph to yield a non-vanishing contribution. Only in the contractions the non-trivial canonical anti-commutation rules show up.
In order to make these diagrammatic rules more transparent we give an example. The graph shown in Fig. 8 possesses one pair of equivalent lines. The labeled version shown in Fig. 9 has two loops if \( \psi_k \) and \( \psi^\dagger_{k'} \) are paired \((i = 1, 2)\). Therefore it gives the following contribution to the differential equation for \( \langle \psi_{i_1} \psi_{i_2} \psi^\dagger_{k_1} \psi^\dagger_{k_2} \rangle_t \) (cf. Eq. (14)):

\[
- \frac{i}{2} \sum_{i_1, i_2, j_1, j_2} v_{i_1 i_2 j_1 j_2} \left( \langle \psi_{i_1} \psi^\dagger_{i_2} \psi_{k_1} \rangle_t \langle \psi_{k_2} \psi^\dagger_{j_2} \psi^\dagger_{k_1} \rangle_t - \langle \psi^\dagger_{i_1} \psi_{i_2} \psi_{k_1} \rangle_t \langle \psi^\dagger_{j_1} \psi_{j_2} \psi^\dagger_{k_1} \psi^\dagger_{k_2} \rangle_t \right).
\]

(31)

The diagrammatic rules for the correlations are the same as those for the corresponding 2n-point functions except that only connected diagrams must be considered (linked cluster theorem). The fact that the correlations are independent of the order of creation and annihilation operators is of importance only in contractions connecting two external vertices. And these contractions do not appear in connected diagrams.

The linked cluster theorem can be proved in the following way. To each graph for a 2n-point function belongs a partition of the external vertices into connected components, e.g. the graph shown in Fig. 10 gives the partition \( \{ \psi_{i_1}^\dagger, \psi_{k_1} \}, \{ \psi_{i_2}^\dagger, \psi_{k_1}, \psi_{k_2}, \psi_{k_3} \}, \{ \psi_{k_1}^\dagger, \psi_{k_2} \} \). The diagrammatic partition determines exactly one term in the cluster expansion of the 2n-point function. In addition, there is one and only one connected component containing the interaction vertex, in the example it is \( \{ \psi_{i_1}^\dagger, \psi_{k_1} \} \). We call this component the marked component. The term in the cluster expansion with this marked component determines one term in the temporal evolution of the 2n-point function. In order to reduce the formalism this is explained for the example:

\[
\left[ \frac{d}{dt} + i (\epsilon_{k_1} + \cdots + \epsilon_{k_4} - \epsilon_{k_1}' - \cdots - \epsilon_{k_4}') \right] \langle \psi_{k_1} \cdots \psi_{k_4} \psi^\dagger_{k_1} \cdots \psi^\dagger_{k_4} \rangle_t = \cdots + \left\{ \left[ \frac{d}{dt} + i (\epsilon_{k_1} - \epsilon_{k_1}') \right] \langle \psi_{k_1} \psi^\dagger_{k_1} \rangle_t \right\} \langle \psi_{k_2} \psi_{k_3} \psi^\dagger_{k_2} \psi^\dagger_{k_3} \psi^\dagger_{k_1} \rangle_t + \cdots,
\]

i.e. the time derivative and the one-particle Hamiltonian act on the marked component according to Leibniz’s rule.

We will prove the linked cluster theorem by induction on the order of the correlations, corresponding to their recursive definition in Eq. (5). Obviously only connected diagrams contribute to the time evolution of the contractions as at least one external vertex must be connected with the interaction vertex (and the other one must be connected to the interaction vertex because of the fermionic particle conservation). We consider now a correlation \( \langle \psi_{k_1} \cdots \psi_{k_n} \psi^\dagger_{k_n} \cdots \psi^\dagger_{k_1} \rangle_t \) of order \( n \geq 2 \) and assume by induction that the linked cluster theorem holds for all correlations of order less than \( n \). The set of all diagrams for the corresponding 2n-point function \( \langle \psi_{k_1} \cdots \psi_{k_n} \psi^\dagger_{k_n} \cdots \psi^\dagger_{k_1} \rangle_t \) is decomposed into classes of diagrams with the same partition of the external vertices and the same marked component. To each of the classes belongs a term in the cluster expansion of the differential equation, as described above. By induction, this term is described by the corresponding class of diagrams if the marked component is of order less than \( n \). But the total of these diagrams are all
unconnected diagrams. Thus, the remaining term in the cluster expansion of the differential equation
\[
\frac{d}{dt} + t \left( \epsilon_{k_1} + \cdots + \epsilon_{k_n} - \epsilon_{k_1'} - \cdots - \epsilon_{k_n'} \right) \left\langle \psi_{k_1} \cdots \psi_{k_n} \psi_{k_1'}^\dagger \cdots \psi_{k_n'}^\dagger \right\rangle_c
\]  
(33)
is represented by the connected diagrams. This completes the proof. Of course, it is necessary to check the sign and the prefactor as well. As far as the factor \((-i)^{1/2}n_e\) is concerned, this is clear because the factor belongs to the component containing the interaction vertex. We will not give a formalized proof for the correctness of the sign, which should nonetheless be apparent as the sign only reflects the necessary permutation to bring the fermionic operators into the given order. We close with the remark that the proof is the same for the case of a non-diagonal one-particle Hamiltonian \(h_{ij}(t)\) and that for bosons the induction starts with the correlations of lowest order \(\langle B^{(1)} \rangle_t^c\) and no argument about particle-conservation is needed.

The fact that only connected diagrams contribute to the time evolution of correlations is explained by the definition of the correlations because we allowed for all possible partitions of the creation and annihilation operators. Therefore, it is necessary to define the cluster expansion for bosonic systems with non-vanishing expectation values \(\langle B^{(1)} \rangle_t\) as in Eq. (5) and not as sometimes defined:
\[
\begin{align*}
\langle B_1 \rangle_t &= \langle B_1 \rangle_t^c, \\
\langle B_1 B_2 \rangle_t &= \langle B_1 B_2 \rangle_t^c, \\
\langle B_1 B_2 B_3 \rangle_t &= \langle B_1 B_2 \rangle_t^c \langle B_3 \rangle_t^c + \langle B_2 \rangle_t^c \langle B_1 B_3 \rangle_t^c + \langle B_1 \rangle_t^c \langle B_2 B_3 \rangle_t^c + \langle B_1 B_2 B_3 \rangle_t^c \\
&\vdots
\end{align*}
\]  
(34)
Otherwise, also unconnected diagrams give contributions to correlations.

We now return to the example given in section II and present the diagrams for the correlations of one, two, and three particles. The diagrams for the one-particle distribution function representing the Hartree-Fock contribution and the “real” collision term in Eq. (12) are shown in Fig. 11. In order to greatly reduce the number of diagrams, we draw the diagrams for higher-order correlations unlabeled and without arrows. These diagrams are to be seen as representatives for all the diagrams which arise by labeling the external vertices in all possible ways and attaching arrows consistently with the conservation of the particle number. The last two graphs in Fig. 11, for example, are represented by the single graph in Fig. 12. With this simplification there are four types of diagrams for the two-particle correlations (cf. Eq. (15)) shown in Fig. 13. The numbers of resulting diagrams with external labels and arrows are indicated in parentheses. For the three-particle correlations we show the diagrams in Fig. 14 without writing down the corresponding equations. To cut off the hierarchy at this order the four-particle correlations are ignored as described in section II.

IV. SUMMARY

We have described the general formalism for a new method of deriving transport equations for quantum many-body systems. It is based on the equation-of-motion technique and
a cluster expansion of many-particle expectation values. Combining these two elements one obtains an exact infinite hierarchy of EOM in terms of correlations which allows a consistent, unambiguous breaking at any order in contrast to the usual hierarchy. The transport equations consist of a set of ordinary differential equations for the one-particle distribution functions and many-particle correlations up to a given order. By the initial values of these dynamical quantities information (initial correlations) of the initial statistical operator enters the quantum kinetics of the system. In contrast to real-time Green’s function methods our method involves only single-time quantities from the beginning. There is no need for a generalized Kadanoff-Baym ansatz and the separate determination of retarded/advanced Green’s functions. A diagrammatic representation of the equations of motion for the correlations was derived. It simplifies the calculations in the same way as Feynman diagrams do in equilibrium theory. The definition of the correlations by a cluster expansion leads to a linked cluster theorem for the corresponding diagrams.

In this first part of a series of two papers we developed the general formalism. The application of the transport equations to physical systems is left to the second part.

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FIG. 1. An interaction vertex.

FIG. 2. An interaction vertex with paired creation and annihilation operators.

FIG. 3. External vertices.

FIG. 4. A contraction.

FIG. 5. A correlation bubble representing $\langle \psi_{k_1} \cdots \psi_{k_n} \psi_{k_1}^\dagger \cdots \psi_{k_n}^\dagger \rangle_c$.

FIG. 6. A correlation bubble with paired creation and annihilation operators.
FIG. 7. The graph for the explanation of the Pauli factors for a general $n$-body vertex. There are $r + s$ lines connecting the interaction vertex with external vertices. The remaining lines go to correlation bubbles.

FIG. 8. A graph contributing to the 4-point function.

FIG. 9. A labeled version of the graph in Fig. 8 with paired creation and annihilation operators.

FIG. 10. An unconnected graph for the 8-point function.
FIG. 11. The diagrams for the one-particle distribution function.

FIG. 12. The diagram representing the last two diagrams in Fig. [11].

FIG. 13. The diagrams for the two-particle correlations.
FIG. 14. The diagrams for the three-particle correlations.