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

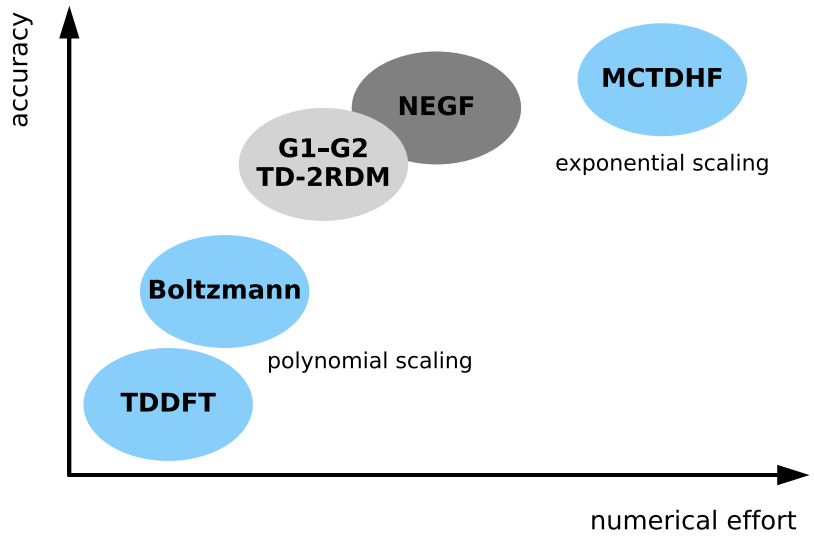

Abbildung 5.1: Qualitative overview of different many-body methods: comparison of accuracy versus numerical effort (computing time). MCTDHF represents wave function-based methods; TDDFT: time-dependent density functional theory; Boltzmann: Markovian kinetic equations, NEGF: Nonequilibrium Green functions; 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