Chapter 5

Dynamics of the creation and annihilation operators

After considering the description of a many-particle system in thermodynamic equilibrium we now extend the formalism of second quantization to nonequilibrium. We obtain the equations of motion for the second quantization operators where we consider fermions and bosons in a common approach. The only distinction will enter through the different (anti-)commutation properties of the respective operators.

Before discussing the dynamics of the field operators we recall that in quantum mechanics there exist two (main) pictures of studying time-dependent processes—the Schrödinger and the Heisenberg picture. In the Schrödinger picture the quantum mechanical states (or wave functions) evolve in time, starting from an initial state,

$$\langle \Psi(t) \rangle = U(t, t_0) \langle \Psi(t_0) \rangle$$  \hspace{1cm} (5.1)
$$\langle \Psi(t_0) \rangle = \langle \Psi_0 \rangle.$$  \hspace{1cm} (5.2)

where the dynamics are governed by the time evolution operator $U(t, t')$ that obeys a Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} U(t, t') - \hat{H}(t)U(t, t') = 0,$$ \hspace{1cm} (5.3)
$$U(t, t) = \hat{1},$$ \hspace{1cm} (5.4)

where $\hat{H}$ is the full $N$-particle hamiltonian. We recall the main properties of the time evolution operator:

1. The explicit solution of Eq. (5.3) with the initial condition (5.4), for the case of a time-independent hamiltonian, is given by

$$U(t, t') = e^{-i\hat{H}(t-t')},$$ \hspace{1cm} (5.5)
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If the hamiltonian depends on time the solution is generalized to

$$U(t, t') = T e^{-\frac{i}{\hbar} \int_{t'}^{t} dt' \hat{H}(t')}.$$  

(5.6)

2. If the hamiltonian is hermitean, $\hat{H}^\dagger = \hat{H}$, then $U$ is unitary, $U^\dagger = U^{-1}$.

3. The backward evolution is equivalent to hermitean conjugation of $U$,

$$[U(t, t')]^\dagger = U(t', t)$$  

(5.7)

4. $U$ has a semi-group property, i.e. for $t_2 \geq t_1 \geq t_0$, it follows $U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$.

5. Since $U$ depends on two times we should also consider the dynamics with respect to the second time argument, in addition to the equation of motion (5.3). To this end we compute the adjoint of this equation,

$$0 = -i\hbar \partial_t U(t, t') - U^\dagger(t, t') \hat{H}(t) = -i\hbar \partial_t U(t', t) - U(t', t) \hat{H}(t)$$

$$= -i\hbar \partial_{t'} U(t, t') - U(t, t') \hat{H}(t'),$$  

(5.8)

where, in the last line, we used (5.7), renamed the time arguments $t \leftrightarrow t'$ and understand $H$ to act to the left.

5.1 Equation of motion of the field operators

Let us now consider the dynamics of the field operators. Their time-dependent form is obtained by transforming to the Heisenberg representation of quantum mechanics according to

$$\hat{\psi}_H(x, t) = U^\dagger(t, t_0)\hat{\psi}(x)U(t, t_0)$$  

(5.9)

where $\hat{\psi}(x)$ is the (time-independent) field operator in the Schrödinger picture, i.e. the value of the Heisenberg operator $\hat{\psi}_H(x, t)$ at a chosen initial time $t_0$.

The time evolution of the field operators is governed by the hamiltonian for which we use a general expression containing kinetic energy, potential energy

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1. The derivation was given in quantum mechanics in the context of the interaction picture.
2. A critical discussion of the Heisenberg representation of the field operators is given in Sec. 5.6.
and pair interaction energy which we write in second quantization \((x = (r, \sigma))\), see chapter 3)

\[
\hat{H} = \hat{T} + \hat{V} + \hat{W} = \int dx' \hat{\psi}^\dagger(x') \left( -\frac{\hbar^2}{2m} \nabla'^2 + v(r') \right) \hat{\psi}(x') + \frac{1}{2} \int dx' \int dx'' \hat{\psi}^\dagger(x') \hat{\psi}^\dagger(x'') \hat{\psi}(x'') \hat{\psi}(x').
\]

The evolution equation of the field operators is given by Heisenberg’s equation (see problem 5.1, Sec. 5.10)

\[
\mathrm{i}\hbar \partial_t \hat{\psi}_H(x, t) = -[\hat{H}_H, \hat{\psi}_H(x, t)] = -U^\dagger(t, t_0) \{ [\hat{H}, \hat{\psi}(x)] \} U(t, t_0).
\]

We now evaluate the commutator which is the sum of three commutators involving \(\hat{T}, \hat{V}\) and \(\hat{W}\), respectively. This will lead to commutators of different combinations of field operators which we will simplify using the commutation (anticommutation) relations for bosonic (fermionic) operators.

We start the derivation by noting the following properties of commutators,

\[
[\hat{A} \hat{B}, \hat{C}] = \hat{A} [\hat{B}, \hat{C}] + [\hat{A}, \hat{C}] \hat{B},
\]

\[
[\hat{A} \hat{B}, \hat{C}] = \hat{A} [\hat{B}, \hat{C}] \mp [\hat{A}, \hat{C}] \hat{B},
\]

\[
[\hat{\psi}^\dagger(x'), \hat{\psi}(x)] = \mp \delta(x - x'),
\]

where the first two are verified by direct evaluation of the left and right-hand sides (see problem 5.2, Sec. 5.10) and the third follows from the standard (anti-)commutation relations.

Consider first the commutator with the external potential which is simplified with the help of Eq. (5.14),

\[
[\hat{V}, \hat{\psi}(x)] = \int dx' [\hat{\psi}^\dagger(x') v(r') \hat{\psi}(x'), \hat{\psi}(x)] = \\
\int dx' v(r') \left\{ [\hat{\psi}^\dagger(x'), \hat{\psi}(x)] \mp [\hat{\psi}^\dagger(x'), \hat{\psi}(x)] \right\} = -v(r) \hat{\psi}(x).
\]

\[\text{The derivation starts from the r.h.s. of Heisenberg’s equation that involves two Heisenberg operators}
\]

\[\text{and uses the property } U(t, t_0) U^\dagger(t, t_0) = 1.
\]

\[\text{In the second and third line the upper (lower) sign refers to bosons (fermions), i.e. to the commutator (anti-commutator).}\]
where we took into account that the first commutator vanishes and the second is evaluated according to Eq. (5.15). The same derivation applies to the kinetic energy term with the result

\[ [\hat{T}, \hat{\psi}(x)] = -\left(-\frac{\hbar^2}{2m} \nabla^2\right) \hat{\psi}(x). \]

(5.17)

Finally, we transform the commutator with the interaction energy using relation (5.13),

\[ 2[\hat{W}, \hat{\psi}(x)] = \int dx' \int dx'' [\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x'')w(r', r'')\hat{\psi}(x'')\hat{\psi}(x'), \hat{\psi}(x)] = \]

\[ = \int dx' \int dx'' w(r', r'')\left\{\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x'')[\hat{\psi}(x'')\hat{\psi}(x'), \hat{\psi}(x)] + \right. \]

\[ + \left. [\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x''), \hat{\psi}(x)]\hat{\psi}(x'')\hat{\psi}(x')\right\}. \]

(5.18)

The first commutator vanishes as it involves only annihilation operators whereas the second is transformed, using Eqs. (5.14) and (5.15),

\[ [\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x''), \hat{\psi}(x)] = \hat{\psi}^\dagger(x')[\hat{\psi}^\dagger(x''), \hat{\psi}(x)]_{\pm} \pm [\hat{\psi}^\dagger(x'), \hat{\psi}(x)]_{\mp}\hat{\psi}^\dagger(x'') \]

\[ = \mp\hat{\psi}^\dagger(x')\delta(x'' - x) - \delta(x' - x)\hat{\psi}^\dagger(x''), \]

(5.19)

and the second term in the integral (5.18) becomes

\[ [\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x''), \hat{\psi}(x)]\hat{\psi}(x') = -2\delta(x' - x)\hat{\psi}^\dagger(x'')\hat{\psi}(x''), \]

where the first term in Eq. (5.19) is transformed by exchanging \(x' \leftrightarrow x''\), after which it becomes identically equal to the second one\(^5\). With this the final result for the commutator becomes

\[ [\hat{W}, \hat{\psi}(x)] = -\int dx'' w(r, r'')\hat{\psi}^\dagger(x'')\hat{\psi}(x''). \]

(5.20)

Inserting the results for the three commutators into Eq. (5.12) and applying the time evolution operators (assuming \(\partial H/\partial t = 0\), it follows \(U^\dagger v(r) = v(r)U^\dagger\); for the general case, see Sec. 5.5 and problem 2) we obtain the equation of motion of the field operator,

\[ i\hbar \partial_t \hat{\psi}_H(x, t) = \left\{-\frac{\hbar^2}{2m} \nabla^2 + v(r) + \hat{U}_H^{\text{ind}}(x, t)\right\} \hat{\psi}_H(x, t) \]

(5.21)

\[ \hat{U}_H^{\text{ind}}(x, t) = \int dx'' w(r, r'')\hat{\psi}^\dagger(x'', t)\hat{\psi}_H(x'', t). \]

(5.22)

\(^5\)The derivation assumes \(w(r', r'') = w(r'', r')\), and the sign change, in the case of fermions, arises from exchanging the order of the two annihilation operators.
Let us briefly discuss this result. The notion “induced” potential in Eq. (5.22) indicates a similarity to the induced electrostatic potential of charged particles. Indeed, when \( w \) is a Coulomb potential, \( w(r, r') = e^2 |r - r'|^{-1} \), then the induced potential becomes \( \hat{U}^{\text{ind}}_H(x, t) = e\hat{\phi}^{\text{ind}}_H(x, t) \), where the potential \( \hat{\phi}^{\text{ind}}_H \) is the operator generalization of the electrostatic potential produced by a charge density \( \hat{\rho}^{\text{ind}}_H(x', t) = e\hat{\psi}^{\dagger}_H(x', t)\hat{\psi}_H(x', t) \) which obeys Poisson’s equation\(^6\)

\[
\Delta \hat{\phi}^{\text{ind}}_H(x, t) = -4\pi \hat{\rho}^{\text{ind}}_H(x', t) \tag{5.23}
\]

Thus the field operator is subject to an effective single-particle potential \( \hat{v}^{\text{eff}}_H = v(r) + \hat{U}^{\text{ind}}_H \).

This is an exact result, valid both for fermions and bosons. Remarkably, this equation which was derived from the Heisenberg equation (5.12) has the form of a one-particle time-dependent Schrödinger equation, just as for the wave function, and it shares the same basic properties. First, the equation for the creation operator is obtained by hermitean conjugation of Eq. (5.21):

\[
i\hbar \partial_t \hat{\psi}^{\dagger}_H(x, t) = -\frac{\hbar^2}{2m} \nabla^2 + v(r) + \hat{U}^{\text{ind}}_H(x, t) \tag{5.24}
\]

where the operators \( \nabla \) and \( \hat{U}^{\text{ind}}_H \) act on the field operator to the left, and we took into account that \((\hat{U}^{\text{ind}}_H)\) is hermitean.

Theorem: As the Schrödinger equation in quantum mechanics, Eq. (5.21) is associated with an operator continuity equation describing local particle number conservation,

\[
\partial_t \hat{n}_H(x, t) + \nabla \hat{j}_H(x, t) = 0 \tag{5.25}
\]

where

\[
\hat{n}_H = \hat{\psi}^{\dagger}_H \hat{\psi}_H, \quad \hat{j}_H(x, t) = \frac{\hbar}{2im} \left\{ \hat{\psi}^{\dagger}_H \nabla \hat{\psi}_H - \left( \nabla \hat{\psi}^{\dagger}_H \right) \hat{\psi}_H \right\} \tag{5.26}
\]

While in the continuity equation for the single-particle wave function of standard quantum mechanics the quantities \( n \) and \( j \) describe the probability density and probability current density, here the analogous quantities refer to an \( N \)-particle system\(^7\).

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\(^6\)Note that, with this, we have obtained a quantization of the electrostatic potential which is done more systematically in quantum electrodynamics.

\(^7\)While the probability density is normalized to 1 (the particle number equals one), here the integral of \( \hat{n} \) over the volume yields the total particle number operator \( \hat{N} \).
Proof: We compute the time-derivative of the density operator and use the equations of motion (5.21), (5.24), dropping the arguments \(x,t\)

\[
\dot{n}_H = \hat{\psi}_H^\dagger \hat{\psi}_H + \hat{\psi}_H^\dagger \hat{\psi}_H = -\frac{\hbar}{2im} \left\{ \hat{\psi}_H^\dagger \nabla^2 \hat{\psi}_H - \left( \nabla^2 \hat{\psi}_H^\dagger \right) \hat{\psi}_H \right\} = -\frac{\hbar}{2im} \nabla \left\{ \hat{\psi}_H^\dagger \nabla \hat{\psi}_H - \left( \nabla \hat{\psi}_H^\dagger \right) \hat{\psi}_H \right\},
\]

and the expression in the brackets is just the current density operator (5.26)\(^8\) which completes the proof.

The key difference between the familiar one-particle Schrödinger equation and Eq. (5.21) for the field operator is the appearance of an effective potential \(\hat{U}_H^{\text{eff}} = v + \hat{U}_H^{\text{ind}}\) instead of the external potential \(v\). This “induced” potential includes the whole many-body problem. It has exactly the form of a mean field (Hartree) potential that is created by all particles, as in the case of the quantum Vlasov equation (Hartree equation)\(^9\). Thus this equation is the simplest formulation of the nonequilibrium many-body problem for fermions and bosons in its full generality. This simple form arises from the nature of the creation and annihilation operators that are well adapted to this problem. One should, however, note that this single-particle Schrödinger equation is nonlinear in the field operators, since in the induced potential two additional operators appear.

Unfortunately, a direct solution of Eq. (5.21) is impossible due to its operator character. The standard procedure is, therefore, to introduce suitable expectation values. This will be considered in Sec. 5.8. An independent approach that is based on a stochastic treatment of this equation will be discussed in Sec. 5.6. But before that we generalize the equation of motion for the field operators to a general basis and derive the equations of motion for the general creation and annihilation operators.

### 5.2 Dynamics of the creation and annihilation operators in an arbitrary representation

After considering the dynamics of the second quantization operators in coordinate representation, we now generalize this result to an arbitrary basis of single-particle states \(\{|i\}\}. The \(N\)-particle states belong to the Fock space and are again written in occupation number representation \(|n_1n_2\ldots\rangle\), cf. Chapter

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\(^8\)In the derivation we took into account that the terms with the potentials cancel.

\(^9\)Interestingly, the same general structure of an exact mean-field type form of the many-body problem was obtained before in Ch. 2 for classical systems when we discussed the phase space density \(N(r,p,t)\), cf. Eq. (2.20).
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3. The creation and annihilation operators associated to orbital $i$ are $a_i$ and $a_i^\dagger$ and obey the standard (anti-)commutation relations.

We start with the same Hamiltonian as before, Eq. (5.10), for which we use the general second quantization representation,

$$\hat{H} = \hat{T} + \hat{V} + \hat{W},$$

(5.27)

$$\hat{T} + \hat{V} = \sum_{i,j=1}^{\infty} a_i^\dagger (t_{ij} + v_{ij}) a_j = \sum_{i,j=1}^{\infty} h_{ij} a_i^\dagger a_j,$$

(5.28)

$$\hat{W} = \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} a_i^\dagger a_j^\dagger a_k a_l.$$

(5.29)

Proceeding as in Sec. 5.1 we introduce Heisenberg operators (we omit the subscript “H” – when the time dependence is written this implies the Heisenberg form),

$$\hat{a}_i(t) = U^\dagger(t,t_0)\hat{a}_i U(t,t_0),$$

and consider the Heisenberg equation of motion\(^{10}\)

$$i \hbar \partial_t \hat{a}_i(t) = -U^\dagger(t,t_0)[\hat{H}, a_i(t)] U(t,t_0), \quad a_i(t_0) = a_i.$$

(5.30)

Evaluating the three commutators in Eq. (5.30) we finally obtain (see problem 5.4, Sec. 5.10)

$$i \hbar \partial_t \hat{a}_i(t) = \sum_l \{ (t_{il} + v_{il}) a_l(t) + \sum_{mn} w_{imln} a_m^\dagger(t) a_n(t) a_l(t) \}$$

(5.31)

where all operators are now Heisenberg operators. This is the generalization of the coordinate space result (5.21) to a general basis representation. All the results discussed before (induced potential, adjoint equation, continuity equation etc.) remain valid. Again we may introduce an effective potential and rewrite the equation of motion in the form of an effective single-particle problem

$$i \hbar \partial_t \hat{a}_i(t) = \sum_l \{ t_{il} + \hat{v}_{H,l}^{\text{eff}}(t) \} a_l(t),$$

(5.32)

$$\hat{v}_{H,l}^{\text{eff}}(t) = v_{il} + \sum_{mn} w_{imln} \hat{n}_{mn}(t).$$

(5.33)

Consider now a few special cases:

a. basis in which kinetic energy is diagonal

b. basis in which single-particle energy is diagonal

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\(^{10}\)As before, we assume $\partial_t H = 0$. For the general case, see Sec. 5.5.
5.3 Solution of the field equations 1: Bose condensates. Gross-Pitaevskii equation

For the case of weakly interacting bosons at temperatures below the condensation temperature the field equations simplify considerably. Since (almost) all particles occupy the lowest orbital (there is no Pauli principle), in the thermodynamic limit, $N \to \infty$, one can approximately replace

$$
\lim_{N \to \infty} \langle m,N | \hat{\Psi} | m,N + 1 \rangle \approx \chi(r,t),
$$

(5.34)

where $\chi(r,t)$ is the condensate wave function that is macroscopically populated with the normalization $\int d^3r |\chi(r,t)|^2 = N$. Replacing the field operator in Eq. (5.21) by the condensate wave function gives rise to a nonlinear Schrödinger equation

$$
i\hbar \frac{\partial}{\partial t} \chi(r,t) = \left\{-\frac{\hbar^2}{2m} \nabla^2 + V(r)\right\} + \chi(r,t) \int d^3r' |\chi(r,t)|^2 w(r-r'),
$$

(5.35)

which was independently derived by Gross and Pitaevskii in 1961 and carries their name. This equation can also be derived from the N-particle Schrödinger equation making a factorization ansatz in N single-particle orbitals that are all coinciding with the ground state orbital. Integration over all particle indices except that of particle one yields immediately Eq. (5.35). This means that the Gross-Pitaevskii equation has to be understood as a pure mean field (Hartree) approximation to the full many-body problem that even neglects exchange effects\(^{11}\). We return to this problem in Sec. 5.9.

5.4 Solution of the field equations 2: Basis of coherent states

Another approach to the solution of the field equation (5.31) for the annihilation operators $\hat{a}_i$ consists in conversion to an equation for the eigenvalues $a_i$ of the operators. This can be done by choosing a basis of coherent states $|i\rangle$.

Assuming that these states exist, are complete in the single-particle Hilbert space and orthonormal we obtain

$$
\langle i | \hat{a}_i | j \rangle = a_j \delta_{i,j} \delta_{i,j}
$$

(5.36)

\(^{11}\)For more details, see the diploma thesis of Jens Böning, Kiel University 2007. pdf-file available from the web page of M. Bonitz (link Arbeitsgruppe)
What remains is to construct anti-symmetrized N-particle state (Slater determinants or permanents) of these orbitals and then compute the matrix elements of $\hat{a}_i$ in this N-particle basis.

**Problem:** perform this procedure and analyze the resulting system of equations for the eigenvalues.

We will continue the discussion of the solution of the field equations in Sec. 5.7.

## 5.5 Extension to time-dependent hamiltonians

So far we have assumed that the hamiltonian does not depend explicitly on time. This was used when applying the time evolution operator, on the final step of the derivation. We now remove this restriction and generalize our results to the case of a time-dependent single-particle potential, such as an external electromagnetic field. Then the only term that changes is the one involving the potential $\hat{V}(t)$, cf. Eq. (5.28), and the contribution to the r.h.s. of Eq. (5.30) becomes

$$-
\hat{U}^\dagger(t,t_0)[\hat{V}, a_i] \hat{U}(t,t_0) = \hat{U}^\dagger(t,t_0) \sum_l v_{il}(t) a_l \hat{U}(t,t_0)$$

$$= \sum_l \hat{U}^\dagger(t,t_0) v_{il}(t) \hat{U}(t,t_0) a_l(t) = \sum_l \hat{v}_{H,il}(t) a_l(t).$$

where, in the last line we inserted a unity operator between $v_{il}$ and $a_l$. Note that, for the general case of a time-dependent potential $v(t)$ does not necessarily commute with the time evolution operator, $v(t)\hat{U}(t,t_0) \neq \hat{U}(t,t_0)v(t)$, and the result, therefore, contains the Heisenberg operator $\hat{v}_{H,il}(t)$. Thus, our previous result, Eq. (5.33) is generalized to

$$i\hbar \partial_t a_i(t) = \sum_l \left\{ t_{il} + \hat{v}_{H,il}^{\text{eff}}(t) \right\} a_l(t),$$

$$\hat{v}_{H,il}^{\text{eff}}(t) = \hat{v}_{H,il}(t) + \sum_{mn} w_{ilmn} \hat{n}_{mn}(t),$$

where the time dependence of the new potential operator,

$$\hat{v}_{H,il}(t) = \hat{U}^\dagger(t,t_0) v_{il}(t) \hat{U}(t,t_0),$$

is due, both, to the explicit time dependence of the potential $v$ and the two time evolution operators.
5.6 Schrödinger dynamics of the creation and annihilation operators

In the previous sections we used the Heisenberg picture for the creation and annihilation operators\textsuperscript{12}. While this is common practice in many textbooks, this approach has to be critically assessed. The problem is that the “standard” Heisenberg operator $\hat{a}_H(t) = U(t_0) \hat{a} U(t t_0)$ has, strictly speaking, no clear mathematical meaning if the Hamilton operator (and, similarly, the evolution operator $U$) refers to a fixed particle number $N$. Suppose we act with $\hat{a}_H(t)$ on an arbitrary state $|\psi_N\rangle$ of the $N$-particle Hilbert state $\mathcal{H}_N$. Then we will, obviously, understand $U$ as an $N$-particle time evolution operator associated with the $N$-particle Hamiltonian $\hat{H}_N$. The action of $U$ produces again a state from $\mathcal{H}_N$. Acting now with $\hat{a}$ produces a state from the Hilbert space $\mathcal{H}_{N-1}$. The final action of $U^\dagger$, which is again associated with $\hat{H}_N$, is then, however, ill-defined. Thus, the use of the standard Heisenberg picture for the operators $\hat{a}$ and $\hat{a}^\dagger$ is only possible if $\hat{H}_N$ and $U$ do not refer to a fixed $N$ but are defined

\textsuperscript{12}This aspect and the following results have been worked out together with S. Hermanns and C. Hinz.
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in Fock space\(^\text{13}\).

Alternatively, if the Hamiltonian is defined in Hilbert space \(\mathcal{H}_N\), the dynamics of creation and annihilation operators should be formulated in the Schrödinger picture where no such problem occurs since it involves only a single evolution operator \(U_N\). Let us now consider how this is accomplished and compare the results with those of the previous sections of this chapter.

We start with an arbitrary complete set of single-particle states \(|i\rangle\) for which the operators \(\hat{a}_i\) and \(\hat{a}_i^\dagger\) are defined as before. With these operators we can again produce the second quantization representation of arbitrary operators, in particular, for the generic \(N\)-particle Hamiltonian \(\hat{H}\), cf. Eq. (5.27). We proceed by constructing properly (anti-)symmetrized \(N\)-particle states \(|\{\alpha\}\rangle\) and defining the \(N\)-particle evolution operator \(U\), as before, via Eq. (5.21).

Now we define the time-dependent annihilation and creation operators that evolve from the operators \(\hat{a}_i\) and \(\hat{a}_i^\dagger\), leaving out the hats
\[
\begin{align*}
\hat{a}_i(t) &= a_i U(t, t_0) \\
\hat{a}_i^\dagger(t) &= U^\dagger(t, t_0) a_i^\dagger
\end{align*}
\]
(5.45) (5.46)

\(^{13}\)One possible way to define Heisenberg-type operators with Hamiltonians for a fixed \(N\) is to work with different Hilbert spaces:
\[
\hat{a}^H_k(t) = U^\dagger_{N-1}(t, t_0) a_k U_N(t, t_0).
\]
(5.41)

Then, the equation of motion is given by
\[
\begin{align*}
i\partial_t \hat{a}^H_k(t) &= i\partial_t U^\dagger_{N-1} a_k U_N + U^\dagger_{N-1} a_k i\partial_t U_N \\
&= -U^\dagger_{N-1} H_{N-1} a_k U_N + U^\dagger_{N-1} a_k H_N U_N \\
&= -H^H_{N-1}(t) \hat{a}^H_k(t) + \hat{a}^H_k(t) H^H_N(t)
\end{align*}
\]
(5.42)

where, in the third line, we inserted unity according to \(U^\dagger_{N-1} U_N = 1\). The density matrix operator is then given by
\[
n^H_{kl}(t) = a^\dagger_{k,H}(t) a^H_l(t) = U^\dagger_{N} a^\dagger_{k} U_{N-1} U^\dagger_{N-1} a_l U_N = U^\dagger_{N} n_{kl} U_N,
\]
(5.43)

which is a proper Heisenberg operator in \(N\)-particle Hilbert space that evolves according to the Heisenberg equation of motion
\[
\begin{align*}
i\hbar \partial_t n^H_{kl}(t) &= [n^H_{kl}(t), H^H_{kl}(t)].
\end{align*}
\]
(5.44)

Thus this modified Heisenberg dynamics of the creation and annihilation operators lead to the same equations of motion for the density matrix operator. Furthermore, it is clear that this modified Heisenberg dynamics will approach the standard definition in the macroscopic limit, \(N \to \infty\) when \(N-1 \to N\), and the r.h.s. of Eq. (5.42) approaches the commutator \([a^H_k(t), H^H_N(t)]\).
where the second line follows by hermitean adjungation of the first one. These definitions mean that the annihilation and creation operators behave like wave functions of first quantization evolving according to the time-dependent $N$-particle Schrödinger equation,

\begin{align}
  i\hbar \partial_t a_i(t) &= a_i H(t) U(t, t_0), \\
  -i\hbar \partial_t a_i^\dagger(t) &= U^\dagger(t, t_0) H(t) a_i^\dagger.
\end{align}

These equations are well defined when $U$ is an $N$-particle operator\textsuperscript{14}.

Let us now see how the corresponding density matrix operator looks like and what its properties are. One immediately finds

\begin{align}
  n_{ji}(t) &= a_j^\dagger(t) a_i(t) = U^\dagger(t, t_0) a_j^\dagger a_i U(t, t_0) = n_{ji}^H(t), \\
  n_j^i(t) &= n_{ij}(t).
\end{align}

The first line shows that the density matrix operator defined with Eqs. (5.45) and (5.46) is a proper Heisenberg operator and its equation of motion is given by the Heisenberg equation (5.44).

This way we have at our disposal two independent dynamical equations of the creation and annihilation operators – a Schrödinger equation and a Heisenberg equation. Both have a different applicability range: the first corresponds to Hamiltonians (and time evolution operators) acting in the $N$-particle Hilbert space, whereas the second involves operators defined in Fock space with a variable particle number. Both approaches have their advantages and disadvantages for numerical applications as we discuss below.

### 5.7 Dynamics of the density matrix operator $\hat{n}_{nm}(t)$

Similar as for the field operators, we can derive equations of motion for any product of field operators. In particular, we wish to consider the dynamics of the operator $\hat{n}_{nm}(t)$. This operator is directly related to observable quantities in quantum many-body systems in nonequilibrium and is, thus, of prime importance. Since $\hat{n}_{nm}(t)$ is a Heisenberg operator the ambiguity in the dynamics of the field operators – Heisenberg vs. Schrödinger dynamics – does not play a role here, as we showed above. Both representations lead to the same result for the density matrix operator.

\textsuperscript{14}This is not a restriction. $N$ can be chosen arbitrary, only $U$ has to be chosen correspondingly.
5.7. DYNAMICS OF THE DENSITY MATRIX OPERATOR

5.7.1 Equation of motion for \( \hat{n}_{nm}(t) \)

We start from the Heisenberg equation

\[
i \hbar \partial_t \hat{n}_{ij}(t) = -U^\dagger(t, t_0) [\hat{H}_s(t), \hat{n}_{ij}] U(t, t_0), \quad \hat{n}_{ij}(t_0) = \hat{n}_{ij}. \tag{5.51}
\]

and evaluate the three commutators in Eq. (5.51), using again the relations (5.13), (5.14) and \([a^\dagger_i, a_j]_\mp = \mp \delta_{ij},\]

\[
[\hat{T} + \hat{V}, \hat{n}_{ij}] = \sum_{kl} h_{kl}(t) a^\dagger_k a_l, a^\dagger_i a_j = \tag{5.52}
\]

\[
= \sum_{kl} h_{kl}(t) \left\{ a^\dagger_k [a_l, a^\dagger_i a_j] + [a^\dagger_k, a_l a^\dagger_i a_j] \right\} =
\]

\[
= \sum_{kl} h_{kl}(t) \left\{ \pm a^\dagger_k [a_l, a^\dagger_i a_j] + a^\dagger_l [a_j, a^\dagger_i a_k] \right\} =
\]

\[
= \sum_{kl} h_{kl}(t) \left\{ a^\dagger_k a_j \delta_{ij} - a^\dagger_l a_\delta_{jk} \right\} =
\]

\[
= \sum_k \left\{ h_{ki}(t) a^\dagger_k a_j - h_{kj}(t) a^\dagger_j a_k \right\} =
\]

\[
= - \sum_k \left\{ \hat{n}_{ik} h^*_k(t) - h^*_i(t) \hat{n}_{kj} \right\} = \hbar^*(t) \hat{\mathbf{n}} - \hbar \mathbf{n}^*(t), \tag{5.53}
\]

where, in the last expression, we introduced standard matrix notation.

Finally, the commutator with the interaction energy is transformed similarly,

\[
2[\hat{W}, a^\dagger_i a_j] = \sum_{klmn} w_{klmn} \left\{ a^\dagger_k a^\dagger_l a_n a_m, a^\dagger_i a_j + [a^\dagger_k a^\dagger_l a^\dagger_i a_j] a_n a_m \right\} =
\]

\[
= \sum_{klmn} w_{klmn} \left\{ -a^\dagger_k a^\dagger_l a_n a_m a_j - a^\dagger_l a^\dagger_i a_j a_n a_m a_l a_i \right\} =
\]

\[
= \sum_{klmn} w_{klmn} \left\{ a^\dagger_k a^\dagger_l (a_n \delta_{mi} \pm a_m \delta_{ni}) a_j - a^\dagger_l a^\dagger_i \left( a^\dagger_k \delta_{kj} \pm a^\dagger_l \delta_{lj} \right) a_n a_m \right\} =
\]

\[
= -2 \sum_{kln} \left\{ w_{jnk} a^\dagger_k a^\dagger_n a_l a_k - w^*_{ink} a^\dagger_k a^\dagger_i a_n a_j \right\}. \tag{5.54}
\]

In the third line, the first terms in the parantheses are equal to the second ones – this is shown by exchanging \((k, m) \leftrightarrow (l, n)\) and using the symmetries \(a^\dagger_m a_n = \pm a_n a_m\) and \(w_{klmn} = w_{lknm}\).

What remains now is to apply the time evolution operators. There are two ways to proceed. The first is to apply the evolution operators only to the
outermost field operators. To this end we use the results for the commutators in the form (5.53) and (5.55) and combine them as follows

\[ i\hbar \frac{\partial}{\partial t} \hat{n}_{ij}(t) = U^\dagger(t,t_0)a_i^\dagger \sum_k h^\text{eff}_{jk}(t)a_k U(t,t_0) - \sum_k U^\dagger(t,t_0)a_i^\dagger h^\text{eff}_{ki}(t)a_j U(t,t_0) \]  

(5.56)

\[ h^\text{eff}_{jk} = h_{jk}(t) + \hat{W}_{jk}^\text{ind}, \quad \hat{W}_{jk}^\text{ind} = \sum_{ln} w_{jnk} a_n^\dagger a_l, \]  

(5.57)

where we introduced the same operators of the induced potential (Hartree mean field) and effective single-particle potential as before, cf. Sec. 5.5. Note, however, that here the induced potential is still time-independent. This is our first result. It is particularly useful when we consider computation of suitable averages.

Suppose we are interested in the average dynamics of the density matrix operator, i.e. the dynamics of the density matrix \( n_{ij} \), in a given time-independent \( N \)-particle state \( |\Psi \rangle \). When the density matrix operator is averaged with \( |\Psi \rangle \), we can, for each term, combine the pair of time evolution operators, \( \langle \Psi|U(t_0,t)\ldots U(t,t_0)|\Psi \rangle = \langle \Psi(t)|\ldots|\Psi(t) \rangle \) with the state vectors to yield time-dependent \( N \)-particle states, where the dots denote a time-independent operator, except for the intrinsic time-dependence of \( \hat{h}(t) \). This brings us back to a Schrödinger-type description of the time evolution which is the basis for Configuration Interaction approaches (exact diagonalization). Of course the computational effort of working with and propagation of \( N \)-particle states is tremendous as it scales exponentially with the system size.

5.7.2 Closed equation of motion for \( \hat{n}_{nm}(t) \) in terms of density matrix operators

The second approach consists in re-ordering the field operators in the interaction term such that this term can be expressed via time-dependent density matrix operators. The goal is to get rid of the \( N \)-particle time evolution operators. Eventually we will also try to achieve a compact matrix equation, as was done for the single-particle terms in Eq. (5.54). To this end we transform
the first four-operator product, using $\hat{n}_{nl}a_k = a_k\hat{n}_{nl} - \delta_{kn}a_l$

\[
a_i^\dagger a_i^\dagger a_i a_k = \hat{n}_{ik}\hat{n}_{nl} - \delta_{nk}\hat{n}_{il} = \pm (\hat{n}_{il}\hat{n}_{nk} - \delta_{ln}\hat{n}_{ik}) = \frac{1}{2} (\hat{n}_{ik}\hat{n}_{nl} + \hat{n}_{il}\hat{n}_{nk}) - \frac{1}{2} (\delta_{nk}\hat{n}_{il} + \delta_{ln}\hat{n}_{ik}). \tag{5.58}
\]

The first two lines correspond to the two options to pair the creation and annihilation operators which are both equivalent. Therefore, below we will use the (anti-)symmetrized form given in the third line. Analogously, the second four-operator product becomes

\[
a_i^\dagger a_i^\dagger a_i a_j = \frac{1}{2} (\hat{n}_{ln}\hat{n}_{kj} + \hat{n}_{kn}\hat{n}_{lj}) - \frac{1}{2} (\delta_{nk}\hat{n}_{lj} + \delta_{ln}\hat{n}_{kj}). \tag{5.59}
\]

The next step is to apply the two time evolution operators which simply leads to the replacement of all density matrix operators by time-dependent (Heisenberg) operators. Finally, we take into account the induced potential and transform, using Eq. (5.58),

\[
a_i^\dagger \sum_k \hat{W}_{jk}^{\text{ind}} a_k = \sum_{kl} \frac{w_{jnk}}{2} \left\{ (\hat{n}_{ik}\hat{n}_{nl} + \hat{n}_{il}\hat{n}_{nk}) - (\delta_{nk}\hat{n}_{il} + \delta_{ln}\hat{n}_{ik}) \right\}.
\]

\[
= \sum_k \hat{n}_{ik}\sum_{ln} \frac{w_{kljn}}{2} \hat{n}_{nl} + \sum_k \hat{n}_{il}\sum_{kn} \frac{w_{kijn}}{2} \hat{n}_{nk}
- \sum_k \hat{n}_{ik}\sum_{ln} \delta_{ln} w_{kijn}^* + w_{kijn}^* w_{kljn}^* \frac{1}{2}
= \sum_k \hat{n}_{ik}\sum_{ln} \frac{w_{kljn}^* + w_{kijn}^*}{2} \{\hat{n}_{nl} + \delta_{ln}\}
= \hat{n}\hat{U}^\pm,
\]

with the definition

\[
\hat{U}_{kj}^\pm = \sum_{ln} \frac{w_{kljn}^* + w_{kijn}^*}{2} \{\hat{n}_{nl} + \delta_{ln}\}, \tag{5.60}
\]

where, in the two terms containing $\hat{n}_{il}$, we exchanged the summation indices $l \leftrightarrow k$. In Eq. (5.60) we introduced the operator of the (anti-)symmetrized

\[\text{This follows directly from the commutator } [\hat{n}_{nl}, a_k] = -a_k\delta_{nk}. \text{ It is easy to verify that this holds for bosons and fermions by using the definition of } \hat{n}_{nl}.\]
induced potential that involves the (anti-)symmetrized potential matrix elements \( w_{jnk} = w_{jnkl} \pm w_{jnlk} \) that also appeared in the Slater-Condon rules in Chapter 4.

Similarly, the second term becomes

\[
\sum_k a_k^\dagger \tilde{W}_{ki}^\text{ind} a_j = \sum_{kln} \frac{w_{klin}}{2} \left\{ (\hat{n}_{ln} \hat{n}_{kj} \pm \hat{n}_{kn} \hat{n}_{lj}) - (\delta_{nk} \hat{n}_{lj} \pm \delta_{ln} \hat{n}_{kj}) \right\}.
\]

One readily verifies that the potential \( U^\pm \) is exactly the one introduced in Eq. (5.60).

Collecting all the results, we obtain, after applying the time evolution operators,

\[
i\hbar \partial_t \hat{n}(t) = \left[ \hat{n}(t), \left\{ h^*_{H}(t) + \hat{U}^\pm_{H}(t) \right\} \right] = \left[ \hat{n}(t), h^*_{H}(t) + \hat{U}^\pm_{H}(t) \right]
\]

where all operators are now Heisenberg operators, in particular, the induced potential operator now contains Heisenberg creation and annihilation operators. The term in the curly brackets can again be understood as the operator of an effective (Hartree-Fock-type) potential, \( \hat{h}^*_{H}(t) = h^*_{H}(t) + \hat{U}^\pm_{H}(t) \).

Thus, we have achieved our goal of obtaining a closed equation of motion for the single-particle density matrix operator and to eliminate the N-particle time evolution operator completely.

### 5.8 Ensemble average of the Heisenberg equation. Fluctuations and correlations

Despite the formal simplicity of the dynamical equation (5.62) which has the form of a Hartree-Fock equation, the operator nature of the entering field

\[
\hat{U}^\pm_{ik} = \sum_{ln} \frac{w_{kn} \pm w_{kn}}{2} \left\{ \hat{n}_{ln} \mp \delta_{ln} \right\}
\]

\[
= \sum_{ln} \frac{w_{klin} \pm w_{klin}}{2} \left\{ \hat{n}_{ln} \mp \delta_{ln} \right\} = \sum_{ln} \frac{w_{klin} \pm w_{klin}}{2} \left\{ \hat{n}_{ln} \mp \delta_{ln} \right\}.
\]
operators prohibits a direct access to observable physical quantities. There are (at least) four solutions:

A. Computation of pure state averages using \(N\)-particle states and time propagation of these states (expansion coefficients) in CI-manner, as discussed in the context of Eq. (5.56), or using coherent states, cf. Sec. 5.4.

B. Application of the field operators to suitable many-body states using random initial states. Propagation of individual random trajectories with subsequent ensemble averaging. An example is the stochastic mean field approach of Ayik, Lacroix and others which is discussed in Sec. 5.8.2.

C. Performing a suitable statistical average over field operators yielding results in a mixed ensemble. This approach results in a hierarchy of equations for reduced \(s\)-particle density matrices (BBGKY-hierarchy or for correlation functions of fluctuations) and will be considered in Sec. 5.8.1.

D. Computation of statistical averages of field operator products taken at different times. This leads to the theory of nonequilibrium Green functions and will be discussed in Chapter 7.

### 5.8.1 Fluctuations and correlations (Approach B)

We now perform a statistical average of the operator equation (5.62). We will denote averages of operators by symbols without hat and fluctuations (deviations from the average) by the symbol \(\delta\), i.e.

\[
\langle \hat{n}_{nm} \rangle \equiv n_{nm}, \\
\delta \hat{n}_{nm} \equiv \hat{n}_{nm} - n_{nm}. \tag{5.63}
\]

Since averaging is a linear operation, its application to the operator equation of motion (5.62) does not change the equation, except for terms containing products of density matrix operators. For arbitrary operators (or random variables), the average of a product can be written as \(\langle \hat{A}\hat{B} \rangle = AB + \langle \delta \hat{A}\delta \hat{B} \rangle\).

We now apply these results to the operator equation (5.62):

\[
\begin{aligned}
&\frac{i\hbar}{\partial t} \mathbf{n}(t) - \left[\mathbf{n}(t), \mathbf{h}_H^+(t)\right] = \left\langle \left[\delta \mathbf{n}(t), \delta \mathbf{U}_H^+(t)\right] \right\rangle \equiv \mathbf{I}^+(t) \tag{5.65}
\end{aligned}
\]

Here the l.h.s. contains all (ensemble averaged) mean field terms and constitutes a standard time-dependent Hartree-Fock (TDHF) equation for the density matrix. Since the hamiltonian again contains the density, this is a
nonlinear equation. There exist various approaches (e.g. iterative procedures) for an efficient numerical solution of this equation (without the right-hand side).

The r.h.s., in contrast, contains all terms going beyond TDHF. By definition, these are correlation contributions to the many-body problem. Here we see that these correlation terms have a one to one correspondence with fluctuations of operator pairs\(^{17}\). We have also introduced the short notation \(I^\pm\) for the collision integral.

The solution of this inhomogeneous (formally) linear equation, together with the initial condition, \(n(t_0) = n_0\), is straightforward and given in terms of Hartree-Fock propagators \(U_{HF}\) (these are two-dimensional matrices and everywhere matrix multiplication is implied)

\[
\begin{align}
\mathbf{n}(t) &= U_{HF}^\dagger(t, t_0) \mathbf{n}_0 U_{HF}(t, t_0) + \mathbf{n}_f(t), \\
\mathbf{n}_f(t) &= \frac{1}{i\hbar} \int_{t_0}^{t} dt' U_{HF}^\dagger(t, t') I^\pm(t') U_{HF}(t, t'), \\
i\hbar \partial_t U_{HF}(t, t_0) &= \mathbf{h}_n^\pm(t) U_{HF}(t, t_0), \quad U_{HF}(t, t) = 1.
\end{align}
\]

We now can make further progress in evaluating the collision term \(I^\pm\) by directly computing the fluctuations \(\delta \hat{n}\) and, from it, also the fluctuation of the effective potential (5.60),

\[
\delta U_{kj}^\pm = \frac{1}{2} \sum_{jn} w_{njkl} \delta n_{nl}.
\]

Indeed the equation of motion of \(\delta \hat{n}\) follows immediately by taking the difference of Eqs. (5.62) and (5.65) [we suppress the time arguments]

\[
i\hbar \partial_t (\hat{n} - n) = [\hat{n}, \mathbf{h}_n^\pm] - [n, \mathbf{h}_n^\pm] + \\
+ \left[\hat{n}, \hat{U}_{HF}^\pm\right] - \left[n, U_{HF}^\pm\right] - \left[\delta \hat{n}, \delta \hat{U}_{HF}^\pm\right]
\]

Using the linearity in the density matrix, this can be rewritten as

\[
i\hbar \partial_t \delta \hat{n} - [\delta \hat{n}, \mathbf{h}_n^\pm] = \left[\delta \hat{n}, \delta \hat{U}_{HF}^\pm\right] - \left[\delta \hat{n}, \delta \hat{U}_{HF}^\pm\right] \equiv \mathbf{J}^\pm
\]

The term on the right can be understood as a higher order collision integral or as the fluctuation of the correlator of the fluctuations, \(\mathbf{J}^\pm = \delta \left[\delta \hat{n}, \delta \hat{U}_{HF}^\pm\right]\).

\(^{17}\)This correspondence between correlations and fluctuations is well known from the kinetic theory of classical plasmas and was established by Kadomtsev, Klimontovich and others.
Equation (5.70), together with the initial condition \( \delta \hat{\mathbf{n}}(t_0) = \delta \hat{\mathbf{n}}_0 \), is solved like Eq. (5.65), but using ideal propagators instead of Hartree-Fock propagators:

\[
\delta \hat{\mathbf{n}}(t) = \mathcal{U}^{\text{id}}(t,t_0) \delta \hat{\mathbf{n}}_0 \mathcal{U}^{\text{id}}(t,t_0) + \delta \hat{\mathbf{n}}_f(t), \tag{5.71}
\]

\[
\delta \hat{\mathbf{n}}_f(t) = \frac{1}{i \hbar} \int_{t_0}^{t} dt' \mathcal{U}^{\text{id}}(t,t') \mathcal{J}^\pm(t') \mathcal{U}^{\text{id}}(t,t), \tag{5.72}
\]

\[
i \hbar \partial_t \mathcal{U}^{\text{id}}(t,t_0) = i \hbar H(t) \mathcal{U}^{\text{id}}(t,t_0), \quad \mathcal{U}^{\text{id}}(t,t) = 1. \tag{5.73}
\]

There are several ways how to proceed. One is to evaluate the r.h.s. of Eq. (5.70) by using again the equation of motion (5.70), multiply by \( \delta \hat{\mathbf{n}} \) to derive the equation of motion for the product of fluctuations \( \delta \hat{\mathbf{n}} \delta \hat{\mathbf{n}}_\pm \) and for their commutator. It is easy to see that this equation, on the r.h.s., will contain products of three operator fluctuations. This shows that a hierarchy of equations for the fluctuations emerges which, in fact, is analogous to the BBGKY-hierarchy for the reduced density operators.

As an alternative, we can use the solution \( \delta \hat{\mathbf{n}}(t) \), Eq. (5.71), to compute the commutator \([\delta \hat{\mathbf{n}}(\alpha)(t), \delta \hat{\mathbf{n}}_\pm(\alpha)(t)]\), for a given initial condition \( \delta \hat{\mathbf{n}}_0(\alpha) \). This yields a single random realization of the collision integral \( I^{\pm(\alpha)} \) in Eq. (5.65). Repeating this for a representative set of initial conditions we can compute the expectation value by averaging over an ensemble of initial conditions,

\[
I^{\pm}(t) = \left\langle \left[ \delta \hat{\mathbf{n}}(t), \delta \hat{\mathbf{n}}_\pm(t) \right] \rightangle = \lim_{M \to \infty} \frac{1}{M} \sum_{\alpha=1}^{M} \left\langle \left[ \delta \hat{\mathbf{n}}^{(\alpha)}(t), \delta \hat{\mathbf{n}}^{(\pm)(\alpha)}(t) \right] \rightangle, \tag{5.74}
\]

where \((\alpha)\) denotes the possible realizations that occur with probability \( p_\alpha \), where \( \sum_\alpha p_\alpha = 1 \). This set \((\alpha, p_\alpha)\) specifies the ensemble.

With this, the r.h.s. of Eq. (5.65) is known and this equation can be solved. Two problems remain. The first is how to specify a physically adequate ensemble and the second, how to solve for \( \delta \hat{\mathbf{n}} \), considering the complicated structure of the collision integral \( \mathcal{J}^\pm \). A very simple and successful approach has recently been proposed by Ayik and co-workers [Ayi08, Lac13] and will be considered in the next section.

### 5.8.2 Stochastic Mean Field Approximation

One problem in treating the fluctuations of the density matrix operator and of the mean field potential is their time dependence. A first simplifying attempt to understand the general physics is, therefore, to neglect this dependence entirely. This can be done by approximating the collision integral \( I^\pm \) in Eq. (5.65) by a local function according to \( I^\pm(t) \to I^\pm(t_0) \delta(t-t_0) \). This means
only the initial fluctuations are taken into account. With this the solution for the density matrix, Eq. (5.67) becomes

\[ n_I(t) = \frac{1}{i\hbar} \mathcal{U}^{\text{HF}}(t, t_0) \hat{I}^\pm(t_0) \mathcal{U}^{\text{HF}}(t, t_0), \]

and the total solution for the density matrix is given by

\[ n(t) = \mathcal{U}^{\text{HF}}(t, t_0) \left\{ n_0 + \frac{1}{i\hbar} \left\langle \left[ \delta \hat{n}(t_0), \delta \hat{U}^{\text{HF}}_{\pm}(t_0) \right] \right\rangle \right\} \mathcal{U}^{\text{HF}}(t, t_0). \]

This means that the evolution of the density matrix \( n(t) \) is given by a pure Hartree-Fock dynamics. However, the evolution does not start from the initial value of the density matrix, \( n_0(t_0) \), but from a value that is shifted by the second term in the parentheses. If we forget for a moment the angular brackets we would have random realizations of initial values. Ayik had the idea \([\text{Ayi08}]\) to replace the complicated commutator by a semiclassical ensemble of initial density fluctuations with given mean and variance such that the term in parentheses becomes \( n_0 + \Delta n_0^{(\alpha)} \), for a given realization \( (\alpha) \). The corresponding dynamics, starting from this initial state is given by

\[ \hat{n}^{(\alpha)}(t) = \mathcal{U}^{\text{HF}}_{(\alpha)}(t, t_0) \left\{ n_0 + \Delta n_0^{(\alpha)} \right\} \mathcal{U}^{\text{HF}}_{(\alpha)}(t, t_0), \]

and the full result is then given by the ensemble average, i.e. by the sum over all realizations, for all times,

\[ n(t) = \lim_{M \to \infty} \frac{1}{M} \sum_{\alpha=1}^{M} \hat{n}^{(\alpha)}(t). \quad (5.75) \]

Since only mean field trajectories are involved and the result is obtained from a stochastic sampling over realizations this approach has been called \textit{Stochastic Mean Field (SMF)}. Thereby, the incorporation of fluctuations reproduces (part of) the correlations in the system. The most attractive feature is the conceptional simplicity and computational efficiency: THDF propagations are very simple and fast, and sampling of the initial states is very efficiently realized with Monte Carlo methods. Finally, this sampling an be performed in parallel on a large number of computer cores.

Although the SMF concept is very crude since it restricts the fluctuations to those of the initial state, neglecting decay of initial fluctuations and buildup of correlations due to collisions, this method shows remarkable results. Tests for simple Hubbard clusters have shown that the results are not only better than pure time-dependent Hartree-Fock (TDHF) but also more accurate than NEGF results using selfenergies in second order Born approximation \([\text{LHHB14}]\).
5.8.3 Iterative Improvement of Stochastic Mean Field Approximation

Here we suggest a further improvement of SMF that allows to include the time-dependence of the fluctuations in an iterative manner. A crucial observation is that SMF does not only yield the one-body expectation value $\langle n(t) \rangle$ but a full set of random trajectories. This means, we can also compute fluctuations of the density, correlation functions, higher order density matrices and so on. Using the entire ensemble of trajectories $\{n^{(a1)}\}$ we can immediately compute the ensemble of fluctuations $\{\delta n^{(a1)}\}$ and $\{\delta U^\pm (a1)\}$, cf. Eq. (5.69). Using Eq. (5.74) we can directly evaluate the collision integral and thus compute the evolution of the density matrix.

A further improvement would be to avoid the computation of the ensemble average in Eq. (5.74) but instead, again, to propagate random realizations. Then we would again have access to an ensemble of improved trajectories $\{n^{(a2)}\}$ which can, again, be used as input into the collision integral. This way an iterative procedure can be designed. It remains to be checked how big the computational effort and how good the convergence are.

The open problem is to work out an approximation how to compute the commutator of $\{\delta n^{(a)}\}$ and $\{\delta U^\pm (a)\}$ that enters the collision integral. With this we conclude the discussion of stochastic approaches to the equations of motion for the density matrix operator and turn to an entirely different concept that starts with an ensemble average in the very beginning.

5.9 Ensemble average of the field operators

As we have discussed above, the operator nature of the field operators prohibits their direct evaluation. One way to achieve measurable results is, therefore, to perform a suitable averaging of the operators. Suppose our many-body system is in a mixed state characterized by some time-independent probability distribution. In the most general case this is the $N$-particle density operator $\rho_N$. Then we can compute averages, $\langle \cdots \rangle_{\rho_N} = \text{Tr} \cdots \rho_N$, 

\[
\langle \hat{\psi}(r, \sigma, t) \rangle_{\rho_N} = \psi(r, \sigma, t) \quad (5.76)
\]

\[
\langle \hat{\psi}^\dagger(r, \sigma, t) \rangle_{\rho_N} = \psi^*(r, \sigma, t) \quad (5.77)
\]

which are already regular functions of coordinate, spin and time. Similarly, in an arbitrary basis the expectation value of the second quantization operators
become,
\[ \langle \hat{a}_i(t) \rangle_{\rho_N} = a_i(t) \]  
(5.78)
\[ \langle \hat{a}_i^\dagger(t) \rangle_{\rho_N} = a_i^*(t) \]  
(5.79)
where we have “absorbed” the spin argument into the orbital label. In most cases of interest, however, these expectation values will vanish. An exception would be if the averaging is performed in a coherent state, which is an eigenstate of the annihilation operator, so the expectation value would be given by the associated eigenvalue.

5.9.1 Bose-Einstein condensates

Another example with a nontrivial expectation value would be a state that is occupied by a macroscopically large number of particles. This is, obviously, possible only for bosons, and a macroscopic occupation would be most easily achieved for the ground state, i.e., for a Bose-Einstein condensate. The action of the second quantization operator on such a state would change the occupation by one—which would be only a small modification leading to small fluctuations around the mean value. In fact, replacing the field operators by their mean values, i.e., by wave functions transforms Eq. (5.21) into a nonlinear Schrödinger equation

\[ i\hbar \partial_t \psi(x, t) = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + v(r) + U^{\text{ind}}(x, t) \right\} \psi(x, t) \]  
(5.80)

\[ U^{\text{ind}}(x, t) = \int dx'' w(r, r'') \psi^\dagger(x'', t) \psi(x'', t). \]

In the case of atomic Bose systems, usually the interaction is short-range and it is often approximated by contact interaction, \( w(r, r'') \rightarrow g\delta(r-r'') \), and the equation (5.81) becomes

\[ i\hbar \partial_t \psi(x, t) = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + v(r) + g|\psi(x, t)|^2 \right\} \psi(x, t), \]  
(5.81)

which has the name Gross-Pitaevskii equation that was first derived in 1961.\(^{18}\)

and is also a reasonable order parameter, counting the number of particles in the ground state (condensate). This system has the total energy

\[ W[\psi] = \int d^3r \left\{ \frac{\hbar^2}{2m} (\nabla \psi)^2 + v(r)|\psi|^2 + g|\psi|^4 \right\}, \tag{5.82} \]

and equation (5.81) can be derived by minimizing the energy (5.82) with respect to \( \psi^* \) under the constraint of fixed normalization. The stationary Gross-Pitaevskii equation is the eigenvalue problem for the Gross-Pitaevskii hamiltonian [r.h.s. of Eq. (5.81)], \( \hat{H}_{GP} \psi = E \psi \). In the homogeneous case (\( v \equiv 0 \)), we make the ansatz of a plain wave, \( \psi(r) = n^{-1/2} e^{i k r} \), with \( n = N/V \), and obtain the dispersion relation

\[ E = E(k) = N \left\{ \frac{\hbar^2 k^2}{2m} + n g \right\}, \]

which has a gap at zero momentum. This violates the Hugenholtz-Pines theorem (for repulsive interaction)\(^{19}\). The reason is the too simple treatment of the effect of interactions. In fact, the assumption that all particles are in the condensate and that the wave function is a plain wave, as for free particles, is not correct, in the case of interactions. Interactions between the condensate lead to a (possibly small) fraction of particles that leave the condensate (Landau’s two fluid theory) which can be treated in perturbation theory as proposed by Bogolyubov: \( \psi = \psi_0 + \delta \psi \). As before, the appearance of the fluctuating part is equivalent to including correlations whereas its neglect corresponds to a mean field (Hartree) approximation. Then the time-dependent Gross-Pitaevskii equation can be solved with the ansatz

\[ \psi_0 = n^{1/2} e^{-i\mu t} \]

\[ \delta \psi = e^{-i\mu t} \{ u(r) e^{-i\omega t} + v^*(r) e^{i\omega t} \} \]

This is inserted in the equations for \( \psi \) and \( \psi^* \) and leads to the following system of equations by taking the \( e^{\pm i\omega t} \) components as independent

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + v + 2gn - \hbar \mu - \hbar \omega \right) u - gnv = 0 \]

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + v + 2gn - \hbar \mu + \hbar \omega \right) v - gnu = 0 \] \( \tag{5.85} \)

Considering again the homogeneous case, i.e. \( v = \text{const} \), and assuming plain waves one finds the modified energy spectrum by using \( V = \hbar \mu - gn \), from the 0-th order equation,

\[
\epsilon_k = \hbar \omega(k) = \left\{ \frac{\hbar^2 k^2}{2m} \left( \frac{\hbar^2 k^2}{2m} + 2g|\psi|^2 \right) \right\}^{1/2}.
\]

For large \( k \) the dispersion is quadratic, as for free particles, because kinetic energy dominates. In contrast, for small \( k \) there is no energy gap but the dispersion is linear, resembling phonons. In fact the sound speed can be computed to

\[
\epsilon_k = v_s \cdot \hbar k, \quad v_s = \left( \frac{ng}{m} \right)^{1/2}.
\]  (5.86)

Since \( \epsilon_k > v_s \cdot \hbar k \) the energy cannot dissipate into phonons and the system is frictionless (superfluid), as first explained by Landau. In the case of negative \( g \), with increasing \( k \), the energy may decrease, giving rise to a minimum – the so-called roton – minimum that corresponds to different kind of excitations: rotons. This is also reproduced by exact quantum Monte Carlo simulations.

An interesting property of these systems is that \( g \) can be positive (repulsive interaction) or negative which drastically changes the dispersion relation. Another striking feature is that in cold atomic gases the value of \( g \) and even its sign can be tuned by an external magnetic field (Feshbach resonance).

In the case of charged bosons in an external electromagnetic field Eq. (5.81) is modified according to (minimal coupling) \( p \rightarrow p - q_e A \). The resulting equation is the Ginzburg-Landau equation which allows for a phenomenological description of superconductivity.

### 5.9.2 Fermions

Putting these cases aside, a nontrivial expectation value will involve typically pairs of field operators such as the single-particle density-matrix operator, the average of which leads to the single-particle density matrix,

\[
\langle \hat{a}_i^\dagger(t)\hat{a}_j(t) \rangle_{\rho_N} = n_{ij}(t).
\]  (5.87)

This is a special case of a more general class of functions, the reduced \( s \)-particle density matrices. These functions are closely related to the reduced density operators of density operator theory. The relation between these quantities and the second quantization operators is explored in the following section.
5.9.3 Field operators and reduced density matrices

Consider an arbitrary $s$-particle operator, $\hat{B}_s$. To compute its expectation values we have two options. First is to use the (anti-) symmetrized reduced $s$-particle density operator $F^\pm_s$ that are defined via the full $N$-particle density operator according to [Bon]

\begin{align}
F^\pm_s &= F_s \Lambda^\pm_{1..s} \\
F_s &= \frac{N!}{(N-s)!} \text{Tr}_{s+1..N} \rho_N, \quad \text{Tr}_{1..s} F_s = \frac{N!}{(N-s)!}.
\end{align}

Here we introduced the (anti-)symmetrization operator defined in Eq. (3.14) in Sec. 3. Note that $F_s$ is an ensemble averaged quantity since it is computed from $\rho_N$ that incorporates a mixed state description with given probabilities of the individual $N$-particle states.

Using the reduced density operator the expectation value of $\hat{B}_s$ is computed according to

\begin{align}
\langle \hat{B}_s \rangle_{\rho_N} &= \frac{1}{s!} \text{Tr}_{1..s} \hat{B}_s F^\pm_s \\
&= \frac{1}{s!} \sum_{i_1..i_s=1}^{\infty} \sum_{k_1..k_s=1}^{\infty} \langle i_1..i_s | F^\pm_s | k_1..k_s \rangle \langle k_1..k_s | \hat{b}_{1..s} | i_1..i_s \rangle,
\end{align}

where, in the second line, the trace is performed using a complete set of $s$-particle states $|i_1..i_s\rangle$ which we can always construct as products of single-particle orbitals. This expression is equivalent to averaging over the full $N$-particle density operator since the trace over the variables of particles $s+1..N$ is trivially performed.

The second approach to compute this expectation value is to transform the operator $\hat{B}_s$ into second quantization representation, cf. Eq. (3.54),

\begin{align}
\hat{B}_s &= \frac{1}{s!} \sum_{i_1..i_s=1}^{\infty} \sum_{k_1..k_s=1}^{\infty} \langle k_1..k_s | \hat{b}_{1..s} | i_1..i_s \rangle a^\dagger_{i_1}..a^\dagger_{i_s} a_{k_s}..a_{k_1},
\end{align}

where the sums run over the complete set of single-particle orbitals. This is still an operator expression. In order to obtain its expectation value in the relevant statistical ensemble, we average this expression with the density operator $\rho_N$, taking into account that the matrix element of $\hat{b}$ is a regular $c$-function,

\begin{align}
\langle \hat{B}_s \rangle_{\rho_N} &= \frac{1}{s!} \sum_{i_1..i_s=1}^{\infty} \sum_{k_1..k_s=1}^{\infty} \langle k_1..k_s | \hat{b}_{1..s} | i_1..i_s \rangle \langle a^\dagger_{i_1}..a^\dagger_{i_s} a_{k_s}..a_{k_1} \rangle_{\rho_N}.
\end{align}

\footnote{Of course, it is equivalent only if the density operator $F^\pm_s$ is known exactly.}
Now, comparing the two results, Eq. (5.90) and (5.91), we can establish the connection between the creation and annihilation operators and the reduced density operators:

\[
\langle i_1 \ldots i_s | F_s^{\pm} | k_1 \ldots k_s \rangle = \langle a_{i_1}^\dagger \ldots a_{i_s}^\dagger a_{k_s} \ldots a_{k_1} \rangle_{\rho_N}.
\]  (5.92)

This is an important result as it establishes the connection between quantum kinetic theory (reduced density operators) and second quantization and allows us to construct the reduced density operators directly from the second quantization operators. From this we obtain the normalization of the expression (5.92):

\[
\text{Tr}_{1 \ldots s} F_s^{\pm} = \sum_{i_1 \ldots i_s = 1}^\infty \langle a_{i_1}^\dagger \ldots a_{i_s}^\dagger a_{i_s} \ldots a_{i_1} \rangle_{\rho_N} = \frac{N!}{(N - s)!}.
\]  (5.93)

The definition (5.92) contains all relevant cases. Let us discuss some of them explicitly:

i) The single-particle reduced density operator is obtained from setting, in Eq. (5.92), \( s \to 1 \):

\[
\langle i | F_1^{\pm} | k \rangle = \langle a_i^\dagger a_k \rangle_{\rho_N} \equiv n_{ik} \equiv n_i,
\]  (5.94)

and its coordinate representation is obtained by using the field operators, instead of \( a \) and \( a^\dagger \), and a basis of single-particle coordinate-spin states (\( x = r, \sigma \)),

\[
\langle r \sigma | F_1^{\pm} | r' \sigma' \rangle = \langle \psi^\dagger(r, \sigma)\psi(r' \sigma') \rangle_{\rho_N} \equiv n(x, x').
\]  (5.95)

For completeness, we give the normalization condition of the single-particle density matrix in coordinate representation which follows directly from the general relation (5.93),

\[
N = \sum_{\sigma} \int dr \langle r \sigma | F_1^{\pm} | r \sigma \rangle = \sum_{\sigma} \int dr \langle \psi^\dagger(r, \sigma)\psi(r \sigma) \rangle_{\rho_N}.
\]  (5.96)

ii) The diagonal elements of the single-particle density operator (5.94) yield the ensemble averaged occupations of the single-particle orbitals \( |i\rangle \),

\[
\langle a_i^\dagger a_i \rangle_{\rho_N} \equiv n_{ii} = n_i,
\]  (5.97)

whereas the diagonal elements in the coordinate representation yield the local spin density

\[
\langle \psi^\dagger(r, \sigma)\psi(r \sigma) \rangle_{\rho_N} \equiv n_{\sigma}(r) = n_{\sigma}(r).
\]  (5.98)
In contrast, the off-diagonal elements of expression (5.94) describe the statistical probability of transitions between orbital $|k\rangle$ and $|i\rangle$. Similarly, the off-diagonal elements of the coordinate-space expression (5.95) are related to the probability of a particle undergoing a transition from spin orbital $|r'\sigma'\rangle$ to $|r\sigma\rangle$.

**iii)** The second important case of (5.92) is the two-particle reduced density operator ($s = 2$),

$$
\langle i_1 i_2 | F_{2}^{\pm} | k_1 k_2 \rangle = \langle a_{i_1}^{\dagger} a_{i_2} a_{k_2} a_{k_1} \rangle_{\rho_N} = n_{i_1,i_2;k_1,k_2}^{(2)} = n^{(2)},
$$

(5.99)

whereas its coordinate representation is,

$$
\langle r_1 \sigma_1 r_2 \sigma_2 | F_{2}^{\pm} | r_1' \sigma_1' r_2' \sigma_2' \rangle = \langle \psi^{\dagger}(r_1,\sigma_1) \psi^{\dagger}(r_2,\sigma_2) \psi(r_1',\sigma_1') \psi(r_2',\sigma_2') \rangle_{\rho_N} = n^{(2)}(x_1,x_2;x_1',x_2').
$$

(5.100)

The two-particle density matrix is normalized according to [cf. Eq. (5.93)]

$$
\text{Tr}_{12} n^{(2)} = \sum_{i_1i_2=1}^{\infty} \langle a_{i_1}^{\dagger} \ldots a_{i_s}^{\dagger} a_{i_s} \ldots a_{i_1} \rangle_{\rho_N} = N(N-1).
$$

**iv)** All the above results are directly extended to time-dependent situations. We simply have to introduce the Heisenberg operators in standard manner,

$$
a_i \rightarrow a_{Hi}(t) = U^{\dagger}(t,t_0) a_i U(t,t_0),
$$

and so on. This will give rise to the time-dependent reduced density operators $F_{s}^{\pm}(t)$, $n_{ij}(t)$, $n_{ij}^{(2)}(t)$, time-dependent densities $n_i(t)$ and $n_{\sigma}(r,t)$ etc. Thereby, the underlying dynamics of the Heisenberg operators was computed above: the field operators obey Eqs. (5.21) and (5.24) and the general annihilation operator obeys Eq. (5.31).

As we just discussed, the time-dynamics of a many-body system can be obtained from the time evolution of the second quantization operators in the Heisenberg picture. Alternatively, the dynamics of the reduced density operators $F_{s}^{\pm}(t)$ is known: it is given by the BBGKY-hierarchy which follows from the equation of motion of the $N$-particle density operator $\rho_N$ – the von Neumann equation. Since we found a one-to-one relation between the $F_{s}^{\pm}(t)$ and the second quantization operators, this BBGKY-hierarchy has to follow from the dynamics of $a_i$ and $a_i^{\dagger}$. This will be discussed below.
5.9.4 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 textbook [Bon] and the reader is referred to this reference.

5.10 Problems to Chapter 5

Problem 5.1 Derive the equation
\[ i \partial_t \hat{\psi}_H(x, t) = -U^\dagger(t, t_0)[\hat{H}, \hat{\psi}(x)]U(t, t_0). \]  
(5.101)

Problem 5.2 Prove the identity (5.14): 
\[ [\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] \pm [\hat{A}, \hat{C}][\hat{A}, \hat{B}] \]

Problem 5.3 Discuss the derivation of Eq. (5.21) for the case of a time-dependent Hamiltonian. Consider a time-dependent single-particle potential, \( v(r, t) \).

Problem 5.4 Derive the general equation of motion (5.31) for the creation and annihilation operators for the case of a time-independent external potential.

Problem 5.5 Verify the equation of motion for the density matrix operator, Eq. (5.62)