# Kapitel 6

# BBGKY-hierarchy

The reduced density operators obey a coupled system of equations–the BBGKY hierarchy. The derivation and extensive discussion of this hierarchy are given in the text book [Bon98] and are briefly summarized here. In order to make the following considerations more transparent, we will consider first a quantum system of spinless particles.[1] The effects of the spin statistics will be included explicitly into the final equations of motion below, see Sec. 6.6[2]

## 6.1 Nonequilibrium N-particle density operator

The idea of how to extend a quantum-mechanical pure state description (in terms of wave functions $|\Psi\rangle$) to a mixed state description, in case of a system coupled to a bath, is due to Landau and von Neumann. They defined an incoherent superposition of solutions of the Schrödinger equation which we assume to be orthonormalized. In case of an externally driven system the problem is formulated based on solutions of the time-dependent Schrödinger

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[1] In principle, the equations derived below, are applicable to Bose or Fermi particles also. We would only have to define the trace operations to be performed respectively in the symmetric or antisymmetric subspace of the Hilbert space.

[2] An alternative derivation which includes the spin symmetry from the beginning considers equations of motion of time-dependent field operator products such as $a^\dagger a$, $a^\dagger a^\dagger a a$ and so on, using the results of Sec. 5.2, with a subsequent ensemble average. This, however, generates very lengthy results and the meaning of the different terms is more difficult to identify.

equation[3],

$$\hat{\rho}_N(t) = \sum_{\alpha=1}^{M} W_\alpha \, |\Psi_N^\alpha(t)\rangle\langle\Psi_N^\alpha(t)| \,, \qquad \mathrm{Tr}\,\hat{\rho}_N = 1 \,, \tag{6.1}$$

$$0 \le W_\alpha \le 1 \,, \qquad \sum_{\alpha=1}^{M} W_\alpha = 1 \,,$$

$$i\hbar\frac{\partial}{\partial t}|\Psi_N^\alpha\rangle = \hat{H}_N|\Psi_N^\alpha\rangle \,, \qquad \langle\Psi_N^\alpha|\Psi_N^\beta\rangle = \delta_{\alpha,\beta} \,, \tag{6.2}$$

with the coefficients being standard real probabilities. The density operator is normalized to unity and is the straightforward generalization of the N-particle probability distribution of classical statistical mechanics to the quantum case. The present definition applies to thermodynamic equilibrium (special cases are the canonical or grand-canonical density operator) and to nonequilibrium as well. In the latter case the time dependence enters via the wave functions, cf. Eq. (6.2). The resulting equation of motion of $\rho_N(t)$ – the von Neumann equation – will be discussed in Sec. 6.3.

Our ultimate goal, in most cases, is the computation of time-dependent averages of $s$-particle operators. In quantum statistics this can now be done with the density operators,

$$\langle\hat{B}_s\rangle(t) = \mathrm{Tr}_{1\dots N}\hat{B}_s\,\rho_N(t) = \mathrm{Tr}_{1\dots s}\hat{B}_s\,\mathrm{Tr}_{s+1\dots N}\,\rho_N(t) \,, \tag{6.3}$$

where, in the last expression, we split the trace in two contributions. Evidently, for the s-particle average the full N-particle density operator is not needed, but only its trace over the remaining indices $s+1,\dots N$, which constitutes an s-particle operator. This suggests to introduce additional simpler quantities – the reduced density operators.

**Problem:** prove the normalization of the density operator by using the coordinate representation for computing the trace.

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[3] The (anti-)symmetrization of theses states will be considered later, in Sec. 6.6.

## 6.2 Reduced density operators

### 6.2.1 Main definitions

We define the reduced $s$-particle density operator by a partial trace of the full $N$-particle density operator, the latter being normalized to unity,

$$F_{1\dots s} = \frac{N!}{(N-s)!}\mathrm{Tr}_{s+1\dots N}\rho_N, \quad \mathrm{Tr}_{1\dots s}F_{1\dots s} = \frac{N!}{(N-s)!}. \tag{6.4}$$

Note that $F_s$ is an ensemble-averaged quantity since it is computed from $\rho_N$ that, in general, incorporates a mixed state description with given probabilities of the individual $N$-particle states. The three lowest operators are

$$F_1 = N\mathrm{Tr}_{2\dots N}\,\rho_N, \quad \mathrm{Tr}_1 F_1 = N\,, \tag{6.5}$$

$$F_{12} = N(N-1)\mathrm{Tr}_{3\dots N}\,\rho_N, \quad \mathrm{Tr}_{12}F_{12} = N(N-1)\,, \tag{6.6}$$

$$F_{123} = N(N-1)(N-2)\mathrm{Tr}_{4\dots N}\,\rho_N, \quad \mathrm{Tr}_{123}F_{123} = N(N-1)(N-2)\,. \tag{6.7}$$

The normalization of these operators differs from a probability density. It is chosen such that it accounts for statistical factors – the number of possibilities to select one particle ($F_1$), particle pairs ($F_{12}$) and so on.

### 6.2.2 Trace consistency

The definitions of different reduced density operators have to be consistent with each other because they all follow from the same N-particle operator. Therefore, for $k, s \geq 1$, the different operators have to satisfy[4]

$$F_{1\dots s} = [(N-s+1)\dots(N-s+k-1)]^{-1}\,\mathrm{Tr}_{s+1\dots s+k}\,F_{1\dots s+k}. \tag{6.9}$$

In particular, the lowest order operators are related by

$$F_1 = (N-1)^{-1}\,\mathrm{Tr}_2\,F_{12} = (N-1)^{-1}(N-2)^{-1}\,\mathrm{Tr}_{23}\,F_{123}\,. \tag{6.10}$$

$$F_{12} = (N-2)^{-1}\,\mathrm{Tr}_3\,F_{123}\,. \tag{6.11}$$

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[4] From the normalization conditions for the two operators it follows:

$$\mathrm{Tr}_{1\dots s}F_{1\dots s} = \frac{N!}{(N-s)!}$$

$$\mathrm{Tr}_{1\dots s+k}F_{1\dots s+k} = \frac{N!}{(N-s-k)!}$$

and, therefore,

$$N! = (N-s)!\,F_{1\dots s} = (N-s-k)!\,\mathrm{Tr}_{s+1\dots s+k}F_{1\dots s+k}\,. \tag{6.8}$$

Trace consistency is obvious for the exact density operators whereas, for approximations, it provides an important consistency criterion. For example, for *independent particles*, we will show below that

$$F_{1\dots s} \to F^{\text{ideal}}_{1\dots s} = F_1 \cdot F_2 \cdot \dots \cdot F_s \,, \tag{6.12}$$

where the subscripts refer to the Hilbert spaces of the different particles. Then relations (6.10) and (6.11) turn into

$$(N-1)\,F_1 = F_1 \mathrm{Tr}_2\, F_2 = N F_1 \,, \tag{6.13}$$

$$(N-2)\,F_1F_2 = F_1F_2\mathrm{Tr}_3\, F_3 = N F_1F_2 \,, \tag{6.14}$$

i.e. trace consistency is violated. This is surprising because the approximation (6.12) is a physically reasonable choice. We will return to the discussion of trace consistency after we have restored spin symmetry in the operators in Sec. 6.6.

## 6.3 Derivation of the quantum BBGKY-hierarchy for spinless particles

We now consider the general nonequilibrium case where a quantum system is excited by a time-dependent hamiltonian. We first derive the equation of motion for the full $N$-particle density operator which will serve as the basis to derive the equations of motion for the reduced density operators.

### 6.3.1 BBGKY hierarchy

The time evolution of $\hat{\rho}_N$ follows from the time evolution of the underlying $N$-particle wave functions, cf. the definition (6.1). Differentiating this definition with respect to time, we easily derive the *von Neumann equation*,

$$i\hbar\frac{d}{dt}\rho_N - [H_N, \rho_N] = 0 \,, \tag{6.15}$$

$$\rho_N(t_0) = \rho_N^0 \equiv \sum_k W_k \,|\Psi_N^k(t_0)\rangle\langle\Psi_N^k(t_0)| \,,$$

supplemented by an initial condition. Here it is assumed that $\dot{W}_k = 0$. We briefly outline the main steps in the derivation of the equations of motion for the reduced density operators $F_{1\dots s}$. First, the hamiltonian is split into three parts for the two subsystems, $\hat{H}_N = H_{1\dots s} + H_{s+1\dots N} + H^{\rm int}$, where the coupling part contains all pair interactions of two particles from the two parts,

$$H^{\rm int} = \sum_{i=1}^{s} \sum_{k=s+1}^{N} V(r_i, r_k)\,,$$

Now we compute the partial trace over $s+1\dots N$ in all terms of Eq. (6.15). Taking into account the invariance of the trace it is easy to understand that the hamiltonian $H_{s+1\dots N}$ vanishes under the commutator. The trace with $H^{\rm int}$ leads to $N-s$ identical terms. Taking the definitions of $F_{1\dots s}$ and $F_{1\dots s+1}$ into account this factor cancels, and we arrive at[5] the hierarchy of equations of motion for the reduced density operators, the quantum **BBGKY-hierarchy**,

$$i\hbar\frac{\partial}{\partial t}F_{1\dots s} - [H_{1\dots s}, F_{1\dots s}] = {\rm Tr}_{s+1}[V^{(1\dots s),s+1}, F_{1\dots s+1}]\,, \tag{6.16}$$

$$V^{(1\dots s),s+1} = \sum_{\alpha=1}^{s} V^{\alpha,s+1}, \tag{6.17}$$

$$F_{1\dots s}(t_0) = F^0_{1\dots s} = \frac{N!}{(N-s)!}{\rm Tr}_{s+1\dots N}\,\rho^0_N\,. \tag{6.18}$$

Here, $H_{1\dots s}$ is the $s$-particle Hamilton operator which follows from $H_{1\dots N}$ by substituting $N \to s$. The equations of the hierarchy differ from the von Neumann equation due to the terms on the r.h.s, which contain the coupling of the $s$ particles to the remainder of the system via all possible binary interactions. The complete hierarchy is, obviously, equivalent to the von Neumann equation and, therefore, has the same properties. In particular, the system (6.16) is time reversible and conserves the total energy. The individual equations are also connected via the trace relation, Eq. (6.9). This means, by computing a partial trace, a higher order equation can be reduced to a lower-order one. This is trivial for the exact system, however, for approximate solutions, this represents an important consistency criterion, see Sec. 6.3.2.

Each equation of the hierarchy, for $s < N$, is an inhomogeneous first order differential equation which can be solved formally using the time evolution operators, $U_{1\dots s}$, corresponding to the hamiltonian $H_{1\dots s}$, for details see Ref. [Bon98]. Finally, we may ask at what place in our derivation the neglect of Fermi or Bose statistics was required. It is easy to understand that imposing the subdivision into a system of $s$ particles and a second one of $N-s$ particles we implicitly assumed that the two groups are distinguishable. In contrast, for a system of fermions or bosons the interaction between the two subgroups

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[5] See problem 5.5.

will also give rise to exchange effects where particles, in the course of their interaction, will change their association with the two subsystems.

### 6.3.2 Trace consistency of the equations of the BBGKY-hierarchy

Due to the expected trace consistency between different reduced density operators [cf. Eq. (6.9)] there should also exist a consistency between different equations. For example, the second equation should reduce, via a partial trace over one variable to the first equation. Again, this is fulfilled for the exact solution. On the other hand, if approximations are being used, this consistency is an important criterion of the quality of the approximation. We demonstrate this for the two lowest equations that directly follow from the hierarchy (6.16),

$$i\hbar\frac{\partial}{\partial t}F_1 - [H_1, F_1] = \mathrm{Tr}_2[V^{(12)}, F_{12}]\,. \tag{6.19}$$

$$i\hbar\frac{\partial}{\partial t}F_{12} - [H_{12}, F_{12}] = \mathrm{Tr}_3[V^{(12),3}, F_{123}]\,. \tag{6.20}$$

We now compute $(N-1)^{-1}\mathrm{Tr}_2\ldots$ of Eq. (6.20) and use relation (6.10), with the result

$$i\hbar\frac{\partial}{\partial t}F_1 - [H_1, F_1] = \frac{1}{N-1}\mathrm{Tr}_2[V^{(12)}, F_{12}] + \frac{1}{N-1}\mathrm{Tr}_{23}[V^{(12),3}, F_{123}]\,.$$

where we took into account that $[H_2, F_{12}]$ vanishes under the trace. Comparing the right hand side of this equation to the r.h.s. of (6.19) we find the consistency requirement

$$(N-2)\,\mathrm{Tr}_2[V^{(12)}, F_{12}] = \mathrm{Tr}_{23}[V^{(13)}, F_{123}]\,, \tag{6.21}$$

where, on the r.h.s., the contribution with $V^{(23)}$ vanishes under the trace. This can be reformulated as a condition on $F_{123}$. To this end we eliminate $F_{12}$ with the help of Eq. (6.11),

$$\mathrm{Tr}_{23}[V^{(12)}, F_{123}] = \mathrm{Tr}_{23}[V^{(13)}, F_{123}]\,. \tag{6.22}$$

The sufficient condition for this to hold is the permutation symmetry

$$F_{123} = F_{132}\,. \tag{6.23}$$

Since this condition follows from the first hierarchy equation it does not involve any requirement on subscript “1”. We can make this more transparent by choosing a representation in terms of a complete orthonormal set of three-particle states, $\{|123\rangle\}$, and by denoting $V' = V^{(12)} - V^{(13)}$. Then we can rewrite Eq. (6.22) as

$$0 = Y(1,1') = \sum_{23}\sum_{\bar{1}\bar{2}\bar{3}} \{\langle 123|V'|\bar{1}\bar{2}\bar{3}\rangle\langle\bar{1}\bar{2}\bar{3}|F_{123}|1'23\rangle - \\ \langle 123|F_{123}|\bar{1}\bar{2}\bar{3}\rangle\langle\bar{1}\bar{2}\bar{3}|V'|1'23\rangle\}\,.$$

Using the coordinate representation and assuming a distance-dependent interaction with $\langle r_1r_2r_3|V^{(12)}|r_1'r_2'r_3'\rangle = V(r_1-r_2)\delta(r_1-r_1')\delta(r_2-r_2')\delta(r_3-r_3')$, this result becomes

$$0 = Y(r_1,r_1') = \int dr_2dr_3\, F(r_1,r_2,r_3;r_1',r_2,r_3)\times \\ \times\left\{V(r_1-r_2) - V(r_1-r_3) - V(r_1'-r_2) + V(r_1'-r_3)\right\}. \tag{6.24}$$

Again, we confirm the previously found sufficient condition (6.23) (but there can be others)

$$F(r_1,r_2,r_3;r_1',r_2,r_3) = F(r_1,r_3,r_2;r_1',r_3,r_2)\,. \tag{6.25}$$

It is interesting to compare this condition to the condition for total energy conservation which reads [Bon98]:

$$0 = \mathrm{Tr}_{123}V^{(12)}[V^{(13)}+V^{(23)},F_{123}] \\ = \mathrm{Tr}_{123}\left\{V^{(12)}(V^{(13)}+V^{(23)})F_{123} - F_{123}(V^{(13)}+V^{(23)})V^{(12)}\right\}\,. \tag{6.26}$$

A sufficient condition for this to hold is $P_{123}F_{123} = F_{123}$, i.e. a complete permutation symmetry in all indices. Alternatively, energy conservation is fulfilled if the interaction is diagonal in a given basis. An example is, again a distance-dependent potential in the coordinate representation. In this case energy is conserved for any approximation for $F_{123}$, even if trace consistency, Eq. (6.25), is violated.

Trace consistency between the two first equations of the hierarchy is, of course, fulfilled for the exact solution for $F_{123}$. On the other hand, this issue is not trivial for approximations. Two contributions to $F_{123}$ that obviously fulfill condition (6.23) are

$$F_{123} = F_1F_2F_3 + F_1g_{23}\,.$$

We will return to the question of trace consistency of important approximations below, in Sec. 6.5.

### 6.3.3 Matrix representation of the BBGKY-hierarchy

The BBGKY-hierarchy (6.16) is written in an abstract operator notation which has the advantage of a simple and compact structure. At the same time, for practical applications it is necessary to transform this result into a suitable basis representation. Let us present such a result for a general complete orthonormal system of s-particle states, $\{|i_1 \dots i_s\rangle\} \in \mathcal{H}_s$. Without loss of generality, we can assume that these are products of single-particle orbitals. For example, an $s+1$-particle state can be produced from an $s$-particle state multiplied with single-particle orbitals[6]. Denoting matrix elements of operators by

$$F^{(s)}_{i_1 \dots i_s, j_1 \dots j_s} = \langle i_1 \dots i_s | F_{1 \dots s} | j_1 \dots j_s \rangle \,, \tag{6.27}$$

we obtain the basis representation of Eq. (6.16),

$$i\hbar \frac{\partial}{\partial t} F^{(s)}_{i_1 \dots i_s, j_1 \dots j_s} - [H^{(s)}, F^{(s)}]_{i_1 \dots i_s, j_1 \dots j_s} = \sum_{i_{s+1}} [V^{(1 \dots s), s+1}, F^{(s+1)}]_{i_1 \dots i_{s+1}, j_1 \dots j_s, i_{s+1}} \,, \tag{6.28}$$

$$\begin{aligned} [A, B]_{i_1 \dots i_s, j_1 \dots j_s} &= (AB)_{i_1 \dots i_s, j_1 \dots j_s} - (BA)_{i_1 \dots i_s, j_1 \dots j_s} \\ (AB)_{i_1 \dots i_s, j_1 \dots j_s} &= \sum_{k_1 \dots k_s} A_{i_1 \dots i_s, k_1 \dots k_s} B_{k_1 \dots k_s, j_1 \dots j_s} \\ V^{1, s+1}_{i_1 \dots i_{s+1}, j_1 \dots j_s, j_{s+1}} &= V_{i_1, i_{s+1}; j_1, j_{s+1}} \delta_{i_2; j_2} \cdot \delta_{i_2; j_2} \dots \delta_{i_s; j_s} \end{aligned} \tag{6.29}$$

Note that the commutator term on the l.h.s. contains, in general an s-fold sum, whereas the collision term on the r.h.s. contains two additional sums that involve the matrix indices of the pair potential.

Important special cases of basis sets, including the coordinate, momentum and Wigner representations, are discussed in Ref. [Bon98].

## 6.4 Decoupling of the BBGKY-hierarchy. Cluster expansion. Correlation operators

The fruitfulness of the concept of the hierarchy is due to the fact, that the vast majority of physical phenomena and observables of the $N$-particle system, can be described by a quite limited number of reduced density operators, typically not exceeding the order $s$=4. Therefore, it is reasonable to decouple the hierarchy at some appropriate level, thereby drastically reducing the complexity

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[6] Note that we do not use (anti-)symmetrized states [Slater determinants/permanents] here because this would lead to more complicated expressions.

of the problem. The influence of the higher order contributions is neglected or treated approximately. Thus, in the following we will concentrate on the first three equations:

$$i\hbar\frac{\partial}{\partial t}F_1 - [H_1, F_1] = \mathrm{Tr}_2[V_{12}, F_{12}], \tag{6.30}$$

$$i\hbar\frac{\partial}{\partial t}F_{12} - [H_{12}, F_{12}] = \mathrm{Tr}_3[V^{(12),3}, F_{123}], \tag{6.31}$$

$$i\hbar\frac{\partial}{\partial t}F_{123} - [H_{123}, F_{123}] = \mathrm{Tr}_4[V^{(123),4}, F_{1234}]. \tag{6.32}$$

It is tempting to decouple the hierarchy by neglecting the right hand side of a chosen equation, say for $F_{1\dots s}$. Then we have a closed equation for $F_{1\dots s}$ which can be solved and the result inserted into the r.h.s. of the equation for $F_{1\dots s-1}$ and so on. While this is done by many authors, such a decoupling scheme has to be questioned. Let us illustrate this on the example of the first hierarchy equation, Eq. (6.30). In what cases will the r.h.s. be small? Low density (small particle number $N$) is not a relevant case. $F_{12}$ describes the joint probabilities of two particles to be in certain two-particle states and it is normalized to $N(N-1)$. On the other hand, $F_1$ on the l.h.s. is normalized to $N$. So, even in the limit of small particle number or low density, the r.h.s. will remain finite.

## 6.4.1 Mean field approximation. Hartree potential

The second case where it could be argued the r.h.s. of the system (6.30), (6.31), 6.32) might vanish is the case of weak interaction. However, in that case the joint probability described by $F_{12}$ does not vanish but, rather, the two particles will not be correlated, i.e. behave independently. This means, obviously[7], that the ideal two-particle RDO has the form

$$F_{12} \approx F_{12}^{\mathrm{id}} = F_1 F_2. \tag{6.33}$$

In a spatially uniform system, this becomes, in the coordinate representation,

$$\langle r_1 r_2|F_{12}|r_1 r_2\rangle \approx F(r_1)F(r_2)\,, \tag{6.34}$$

which is normalized to $N^2$. By introducing center of mass and relative coordinates, $R = (r_1 + r_2)/2$ and $r = r_1 - r_2$, this can also be related to the pair distribution function (PDF) $f_{12}$,

$$\langle r_1 r_2|F_{12}|r_1 r_2\rangle = Cf_{12}(R, r) \approx Cf_{12}(r)\,, \tag{6.35}$$

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[7] Recall that we have neglected the bosonic/fermionic nature of the particles. If this is taken into account, in addition to the product, there appears an exchange term. This will be considered in Sec. 6.6.

which, is due to homogeneity. In the ideal case, this becomes, $f_{12}^{\mathrm{id}}(r) = \mathrm{C}$ where the constant follows from the normalization. If we regard the PDF as a probability density, the normalization is $\int d^3r f_{12}^{\mathrm{id}}(r) \equiv 1$, therefore the constant equals $C = 1/V$.

Inserting expression (6.33) into the r.h.s of Eq. (6.30) leads, in general, to a finite expression,

$$\begin{aligned}\mathrm{Tr}_2[V_{12}, F_1F_2] = &(\mathrm{Tr}_2 V_{12} F_2)\, F_1 - F_1 \mathrm{Tr}_2 F_2 V_{12} = \\ =&U_1^{\mathrm{H}} F_1 - F_1 U_1^{\mathrm{H}}\,,\end{aligned} \tag{6.36}$$

where we introduced an effective potential

$$U_1^{\mathrm{H}} = \mathrm{Tr}_2 V^{(12)} F_2\,, \tag{6.37}$$

that will appear frequently below[8]. This potential can be understood as the mean potential created by all particles (*Hartree mean field*).

$$i\hbar \frac{\partial}{\partial t} F_1 - [\bar{H}_1, F_1] = 0\,, \tag{6.38}$$

where the effective single-particle hamiltonian is defined as $\bar{H}_1 = H_1 + U_1^{\mathrm{H}}$. For now it is important to note that the case of non-interacting particles does not lead to a vanishing r.h.s. of Eq. (6.30) but to an additional potential energy that can, in general, not be neglected. The same argument applies to the three-particle density operator $F_{123}$ which, in the case of weak interaction, will not vanish but retain an elementary contribution $F_1F_2F_3$. The same applies to all higher order density operators.

### 6.4.2 Cluster expansion of the reduced density operators

The effect of a non-vanishing interaction then will be a deviation of the $s$-particle density operator from the primitive factorization into $s$ single-particle operators. These deviations are called *correlation operators.* The corresponding expansion of the density operators is called **cluster expansion for the reduced density operators** (or Ursell-Mayer expansion)[9]. This expansion will turn out to be the proper starting point to develop systematic approximations

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[8] In fact, this potential coincides with the induced potential that was discussed in the dynamics of the field operators.

[9] We still neglect spin statistics, generalizations will be discussed below.

to the BBGKY-hierarchy, Eq. (6.16). The cluster expansion is given by[10]

$$
\begin{aligned}
F_{12} &= F_1F_2 + g_{12}\,, && (6.39)\\
F_{123} &= F_1F_2F_3 + g_{23}F_1 + \dots + g_{123}\,, && (6.40)\\
F_{1234} &= F_1F_2F_3F_4 + g_{34}F_1F_2 + \dots + g_{12}g_{34} + \dots + g_{234}F_1 + \dots + g_{1234}\,.\\
&\dots
\end{aligned}
$$

The dots denote contributions arising from permutations of the particle indices in the previous term. As one can see, the density operators $F_{12}, F_{123}$ etc. contain one-particle and higher order contributions. As discussed above, products of one-particle density operators $F_1F_2\dots F_s$ correspond to the uncorrelated superposition of $s$ particles, whereas $g_{12}$, $g_{123}, \dots$ describe correlations of two, three or more particles which are caused by their interaction [additional correlations due to the spin statistics, entanglement and similar phenomena will only emerge after (anti-)symmetrization of the hierarchy, cf. Sec. 6.6].

Before we proceed to the equations of motion for the correlation operators let us consider some of their properties.

**Normalization of the correlation operators.** First, we consider the question how these operators are normalized. This follows directly from the normalization of the reduced density operators, Eq. (6.4) and of operator products,

$$
\mathrm{Tr}_{1\dots s}F_1F_2\dots F_s = N^s. \tag{6.41}
$$

In particular, we obtain for the two-particle correlation operator

$$
\mathrm{Tr}_{12}\,g_{12} = \mathrm{Tr}_{12}(F_{12} - F_1F_2) = N(N-1) - N^2 = -N\,. \tag{6.42}
$$

This can be used to compute the normalization of the three-particle correlation operator

$$
\begin{aligned}
\mathrm{Tr}_{123}\,g_{123} &= \mathrm{Tr}_{12}(F_{123} - F_1F_2F_3 - 3F_1g_{23}) =\\
&= N(N-1)(N-2) - N^3 - 3N(-N) = 2N\,,
\end{aligned} \tag{6.43}
$$

and so on. The results (6.42) and (6.43) are unexpected because the particle number (norm) should not change with the interaction. This means the trace of $F_{1\dots s}$ should coincide with the uncorrelated limit, i.e. the trace of $F^s$. This is indeed fulfilled in the thermodynamic limit because the correction of $g_{12}$ ($g_{123}$) to the normalization is of order $1/N$ ($1/N^2$). However, for finite systems the normalization of the correlation operators has to be taken into account.[11]

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[10] A modified cluster expansion is analyzed in Sec. ??.

[11] Again, this difficulty arises from the assumption of distinguishable particles and will be naturally resolved when we consider fully (anti-)symmetrized versions of the reduced density and correlation operators in Sec. 6.6.

**Trace consistency in terms of correlation operators.** Another consistency test is to verify the trace relations that were discussed in Secs. 6.2 and 6.3.2. In fact, starting from the trace consistency between $F_1$ and $F_{12}$, we obtain

$$\begin{aligned}(N-1)F_1 &= \mathrm{Tr}_2(F_1F_2 + g_{12})\,,\\ \to \mathrm{Tr}_2\, g_{12} &= -F_1\end{aligned} \tag{6.44}$$

Now, doing the same on the next level, we have

$$(N-2)F_{12} = \mathrm{Tr}_3\left\{F_3F_{12} + F_1g_{23} + F_2g_{13} + g_{123}\right\}\,.$$

Using the result (6.44) we obtain

$$\mathrm{Tr}_3\, g_{123} = -2g_{12}\,. \tag{6.45}$$

The results (6.44) [(6.45)] are consistent with the normalization conditions that were found above, as is easily checked by performing the trace over 1 [1 and 2]. Redoing the derivations that led to Eqs. (6.44) and (6.45) in the *thermodynamic limit*, i.e. replacing $N-1 \to N$ and $N-2 \to N$ we obtain

$$\mathrm{Tr}_2\, g_{12} = \mathrm{Tr}_3\, g_{123} = 0\,, \quad N \gg 1\,.$$

### 6.4.3 BBGKY-hierarchy for the correlation operators

Using the cluster expansion it is straightforward to derive equations of motion for the correlation operators[12],

$$\begin{gathered}
i\hbar\frac{\partial}{\partial t}F_1 - [\bar{H}_1, F_1] = \mathrm{Tr}_2[V_{12}, g_{12}]\\[2ex]
i\hbar\frac{\partial}{\partial t}g_{12} - [\bar{H}_{12}, g_{12}] = [V_{12}, F_1F_2] +\\
\mathrm{Tr}_3\Big\{[V_{13}, F_1g_{23}] + [V_{23}, F_2g_{13}] + [V^{(12),3}, g_{123}]\Big\}\\[2ex]
i\hbar\frac{\partial}{\partial t}g_{123} - [\bar{H}_{123}, g_{123}] = [V^{(123)}, F_1F_2F_3] +\\
[V^{(12),3}, F_3g_{12}] + [V^{(13),2}, F_2g_{13}] + [V^{(23),1}, F_1g_{23}] +\\
\mathrm{Tr}_4[V^{(12),4}, g_{12}g_{34}] + \mathrm{Tr}_4[V^{(13),4}, g_{13}g_{24}] + \mathrm{Tr}_4[V^{(23),4}, g_{23}g_{14}]\\
+\mathrm{Tr}_4[V_{14}, F_1g_{234}] + \mathrm{Tr}_4[V_{24}, F_2g_{134}] + \mathrm{Tr}_4[V_{34}, F_3g_{124}]\\
+\mathrm{Tr}_4[V^{(123),4}, g_{1234}]
\end{gathered} \tag{6.46}$$

---

[12] see problem 5.7

where we introduced the effective Hamiltonians which contain an effective potential (Hartree potential or mean field) $U^{\mathrm{H}}$ that we discussed above:

$$U_1^{\mathrm{H}} = \mathrm{Tr}_2\, V_{12}\, F_2\,, \tag{6.47}$$

$$\bar{H}_1 = H_1 + U_1^{\mathrm{H}}, \tag{6.48}$$

$$\bar{H}_{12} = \bar{H}_1 + \bar{H}_2 + V_{12} = \bar{H}_{12}^0 + V_{12}, \tag{6.49}$$

$$\bar{H}_{123} = \bar{H}_1 + \bar{H}_2 + \bar{H}_3 + V^{(123)}, \tag{6.50}$$

$$V^{(123)} = V_{12} + V_{13} + V_{23} \tag{6.51}$$

where the superscript “0” indicates the noninteracting (mean field) contributions to the hamiltonians, e.g. $\bar{H}_{12}^0 = \bar{H}_1 + \bar{H}_2$, and so on. The external field $\mathcal{U}$ is contained in the single-particle hamiltonians, and will not be written explicitly.

Let us rewrite the above results for an arbitrary basis representation.

$$\begin{aligned}
\bar{H}_{ij} &= H_{ij} + U_{ij}^{\mathrm{H}}, \\
\bar{H}_{ij,kl}^{(2)} &= \bar{H}_{i,k}\delta_{jl} + \bar{H}_{jl}\delta_{ik} + V_{ij,kl} = \bar{H}_{ij,kl}^{(2)0} + V_{ij,kl}, \\
\bar{H}_{ijk,lmn}^{(3)} &= \bar{H}_{il}\delta_{jm}\delta_{kn} + \bar{H}_{jm}\delta_{ik}\delta_{kn} + \bar{H}_{kn}\delta_{jm}\delta_{il} + \\
&\quad + V_{ij,lm}\delta_{kn} + V_{ik,ln}\delta_{jm} + V_{jk,mn}\delta_{il}, \\
U_{ij}^{\mathrm{H}} &= \sum_{kl} V_{ik,jl}\, F_{lk} \\
V_{ijk,opq}^{(123)} &= V_{ij,op}\delta_{kq} + V_{ik,oq}\delta_{jp} + V_{jk,pq}\delta_{io}.
\end{aligned} \tag{6.52}$$

With these results we now transform the operator equations for $F_1$, $g_{12}$ and $g_{123}$ into a general matrix representation, in analogy to Eq. (6.28):

$$i\hbar\frac{\partial}{\partial t}F_{ij} - [\bar{H}_1, F]_{ij} = \sum_{klm}\{V_{ik,lm}g_{lm,jk} - g_{ik,lm}V_{lm,jk}\} \tag{6.53}$$

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}g_{ij,kl} - [\bar{H}^{(2)}, g]_{ij,kl} &= \sum_{op}\left(V_{ij,op}F_{ok}F_{pl} - F_{io}F_{jp}V_{op,kl}\right) + \\
&\quad + \sum_{mop}\left\{V_{im,op}F_{ok}g_{jp,lm} - F_{io}g_{jm,lp}V_{ok,pm}\right\} \\
&\quad + \sum_{mop}\left\{V_{jm,po}F_{pl}g_{io,km} - F_{jo}g_{im,kp}V_{ol,pm}\right\} \\
&\quad + \sum_{mopq}\left\{V_{ijm,opq}^{(12)3}g_{opq,klm}^{(3)} - g_{ijm,opq}^{(3)}V_{opq,klm}^{(12)3}\right\}.
\end{aligned} \tag{6.54}$$

The term on the r.h.s. of Eq. (6.53) is the collision integral. The first term on the r.h.s. of Eq. (6.54) is the inhomogeneity whereas lines two and three contain the polarization contributions. Finally, in the last term that couples to three-particle correlations, one sum can be taken due to the Kronecker symbols contained in the potential $V^{(12)3}$, cf. the definition (6.29).

For completeness we also present the matrix form of the equation for the three-particle correlation operator, cf. the third equation of the system (6.46),

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}g^{(3)}_{ijk,lmn} - [\bar{H}^{(3)}, g^{(3)}]_{ijk,lmn} =& \sum_{opq}\left\{V^{(123)}_{ijk,opq}F_{ol}F_{pm}F_{qn} - F_{io}F_{jp}F_{kq}V^{(123)}_{opq,lmn}\right\}+\\
&\sum_{opq}\left\{V^{(12)3}_{ijk,opq}F_{qn}g_{op,lm} - F_{kq}g_{ij,op}V^{(12)3}_{opq,lmn}\right\}+\\
&\sum_{opq}\left\{V^{(13)2}_{ijk,opq}F_{pm}g_{oq,ln} - F_{jp}g_{ik,oq}V^{(13)2}_{opq,lmn}\right\}+\\
&\sum_{opq}\left\{V^{(23)1}_{ijk,opq}F_{ol}g_{pq,mn} - F_{io}g_{jk,pq}V^{(23)1}_{opq,lmn}\right\}+\\
&\sum_{opqr}\left\{V^{(12)4}_{ijo,pqr}g_{pq,lm}g_{kr,no} - g_{ij,pq}g_{ko,nr}V^{(12)4}_{pqr,lmo}\right\}+\\
&\sum_{opqr}\left\{V^{(13)4}_{iko,pqr}g_{pq,ln}g_{jr,mo} - g_{ik,pq}g_{jo,mr}V^{(13)4}_{pqr,lno}\right\}+\\
&\sum_{opqr}\left\{V^{(23)4}_{jko,pqr}g_{pq,mn}g_{ir,mn} - g_{jk,pq}g_{io,lr}V^{(23)4}_{pqr,mno}\right\}+\\
&\sum_{opr}\left\{V_{io,pr}F_{pl}g^{(3)}_{jkr,mno} - F_{ip}g^{(3)}_{jko,mnr}V_{pr,lo}\right\}+\\
&\sum_{opr}\left\{V_{jo,pr}F_{pm}g^{(3)}_{ikr,lno} - F_{jp}g^{(3)}_{iko,lnr}V_{pr,mo}\right\}+\\
&\sum_{opr}\left\{V_{ko,pr}F_{pn}g^{(3)}_{ijr,lmo} - F_{kp}g^{(3)}_{ijo,lmr}V_{pr,no}\right\}+\\
&\sum_{opqrs}\left\{V^{(123)4}_{ijko,pqrs}\,g^{(4)}_{pqrs,lmno} - g^{(4)}_{ijko,pqrs}\,V^{(123)4}_{pqrs,lmno}\right\},
\end{aligned}
\tag{6.55}
$$

where most of the multiple sums can be reduced by one summation index because of the Kronecker deltas contained in $V^{(ab)c}_{ijk,lmn}$ and $V^{(abc)}_{ijk,lmn}$, whereas the matrix elements $V^{(abc)d}_{ijkl,mnop}$ contain even two delta symbols.

While this matrix form of the first three hierarchy equations is completely general, it is instructive to consider also the special cases of a Hubbard basis, cf. Chapter 7, or of a momentum basis, as these cases are relevant for strongly correlated systems and jellium (spatially uniform systems), respectively.

## 6.5 Important approximations to the hierarchy

Let us first rewrite the first two hierarchy equations introducing definitions for some of the terms,

$$i\hbar\frac{\partial}{\partial t}F_1 - [\bar{H}_1, F_1] = \mathrm{Tr}_2[V_{12}, g_{12}]$$

$$i\hbar\frac{\partial}{\partial t}g_{12} - [\bar{H}_1^0 + \bar{H}_2^0, g_{12}] = [V_{12}, F_1F_2] + L_{12} + \Pi_{12} + \mathrm{Tr}_3[V^{(12),3}, g_{123}]\,, \quad (6.56)$$

$$L_{12} = [V_{12}, g_{12}], \quad \Pi_{12} = \hat{P}_{12}\left(\mathrm{Tr}_3[V_{13}, F_1 g_{23}]\right)\,. \quad (6.57)$$

We now summarize the most important approximations for the decoupling of the BBGKY hierarchy.

1. Mean field (Hartree) approximation: $g_{12} \to 0$, i.e. neglect of all correlations. Closed mean field equation for $F_1$.

2. Solution of an effective two-particle problem for $F_1$ and $g_{12}$, with $g_{123} \to 0$ and different additional approximations.

   **a.** Second Born approximation (SOA): neglect of ladder and polarization contributions, $L_{12} = \Pi_{12} \to 0$.

   **b.** Third Born approximation (TOA): in addition to item a., inclusion of first polarization contributions and ladder terms. This means, $L_{12} \to L_{12}^{\mathrm{TOA}} = [V_{12}, g_{12}^{\mathrm{SOA}}]$ and $\Pi_{12} \to \Pi_{12}^{\mathrm{TOA}} = \hat{P}_{12}\left(\mathrm{Tr}_3[V_{13}, F_1 g_{23}^{\mathrm{SOA}}]\right)$

   **c.** Static T-matrix approximation: neglect of polarization contributions, $\Pi_{12} \to 0$, summation of an infinite "ladder" sum[13]. Thereby account of arbitrary strong coupling effects on the two-particle level with static pair interaction, cf. second line of Fig. 6.1.

   **d.** Polarization approximation: neglect of "ladder" contributions, $L_{12} \to 0$, summation of an infinite "bubble" sum, thereby account of dynamical screening effects in the weak coupling limit, cf. third line of Fig. 6.1.

---

[13] If spin statistics are taken into account it turns out that there are two independent T-matrix contributions: particle-particle ladders and particle-hole ladders, e.g. [JSB20, JSO$^+$22].

**e.** Gould-DeWitt or FLEX approximation: linear combination of items c. and d, $g_{12}^{\mathrm{FLEX}} = g_{12}^{L} + g_{12}^{\Pi} - g_{12}^{\mathrm{SOA}}$ where approximation a. is subtracted to avoid double counting.

**f.** Dynamically screened ladder approximation: complete solution of the second equation with ladder and polarization terms included (sometimes also called Wang-Cassing [WC85, Cas09] or Valdemoro approximation [CPdVV93]). For a detailed analysis, see Ref. [JSO$^{+}$22].

The physical meaning of these approximations, in particular c. and d., can be understood from a diagrammatic representation and from an iterative solution of the second equation, using the Born approximation a. as the starting point. This is illustrated in Fig. 6.1.

3. Partial account of three-particle correlations. Generally, on this level, one would neglect four-particle correlations, $g_{1234} \to 0$.

**a.** Partial account of inhomogeneity contributions, whereas three-particle ladder terms ($V$ contributions to $\bar{H}_{123}$) and polarization contributions [third line of Eq. (6.46)] are neglected.

**b.** selfenergy effects

**c.** additional approximations. There is a broad class of additional approximations on three-particle correlations that have been proposed in various fields that are presently being actively investigate. We only mention a few examples: the Nakatsuji-Yasuda approximation [NY96], the selfconsistent RPA by Schuck and Tohyama [ST16].

## 6.6 Restoring spin statistics in the hierarchy

So far we have considered reduced density operators that describe the behavior of a selection of 1, 2, 3 or more particles, in the presence of the rest of the system. During this selection process we essentially "marked" these particles which is only possible if Fermi or Bose statistics do not play a role. Among the problems that we observed are the normalization of the correlation operators. Furthermore, we observed that important exchange corrections, e.g. to the Hartree mean field (the Fock term), and Pauli blocking, are missing in our theory.

We now drop this restriction and extend the BBGKY hierarchy to density operators that are fully (anti-)symmetrized. While the operator form of the hierarchy is still completely general, symmetry properties are introduced in

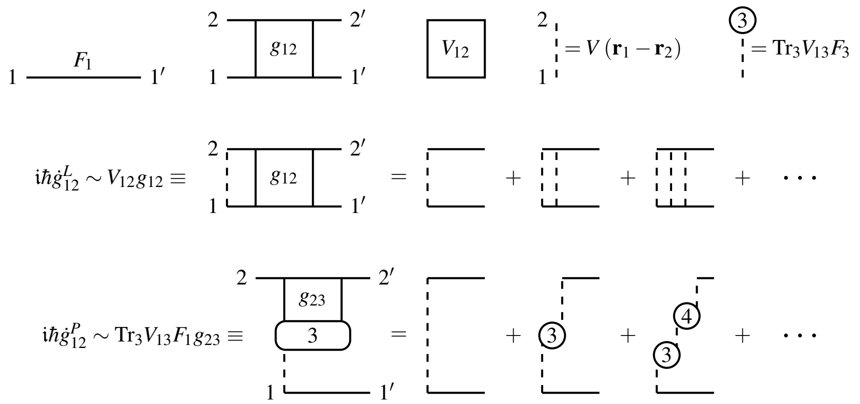

Abbildung 6.1: Graphical representation of important approximations to the BBGKY-hierachy. **First line**: $F_1$, $g_{12}$, $V_{12}$, $V(r_1 - r_2)$ (distance dependent potential in coordinate representation) and the Hartree mean field $U_1^{\mathrm{H}}$. **2nd/3rd line**: the "ladder"/"polarization" terms. Both series start with the first Born approximation, $\sim V_{12} F_1 F_2$ (only first term of commutator shown), each successive term follows by iteratively inserting the previous one into the ladder/polarization term. Figure from Ref. [Bon98].

the calculation of the trace. Until now we had assumed that all traces are over a complete set of $s$-particle states that are constructed as products of single-particle states belonging to the $s$-particle Hilbert space. As we discussed in detail in Ch. 3, for bosons (fermions), instead, (anti-)symmetric states have to be used that belong to the (anti-)symmetric subspace $\mathcal{H}_s^+$ ($\mathcal{H}_s^-$). The straightforward way of doing this is, to define all trace operations which appear in the hierarchy equations in such a way that they are carried out in the corresponding subspace of $s$-particle states[14]. However, it turns out that working with matrix elements of operators that are computed with (anti-)symmetric states (i.e. Slater determinants or permanents[15]) is very cumbersome. Therefore, we will follow a different strategy: we will carry over the (anti-)symmetry from the states to the operators.

### 6.6.1 (Anti-)Symmetrized density operators

Let us explain this procedure which we apply to the general nonequilibrium case. The projection onto the (anti-)symmetric subspace of the Hilbert space

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[14] This procedure was demonstrated in Sec. 3.10, see also Ref. [SBF$^+$11].

[15] This approach has been used in configuration path integral Monte Carlo (CPIMC), introduced in Ref. [SBF$^+$11]. For details see Sec. 4.3

is achieved by acting with an (anti-)symmetrization operator $\Lambda^\pm$ (see Sec. 3.2)

$$|\Psi_{1\dots N}(t)\rangle^\pm = \Lambda^\pm_{1\dots N}|\Psi_{1\dots N}(t)\rangle \,. \tag{6.58}$$

$$\Lambda^\pm_{1\dots N} = \frac{1}{\sqrt{N!}}\,\lambda^\pm_{1\dots N}\,, \tag{6.59}$$

$${}^\pm\langle\Psi_{1\dots N}(t)|\Psi_{1\dots N}(t)\rangle^\pm = \langle\Psi_{1\dots N}(t)|\Psi_{1\dots N}(t)\rangle = 1\,, \tag{6.60}$$

where we introduced a new definition, $\lambda^\pm$, for the (anti-)symmetrization operators that does not contain the normalization pre-factor, which will be used throughout this section. From this we can construct the (anti-)symmetrized $N$-particle density operator of the full system (recall that the probabilities obey $0 \le W_a \le 1$ and $\sum_a W_a = 1$),

$$\begin{aligned}\rho^\pm_N(t) &= \sum_a W_a|\Psi^{(a)}_{1\dots N}(t)\rangle^{\pm}\,{}^{\pm}\langle\Psi^{(a)}_{1\dots N}(t)| = \frac{1}{N!}\sum_a W_a|\Psi^{(a)}_{1\dots N}\rangle(\lambda^\pm_{1\dots N})^2\langle\Psi^{(a)}_{1\dots N}| \\ &= \frac{1}{N!}\sum_a W_a|\Psi^{(a)}_{1\dots N}(t)\rangle\langle\Psi^{(a)}_{1\dots N}(t)|(\lambda^\pm_{1\dots N})^2 = \rho_N(t)\lambda^\pm_{1\dots N}\,,\end{aligned} \tag{6.61}$$

where the final steps will become clear from the properties of the (anti-)symmetrization operators below, cf. Eq. (6.78). The (anti-)symmetrized density operator[16] should obey the standard normalization condition, as in the spinless case, which is easily verified,

$$\mathrm{Tr}_{1\dots N}\,\rho^\pm_N(t) = \sum_{i_1\dots i_N}\langle i_1\dots i_N|\rho^\pm_N(t)|i_1\dots i_N\rangle = 1\,, \tag{6.62}$$

as it follows directly from the definition of $\rho^\pm_N$ in terms of the states $|\Psi^{(a)}_{1\dots N}\rangle^\pm$, Eq. (6.58), which are each normalized to unity[17].

Let us now compute the expectation value of an arbitrary $s-$particle ope-

---

[16] This result agrees with the previous equilibrium result, see Sec. 4.1, and extends it to arbitrary nonequilibrium situations.

[17] The only difference to the spinless case is that, now, the trace is restricted to states of the (anti-)symmetric subspace of the Hilbert space.

rator for the case of fermions or bosons, in a general mixed state

$$
\begin{aligned}
\langle\hat{B}_s\rangle^{\pm}(t) &= \frac{1}{s!}\mathrm{Tr}^{\pm}\hat{B}_s\hat{F}_{1\ldots s}(t) \\
&= \frac{1}{(s!)^2}\sum_{i_1\ldots i_s}\langle i_1\ldots i_s|\Lambda^{\pm}_{1\ldots s}\hat{B}_s\hat{F}_{1\ldots s}(t)\Lambda^{\pm}_{1\ldots s}|i_1\ldots i_s\rangle && (6.63)\\
&= \frac{1}{(s!)^2}\sum_{i_1\ldots i_s}\langle i_1\ldots i_s|\hat{B}_s\hat{F}_{1\ldots s}(t)(\Lambda^{\pm}_{1\ldots s})^2|i_1\ldots i_s\rangle && (6.64)\\
&= \frac{1}{s!}\sum_{i_1\ldots i_s}\sum_{k_1\ldots k_s}\langle i_1\ldots i_s|\hat{B}_s|k_1\ldots k_s\rangle\langle k_1\ldots k_s|\hat{F}^{\pm}_{1\ldots s}(t)|i_1\ldots i_s\rangle\,. && (6.65)
\end{aligned}
$$

This result means (we discuss the key transformations below) that the computation of expectation values in the (anti-)symmetric subspace of the Hilbert space can be performed in the full Hilbert space with normal product states whereas the (anti-)symmetrization is carried over to the density operators[18],

$$
\hat{F}_{1\ldots s}(t) \to \hat{F}^{\pm}_{1\ldots s}(t) = \hat{F}_{1\ldots s}(t)\Lambda^{\pm}_{1\ldots s}\,, \tag{6.66}
$$

exactly as in the case of the full $N$-particle density operator, Eq. (6.61).

### 6.6.2 Relation between reduced density operators and field operators

Our result for the (anti-)symmetrized expectation value of an s-particle operator, Eq. (6.65) can now be compared to the result in terms of field operators that we established earlier, cf. Eq. (5.89). Since both expressions are identical and contain the same matrix element of the operator $\hat{B}_s$, we can directly read-off the connection between RDO and second quantization operators:

$$
\langle i_1\ldots i_s|\hat{F}^{\pm}_{1\ldots s}(t)|k_1\ldots k_s\rangle = \langle a^{\dagger}_{k_1}\ldots a^{\dagger}_{k_s}a_{i_s}\ldots a_{i_1}\rangle_{\rho_N}(t)\,, \tag{6.67}
$$

where the time argument on the r.h.s. indicates that Heisenberg operators are being used. This relation has far reaching consequences because we have connected two completely independent approaches.

One application is to verify the normalization of the (anti-)symmetrized

---

[18] This idea was first realized by Dufty and Boercker [BD79].

reduced density operators[19] which is done as for $\rho_N^\pm$ above:

$$\begin{aligned}\mathrm{Tr}_{1\dots s}\,\hat{F}^{\pm}_{1\dots s} &= \sum_{i_1\dots i_s}\langle i_1\dots i_s|\hat{F}^{\pm}_{1\dots s}|i_1\dots i_s\rangle = \\ &= \sum_{i_1\dots i_s}\langle a^\dagger_{i_1}\dots a^\dagger_{i_s}a_{i_s}\dots a_{i_1}\rangle_{\rho_N} \qquad (6.68)\\ &= \mathrm{Tr}^{\pm}_{1\dots s}\,\hat{F}_{1\dots s} = \mathrm{Tr}_{1\dots s}\,\hat{F}_{1\dots s} = \frac{N!}{(N-s)!}\,. \qquad (6.69)\end{aligned}$$

Therefore, all our previous results remain in place if we replace, everywhere, $\hat{F}_{1\dots s}\to\hat{F}^{\pm}_{1\dots s}$. At the same time we eliminated the need to work with matrix elements in terms of Slater determinants or permanents as well as partial traces thereof, but can continue to use simple product states.

Before continuing with an (anti-)symmetrization of the BBGKY-hierarchy, we first consider the above derivations and the properties of the (anti-)symmetrization operators $\lambda^\pm$ more in detail.

### 6.6.3 Properties of the (anti-)symmetrization operators

1. The operators are defined according to

$$\lambda^{\pm}_{1\dots s} = \sum_{P^{(s)}}\epsilon^{N(P^{(s)})}\,P^{(s)}, \qquad (6.70)$$

with $\epsilon = 1$ for bosons, $-1$ for fermions, and zero for spinless particles. For fermions, the sign of each contribution depends on whether $P^{(s)}$ is an even or odd permutation, i.e. if $P^{(s)}$ can be decomposed into an even or odd number $N(P^{(s)})$ of binary permutations. For bosons, all contributions have the same prefactor $+1$.

2. The lowest order operators are

$$\begin{aligned}\lambda^{\pm}_{12} &= 1+\epsilon P_{12}\,, \qquad (6.71)\\ \lambda^{\pm}_{123} &= \lambda^{\pm}_{12}\,(1+\epsilon P_{13}+\epsilon P_{23}), \qquad (6.72)\\ \lambda^{\pm}_{1234} &= \lambda^{\pm}_{123}\,(1+\epsilon P_{14}+\epsilon P_{24}+\epsilon P_{34}), \qquad (6.73)\\ &\dots\end{aligned}$$

This is verified by direct computation.

---

[19] Problem: prove this directly for $\hat{F}^{\pm}_{12}$ using the definition.

3. The permutation operator has the following properties, which are easily verified,

$$\begin{aligned} P_{ij}^2 &= \hat{1}, \\ \mathrm{Tr}_j P_{ij} &= \hat{1}, \qquad (6.74) \\ P_{ij} A_{ij} P_{ij} &= A_{ji}, \\ P_{ij} B_{ij} &= B_{ji} P_{ij}, \qquad (6.75) \end{aligned}$$

4. Pair permutations of different particles don't commute, i.e., $P_{ij}P_{jk} \neq P_{jk}P_{ij}$. For the case of three-particle states, the three different permutations, labeled by $\alpha, \beta, \gamma$, have the properties

$$P_\beta P_\gamma = P_\alpha P_\beta \,, \qquad (6.76)$$

$$P_\gamma P_\beta = P_\beta P_\alpha \,. \qquad (6.77)$$

5. Important properties of $\lambda^\pm$ are

$$\begin{aligned} (1 - \epsilon P_{ij})\lambda^\pm_{12} &= 0, \quad \epsilon \neq 0 \,, \\ \lambda^\pm_{12}(1 + \epsilon P_{12} + \epsilon P_{13}) &= (1 + \epsilon P_{12} + \epsilon P_{13})\lambda^\pm_{12} \\ P_{23}\lambda^\pm_{13} &= \lambda^\pm_{12} P_{23} \\ (\lambda^\pm_{1\dots s})^2 &= s!\lambda^\pm_{1\dots s} \,. \qquad (6.78) \end{aligned}$$

The first property means that Fermi and Bose statistics are incompatible. The property (6.78) has been used above, in Eqs. (6.61) and (6.65). Let us prove it for the simplest cases, starting with $s = 2$,

$$(\lambda^\pm_{12})^2 = (1 + 2\epsilon P_{12} + P_{12}^2) = 2(1 + \epsilon P_{12}) = 2\lambda^\pm_{12} \,.$$

For the case $s = 3$, we have

$$\begin{aligned} (\lambda^\pm_{123})^2 &= \lambda^\pm_{12}(1 + \epsilon P_{13} + \epsilon P_{23})(1 + \epsilon P_{12} + \epsilon P_{13} + \epsilon P_{23} + P_{12}P_{13} + P_{12}P_{23}) \\ &= 3(\lambda^\pm_{12})^2(1 + \epsilon P_{13} + \epsilon P_{23}) = 3!\lambda^\pm_{123} \,, \end{aligned}$$

where, during the transformations, expressions (6.76) and (6.77) have been used. It remains to generalize this to the $N$-particle case, see problem 2, Sec. 6.6.9.

We conclude that, due to the property (6.78), in computing expectation values and traces we need to perform an (anti-)symmetrization only once.

We now return to the BBGKY-hierarchy. All reduced s-particle operators will now be replaced by $F_{1\dots s} \to F_{1\dots s}\lambda^\pm_{1\dots s}$, and the same with the correlation operators, products of single-particle operators, and products of single-particle and correlation operators and so on.

### 6.6.4 Trace consistency for (anti-)symmetrized RDO

Let us now return to the problem of trace consistency that we discussed in Sec. 6.2.2 and investigate how the results are modified if the density operators are (anti-)symmetrized. Consider again the case of an ideal two-particle operator which now becomes an Hartree-Fock operator, $F_{12}^{\text{ideal}} = F_1 F_2 \lambda_{12}^{\pm}$. We recompute the partial trace (6.13) using matrix notation

$$\begin{aligned}(N-1)\,\langle i_1|F|k_1\rangle &= \sum_{i_2}\langle i_1 i_2|F_1F_2|k_1 i_2\rangle \pm \sum_{i_2}\langle i_1 i_2|F_1F_2|i_2 k_1\rangle \\ &= N\langle i_1|F|k_1\rangle \pm \sum_{i_2}\langle i_1|F|i_2\rangle\langle i_2|F|k_1\rangle \\ &= N\langle i_1|F|k_1\rangle \pm \langle i_1|F^2|k_1\rangle \qquad (6.79)\end{aligned}$$

After cancellation we obtain the condition for trace consistency:

$$\langle i_1|F|k_1\rangle = F_{i_1k_1} = \mp\langle i_1|F^2|k_1\rangle = \mp F^2_{i_1k_1}\,, \qquad (6.80)$$

where we also introduced a short matrix notation. This equation can be satisfied only for fermions (lower sign) if the matrix of $F^2$ equals the matrix of $F$, i.e. the single-particle density operator is idempotent.

If the trace relation is not fulfilled, this also leads to inconsistencies in the normalization. Indeed, performing in Eq. (6.80) also the trace over the variable “1”, we obtain

$$N = \mp\sum_i F^2_{ii}\,. \qquad (6.81)$$

For fermions and, in case of idempotency, the r.h.s. also gives $N$.

**Trace consistency of $F_{12}$ with spin components resolved.** We now extend this analysis to an explicit treatment of the spin components.[20] We consider only fermions with spin 1/2 for which only two spin projections exist. For the trace relation of the spin-up component this leads to

$$(N-1)\,F_{ij}^{\uparrow\uparrow} = \sum_p \left(F_{ipjp}^{\uparrow\uparrow\uparrow\uparrow} + F_{ipjp}^{\uparrow\downarrow\uparrow\downarrow}\right)\,. \qquad (6.82)$$

The spin components of the Hartree–Fock two-particle density matrix are

$$F_{ijkl}^{\uparrow\uparrow\uparrow\uparrow} = F_{ik}^{\uparrow\uparrow}F_{jl}^{\uparrow\uparrow} - F_{il}^{\uparrow\uparrow}F_{jk}^{\uparrow\uparrow}\,, \qquad (6.83)$$

$$F_{ijkl}^{\uparrow\downarrow\uparrow\downarrow} = F_{ik}^{\uparrow\uparrow}F_{jl}^{\downarrow\downarrow}\,. \qquad (6.84)$$

---

[20] Result of Jan-Philip Joost.

Note that the Fock contribution of the $\uparrow\downarrow\uparrow\downarrow$-component vanishes since spin flips are not allowed, i.e. $F^{\uparrow\downarrow} = 0$. Inserting Eqs. (6.83) and (6.84) in Eq. (6.82) results in

$$\begin{aligned}(N-1)\,F_{ij}^{\uparrow\uparrow} &= \sum_p \left( F_{ij}^{\uparrow\uparrow} F_{pp}^{\uparrow\uparrow} - F_{ip}^{\uparrow\uparrow} F_{pj}^{\uparrow\uparrow} + F_{ij}^{\uparrow\uparrow} F_{pp}^{\downarrow\downarrow} \right) && (6.85)\\ &= N F_{ij}^{\uparrow\uparrow} - \sum_p F_{ip}^{\uparrow\uparrow} F_{pj}^{\uparrow\uparrow} \,, && (6.86)\end{aligned}$$

where we took into account the normalization $\sum_p F_{pp}^{\uparrow\uparrow} = \sum_p F_{pp}^{\downarrow\downarrow} = \frac{N}{2}$. Consequently, trace consistency holds if

$$F_{ij}^{\uparrow\uparrow} = \sum_p F_{ip}^{\uparrow\uparrow} F_{pj}^{\uparrow\uparrow} = [F^{\uparrow\uparrow\,2}]_{ij} \,. \tag{6.87}$$

Eq. (6.87) holds if the spin-up single-particle density matrix is idempotent. (The same must hold for the the spin-down component.) This means that in the case that the single-particle density matrix is idempotent the Fock contribution provides the '$-1$'-term that is missing in Eq. (6.13).

**Comments**: This result is directly extended to the case of spin-unsymmetric systems where $N^{\uparrow} \neq N^{\downarrow}$. For bosons, the Fock term, apparently does not solve the trace consistency problem. For spin-0 bosons the previous (spin-less) treatment applies. The next case to study would be spin-1 bosons, but there we cannot directly use the present derivation, as we need to include three spin projections.

**Idempotency for a mixed state and in case of correlations.** Here we show that the single-particle density matrix can be idempotent only in a pure state[21] and in the absence of correlations.

Let $\rho$ be the $N$-particle density operator of a mixed state, as introduced in the beginning,

$$\rho = \sum_k W_k |\Psi_k\rangle\langle\Psi_k| \,,$$

with $\sum_k W_k = 1$. We now show that $\rho$ is idempotent if and only if the corresponding state is pure. We compute the square and use the orthonormality of the states,

$$\rho^2 = \sum_{kl} W_k W_l |\Psi_k\rangle\langle\Psi_k|\Psi_l\rangle\langle\Psi_l| = \sum_k W_k^2 |\Psi_k\rangle\langle\Psi_k| \,. \tag{6.88}$$

---

[21] Result of Jan-Philip Joost.

Thus, the idempotency of $\rho$, i.e. $\rho = \rho^2$, is only fulfilled if $W_k = W_k^2$ for all $k$. The latter equation is fulfilled only by $W_k = 0$ and $W_k = 1$, and the sum over all $W_k$ is normalized to one. Therefore, all but one $W_k$ have to vanish, leading to a pure state.

Let us now discuss application of this result to the single-particle density operator, $\rho \to F_1$. In this case, the states $|\psi_k\rangle$ have to be understood as natural orbitals. For an ideal system, this are Slater determinants. Then the same derivation applies, and the results for the eigenvalues hold.

Let us now consider a correlated system in the ground state. Then we again can write $F$ as a superposition of natural orbitals. Consider as an example jellium. There the natural orbitals are plane waves, the single-particle density matrix is diagonal, $F_{kk'} = n_k \delta_{k,k'}$, and the eigenvalues $p_k$ can be understood as occupation numbers (momentum distribution $n_k$). The density matrix in coordinate space will then be a superposition of these orbitals. For an ideal system in the ground state, the momentum distribution is a step function which indeed satisfies the idempotency condition. In contrast, in case of correlations, the density matrix is still diagonal, but the momentum distribution is softened around the Fermi edge which means that the occupation numbers around the Fermi edge will violate the idempotency condition. At finite temperatures, the distribution will be even more softened, and the idempotency condition will be even more strongly violated.

As a historical remark we note that trace consistency and the related concept of so-called N-representability have been studied by Coleman [CY00]. This is presently actively discussed in reduced density matrix theory of atoms, e.g. by Maziotti [Maz07]. More details are discussed in the appendix **??**.

### 6.6.5 (Anti-)Symmetrization of the first equation. Exchange and Hartree-Fock

Let us now start with the (anti-)symmetrization of the equation for $F_1$, Eq. (6.30). It follows if we use, on the r.h.s., the trace over (anti-)symmetric two-particle states. As we have seen above, this can be transformed into a trace over product states where the (anti-)symmetrization is, instead, carried over to $F_{12}$. This means $F_{12}$ is replaced by the (anti-)symmetrized expression (6.66) together with the (anti-)symmetrized cluster expansion,

$$F_{12}^{\pm} = (F_1 F_2 + g_{12})\lambda_{12}^{\pm}\,, \tag{6.89}$$

which leads to the modified equation

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}F_1 - [H_1, F_1] &= \mathrm{Tr}_2\left([V_{12}, F_1F_2 + g_{12}]\lambda^{\pm}_{12}\right) \\ &= \mathrm{Tr}_2[V_{12}, F_1F_2\lambda^{\pm}_{12} + g^{\pm}_{12}]\,, \end{aligned}$$

where we have introduced the (anti-)symmetrized pair correlation operator. Let us now consider the product of two single-particle operators which previously led to the Hartree mean field. Now we have

$$\begin{aligned} \mathrm{Tr}_2[V_{12}, F_1F_2\lambda^{\pm}_{12}] &= \mathrm{Tr}_2[V_{12}\lambda^{\pm}_{12}, F_1F_2] = [H^{\mathrm{HF}}_1, F_1], \\ \text{with} \quad H^{\mathrm{HF}}_1 &= \mathrm{Tr}_2 V^{\pm}_{12}\, F_2; \quad V^{\pm}_{12} = V_{12}\lambda^{\pm}_{12} = V_{12}(\hat{1} + \epsilon\hat{P}_{12}), \end{aligned} \tag{6.90}$$

where we introduced the Hartree-Fock Hamiltonian and the (anti-)symmetrized pair potential. The expression for $H^{\mathrm{HF}}$ generalizes the previously introduced mean-field operator (Hartree field) $U^{\mathrm{H}}$, Eq. (6.47). So everywhere we may replace $U^{\mathrm{H}} \to H^{\mathrm{HF}}$. The matrix form of the Hartree-Fock hamiltonian becomes,

$$\begin{aligned} H^{\mathrm{HF}}_{ij} &= \sum_{kl} V^{\pm}_{ik,jl} F_{lk}\,, \\ V^{\pm}_{ik,jl} &= V_{ik,jl} + \epsilon V_{ik,lj}\,. \end{aligned}$$

Using the definition of the Hartree-Fock Hamiltonian (6.90), the product of one-particle density operators can be included into an effective hamiltonian, and we obtain the **(anti-)symmetrized first hierarchy equation**

$$i\hbar\frac{\partial}{\partial t}F_1 - [\bar{H}_1, F_1] = \mathrm{Tr}_2[V_{12}, g^{\pm}_{12}]\,, \tag{6.91}$$

$$\bar{H}_1 = H_1 + H^{\mathrm{HF}}_1 = H_1 + \mathrm{Tr}_2 V^{\pm}_{12} F_2\,. \tag{6.92}$$

The term on the r.h.s. of Eq. (6.91) is the collision integral and involves the (anti-)symmetrized pair correlation operator the equation of which we need to derive next.

### 6.6.6 (Anti-)Symmetrization of the second hierarchy equation

For the (anti-)symmetrization of the second hierarchy equation, we cannot start from the previous equation for $g_{12}$ because it was derived using the cluster expansion for distinguishable particles. Instead, we have to go back to the equation for $F_{12}$, Eq. (6.31), and apply the (anti-)symmetrized versions of the cluster (Ursell-Mayer) expansions for $F_{12}^{\pm}$, Eq. (6.89), and of $F_{123}^{\pm}$:

$$F_{123}^{\pm} = \Big[ F_1 F_2 F_3 + \hat{P}_{123}(F_1 g_{23}) + g_{123} \Big] \lambda_{123}^{\pm} , \tag{6.93}$$

which yields

$$\begin{aligned} & i\hbar \frac{\partial}{\partial t} \Big( F_1 F_2 \lambda_{12}^{\pm} + g_{12}^{\pm} \Big) - [H_{12}, F_1 F_2 \lambda_{12}^{\pm} + g_{12}^{\pm}] \\ & = \mathrm{Tr}_3 \Big\{ [V_{13} + V_{23}, F_1 F_2 F_3] + [V_{13} + V_{23}, F_1 g_{23}] \\ & \quad + [V_{13} + V_{23}, F_2 g_{13}] + [V_{13} + V_{23}, F_3 g_{12}] \\ & \quad + [V_{13} + V_{23}, g_{123}] \Big\} (1 + \epsilon P_{13} + \epsilon P_{23}) \lambda_{12}^{\pm} , \end{aligned} \tag{6.94}$$

where we factorized the operator[22] $\lambda_{123}^{\pm}$. Let us now transform some of the terms appearing in this equation.

**Hartree-Fock and Pauli blocking:** The r.h.s. contains the trace over three-operator products, $F_1 F_2 F_3$, which now becomes the trace over $F_1 F_2 F_3 (1 + \epsilon P_{13} + \epsilon P_{23}) \lambda_{12}^{\pm}$. First, we notice that

$$\mathrm{Tr}_3 V_{13} (1 + \epsilon P_{13}) F_3 F_1 F_2 \lambda_{12}^{\pm} = H_1^{\mathrm{HF}} F_1 F_2 \lambda_{12}^{\pm} , \tag{6.95}$$

and similarly for 1 $\Longleftrightarrow$ 2. Now we transform the remaining terms, i.e. the two terms containing $V_{13}\, P_{23}$ and $V_{23}\, P_{13}$. Starting with $P_{23}$ we obtain

$$\begin{aligned} \mathrm{Tr}_3 V_{13} F_1 F_2 F_3 P_{23} \lambda_{12}^{\pm} &= F_2 \mathrm{Tr}_3 V_{13} F_1 F_3 P_{23} \lambda_{12}^{\pm} \\ F_2 \mathrm{Tr}_3 P_{23} V_{12} F_1 F_2 \lambda_{12}^{\pm} &= F_2 \mathrm{Tr}_3 P_{23} V_{12} \lambda_{12}^{\pm} F_1 F_2 = \\ &= F_2 V_{12}^{\pm} F_1 F_2 \end{aligned} \tag{6.96}$$

where, in the last equality, we used the property (6.74) of the permutation operator. The second term follows by interchanging 1 ↔ 2, with the result $F_1 V_{12}^{\pm} F_1 F_2$. Thus the entire trace term, together with the commutator $[V_{12}, F_1 F_2 \lambda_{12}^{\pm}]$, becomes

$$\begin{aligned} V_{12} F_1 F_2 \lambda_{12}^{\pm} + \mathrm{Tr}_3 (V_{13} + V_{23}) F_1 F_2 \lambda_{12}^{\pm} F_3 (1 + \epsilon P_{13} + \epsilon P_{23}) \\ = (H_1^{\mathrm{HF}} + H_2^{\mathrm{HF}}) F_1 F_2 \lambda_{12}^{\pm} + \hat{V}_{12}^{\pm} F_1 F_2 , \end{aligned} \tag{6.97}$$

$$\hat{V}_{12}^{\pm} = \hat{V}_{12} \lambda_{12}^{\pm} , \quad \hat{V}_{12} = (1 + \epsilon F_1 + \epsilon F_2) V_{12} . \tag{6.98}$$

---

[22] In Refs. [BD79] and [Bon98] the overall factor $\lambda_{12}^{\pm}$ occuring in each term was cancelled. This factor is retained here and applied to all terms.

This means exchange effects modify the pair interaction in the presence of other particles, $V_{12} \to \hat{V}^{\pm}_{12}$: the potential contains a blocking factor ($\epsilon = -1$ for fermions) that takes into account the occupation of the two-particle states by other particles. In case of bosons, one observes the familiar enhancement of the scattering process.

The second part of the commutator is transformed in the same way[23],

$$
\begin{aligned}
F_1F_2\lambda^{\pm}_{12}V_{12} + \mathrm{Tr}_3 F_1F_2F_3\lambda^{\pm}_{12}(1+\epsilon P_{13}+\epsilon P_{23})(V_{13}+V_{23}) \\
= F_1F_2\lambda^{\pm}_{12}(H_1^{\mathrm{HF}} + H_2^{\mathrm{HF}}) + F_1F_2\hat{V}^{\pm\dagger}_{12}\,, \\
\hat{V}^{\pm\dagger}_{12} = \hat{V}^{\dagger}_{12}\lambda^{\pm}_{12}\,, \quad \hat{V}^{\dagger}_{12} = V_{12}(1+\epsilon F_1+\epsilon F_2)\,. \qquad (6.99)
\end{aligned}
$$

The Hartree-Fock terms cancel when we subtract the equation for $F_1F_2\lambda^{\pm}_{12}$ below. Finally, the entire scattering term $\hat{\Psi}_{12}$ (inhomogeneity in the equation for $g_{12}$) arises from the commutator of both terms and can be rewritten in a form familiar from Green functions theory:

$$
\begin{aligned}
&\hat{V}^{\pm}_{12}F_1F_2 - F_1F_2\hat{V}^{\pm\dagger}_{12} \equiv \hat{\Psi}^{\pm}_{12} = \\
=&(1+\epsilon F_1)(1+\epsilon F_2)V^{\pm}_{12}F_1F_2 - F_1F_2V^{\pm}_{12}(1+\epsilon F_1)(1+\epsilon F_2) = \\
=&F_1^{>}F_2^{>}V^{\pm}_{12}F_1^{<}F_2^{<} - F_1^{<}F_2^{<}V^{\pm}_{12}F_1^{>}F_2^{>} \qquad (6.100)\\
&F_1^{<} = F_1, \quad F_1^{>} = 1+\epsilon F_1\,,
\end{aligned}
$$

where the latter two notations resemble the single-particle correlation functions on the time diagonal, $G^{\gtrless}(t,t)$.

**Pauli blocking in the particle-particle ladder terms:** The right hand side of the second hierarchy equation also contains the following contribution
$\mathrm{Tr}_3[V_{13}, F_2g_{13}(1+\epsilon P_{13}+\epsilon P_{23})\lambda^{\pm}_{12}]$ and permutations $1 \Longleftrightarrow 2$. They are transformed exactly as in the previous case, with the result

$$
\begin{aligned}
\mathrm{Tr}_3 V_{13}F_2g_{13}P_{23}\lambda^{\pm}_{12} &= F_2\mathrm{Tr}_3 P_{23}V_{12}g_{12}\lambda^{\pm}_{12} = F_2V_{12}g^{\pm}_{12}, \\
\mathrm{Tr}_3 V_{23}F_1g_{23}P_{13}\lambda^{\pm}_{12} &= F_1V_{12}g^{\pm}_{12}, \\
\mathrm{Tr}_3 \lambda^{\pm}_{12}P_{23}F_2g_{13}V_{13} &= g^{\pm}_{12}V_{12}F_2, \\
\mathrm{Tr}_3 \lambda^{\pm}_{12}P_{13}F_1g_{23}V_{23} &= g^{\pm}_{12}V_{12}F_1. \qquad (6.101)
\end{aligned}
$$

The first expression again used the property (6.74) of the permutation operator, and the other expressions are transformed in similar manner.

---

[23] Note that the action of the (anti-)symmetrization operator could also be shifted from the potential $\hat{V}$ to the operator pair $F_1F_2$. This does not change matrix elements of the entire expression.

The first two expressions can be combined with the classical ladder term, $V_{12}g^{\pm}_{12}$, to $\hat{V}_{12}g^{\pm}_{12}$, whereas the second two yield the replacement $g^{\pm}_{12}V_{12} \to g^{\pm}_{12}\hat{V}^{\dagger}_{12}$. Thus the complete ladder term becomes

$$[V_{12}, g^{\pm}_{12}] \to \hat{V}_{12}g^{\pm}_{12} - g^{\pm}_{12}\hat{V}^{\dagger}_{12}\,. \tag{6.102}$$

Note that, in the ladder terms, the operator $\lambda^{\pm}_{12}$ has to act on the operator $g_{12}$, rather than on the pair potential, because we need to obtain an equation of motion for $g^{\pm}_{12}$, as this quantity has physical meaning and enters the collision term of the first equation.

**Cancellation of the uncorrelated terms in $F^{\pm}_{12}$.** From equation (6.94) we now subtract the equation of motion for the product $F_1F_2\lambda^{\pm}_{12}$ that follows from (6.91),

$$i\hbar\frac{\partial}{\partial t}F_1F_2\lambda^{\pm}_{12} - [\bar{H}^0_{12}, F_1F_2\lambda^{\pm}_{12}] = F_2\mathrm{Tr}_3[V_{13}, g^{\pm}_{13}]\lambda^{\pm}_{12} + F_1\mathrm{Tr}_3[V_{23}, g^{\pm}_{23}]\lambda^{\pm}_{12}\,, \tag{6.103}$$

$$\bar{H}^0_{12} = \bar{H}_1 + \bar{H}_2 = H_1 + H_2 + H^{\mathrm{HF}}_1 + H^{\mathrm{HF}}_2\,,$$

which eliminates, from the r.h.s. of Eq. (6.94), the terms $\mathrm{Tr}_3[V_{13}, F_2g_{13}(1 + \epsilon P_{13})]$ and $\mathrm{Tr}_3[V_{23}, F_1g_{23}(1 + \epsilon P_{23})]$, and adds to the r.h.s. the term $[V_{12}, F_1F_2]$ which is absent in Eq. (6.94). We now identify (and cancel) the Hartree-Fock hamiltonians, on the r.h.s., because they are included in $\bar{H}^0_{12}$ but not in $H_{12}$, in Eq. (6.94). As we just showed, cf. Eq. (6.99), these are the terms $\mathrm{Tr}_3V_{13}F_1F_2F_3(1 + \epsilon P_{13})\lambda^{\pm}_{12}$, where we only wrote one half of the commutator, and the term with $1 \Longleftrightarrow 2$ has to be added as well. Finally there are the terms of the form $\mathrm{Tr}_3V_{13}F_1F_2F_3\epsilon P_{23}\lambda^{\pm}_{12} = F_2V^{\pm}_{12}F_1F_2$ that contribute to Pauli blocking in the pair interaction, as shown above in Eq. (6.99). As a result, all terms containing the product $F_1F_2F_3$, are absorbed in different terms.

In similar manner we transform products of the form $F_1g_{23}$, i.e.

$$\mathrm{Tr}_3V_{13}F_3g_{12}(1 + \epsilon P_{13} + \epsilon P_{23})\lambda^{\pm}_{12}\,,$$
$$\mathrm{Tr}_3(V_{13} + V_{23})F_2g_{13}(1 + \epsilon P_{13} + \epsilon P_{23})\lambda^{\pm}_{12}\,,$$

plus terms ↔ 2. In the first line, the term with the 1 gives the Hartree term, $H^{\mathrm{H}}_1g^{\pm}_{12}$, whereas the remaining terms will be considered below, in Eq. (6.105). In the second line, the term $\sim V_{23}\ldots\epsilon P_{23}$ yields the Fock hamiltonian $H^{\mathrm{F}}_2g^{\pm}_{12}$, whereas the terms with the potential $V_{13}\ldots(1 + \epsilon P_{13})\lambda^{\pm}_{12}$ compensate the collision integrals in the equation for $F_1F_2\lambda^{\pm}_{12}$. Further, $V_{13}\ldots\epsilon P_{23}\lambda^{\pm}_{12}$ produces the Pauli blocking contribution, $F_2V_{12}g^{\pm}_{12}$, in the ladder term, see Eq. (6.102). The remainder in the second equation is the term $\sim V_{23}\ldots(1 + \epsilon P_{13})\lambda^{\pm}_{12}$ that is also included in Eq. (6.105) below.

With these identifications we can gather the terms in the equation for $g^{\pm}_{12}$:

$$i\hbar\frac{\partial}{\partial t}g^{\pm}_{12} - [\bar{H}^0_{12}, g^{\pm}_{12}] - (\hat{V}_{12}\, g^{\pm}_{12} - g^{\pm}_{12}\, \hat{V}^{\dagger}_{12}) = (\hat{V}^{\pm}_{12}F_1F_2 - F_1F_2\hat{V}^{\pm\dagger}_{12})$$

$$+ \tilde{\Pi}^{(1)}_{12} + \tilde{\Pi}^{(2)}_{12} + \mathrm{Tr}_3[V_{13} + V_{23}, g^{\pm}_{123}]\,, \tag{6.104}$$

where $\tilde{\Pi}^{(1,2)}$ denote the remaining terms [$\tilde{\Pi}^{(2)}_{12}$ follows from the substitution $1 \longleftrightarrow 2$] that are collected in Eq. (6.105) and will be transformed below.

**Preliminary Summary**. Before proceeding, let us summarize the new effects obtained so far, compared to the previous version for distinguishable particles:

1. The correlation operators are replaced by properly (anti-)symmetrized operators, i.e. $g_{12} \to g^{\pm}_{12}$ and $g_{123} \to g^{\pm}_{123}$.
2. Exchange effects appear in the mean field terms, i.e. the Hartree mean field is replaced by the Hartree-Fock operators.
3. Pauli blocking and exchange appear in the inhomogeneity of the second equation, i.e. $V_{12}F_1F_2 \to \hat{V}^{\pm}_{12}F_1F_2$, ultimately giving rise to Pauli blocking and exchange in the scattering integrals of the first hierarchy equation.
4. Pauli blocking factors appear in the ladder terms, i.e. $V_{12}\, g_{12} \to \hat{V}_{12}\, g^{\pm}_{12}$, giving rise to Pauli blocking in the T-matrices. Note that no exchange terms appear.

**Polarization and particle-hole ladder terms:** What is left is to identify the polarization terms that were present in the previous (spinless) equation for $g_{12}$, Eq. (6.57), and to establish their modification arising from the (anti)-symmetrization. It is clear that these terms must be contained in the remainder of the $F \cdot g$ terms that we noted before and summarize in the following:

$$\mathrm{Tr}_3 \left\{V_{13}F_3g_{12}(\epsilon P_{13} + \epsilon P_{23})\lambda^{\pm}_{12} + V_{23}F_2g_{13}(1 + \epsilon P_{13} + \epsilon P_{12} + P_{13}P_{12})\right\}\,, \tag{6.105}$$

to which the symmetric term with $1 \leftrightarrow 2$ and the other half of the commutators have to be added.

**Classical polarization term. GW (red)**. First, we realize that the term with the 1 is the only one that is present in the spinless case ($\epsilon \to 0$) and, indeed, it coincides with the classical polarization term. Replacing $1 \to 1 + \epsilon P_{13}$ "upgrades" the classical polarization term to the classical-type expression,

$\mathrm{Tr}_3 V_{23} F_2 g^{\pm}_{13}$, but now containing the fully (anti-)symmetric pair correlation operator.

**Exchange corrections to the polarization terms.** Let us now analyze the remaining six terms in Eq. (6.105). We start with the first two contributions from the first term (of the total of four terms):

$$
\begin{aligned}
\mathrm{Tr}_3 V_{13} F_3 g_{12} \epsilon P_{13} &= \mathrm{Tr}_3 V_{13} \epsilon P_{13} F_1 g_{23}\,, \\
\mathrm{Tr}_3 V_{13} F_3 g_{12} \epsilon P_{23} \epsilon P_{12} &= \mathrm{Tr}_3 V_{13} \epsilon P_{13} F_1 g_{23} \epsilon P_{23}\,,
\end{aligned}
$$

where, in the second expression, we used $P_{23}P_{12} = P_{13}P_{23}$. Adding these two expressions and the classical polarization term discussed above (where we exchange 1 ↔ 2) yields

$$
\Pi^{(1)}_{12} = \mathrm{Tr}_3 [V^{\pm}_{13}, F_1] g^{\pm}_{23}\,, \tag{6.106}
$$

thus the previous result was “upgraded” once more, by replacing $V_{12} \to V^{\pm}_{12}$. This is the result that was derived in Refs. [DKBB97] and [Bon98] and describes polarization effects including exchange effects (in the Green functions language this corresponding to GW with exchange).

**Residual polarization terms. Connection to particle-hole ladder terms.** There are four terms left from Eq. (6.105) which we transform such that an (anti-)symmetric pair correlation operator is produced (note that we have to retain the index change 1 ↔ 2 in the second term)

$$
R^{(1)x} = \mathrm{Tr}_3 V_{13} F_3 g_{12} (P_{13}P_{12} + \epsilon P_{23}) + \mathrm{Tr}_3 V_{13} F_1 g_{23} (P_{23}P_{12} + \epsilon P_{12}) \tag{6.107}
$$

Transforming the two parantheses according to

$$
\begin{aligned}
\hat{P}_{13}\hat{P}_{12} + \epsilon \hat{P}_{23} &= \epsilon \hat{P}_{13} \epsilon \hat{P}_{12} + \epsilon^3 \hat{P}^2_{13} \hat{P}_{23} = \\
&= (\epsilon \hat{P}_{13} + \epsilon^2 \hat{P}_{13} \hat{P}_{23}) \epsilon \hat{P}_{12} = \epsilon \hat{P}_{13} \lambda^{\pm}_{23} \cdot \epsilon \hat{P}_{12}\,, \\
\hat{P}_{23}\hat{P}_{12} + \epsilon \hat{P}_{12} &= \lambda^{\pm}_{23} \cdot \epsilon \hat{P}_{12}\,,
\end{aligned}
$$

Inserting these results into Eq. (6.107) and using Eq. (6.75), an overall factor $\epsilon \hat{P}_{12}$ can be taken out to the right, with the result

$$
\begin{aligned}
R^{(1)x} =& \big\{ \mathrm{Tr}_3 V_{13} \epsilon \hat{P}_{13} F_1 g_{23} \lambda^{\pm}_{23} + \mathrm{Tr}_3 V_{13} F_1 g_{23} \lambda^{\pm}_{23} \big\} \cdot \epsilon \hat{P}_{12} \\
=& \mathrm{Tr}_3 V^{\pm}_{13} F_1 g^{\pm}_{23} \cdot \epsilon \hat{P}_{12}
\end{aligned} \tag{6.108}
$$

Together with the second part of the commutator, this yields exactly the polarization term, Eq. (6.106) times $\epsilon \hat{P}_{12}$. Analogously, the symmetric term arising from exchanging 1 ↔ 2 yields $\Pi^{\pm(2)}_{12,\mathrm{DO}} \cdot \epsilon \hat{P}_{12}$.

Comparison to Green functions approaches and to the G1–G2 scheme suggests that these terms describe particle-hole ladder contributions and are equivalent to the particle-hole T-matrix approximation for the selfenergy $\Sigma^{\rm TPH}$. This has been demonstrated by a direct calculation, starting from the Keldysh-Kadanoff-Baym equations using the selfenergy $\Sigma^{\rm TPH}$ [JSB20].

Thus, all terms of Eq. (6.105), together with the permuted terms $(1 \leftrightarrow 2)$ and the second halfs of the commutators, can be combined into

$$\text{Eq. (6.105)} = \left(\Pi^{\pm(1)}_{12,\rm DO} + \Pi^{\pm(2)}_{12,\rm DO}\right)\lambda^{\pm}_{12}\,. \tag{6.109}$$

**Summary and discussion.** The system of the (anti-)symmetrized first and second hierarchy equations (6.91) and (6.104) is exact. Dropping the term $g^{\pm}_{123}$ corresponds to the dynamically screened ladder approximation[24] and is expected to be conserving. With the proper replacement of quantities,

$$\begin{aligned} F_{ij} &= \pm i\hbar\, G^{<}_{ij}\,, \\ g^{\pm}_{12} &= (i\hbar)^2\, \mathcal{G}_{12}\,, \end{aligned}$$

this approximation is equivalent to (the most general version of) the G1-G2 equations of Ref. [JSB20] that follow from the time-diagonal version of the Kadanoff-Baym equations using the Hartree-Fock-GKBA.

With this we achieved our goal and present the final result for the (anti-)symmetrized first and second equations of the BBGKY-hierarchy:

$$i\hbar\frac{\partial}{\partial t}F_1 - [\bar H_1, F_1] = \mathrm{Tr}_2[V_{12}, g^{\pm}_{12}]\,, \tag{6.110}$$

$$i\hbar\frac{\partial}{\partial t}g^{\pm}_{12} - [\bar H^0_{12}, g^{\pm}_{12}] = \Psi^{\pm}_{12} + L_{12} + \Pi^{\pm}_{12} + \mathrm{Tr}_3[V^{(12),3}, g^{\pm}_{123}]\,, \tag{6.111}$$

$$\Psi^{\pm}_{12} = \hat V^{\pm}_{12}F_1F_2 - F_1F_2\hat V^{\pm\dagger}_{12} = \Psi_{12}\lambda^{\pm}_{12}\,, \tag{6.112}$$

$$L_{12} = (\hat V_{12}\, g^{\pm}_{12} - g^{\pm}_{12}\, \hat V^{\dagger}_{12})\,, \tag{6.113}$$

$$\Pi^{\pm}_{12} = \Pi_{12}\lambda^{\pm}_{12}\,, \quad \Pi_{12} = \mathrm{Tr}_3[V^{\pm}_{13}, F_1]g^{\pm}_{23} + (1 \leftrightarrow 2)\,. \tag{6.114}$$

where $\Psi^{\pm}_{12}$ denotes the inhomogeneity and $L_{12}$ the complete pp-ladder term. Finally, $\Pi^{\pm}_{12} = \Pi_{12} + \Pi^{x}_{12}$ is the complete polarization term that is comprised of the bubble sum ($\Pi_{12}$, $\lambda^{\pm}_{12} \to 1$) and the exchange term, $\Pi^{x}_{12} = \epsilon P_{12}\Pi_{12}$, i.e. the particle-hole T-matrix ($\lambda^{\pm}_{12} \to \epsilon P_{12}$).

---

[24] abbreviated DSL. As mentioned before, in other fields the alternative names are being used such as Wang-Cassing approximation or Valdemoro approximation.

Let us discuss possible conserving closure approximations[25], extending our discussion before the (anti-)symmetrization, restricting ourselves to $g_{123} \to 0$. As before, we can neglect $L_{12}$ and/or $\Pi^{\pm}_{12}$ completely. In addition, it is possible to eliminate from all terms the factor $\lambda^{\pm}_{12}$. This would eliminate, in particular, the particle-hole ladder term $\Pi^{x}_{12}$, but the solution $g_{12}$ would not necessarily be (anti-)symmetric. Another valid approximation is to neglect, separately, in any term (or part of terms) the exchange contribution(s). For a discussion of energy conserving approximations, see Refs. [Bon98] and [JSO$^+$22].

### 6.6.7 Matrix form of the equations and comparison to the G1-G2 scheme

It is straightforward to bring the system of equations (6.110)–(6.114) into a matrix form[26] with respect to an arbitrary basis of one and two-particle states including also the different spin combinations. This also allows for a direct comparison with the recently developed G1-G2 scheme [SJB20, JSB20] and other methods based on reduced density matrix theory.

*(to be completed).*

### 6.6.8 (Anti-)Symmetrization of the third equation

To make further progress we need to develop improved many-body approximations. This can be done by including (in part) contributions from three-particle correlations, $g_{123}$. For this it is crucial to perform an anti-symmetrization of Eq. (6.46)[27]

*to be completed*

### 6.6.9 Problems

Problem 1: Compute the normalization of $F^{\pm}_{1\dots s}$ for non-interacting particles. Apply the Hartree-Fock approximation.

Problem 2: Prove Eq. (6.78) for the case $s > 3$.

Problem 3: Derive the matrix representation of the second hierarchy equation, Eq. (6.111). Compare each term with the ones of the G1-G2 scheme of Ref. [JSB20].

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[25] this is still preliminary

[26] see Problem 3.

[27] see Problem 4.

Problem 4: Derive the (anti-)symmetrized equation for the three-particle correlation operator, $g^{\pm}_{123}$. Start from the equation of motion for $F_{123}$ and perform the (anti-)symmetrized cluster expansion.