Kapitel 5

Dynamics of the creation and annihilation operators

5.1 Introduction to many-particle dynamics. Overview of methods

After considering the description of a many-particle system in a pure state in Chapter 3 or in thermodynamic equilibrium, in Chapter 4, we now move on to time-dependent phenomena. In fact, the nonequilibrium dynamics of interacting many-body systems is presently among the most actively developing fields of physics. This is driven by tremendous recent progress in experimental approaches to rapidly excite quantum systems, and to accurately diagnose these dynamics with femtosecond and – in case of laser excitation – even sub-fs time resolution. Examples include atomic physics (laser excitation and ionization of atoms and molecules, dynamics of cold atoms in optical lattices and traps), nuclear matter (dynamics following nuclear collisions), condensed matter systems (laser or free electron laser excitation of solids), or plasma physics (including shock compression of matter and inertial confinement fusion).

All these developments pose a big challenge to theory and simulations. Even though the governing equations are known for almost a century – the time-dependent Schrödinger equation,

$$i\hbar\partial_t \Psi(r_1, r_2, \dots r_N; t) = \hat{H}(t)\Psi(r_1, r_2, \dots r_N; t)\,, \tag{5.1}$$

$$\Psi(r_1, r_2, \dots r_N; 0) = \Psi_0(r_1, r_2, \dots r_N)\,, \tag{5.2}$$

and computer technology has progressed dramatically, a numerical solution of Eq. (5.2) is limited to rather small systems. The reason is the exponential scaling of the required computation time with the system size (basis dimension). There has been tremendous activity in the development of theoretical and

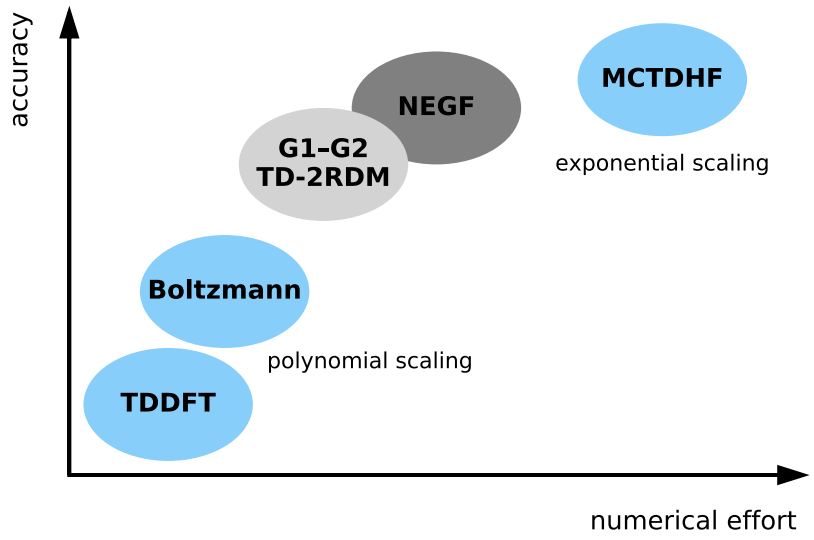

Abbildung 5.1: Qualitative overview of different many-body methods: comparison of accuracy versus numerical effort (computing time). MCTDHF represents wave function-based methods; TDDFT: time-dependent density functional theory; Boltzmann: Markovian kinetic equations, NEGF: Nonequilibrium Green functions; TD-2RDM: time-dependent reduced density matrices [Bon98]; G1-G2: Hartree-Fock-GKBA based NEGF scheme derived in Ref. [SJB20].

computational strategies to overcome this bottleneck. The approaches to the quantum dynamics of correlated many-body systems are extremely diverse, and can be sorted in the following way:

1. **Wave function-based methods.** These include[1]

   (a) perturbative approaches (time-dependent perturbation theory), "coupled cluster" theory, R-matrix methods, or multiconfiguration time-dependent Hartree or Hartree-Fock methods, e.g. [MMC90, HB11];

   (b) approaches that restrict the excitation processes (such as the "single-active electron" approximation, CI-singles, or CI-singles/doubles etc.);

[1]The list is incomplete. There exist many more names for similar concepts in different areas of physic and quantum chemistry, see for example Ref. [HHB14], for an overview.

   (c) approaches that impose different approximations to different spectral (energy) ranges such as time-dependent restricted active space (TD-RASCI) [HB12, HHB14, LBSB16], time-dependent "generalized active space" (TD-GASCI) [BSM14b], or "complete active space" [SI13];

2. **Propagation of reduced quantities**. The idea is to transform the wave function into a suitably averaged quantity of lower complexity.

   (a) Time-dependent density functional theory where the density $n(\mathbf{r}, t)$ is propagated, or kinetic equations where the phase space distribution, $f(\mathbf{r}, \mathbf{p}, t)$, is evolved in time;

   (b) Reduced density operators (density matrices, RDM), where an infinite hierarchy of equations (BBGKY[2]-hierachy) for the time-dependent RDM of different orders, $F_1(t), F_{12}(t), \ldots$ is derived and solved approximately, e.g. [Bon98];

   (c) Nonequilibrium Green functions (NEGF), where a hierarchy of equations (Martin-Schwinger hierarchy) for the many-particle Green functions, $G_1(t_1, t_1'), G_{12}(t_1, t_2; t_1', t_2'), \ldots$ is derived that depend on multiple times. NEGF yield, as a limiting case, the dynamics of single-time quantities that are closely related to RDM.

3. **Other time-dependent approaches** include time-dependent Density matrix renormalization group approaches (DMRG), quantum molecular dynamics (path integral MD), semiclassical approaches such as Wigner function MD [FTV$^+$02], stochastic mean field approximation [LHHB14], quantum fluctuations approaches, e.g. [SJB22, SWJB23, SB24a] hydrodynamics and more.

Here will concentrate on the approaches falling into class two. To develop the foundation for these methods, we now extend the formalism of second quantization to nonequilibrium. We will derive 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 and the different occupation numbers.

Time evolution operator. 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

[2]The shortcut stands for the names Bogolyubov-Born-Green-Kirkwood-Yvon, see Ch. 6

picture[3]. In the Schrödinger picture the quantum mechanical states (or wave functions) evolve in time, starting from an initial state at time t_0,

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle\,, \tag{5.3}$$
$$|\Psi(t_0)\rangle = |\Psi_0\rangle, \tag{5.4}$$

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

$$i\hbar\partial_t U(t,t') - \hat{H}(t)U(t,t') = 0, \tag{5.5}$$
$$U(t,t) = \hat{1}, \tag{5.6}$$

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. (5.5) with the initial condition (5.6), for the case of a time-independent hamiltonian, is given by

$$U(t,t') = e^{-\frac{i}{\hbar}\hat{H}(t-t')}\,, \tag{5.7}$$

   and U depends only on the time difference, $\tau = t - t'$, but not on the center of mass time $T = (t+t')/2$, i.e., the system is time-translation invariant[4]

2. If the hamiltonian depends on time the solution is generalized to[5]

$$U(t,t') = \hat{T}\, e^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\,\hat{H}(\bar{t})}\,, \tag{5.8}$$

   and we observe a dependence on, both, the relative and center of mass times. Since the hamiltonian $\hat{H}(t_1)$, not necessarily commutes with $\hat{H}(t_2)$, the solution involve a time ordering operator $\hat{T}$ tha orders operator with a "later" time argument left of those with earlier times (this will be discussed in more detail below).

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

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

$$[U(t,t')]^\dagger = U(t',t) \tag{5.9}$$

[3]Of course, there exist intermdediate concepts such as the interaction (Dirac) picture

[4]This is a consequence of energy conservation, as expressed in Noether's theorems.

[5]The derivation was given in quantum mechanics in the context of the interaction picture. Recall that $\hat{T}$ is the time-ordering operator that orders products of time-dependent operators such that the latest time appears at the left end and so on.

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

6. Since U, in general, depends on two times we also need to consider the dynamics with respect to the second time argument, in addition to the equation of motion (5.5). To this end we compute the adjoint of this equation,

$$\begin{aligned} 0 &= -i\hbar\partial_t U^\dagger(t,t') - U^\dagger(t,t')\hat{H}(t) = -i\hbar\partial_t U(t',t) - U(t',t)\hat{H}(t) \\ &= i\hbar\partial_{t'} U(t,t') + U(t,t')\hat{H}(t'), \end{aligned} \tag{5.10}$$

where, in the last line, we used Eq. (5.9), multiplied by -1, renamed the time arguments $t \longleftrightarrow t'$ and understand $\hat{H}$ to act to the left.

5.2 Equation of motion of the field operators

Let us now consider the dynamics of the field operators (we start with the coordinate-spin representation). Their time-dependent form is obtained by transforming to the Heisenberg representation of quantum mechanics according to[6]

$$\boxed{\hat{\psi}_H(x,t) = U^\dagger(t,t_0)\hat{\psi}(x)U(t,t_0)} \tag{5.11}$$

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. This holds for fermions and bosons simultaneously.

The time evolution of the field operators is governed by the hamiltonian for which we use a general expression containing kinetic energy, potential energy and pair interaction energy which we write in second quantization ($x = (\mathbf{r}, \sigma)$, see chapter 3)

$$\begin{aligned} \hat{H} = \hat{T} + \hat{V} + \hat{W} = &\int dx'\, \hat{\psi}^\dagger(x') \left(-\frac{\hbar^2}{2m}\nabla'^2 + v(\mathbf{r}') \right) \hat{\psi}(x') + \\ &\frac{1}{2}\int dx' \int dx''\, \hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x'')w(\mathbf{r}', \mathbf{r}'')\hat{\psi}(x'')\hat{\psi}(x'). \end{aligned} \tag{5.12}$$

[6] A critical discussion ot the Heisenberg representation of the field operators is given in Sec. 5.7.

The evolution equation of the field operators is given by Heisenberg's equation (see problem 5.1, Sec. 5.11) [7]

$$i\hbar\partial_t\hat{\psi}_H(x,t) = -[\hat{H}_H, \hat{\psi}_H(x,t)] = -U^\dagger(t,t_0)[\hat{H}, \hat{\psi}(x)]U(t,t_0)\,, \tag{5.14}$$

which always involves a commutator, regardless of the spin statistics. 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,

$$\begin{aligned}
[\hat{A}\hat{B}, \hat{C}] &= \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}, &(5.15)\\
[\hat{A}\hat{B}, \hat{C}] &= \hat{A}[\hat{B}, \hat{C}]_\mp \pm [\hat{A}, \hat{C}]_\mp\hat{B}, &(5.16)\\
[\hat{\psi}^\dagger(x'), \hat{\psi}(x)]_\mp &= \mp\delta(x-x'), &(5.17)
\end{aligned}$$

where the first two are verified by direct evaluation of the left and right-hand sides (see problem 5.2, Sec. 5.11), whereas the third follows from the standard (anti-)commutation relations[8].

Consider first the commutator with the external potential which is simplified with the help of Eq. (5.16),

$$\begin{aligned}
[\hat{V}, \hat{\psi}(x)] &= \int dx'\,[\hat{\psi}^\dagger(x')v(\mathbf{r}')\hat{\psi}(x'), \hat{\psi}(x)] = \\
&= \int dx'\,v(\mathbf{r}')\left\{\hat{\psi}^\dagger(x')[\hat{\psi}(x'), \hat{\psi}(x)]_\mp \pm [\hat{\psi}^\dagger(x'), \hat{\psi}(x)]_\mp\hat{\psi}(x')\right\}\\
&= -v(\mathbf{r})\hat{\psi}(x), &(5.18)
\end{aligned}$$

where we took into account that the first commutator vanishes and the second is evaluated according to Eq. (5.17). The same derivation applies to the kinetic

[7] The derivation starts from the r.h.s. of Heisenberg's equation that involves two Heisenberg operators

$$-[U^\dagger(t,t_0)\hat{H}U(t,t_0), U^\dagger(t,t_0)\hat{\psi}(x)U(t,t_0)], \tag{5.13}$$

and uses the property $U(t,t_0)U^\dagger(t,t_0) = 1$.

[8] In the second and third line the upper (lower) sign refers to bosons (fermions), i.e. to the commutator (anti-commutator).

energy term with the result (see problems)[9]

$$[\hat{T},\hat{\psi}(x)] \;=\; -\left(-\frac{\hbar^2}{2m}\nabla^2\right)\hat{\psi}(x). \tag{5.19}$$

Finally, we transform the commutator with the interaction energy using relation (5.15),

$$\begin{aligned} 2[\hat{W},\hat{\psi}(x)] &= \int dx' \int dx''\,[\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x'')w(\mathbf{r}',\mathbf{r}'')\hat{\psi}(x'')\hat{\psi}(x'),\hat{\psi}(x)] = \\ &= \int dx' \int dx''\, w(\mathbf{r}',\mathbf{r}'')\Big\{\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x'')[\hat{\psi}(x'')\hat{\psi}(x'),\hat{\psi}(x)] + \\ &\quad + \quad [\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x''),\hat{\psi}(x)]\hat{\psi}(x'')\hat{\psi}(x')\Big\}. \end{aligned} \tag{5.20}$$

The first commutator vanishes as it involves only annihilation operators whereas the second is transformed, using Eqs. (5.16) and (5.17),

$$\begin{aligned} [\hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x''),\hat{\psi}(x)] &= \hat{\psi}^\dagger(x')[\hat{\psi}^\dagger(x''),\hat{\psi}(x)]_\mp \pm [\hat{\psi}^\dagger(x'),\hat{\psi}(x)]_\mp\hat{\psi}^\dagger(x'') \\ &= \mp\hat{\psi}^\dagger(x')\delta(x''-x) - \delta(x'-x)\hat{\psi}^\dagger(x''), \end{aligned} \tag{5.21}$$

and the second term in the integral (5.20) becomes

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

where the first term in Eq. (5.21) is transformed by exchanging $x' \leftrightarrow x''$, after which it becomes identically equal to the second one[10]. With this the final result for the commutator becomes

$$[\hat{W},\hat{\psi}(x)] \;=\; -\int dx''\, w(\mathbf{r},\mathbf{r}'')\hat{\psi}^\dagger(x'')\hat{\psi}(x'')\hat{\psi}(x). \tag{5.22}$$

[9]The derivation follows from considering (contributed by Erik Schroedter)

$$\begin{aligned} -\frac{2m}{\hbar^2}[\psi(x),\hat{T}] &= \int dx'[\psi(x),\psi^\dagger(x')\Delta'\psi(x')] = \\ &= -\int dx'\,\{\psi^\dagger(x')[\Delta'\psi(x'),\psi(x)]_\mp \pm [\psi^\dagger(x'),\psi(x)]_\mp\Delta'\psi(x')\} \\ &= -\int dx'\,\{\psi^\dagger(x')\Delta'[\psi(x'),\psi(x)]_\mp - \delta(x-x')\Delta'\psi(x')\} \\ &= \Delta\psi(x) \end{aligned}$$

[10]The derivation assumes $w(\mathbf{r}',\mathbf{r}'') = w(\mathbf{r}'',\mathbf{r}')$, and the sign change, in the case of fermions, arises from exchanging the order of the two annihilation operators.

Inserting the results for the three commutators into Eq. (5.14) 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. 5.6 and problem 2) we obtain the equation of motion of the field operator,

$$\boxed{i\hbar\partial_t\hat{\psi}_H(x,t) = \left\{-\frac{\hbar^2}{2m}\nabla^2 + v(r) + \hat{U}_H^{\rm ind}(x,t)\right\}\hat{\psi}_H(x,t)} \tag{5.23}$$

$$\hat{U}_H^{\rm ind}(x,t) = \int dx''\, w(\mathbf{r},\mathbf{r}'')\hat{\psi}_H^\dagger(x'',t)\hat{\psi}_H(x'',t). \tag{5.24}$$

Let us briefly discuss this result. The notion "induced" potential in Eq. (5.24) indicates a similarity to the induced electrostatic potential of charged particles. Indeed, when w is a Coulomb potential, $w(\mathbf{r},\mathbf{r}'') = e^2|\mathbf{r}-\mathbf{r}''|^{-1}$, then the induced potential becomes $\hat{U}_H^{\rm ind}(x,t) = e\hat{\phi}_H^{\rm ind}(x,t)$, where the potential $\hat{\phi}_H^{\rm ind}$ is the operator generalization of the electrostatic potential produced by a charge density, $\hat{\rho}_H^{\rm ind}(x'',t) = e\hat{\psi}_H^\dagger(x'',t)\hat{\psi}_H(x'',t)$, which obeys Poisson's equation[11]

$$\Delta\hat{\phi}_H^{\rm ind}(x,t) = -4\pi\hat{\rho}_H^{\rm ind}(x,t)\,. \tag{5.25}$$

Thus the field operator is subject to an effective single-particle operator potential,

$$\hat{U}_H^{\rm eff} = v(r) + \hat{U}_H^{\rm ind}. \tag{5.26}$$

This is an exact result valid, both, for fermions and bosons. Remarkably, this equation which was derived from the Heisenberg equation (5.14) 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. (5.23):

$$\boxed{i\hbar\partial_t\hat{\psi}_H^\dagger(x,t) = -\hat{\psi}_H^\dagger(x,t)\left\{-\frac{\hbar^2}{2m}\nabla^2 + v(r) + \hat{U}_H^{\rm ind}(x,t)\right\}} \tag{5.27}$$

where the operators ∇ and $\hat{U}_H^{\rm ind}$ act on the field operator to the left, and we took into account that $(\hat{U}_H^{\rm ind})^\dagger = \hat{U}_H^{\rm ind}$, which is a consequence of the fact that the density operator, $\hat{n}_H = \hat{\psi}_H^\dagger\hat{\psi}_H$, appearing in $\hat{U}_H^{\rm ind}$, is hermitean.

[11] Note that, with this, we have obtained a quantization of the electrostatic potential which is done more systematically in quantum electrodynamics.

Theorem: As the Schrödinger equation in quantum mechanics, Eq. (5.23) is associated with an *operator continuity equation* describing local particle number conservation,

$$\boxed{\partial_t \hat{n}_H(x,t) + \nabla \hat{\mathbf{j}}_H(x,t) = 0} \tag{5.28}$$

$$\boxed{\hat{n}_H = \hat{\psi}_H^\dagger \hat{\psi}_H, \qquad \hat{\mathbf{j}}_H(x,t) = \frac{\hbar}{2im}\left\{\hat{\psi}_H^\dagger \nabla \hat{\psi}_H - \left(\nabla \hat{\psi}_H^\dagger\right)\hat{\psi}_H\right\}} \tag{5.29}$$

Note that, while in the continuity equation for the single-particle wave function of standard quantum mechanics, the quantities n and $\mathbf{j}$ describe the probability density and probability current density, here the analogous operator quantities refer to an N-particle system[12].

Proof: We compute the time-derivative of the density operator and use the equations of motion (5.23), (5.27), dropping the arguments x, t

$$\begin{aligned}\dot{\hat{n}}_H = \hat{\psi}_H^\dagger \dot{\hat{\psi}}_H + \dot{\hat{\psi}}_H^\dagger \hat{\psi}_H &= -\frac{\hbar}{2im}\left\{\hat{\psi}_H^\dagger \nabla^2 \hat{\psi}_H - \left(\nabla^2 \hat{\psi}_H^\dagger\right)\hat{\psi}_H\right\} = \\ &= -\frac{\hbar}{2im}\nabla\left\{\hat{\psi}_H^\dagger \nabla \hat{\psi}_H - \left(\nabla \hat{\psi}_H^\dagger\right)\hat{\psi}_H\right\},\end{aligned}$$

and the expression in the brackets is just the current density operator (5.29)[13], which completes the proof.

The key difference between the familiar one-particle Schrödinger equation and Eq. (5.23) for the field operator is the appearance of the effective potential $\hat{U}_H^{\text{eff}}$, Eq. (5.26), instead of the external potential v. The "induced" potential contained in $\hat{U}_H^{\text{eff}}$, in addition to v, 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)[14]

Thus equation (5.23) 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 operator Schrödinger equation is nonlinear in the field operators, since

[12]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 $\hat{N}$.

[13]In the derivation we took into account that the terms with the potentials cancel.

[14]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 $N(\mathbf{r}, \mathbf{p}, t)$, cf. Eq. (2.20). The closest expression to N is, for quantum systems, the density operator $\hat{n}(\mathbf{r}, \mathbf{r}', t) = \hat{\Psi}^\dagger(\mathbf{r}, t)\hat{\Psi}(\mathbf{r}', t)$. We will consider its equation of motion in Sec. 5.8.

in the induced potential two additional operators appear. This means that this equation does not obey a superposition principle, in contrast to the (equivalent) N-particle Schrödinger equation which is linear in the wave function ψ_N.

Unfortunately, a direct solution of Eq. (5.23) is impossible due to its operator character. The standard procedure is, therefore, to introduce suitable expectation values. This will be considered in Sec. 5.9. An independent approach that is based on a stochastic treatment of this equation will be discussed in Sec. 5.7. 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.

5.3 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 $\{|i\rangle\}$. The N-particle states belong to the Fock space and are again written in occupation number representation $|n_1 n_2 \dots\rangle$, cf. Chapter 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. (5.12), for which we use the general second quantization representation,

$$\hat{H} = \hat{T} + \hat{V} + \hat{W}, \tag{5.30}$$

$$\hat{T} + \hat{V} = \sum_{i,j=1}^{\infty} a_i^\dagger \left(t_{ij} + v_{ij}\right) a_j = \sum_{i,j=1}^{\infty} h_{ij}\, a_i^\dagger a_j, \tag{5.31}$$

$$\hat{W} = \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} a_i^\dagger a_j^\dagger\, w_{ijkl}\, a_l a_k. \tag{5.32}$$

Proceeding as in Sec. 5.2 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[15]

$$i\hbar\partial_t a_i(t) = -U^\dagger(t,t_0)[\hat{H}, a_i]U(t,t_0), \qquad a_i(t_0) = a_i. \tag{5.33}$$

[15] As before, we assume $\partial_t H = 0$. For the general case, see Sec. 5.6.

Evaluating the three commutators in Eq. (5.33) we finally obtain (see problem 5.4, Sec. 5.11)

$$\boxed{i\hbar\partial_t a_i(t) = \sum_l (t_{il} + v_{il}) a_l(t) + \sum_{lmn} w_{imln} a_m^\dagger(t) a_n(t) a_l(t)} \tag{5.34}$$

where all operators are now Heisenberg operators. This is the generalization of the coordinate space result (5.23) 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

$$i\hbar\partial_t a_i(t) = \sum_l \left\{ t_{il} + \hat{v}_{H,il}^{\text{eff}}(t) \right\} a_l(t), \tag{5.35}$$

$$\hat{v}_{H,il}^{\text{eff}}(t) = v_{il} + \sum_{mn} w_{imln} \hat{n}_{mn}(t). \tag{5.36}$$

Problem: Consider the general result for the following special cases:

a. basis in which kinetic energy is diagonal

b. basis in which single-particle energy is diagonal

c. the Hubbard basis.

5.4 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. We will demonstrate this in the coordinate representation using, as a basis, the eigenstates of the coordinate vector, $|\mathbf{r}, N\rangle$ to represent the states of N particles. Since (almost) all particles occupy the lowest orbital (there is no Pauli principle), in the thermodynamic limit, $N \to \infty$, one can approximately replace

$$\lim_{N\to\infty} \langle \mathbf{r}, N | \hat{\Psi} | \mathbf{r}, N+1 \rangle \approx \chi(\mathbf{r}, t)\,, \tag{5.37}$$

where $\chi(\mathbf{r}, t)$ is the *condensate wave function* that is macroscopically populated, with the normalization $\int d^3r |\chi(\mathbf{r}, t)|^2 = \mathrm{N}$. Replacing the field operator in

Eq. (5.23) by the condensate wave function (this means, we neglect fluctuations around the mean values[16]) gives rise to a nonlinear Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\chi(\mathbf{r},t) = \left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + \int d^3r'|\chi(\mathbf{r},t)|^2 w(\mathbf{r}-\mathbf{r}')\right\}\chi(\mathbf{r},t)\,, \quad (5.38)$$

which was independently derived by Gross and Pitaevskii in 1961 and carries their name. It has become extremely popular in recent years for the description of Bose gases and fluids in traps. The attractive feature is its simplicity: the entire N-particle problem is described by a single-particle wave equation.

The Gross-Pitaevskii equation can also be derived from the N-particle Schrödinger equation making a factorization ansatz into 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. (5.38). 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[17]. We return to this problem in Sec. 5.10.

Finally, note that the only assumption that was made in deriving the Gross-Pitaevskii equation was that the wave function χ is independent of the particle number, i.e. that particle number N fluctuations play a negligible role. While changing the particle number by one may be irrelevant in a state that has a macroscopic population, such as a Bose condensate, the situation is dramatically different in the case of fermions where the occupation cannot exceed one.

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

Another approach to the solution of the field equation (5.34) for the annihilation operators $\hat{a}$ 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 $|i\rangle$. For the case of a single annihilation operator, the eigenvalue problem reads

$$\hat{a}|\Psi_k^c\rangle = a_k|\Psi_k^c\rangle\,. \quad (5.39)$$

[16]When N is large, fluctuations related to few particle excitations will be small. This is similar to the close relation between quantum and classical descriptions of the electromagnetic field in the case of high intensity. Note that the situation is completely different for fermions where each orbital contains not more than one particle.

[17]Spin effects are only taken into account by permitting multiple particles to occupy the individual orbitals. 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)

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

$$\langle \Psi_l^c | \hat{a} | \Psi_k^c \rangle = a_k \delta_{l,k} \,. \tag{5.40}$$

What remains is to extend this to N-particle states with field operators for all orbitals. Here exist various path integral concepts that are related to so-called Grassmann variables[18]. However, no simple solution exists.

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

We will continue the general discussion of the solution of the field equations in Sec. 5.8.

5.6 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 operators, 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. (5.31), and the contribution to the r.h.s. of Eq. (5.33) becomes

$$\begin{aligned} -U^\dagger(t,t_0)[\hat{V}, a_i]U(t,t_0) &= U^\dagger(t,t_0) \sum_l v_{il}(t)\, a_l\, U(t,t_0) \\ &= \sum_l U^\dagger(t,t_0) v_{il}(t) U(t,t_0)\, a_l(t) = \sum_l \hat{v}_{H,il}(t)\, a_l(t)\,, \end{aligned} \tag{5.41}$$

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, $v(t)U(t,t_0) \neq U(t,t_0)v(t)$, and the result, therefore, contains the Heisenberg operator $v_{H,il}(t)$. Thus, our previous result, Eq. (5.36), is generalized to

$$i\hbar\partial_t a_i(t) = \sum_l \left\{ t_{il} + \hat{v}^{\text{eff}}_{H,il}(t) \right\} a_l(t), \tag{5.42}$$

$$\hat{v}^{\text{eff}}_{H,il}(t) = \hat{v}_{H,il}(t) + \sum_{mn} w_{imln} \hat{n}_{mn}(t), \tag{5.43}$$

[18] See for example lecture notes by F. Evertz, TU Graz, available online

where the time dependence of the new potential operator,

$$\hat{v}_{H,il}(t) = U^\dagger(t,t_0) v_{il}(t) U(t,t_0), \tag{5.44}$$

is due, both, to the explicit time dependence of the potential v and the two time evolution operators.

5.7 Schrödinger dynamics of the creation and annihilation operators[19]

In the previous sections we used the Heisenberg picture for the creation and annihilation operators[20]. While this is common practice in many text books, this approach has to be critically assessed. The problem is that the "standard" Heisenberg operator $\hat{a}_H(t) = U^\dagger(tt_0)\,\hat{a}\,U(tt_0)$ 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 in Fock space[21].

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[19] Optional section

[20] This aspect and the following results have been worked out together with S. Hermanns and C. Hinz.

[21] One possible way to define Heisenberg-type operators with hamiltonians for a fixed N is to work with different Hilbert spaces:

$$a_k^H(t) = U_{N-1}^\dagger(t,t_0) a_k U_N(t,t_0). \tag{5.45}$$

Then, the equation of motion is given by

$$\begin{aligned} i\partial_t a_k^H(t) &= i\partial_t U_{N-1}^\dagger a_k U_N + U_{N-1}^\dagger a_k i\partial_t U_N \\ &= -U_{N-1}^\dagger H_{N-1} a_k U_N + U_{N-1}^\dagger a_k H_N U_N \\ &= -H_{N-1}^H(t) a_k^H(t) + a_k^H(t) H_N^H(t) \end{aligned} \tag{5.46}$$

where, in the third line, we inserted unity according to $U_{N-1}U_{N-1}^\dagger = \hat{1}$. The density matrix operator is then given by

$$n_{kl}^H(t) = a_k^{\dagger,H}(t) a_l^H(t) = U_N^\dagger a_k^\dagger U_{N-1} U_{N-1}^\dagger a_l U_N = U_N^\dagger n_{kl} U_N, \tag{5.47}$$

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. (5.30). We proceed by constructing properly (anti-)symmetrized N-particle states $|\{n\}\rangle$ and defining the N-particle evolution operator U, as before, via Eq. (5.23).

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

$$\boxed{a_i(t) = a_i U(t, t_0)} \tag{5.49}$$

$$\boxed{a_i^\dagger(t) = U^\dagger(t, t_0) a_i^\dagger} \tag{5.50}$$

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,

$$\begin{aligned} i\hbar\partial_t a_i(t) &= a_i H(t) U(t, t_0), & (5.51)\\ -i\hbar\partial_t a_i^\dagger(t) &= U^\dagger(t, t_0) H(t) a_i^\dagger. & (5.52) \end{aligned}$$

These equations are well defined when U is an N-particle operator[22].

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

$$\begin{aligned} n_{ji}(t) &= a_j^\dagger(t) a_i(t) = U^\dagger(t, t_0) a_j^\dagger a_i U(t, t_0) = n_{ji}^H(t), & (5.53)\\ n_{ji}^\dagger(t) &= n_{ij}(t). & (5.54) \end{aligned}$$

---

which is a proper Heisenberg operator in N-particle Hilbert space that evolves according to the Heisenberg equation of motion

$$i\hbar\partial_t\, n_{kl}^H(t) = [n_{kl}^H(t), H_{kl}^H(t)]. \tag{5.48}$$

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. (5.46) approaches the commutator $[a_k^H(t), H_N^H(t)]$.

[22] This is not a restriction. N can be chosen arbitrary, only U has to be chosen correspondingly.

The first line shows that the density matrix operator defined with Eqs. (5.49) and (5.50) is a proper Heisenberg operator and its equation of motion is given by the Heisenberg equation (5.48).

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.

5.8 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. While for bosons the dynamics of a single field operator leads to a dynamics of the many-particle wave function, this is not the case for fermions, and the expectation value vanishes, $\langle \hat{a}_n \rangle \sim 0$. Instead, we have to consider the dynamics of two-operator correlation functions, such as 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.

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

We start from the Heisenberg equation[23]

$$i\hbar\partial_t \hat{n}_{ij}(t) = -U^\dagger(t,t_0)[\hat{H}_s(t), \hat{n}_{ij}]U(t,t_0), \qquad \hat{n}_{ij}(t_0) = \hat{n}_{ij}. \tag{5.55}$$

[23] Alternatively, we can start from the equation of motion for $\hat{a}_i$, Eq. (5.34), and multiply it by $\hat{a}_j^\dagger$ and do the same with the adjoint equation. However, the present approach avoids the ambiguity in the definition of the time dependent operators.

and evaluate the three commutators in Eq. (5.55), using again the relations (5.15), (5.16) and $[a_i^\dagger, a_j]_\mp = \mp\delta_{i,j}$,

$$
\begin{aligned}
[\hat{T}+\hat{V}, \hat{n}_{ij}] &= \left[\sum_{kl} h_{kl}(t) a_k^\dagger a_l, a_i^\dagger a_j\right] = && (5.56)\\
&= \sum_{kl} h_{kl}(t) \left\{ a_k^\dagger [a_l, a_i^\dagger a_j] + [a_k^\dagger, a_i^\dagger a_j] a_l \right\} = \\
&= \sum_{kl} h_{kl}(t) \left\{ \mp a_k^\dagger [a_i^\dagger, a_l]_\mp a_j - a_i^\dagger [a_j, a_k^\dagger]_\mp a_l \right\} = \\
&= \sum_{kl} h_{kl}(t) \left\{ a_k^\dagger a_j \delta_{il} - a_i^\dagger a_l \delta_{jk} \right\} = \\
&= \sum_{k} \left\{ h_{ki}(t)\, a_k^\dagger a_j - h_{jk}(t)\, a_i^\dagger a_k \right\} = && (5.57)\\
&= -\sum_{k} \left\{ \hat{n}_{ik}\, h^*_{kj}(t) - h^*_{ik}(t)\, \hat{n}_{kj} \right\} = \mathbf{h}^*(t)\hat{\mathbf{n}} - \hat{\mathbf{n}}\mathbf{h}^*(t), && (5.58)
\end{aligned}
$$

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

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

$$
\begin{aligned}
2[\hat{W}, a_i^\dagger a_j] &= \sum_{klmn} w_{klmn} \left\{ a_k^\dagger a_l^\dagger [a_n a_m, a_i^\dagger a_j] + [a_k^\dagger a_l^\dagger, a_i^\dagger a_j] a_n a_m \right\} = \\
&= \sum_{klmn} w_{klmn} \left\{ -a_k^\dagger a_l^\dagger [a_i^\dagger, a_n a_m] a_j - a_i^\dagger [a_j, a_k^\dagger a_l^\dagger] a_n a_m \right\} = \\
&= \sum_{klmn} w_{klmn} \left\{ a_k^\dagger a_l^\dagger \left(a_n \delta_{mi} \pm a_m \delta_{ni}\right) a_j - a_i^\dagger \left(a_l^\dagger \delta_{kj} \pm a_k^\dagger \delta_{lj} \right) a_n a_m \right\} \\
&= -2 \sum_{kln} \left\{ w_{jnkl} a_i^\dagger a_n^\dagger a_l a_k - w^*_{inkl} a_k^\dagger a_l^\dagger a_n a_j \right\}. && (5.59)
\end{aligned}
$$

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 $a_m a_n = \pm a_n a_m$ 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 (5.57) and (5.59) and combine them as follows

$$\begin{aligned} i\hbar\partial_t \hat{n}_{ij}(t) &= U^\dagger(t,t_0)a_i^\dagger \sum_k h_{jk}^{\text{eff}}(t)a_k U(t,t_0) - \\ &\quad - \sum_k U^\dagger(t,t_0)a_k^\dagger h_{ki}^{\text{eff}}(t)a_j U(t,t_0) \qquad (5.60) \\ h_{jk}^{\text{eff}} &= h_{jk}(t) + \hat{W}_{jk}^{\text{ind}}, \quad \hat{W}_{jk}^{\text{ind}} = \sum_{ln} w_{jnkl}a_n^\dagger a_l, \qquad (5.61) \end{aligned}$$

where we introduced the same *operators of the induced potential (Hartree mean field)* and effective single-particle potential as before, cf. Sec. 5.6. 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, $\langle\Psi|U(t_0,t)\dots U(t,t_0)|\Psi\rangle = \langle\Psi(t)|\dots|\Psi(t)\rangle$ 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 (CI, 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.*

5.8.2 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. (5.58). To this end we transform the

first four-operator product, using[24] $\hat{n}_{nl}a_k = a_k\hat{n}_{nl} - \delta_{kn}a_l$

$$\begin{aligned} a_i^\dagger a_n^\dagger a_l a_k &= \hat{n}_{ik}\hat{n}_{nl} - \delta_{nk}\hat{n}_{il} \\ &= \pm\left(\hat{n}_{il}\hat{n}_{nk} - \delta_{ln}\hat{n}_{ik}\right) \\ &= \frac{1}{2}\left(\hat{n}_{ik}\hat{n}_{nl} \pm \hat{n}_{il}\hat{n}_{nk}\right) - \frac{1}{2}\left(\delta_{nk}\hat{n}_{il} \pm \delta_{ln}\hat{n}_{ik}\right). \end{aligned} \tag{5.62}$$

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

$$a_k^\dagger a_l^\dagger a_n a_j = \frac{1}{2}\left(\hat{n}_{ln}\hat{n}_{kj} \pm \hat{n}_{kn}\hat{n}_{lj}\right) - \frac{1}{2}\left(\delta_{nk}\hat{n}_{lj} \pm \delta_{ln}\hat{n}_{kj}\right). \tag{5.63}$$

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. (5.62),

$$\begin{aligned} a_i^\dagger \sum_k \hat{W}_{jk}^{\mathrm{ind}} a_k &= \sum_{kln} \frac{w_{jnkl}}{2}\left\{\left(\hat{n}_{ik}\hat{n}_{nl} \pm \hat{n}_{il}\hat{n}_{nk}\right) - \left(\delta_{nk}\hat{n}_{il} \pm \delta_{ln}\hat{n}_{ik}\right)\right\}. \\ &= \sum_k \hat{n}_{ik} \sum_{ln} \frac{w^*_{kljn}}{2}\hat{n}_{nl} \pm \sum_l \hat{n}_{il} \sum_{kn} \frac{w^*_{kljn}}{2}\hat{n}_{nk} \\ &\quad - \sum_k \hat{n}_{ik} \sum_{ln} \delta_{ln} \frac{w^*_{lkjn} \pm w^*_{kljn}}{2} \\ &= \sum_k \hat{n}_{ik} \sum_{ln} \frac{w^*_{kljn} \pm w^*_{lkjn}}{2}\left\{\hat{n}_{nl} \mp \delta_{ln}\right\} \\ &= \mathbf{\hat{n}}\mathbf{\hat{U}}^{\pm}, \end{aligned}$$

$$\begin{aligned} \text{with the definition} \quad \hat{U}^{\pm}_{kj} &= \sum_{ln} \frac{w^*_{kljn} \pm w^*_{lkjn}}{2}\left\{\hat{n}_{nl} \mp \delta_{ln}\right\}, \\ &= \sum_{ln} \frac{w_{jnkl} \pm w_{jnlk}}{2}\left\{\hat{n}_{nl} \mp \delta_{ln}\right\}, \\ &= \frac{1}{2}\sum_{ln} w^{\pm}_{jnkl}\left\{\hat{n}_{nl} \mp \delta_{ln}\right\}, \end{aligned} \tag{5.64}$$

where, in the two terms containing $\hat{n}_{il}$, we exchanged the summation indices $l \leftrightarrow k$. In Eq. (5.64) we introduced the operator of the (anti-)symmetrized

[24] This follows directly from the commutator $[\hat{n}_{nl}, a_k] = -a_l\delta_{nk}$. 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 $w^{\pm}_{jnkl} = w_{jnkl} \pm w_{jnlk}$ that also appeared in the Slater-Condon rules in Chapter 4.

Similarly, the second term becomes

$$\begin{aligned}\sum_k a^\dagger_k \hat{W}^{\rm ind}_{ki} a_j &= \sum_{kln} \frac{w_{klin}}{2} \left\{ (\hat{n}_{ln}\hat{n}_{kj} \pm \hat{n}_{kn}\hat{n}_{lj}) - (\delta_{nk}\hat{n}_{lj} \pm \delta_{ln}\hat{n}_{kj}) \right\}. \\ &= \sum_k \sum_{ln} \frac{w_{klin} \pm w_{lkin}}{2} \left\{ \hat{n}_{ln} \mp \delta_{ln} \right\} \hat{n}_{kj}. \\ &= \hat{\mathbf{U}}^{\pm}\hat{\mathbf{n}}. \end{aligned} \tag{5.65}$$

One readily verifies that the potential $U^{\pm}$ is exactly the one introduced in Eq. (5.64).[25]

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

$$\boxed{i\hbar\partial_t \hat{\mathbf{n}}(t) = \left[\hat{\mathbf{n}}(t), \left\{ \mathbf{h}^*_{\rm H}(t) + \hat{\mathbf{U}}^{\pm}_{\rm H}(t) \right\}\right] = \left[\hat{\mathbf{n}}(t), \hat{\mathbf{h}}^{\pm}_{\rm H}(t)\right]} \tag{5.66}$$

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, $\hat{\mathbf{h}}^{\pm}_{\rm H}(t) = \mathbf{h}^*_{\rm H}(t) + \hat{\mathbf{U}}^{\pm}_{\rm H}(t)$.

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.

We underline that the present approach uses a particular ordering of the field operators: all operator products are expressed in terms of single-particle density matrix operators, $a^\dagger a$. This approach can be used to construct equations of motion for correlation functions of fluctuations (see Sec. 5.9.1 below). At the same time, this approach differs from standard density operator and Green functions approaches where a "normal" ordering is being used. Here all

[25] Starting from the definition (5.64) we readily transform to the expression (5.65) by, first, exchanging the summation indices n, l and then using, in the second term, the property of the matrix elements of the interaction, $w_{klni} = w_{lkin}$

$$\begin{aligned}\hat{U}^{\pm}_{ik} &= \sum_{ln} \frac{w_{knil} \pm w_{knli}}{2} \left\{ \hat{n}_{nl} \mp \delta_{ln} \right\} \\ &= \sum_{ln} \frac{w_{klin} \pm w_{klni}}{2} \left\{ \hat{n}_{ln} \mp \delta_{ln} \right\} = \sum_{ln} \frac{w_{klin} \pm w_{lkin}}{2} \left\{ \hat{n}_{ln} \mp \delta_{ln} \right\}. \end{aligned}$$

creators appear to the left of all annihilators (or vice versa) which gives rise to the definition of many-particle density operators or Green functions, see below.

5.9 Ensemble average of the Heisenberg equation. Fluctuations and correlations

Despite the formal simplicity of the dynamical equation (5.66) which has the form of a Hartree-Fock equation, the operator nature of the entering field 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. (5.60), or using coherent states, cf. Sec. 5.5.

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. 5.9.2.

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 or correlation operators (BBGKY-hierarchy [Bon98]) and will be considered in Ch. 6.

D. Computation of statistical averages of field operator products taken at different times, e.g. $\hat{a}_i^\dagger(t)\hat{a}_j(t')$. This leads to the theory of nonequilibrium Green functions (NEGF) and will be discussed in Chapter 8. In the equal-time limit the NEGF reduce to density matrices, and a direct connection to approach C can be established. This is done via the Generalized Kadanoff-Baym ansatz (GKBA) and gives rise to the G1–G2 scheme [SJB20], see Ch. 6 and Sec. 8.10.

5.9.1 Fluctuations and correlations (Approach B)

We now perform a statistical average of the operator equation (5.66). We will denote averages of operators by symbols without hat and fluctuations (deviations from the average) by the symbol δ, i.e.

$$\langle \hat{n}_{nm} \rangle \equiv n_{nm}. \tag{5.67}$$

$$\delta\hat{n}_{nm} \equiv \hat{n}_{nm} - n_{nm}. \tag{5.68}$$

Since averaging is a linear operation, its application to the operator equation of motion (5.66) 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 (5.66):

$$\boxed{i\hbar\partial_t \mathbf{n}(t) - \left[\mathbf{n}(t), \mathbf{h}^{\pm}_{\rm H}(t)\right] = \left\langle \left[\delta\hat{\mathbf{n}}(t), \delta\hat{\mathbf{U}}^{\pm}_{\rm H}(t)\right]\right\rangle \equiv \mathbf{I}^{\pm}(t)} \tag{5.69}$$

This equation is a very general quantum kinetic equation for the one-particle density matrix out of equilibrium. 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 procudures) 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 which is the only nontrivial part of the problem and which constitutes the main focus of quantum kinetic theory, density matrix theory and nonequilibrium Green functions. By definition, these are *correlation contributions* to the many-body dynamics that account for elastic collisions between particles, inelastic collisions associated with excitation or ionization and so on. We will see later that this collision integral involves the pair correlation operator, i.e. the correlated part of the two-particle density operator, e.g. [Bon98]. Here we see that these correlation terms have a *one to one correspondence with fluctuations of operator pairs*[26]. We have also introduced the short notation $\mathbf{I}^{\pm}$ for the collision integral.

The solution of this inhomogeneous (formally) linear equation, together with the initial condition, $\mathbf{n}(t_0) = \mathbf{n}_0$, is straightforward and given in terms of Hartree-Fock propagators $\mathcal{U}^{\rm HF}$ (these are two-dimensional matrices and everywhere matrix multiplication is implied)

$$\mathbf{n}(t) = \mathcal{U}^{\rm HF\dagger}(t,t_0)\,\mathbf{n}_0\,\mathcal{U}^{\rm HF}(t,t_0) + \mathbf{n}_I(t), \tag{5.70}$$

$$\mathbf{n}_I(t) = \frac{1}{i\hbar}\int_{t_0}^{t} d\bar{t}\;\mathcal{U}^{\rm HF\dagger}(t,\bar{t})\,\mathbf{I}^{\pm}(\bar{t})\,\mathcal{U}^{\rm HF}(t,\bar{t}), \tag{5.71}$$

$$i\hbar\partial_t \mathcal{U}^{\rm HF}(t,t_0) = \mathbf{h}^{\pm}_{\rm H}(t)\mathcal{U}^{\rm HF}(t,t_0), \qquad \mathcal{U}^{\rm HF}(t,t) = \mathbf{1}. \tag{5.72}$$

Equation of motion for the fluctuation operators: We now can make further progress in evaluating the collision term $\mathbf{I}^{\pm}$ by directly computing the

[26] This correspondence between correlations and fluctuations is well known from the kinetic theory of classical plasmas and was established by Kadomtsev, Klimontovich and others.

fluctuations $\delta\hat{\mathbf{n}}$ and, from them, also the fluctuation of the effective potential (5.64),

$$\delta\hat{U}^{\pm}_{kj} = \frac{1}{2}\sum_{ln} w^{\pm}_{jnkl}\,\delta\hat{n}_{nl}. \tag{5.73}$$

Indeed the equation of motion of $\delta\hat{\mathbf{n}}$ follows immediately by taking the difference of Eqs. (5.66) and (5.69) [we suppress the time arguments]

$$\begin{aligned} i\hbar\partial_t\left(\hat{\mathbf{n}}-\mathbf{n}\right) &= [\hat{\mathbf{n}},\mathbf{h}^*_{\rm H}]-[\mathbf{n},\mathbf{h}^*_{\rm H}]+ \\ &\quad +\left[\hat{\mathbf{n}},\hat{\mathbf{U}}^{\pm}_{\rm H}\right]-\left[\mathbf{n},\mathbf{U}^{\pm}_{\rm H}\right]-\left\langle\left[\delta\hat{\mathbf{n}},\delta\hat{\mathbf{U}}^{\pm}_{\rm H}\right]\right\rangle . \end{aligned}$$

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

$$\begin{aligned} i\hbar\partial_t\delta\hat{\mathbf{n}}-[\delta\hat{\mathbf{n}},\mathbf{h}^*_{\rm H}] &- \left[\delta\hat{\mathbf{n}},\mathbf{U}^{\pm}_{\rm H}\right]-\left[\mathbf{n},\delta\mathbf{U}^{\pm}_{\rm H}\right]= \\ &= \left[\delta\hat{\mathbf{n}},\delta\hat{\mathbf{U}}^{\pm}_{\rm H}\right]-\left\langle\left[\delta\hat{\mathbf{n}},\delta\hat{\mathbf{U}}^{\pm}_{\rm H}\right]\right\rangle\equiv\hat{\mathbf{J}}^{\pm}. \end{aligned} \tag{5.74}$$

The term on the right can be understood as a higher order collision integral or as the fluctuation of the correlator of the fluctuations, $\hat{\mathbf{J}}^{\pm}=\delta\left[\delta\hat{\mathbf{n}},\delta\hat{\mathbf{U}}^{\pm}_{\rm H}\right]$. Equation (5.74), together with the initial condition $\delta\hat{\mathbf{n}}(t_0)=\delta\hat{\mathbf{n}}_0$, can be solved formally like Eq. (5.69). But this analysis is deferred to later when we develop the quantum theory of fluctuations in Ch. ...

Here we only briefly outline possible ways how to proceed. One is to evaluate the r.h.s. of Eq. (5.74) by using again the equation of motion (5.74), multiply by $\delta\hat{\mathbf{U}}^{\pm}$ to derive the equation of motion for the product of fluctuations $\delta\hat{\mathbf{n}}\cdot\delta\hat{\mathbf{U}}^{\pm}$ and for their commutator. This can be expressed in terms of a correlation function of two-particle fluctuations, $\langle\delta\hat{\mathbf{n}}\cdot\delta\hat{\mathbf{n}}\rangle$. It is easy to see that this equation, on the r.h.s., will contain products of three operator fluctuations, $\langle\delta\hat{\mathbf{n}}\delta\hat{\mathbf{n}}\delta\hat{\mathbf{n}}\rangle$. 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. An alternative approach is to avoid the solution of a hierarchy of equations for the fluctuation operators but instead perform an ensemble average using stochastic methods. This is discussed in the next section. These ideas are discussed in detail in Ch. **??**[27].

5.9.2 Stochastic Mean Field Approximation

As an alternative, we can use the solution of Eq. (5.74) for $\delta\mathbf{n}(t)$, to compute the commutator $[\delta\hat{\mathbf{n}}(t)\delta\hat{\mathbf{U}}^{\rm ind}(t)]$, for a given initial condition $\delta\mathbf{n}^{(\alpha)}_0$. This yields

[27] This idea was implemented by Erik Schroedter in his bachelor thesis in 2020 and, subsequently in Refs. [SJB22, SWJB23, SB24a].

a single random realization of the collision integral $\mathbf{I}^{\pm(\alpha)}$ in Eq. (5.69). Repeating this for a representative set of initial conditions we can compute the expectation value by averaging over an ensemble of initial conditions,

$$\mathbf{I}^{\pm}(t) = \left\langle \left[\delta\hat{\mathbf{n}}(t), \delta\hat{\mathbf{U}}^{\pm}(t)\right] \right\rangle = \lim_{M\to\infty} \frac{1}{M} \sum_{\alpha=1}^{M} \left[\delta\mathbf{n}^{(\alpha)}(t), \delta\mathbf{U}^{\pm(\alpha)}(t)\right] , \qquad (5.75)$$

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

With this, the r.h.s. of Eq. (5.69) 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 $\hat{\mathbf{J}}^{\pm}$. A very simple and successful approach has recently been proposed by Ayik and co-workers [Ayi08, Lac13].

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 intergral $\mathbf{I}^{\pm}$ in Eq. (5.69) by a local function according to $\mathbf{I}^{\pm}(t) \to \mathbf{I}^{\pm}(t_0)\delta(t-t_0)$. This means only the initial fluctuations are taken into account. With this the solution for the density matrix, Eq. (5.71) becomes

$$\mathbf{n}_I(t) = \frac{1}{i\hbar}\, \mathcal{U}^{\mathrm{HF}\dagger}(t,t_0)\, \mathbf{I}^{\pm}(t_0)\, \mathcal{U}^{\mathrm{HF}}(t,t_0),$$

and the total solution for the density matrix is given by

$$\mathbf{n}(t) = \mathcal{U}^{\mathrm{HF}\dagger}(t,t_0) \left\{ \mathbf{n}_0 + \frac{1}{i\hbar} \left\langle \left[\delta\hat{\mathbf{n}}(t_0), \delta\hat{\mathbf{U}}^{\pm}_{\mathrm{H}}(t_0)\right] \right\rangle \right\} \mathcal{U}^{\mathrm{HF}}(t,t_0).$$

This means that the evolution of the density matrix $\mathbf{n}(t)$ is given by a pure Hartree-Fock dynamics. However, the evolution does not start from the initial value of the density matrix, $\mathbf{n}(t_0)$, but from a value that is shifted by the second term in the parantheses. If we forget for a moment the angular brackets we would have random realizations of initial values. Ayik had the idea [Ayi08] to replace the complicated commutator by a semiclassical ensemble of initial density fluctuations with given mean and variance such that the term in parantheses becomes $\mathbf{n}_0 + \Delta\mathbf{n}_0^{(\alpha)}$, for a given realization (α). The corresponding dynamics, starting from this initial state is given by

$$\hat{\mathbf{n}}^{(\alpha)}(t) = \mathcal{U}^{\mathrm{HF}\dagger}_{(\alpha)}(t,t_0) \left\{ \mathbf{n}_0 + \Delta\mathbf{n}_0^{(\alpha)} \right\} \mathcal{U}^{\mathrm{HF}}_{(\alpha)}(t,t_0),$$

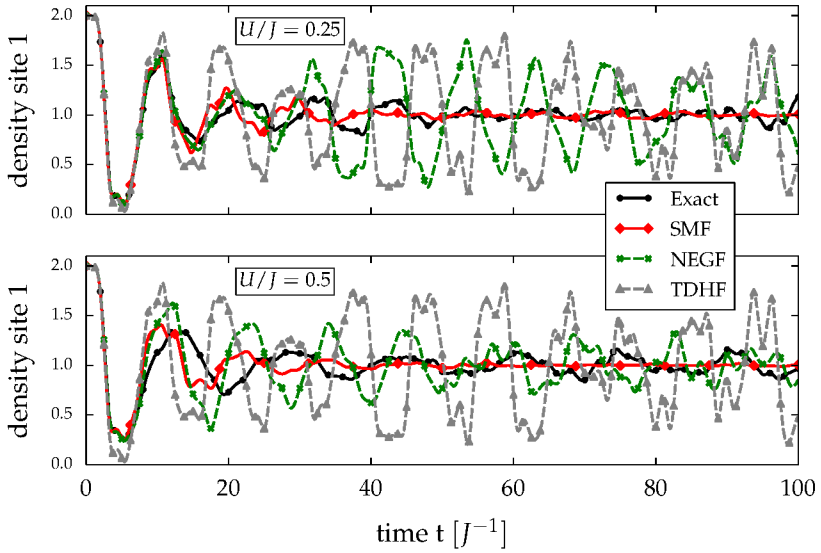

Abbildung 5.2: Time evolution of a Hubbard cluster with $N = N_s = 8$ sites following a confinement quench: sites 1–4 are initially doubly occupied and the others are empty. Top: weak coupling, $U = 0.25J$, bottom: moderate coupling, $U = 0.5J$. SMF results are compared to exact diagonalization, time-dependent HF and NEG results with second order Born selfenergies. From Ref. [LHHB14].

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

$$\mathbf{n}(t) = \lim_{M\to\infty} \frac{1}{M} \sum_{\alpha=1}^{M} \hat{\mathbf{n}}^{(\alpha)}(t). \tag{5.76}$$

Since only mean field trajectories are involved, and the result is obtained from a stochastic sampling over realizations, this approach has been called *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 fluctations 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 are of the same accuracy as NEGF results using selfenergies in second order Born approximation [LHHB14]. An example is shown in Fig. 5.2 for the dynamics of a small Hubbard cluster following a strong perturbation of the system by a confinement quench. The figure also shows the problems of the method: the accuracy quickly fades with increasing time. Furthermore, the accuracy is good for very weak coupling, U/J, but decreases with increasing U.

Concluding this section we note that a systematic quantum fluctuations approach has been recently developed by Schroedter et al. in Refs. [SJB22, SWJB23, SB24b, SB24a]. It starts from the time diagonal limit of the single-particle Green function and then derives equations of motion for the fluctuations of field operator products. More details will be presented in Ch. **??**.

5.10 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 ρ_N. Then we can compute averages, $\langle \dots \rangle_{\rho_N} = \mathrm{Tr} \dots \rho_N$,

$$\langle \hat{\psi}(\mathbf{r}, \sigma, t) \rangle_{\rho_N} = \psi(\mathbf{r}, \sigma, t) \tag{5.77}$$

$$\langle \hat{\psi}^\dagger(\mathbf{r}, \sigma, t) \rangle_{\rho_N} = \psi^*(\mathbf{r}, \sigma, t), \tag{5.78}$$

which are already regular functions of coordinate, spin and time. Similarly, in an arbitrary basis the expectation value of the second quantization operators become,

$$\langle \hat{a}_i(t) \rangle_{\rho_N} = a_i(t) \tag{5.79}$$

$$\langle \hat{a}_i^\dagger(t) \rangle_{\rho_N} = a_i^*(t), \tag{5.80}$$

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.

5.10.1 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,

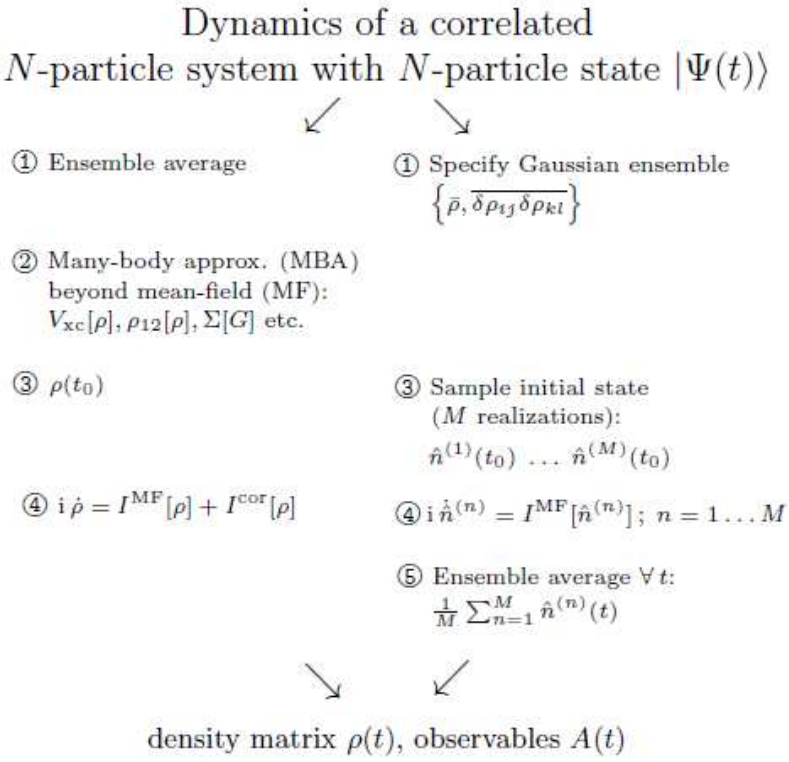

Abbildung 5.3: Schematic comparison of the concepts of standard many-body theories, such as TD-DFT, reduced density matrices and NEGF (left column) with stochastic mean field (right column. From Ref. [LHHB14].

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. We already briefly discussed this problem in Sec. 5.4 and now extend the analysis a bit further.

In fact, replacing the field operators by their mean values, i.e. by wave functions transforms Eq. (5.23) into a nonlinear Schrödinger equation

$$i\hbar\partial_t\psi(x,t) = \left\{-\frac{\hbar^2}{2m}\nabla^2 + v(r) + U^{\rm ind}(x,t)\right\}\psi(x,t)\,, \tag{5.81}$$
$$U^{\rm ind}(x,t) = \int dx''\, w(\mathbf{r},\mathbf{r}'')\psi^*(x'',t)\psi(x'',t).$$

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

$$i\hbar\partial_t\psi(x,t) = \left\{-\frac{\hbar^2}{2m}\nabla^2 + v(r) + g|\psi(x,t)|^2\right\}\psi(x,t)\,, \tag{5.82}$$

which has the name Gross-Pitaevskii equation that was first derived in 1961[28] The wave function is normalized to the total particle number, $\int d^3r|\psi|^2(r) = N$ and is also a reasonable order parameter, counting the number of particles in the ground state (condensate). This system has the total energy

$$W[\psi] = \int d^3r\left\{\frac{\hbar^2}{2m}[\nabla\psi]^2 + v(r)|\psi|^2 + g|\psi|^4\right\}\,, \tag{5.83}$$

and equation (5.81) can be derived by minimizing the energy (5.83) with respect to ψ^* 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 plane wave, $\psi(\mathbf{r}) = n^{-1/2}e^{i\mathbf{kr}}$, with $n = N/V$), and obtain the dispersion relation

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

[28]E. P. Gross, *Structure of a quantized vortex in boson systems*, Il Nuovo Cimento, **20** (1961) 454–457, *Hydrodynamics of a superfluid condensate*, J. Math. Phys. **4**, (1963) 195–207; L.P. Pitaevskii: *Vortex Lines in an Imperfect Bose Gas*, Soviet Physics JETP, **13**, (1961) 451–454.

which has a gap at zero momentum. This violates the Hugenholtz-Pines theorem (for repulsive interaction)[29]. 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 plane 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

$$\psi_0 = n^{1/2} e^{-\frac{i}{\hbar}\mu t} \tag{5.84}$$

$$\delta\psi = e^{-\frac{i}{\hbar}\mu t}\left\{u(\mathbf{r})e^{-i\omega t} + v^*(\mathbf{r})e^{i\omega t}\right\} \tag{5.85}$$

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

$$\begin{aligned}\left(-\frac{\hbar^2}{2m}\nabla^2 + v + 2gn - \hbar\mu - \hbar\omega\right)u - gnv = 0\\ \left(-\frac{\hbar^2}{2m}\nabla^2 + v + 2gn - \hbar\mu + \hbar\omega\right)v - gnu = 0\end{aligned} \tag{5.86}$$

Consdering again the homogeneous case, i.e. v =const, and assuming plane 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

$$\epsilon_k = v_s \cdot \hbar k, \quad v_s = \left(\frac{ng}{m}\right)^{1/2}. \tag{5.87}$$

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

[29]N. M. Hugenholtz; D. Pines. *Ground-state energy and excitation spectrum of a system of interacting bosons*, Physical Review. **116** (3): 489–506 (1959)

so-called roton – minimum that corresponds to different kind of excitations: rotons. This is in good agreement with the experiments with liquid helium and it is also reproduced by numerically exact quantum Monte Carlo simulations [A. Filinov, M. Bonitz, Phys. Rev. A **86**, 043628 (2012)].

An interesting property of cold atomic gases and fluids in an optical trap is that g can be positive (repulsive interaction) or negative which drastically changes the dispersion relation. Another striking feature is that the value of g and even its sign can be tuned by an external magnetic field (Feshbach resonance). Finally, there are qualitative differences between bosons (such as ^{4}He) and fermions (such as ^{3}He). In the latter case, pairing is observed that also leads to superfluidity and large scale vortex formation. These vortices can even crystallize, forming a lattice (Abrikosov lattice).

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

5.10.2 Fermions. Time-dependent expectation values

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,

$$\langle \hat{a}_i^\dagger(t)\hat{a}_j(t)\rangle_{\rho_N} \;=\; n_{ij}(t). \tag{5.88}$$

Here, the expectation value is computed with the density operator of the full system, i.e. the quantum generalization of the N-particle probability that will be discussed below.

Equation (5.88) is a special case of a more general class of functions, the reduced s-particle density matrices (RDM). These functions are the matrix representations of the reduced density operators (RDO) of density operator theory. The relation between these quantities and the second quantization operators is explored in chapter 6.

(Anti-)symmetrized expectation values. Consider an arbitrary s-particle operator, $\hat{B}_s$. To compute its expectation value we transform the operator $\hat{B}_s$ into second quantization representation, cf. Eq. (3.55),

$$\hat{B}_s \;=\; \frac{1}{s!}\sum_{i_1\ldots i_s=1}^{\infty}\sum_{k_1\ldots k_s=1}^{\infty}\langle k_1\ldots k_s|\hat{b}_{1\ldots s}|i_1\ldots i_s\rangle a_{k_1}^\dagger\ldots a_{k_s}^\dagger a_{i_s}\ldots a_{i_1},$$

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 ρ_N (this is denoted by $\langle \dots \rangle_{\rho_N}$), taking into account that the matrix element of $\hat{b}$ is a regular c-function,

$$\langle \hat{B}_s \rangle^{\pm}_{\rho_N} = \frac{1}{s!} \sum_{i_1 \dots i_s=1}^{\infty} \sum_{k_1 \dots k_s=1}^{\infty} \langle k_1 \dots k_s | \hat{b}_{1\dots s} | i_1 \dots i_s \rangle \langle a^{\dagger}_{k_1} \dots a^{\dagger}_{k_s} a_{i_s} \dots a_{i_1} \rangle_{\rho_N}. \tag{5.89}$$

Here we indicated that this is a correctly (anti-)symmetrized expression because of the properties of the field operators. Note that we did not assume any special properties on the basis states that are used to compute the matrix elements and onto which the field operators act. Since the operators guarantee the proper spin statistics we can use the simplest possible form of the basis set, such as products of single-particle orbitals[30], and express $|i_1 \dots i_s\rangle$ as a superposition of $|i_1\rangle \dots |i_s\rangle$.

As we discussed before, the expectation value of the field operator products plays the role of probability density. Here this is extended to the general $s-$particle case. Let us discuss some special cases explicitly.

i) The single-particle RDM is obtained from setting $s \to 1$:

$$\langle a^{\dagger}_i a_k \rangle_{\rho_N} \equiv n_{ik} \equiv \mathbf{n}, \tag{5.90}$$

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

$$\langle \psi^{\dagger}(\mathbf{r}, \sigma) \psi(\mathbf{r}'\sigma') \rangle_{\rho_N} \equiv n(x, x'). \tag{5.91}$$

For completeness, we give the normalization condition of the single-particle density matrix in coordinate representation

$$N = \sum_{\sigma} \int d\mathbf{r} \, \langle \psi^{\dagger}(\mathbf{r}, \sigma) \psi(\mathbf{r}\sigma) \rangle_{\rho_N}. \tag{5.92}$$

ii) The diagonal elements of the single-particle density operator (5.90) yield the ensemble averaged occupations of the single-particle orbitals $|i\rangle$,

$$\langle a^{\dagger}_i a_i \rangle_{\rho_N} \equiv n_{ii} = n_i \,, \tag{5.93}$$

[30]Note that it is not necessary to use (anti-)symmetrized states, because it is sufficient to perform (anti-)symmetrization once. This follows from the properties of $\Lambda^{\pm}$.

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

$$\langle \psi^\dagger(\mathbf{r},\sigma)\psi(\mathbf{r}\sigma)\rangle_{\rho_N} \equiv n_\sigma(\mathbf{r},\mathbf{r}) = n_\sigma(\mathbf{r}). \tag{5.94}$$

In contrast, the off-diagonal elements of expression (5.90) describe the statistical probability of transitions between orbital $|k\rangle$ and $|i\rangle$. Similarly, the off-diagonal elements of the coordinate-space expression (5.91) are related to the probability of a particle undergoing a transition from spin orbital $|\mathbf{r}'\sigma'\rangle$ to $|\mathbf{r}\sigma\rangle$.

iii) The second important case is the two-particle RDM,

$$\langle a_{i_1}^\dagger a_{i_2}^\dagger a_{k_2} a_{k_1}\rangle_{\rho_N} \equiv n^{(2)}_{i_1,i_2;k_1,k_2} \equiv \mathbf{n}^{(2)}, \tag{5.95}$$

whereas its coordinate representation is,

$$\langle \psi^\dagger(\mathbf{r}_1,\sigma_1)\psi^\dagger(\mathbf{r}_2,\sigma_2)\psi(\mathbf{r}_2'\sigma_2')\psi(\mathbf{r}_1'\sigma_1')\rangle_{\rho_N} \equiv n^{(2)}(x_1,x_2;x_1',x_2'). \tag{5.96}$$

The two-particle density matrix is normalized according to

$$\mathrm{Tr}_{12}\,\mathbf{n}^{(2)} = \sum_{i_1 i_2=1}^{\infty} \langle a_{i_1}^\dagger a_{i_2}^\dagger a_{i_2} a_{i_1}\rangle_{\rho_N} = N(N-1).$$

which we will derive in Ch. 6.

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

$$a_i \to a_{Hi}(t) \equiv U^\dagger(t,t_0) a_i U(t,t_0),$$
$$\psi(x) \to \psi_H(x,t) \equiv U^\dagger(t,t_0)\psi(x)U(t,t_0),$$

and so on. This will give rise to the time-dependent densities $n_i(t)$ and $n_\sigma(\mathbf{r},t)$ etc. Thereby, the underlying dynamics of the Heisenberg operators were computed above: the field operators obey Eqs. (5.23) and (5.27) and the general annihilation operator obeys Eq. (5.34). Thereby the basis states are not changed, they remain time-independent.

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 can be derived from the equation of motion of the N-particle density operator ρ_N – the von Neumann equation which leads to the theory of reduced density operators. The equations of motion is given by the BBGKY-hierarchy. This will be discussed in detail in chapter 6. There we also establish the connection between the two approaches.

5.11 Problems to Chapter 5

Problem 5.1 Derive the equation

$$i\partial_t \hat{\psi}_H(x,t) = -U^\dagger(t,t_0)[\hat{H},\hat{\psi}(x)]U(t,t_0). \tag{5.97}$$

Problem 5.2 Prove the identity (5.16): $[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}]_\mp \pm [\hat{A},\hat{C}]_\mp \hat{B}$

Problem 5.3 Discuss the derivation of Eq. (5.23) for the case of a time-dependent hamiltonian. Consider a time-dependent single-particle potential, $v(\mathbf{r},t)$.

Problem 5.4 Derive the general equation of motion (5.34) 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. (5.66)