Chapter 2
Theoretical Concepts and Numerical Methods

Being ignorant is not so much a shame, as being unwilling to learn.

Benjamin Franklin

The scope of this chapter is to give an overview of the various methods available to tackle the problem of solving the TDSE for a system of many bosons. In the rich variety of literature on this problem, References [1, 2] provide a good starting point. Here, special attention is devoted to the motivation and illustration of the mean-field methods and their multiconfigurational generalizations, because these are the methods within which most of the numerical results in the present study have been obtained. To give a self-contained picture, it is a good approach to review the basics of the second quantized formulation of the quantum mechanics of bosons, as well as some of the theoretical concepts used in the field. The approximations considered here fall into two different categories: the first set relies on making assumptions solely on the ansatzes and intends to solve the *full many-body* Hamiltonian (the Gross–Pitaevskii theory, best mean-field theory, and, MCTDHB). The second set relies on making assumptions on the physical situation and constructing model Hamiltonians and possibly also ansatzes for the wave functions (such as the Bose–Hubbard Hamiltonian (BHH), and the discrete non-linear Schrödinger equation (DNLS)). All these approximations allow for an analytical description only in very rare and special cases or under additional assumptions—it is therefore inevitable to construct methods to solve them numerically in order to avoid the necessity of further idealizations. The above points are discussed in this chapter.

2.1 The Schrödinger Equation from a Many-Body Perspective

The many-body Schrödinger equation reads:

$$\hat{H}(\vec{r}_1, ..., \vec{r}_N, t)\Psi(\vec{r}_1, ..., \vec{r}_N, t) = i\,\partial_t \Psi(\vec{r}_1, ..., \vec{r}_N, t). \tag{2.1}$$

A. U. J. Lode, *Tunneling Dynamics in Open Ultracold Bosonic Systems*,
Springer Theses, DOI: 10.1007/978-3-319-07085-8_2,

Here, both, $\hat{H}$ and the wave function Ψ depend on the positions of the N particles. In many cases, the Hamiltonian $\hat{H}$ is an Hermitian operator in the N-particle Hilbert space. For N identical bosons, both $\hat{H}$ and Ψ are symmetric when interchanging any two of the coordinates in Eq. (2.1). Hereafter, a Hamiltonian with a single particle potential for each particle and two-body interactions for every pair of particles is considered,

$$\begin{aligned}\hat{H} &= \sum_{i=1}^{N} \hat{h}(\vec{r}_i) + \sum_{i<j}^{j=N} \hat{W}(\vec{r}_j, \vec{r}_i, t),\\ \hat{h}(\vec{r}) &= \hat{T}(\vec{r}) + V(\vec{r}, t),\\ \hat{T}(\vec{r}) &= -\frac{1}{2}\partial_{\vec{r}}^2,\end{aligned} \tag{2.2}$$

unless otherwise specified. Here $\hat{W}$ is the two-body interaction, V is the one-body potential, and $\hat{T}$ is the usual kinetic energy in dimensionless units with $\hbar = m = 1$. Both, $\hat{W}$ and V, can be time-dependent but for most of the problems they will be considered as time-independent. For ultracold bosons it is usually assumed that the two-body physics are well-described by s-wave scattering. Ultracold temperatures imply very low kinetic energies. Hence, only the s-wave is contributing to the partial wave expansion of the scattering processes. In this case:

$$\hat{W}(\vec{r}_i, \vec{r}_j) = \lambda_0 \delta(\vec{r}_i - \vec{r}_j), \tag{2.3}$$

where λ_0 relates to the s-wave scattering length [3, 4]. Already from Eqs. (2.1), and (2.2) it is obvious that this problem becomes high-dimensional for several particles $N > 1$. It is hence difficult to solve and approximations are a must in the many particle case. A very efficient formalism for treating systems of N identical particles is called second quantization. It is explained below.

2.1.1 Second Quantization

The space of many-boson wave functions is the N-particle Hilbert space [5]. Conventionally, a complete and orthonormal set of single-particle states,[1] $\{|a_i\rangle, i = 1, ..., N\}$ is chosen to describe this N-particle Hilbert space. In this basis, a state of N distinguishable particles is the product

$$|a_1\rangle \cdots |a_N\rangle = |a_1, ..., a_N\rangle,$$

where the subscript identifies the particle. Straightforwardly, symmetrized products, the so-called permanents, can be formed by summing all possible permutations of this

[1] For didactical reasons, the time-dependencies are omitted in various places in this section.

expression. This summation is denoted as the action of the so-called symmetrization operator $\hat{\mathcal{S}}_+$. Hence, the permanent has the following properties:

$$\hat{\mathcal{S}}_+ \left[|a_1, ..., a_N\rangle\right] = \frac{1}{N!} \sum_{\{\vec{a}\}} |\vec{a}\rangle. \tag{2.4}$$

Here $\{\vec{a}\} = \{|a_\alpha, ..., a_\omega\rangle\}$ denotes all possible permutations of the indices $\alpha, ..., \omega$, and $\hat{\mathcal{S}}_+$ is the symmetrization operator for bosons. Permanents are fully symmetric, N-dimensional, orthogonal functions. If one assumes, that one of the single particle states $|a_i\rangle$ is occupied by n_i bosons, the symmetrization with $\hat{\mathcal{S}}_+$ will make it occur $n_i!$ times in the right hand side of Eq. (2.4). To obtain a proper normalization, one has to divide by the square root of $n_i!$ for all i. Hence, it follows for the permanent $|n_1, n_2, ...\rangle$:

$$|n_1, n_2, ...\rangle = \frac{1}{\sqrt{n_1! n_2! \cdots}} \hat{\mathcal{S}}_+ \left[|a_1, ..., a_N\rangle\right] \tag{2.5}$$

$$\langle n_1, n_2, ...|n_1', n_2', ...\rangle = \delta_{n_1,n_1'} \delta_{n_2,n_2'} \cdots \tag{2.6}$$

$$\sum_{n_1,n_2,...} |n_1, n_2, ...\rangle\langle n_1, n_2, ...| = \mathbf{1}. \tag{2.7}$$

Here, a constant particle number, i.e. $\sum_{i=1}^{\infty} n_i = N$ was assumed. By introducing the conventional creation and annihilation operators, respectively:

$$\hat{a}_i^\dagger |..., n_i, ...\rangle = \sqrt{n_i + 1} |..., n_i + 1, ...\rangle$$
$$\hat{a}_i |..., n_i, ...\rangle = \sqrt{n_i} |..., n_i - 1, ...\rangle,$$

it is possible to write a general single-permanent many-boson state as:

$$|n_1, n_2, ...\rangle = \frac{1}{n_1! n_2! \cdots} \left(\hat{a}_1^\dagger\right)^{n_1} \left(\hat{a}_2^\dagger\right)^{n_2} \cdots |vac\rangle, \tag{2.8}$$

where $|vac\rangle \equiv |0, 0, ..., 0\rangle$ denotes the vacuum state in which there is no particle present. The commutation relations of the operators $\hat{a}_j$ are of bosonic nature:

$$\left[\hat{a}_i, \hat{a}_j\right] = 0; \qquad \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0; \qquad \left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij}. \tag{2.9}$$

With this, the description of a general basis set of a many-boson system with constant particle number is complete. Section 2.1.1.1 covers how to transform the set of single-particle states building up the permanent given in Eq. (2.8).

2.1.1.1 Unitary Tranformations of Permanents

Usually, unitary transformations are specified on the boson creation and annihilation operators. This paragraph closely follows the considerations made in Refs. [6, 7]. An M-mode Fock state is considered,

$$|\vec{n}\rangle = |n_1, n_2, ..., n_M\rangle = \frac{1}{\sqrt{n_1! n_2! \cdots n_M!}} \left(\hat{a}_1^\dagger\right)^{n_1} \left(\hat{a}_2^\dagger\right)^{n_2} \cdots \left(\hat{a}_M^\dagger\right)^{n_M} |vac\rangle. \tag{2.10}$$

If the following (unitary) transformation to the $\{\hat{a}_k^\dagger; k = 1, ..., M\}$ is applied:

$$\hat{a}_i^\dagger \rightarrow \tilde{\hat{a}}_i^\dagger = \sum_{k=1}^{M} U_{ki} \hat{a}_k^\dagger. \tag{2.11}$$

In general, the matrix elements of U_{ki} are given by the overlap integrals of the new basis with the old single-particle basis functions $\{\phi_k, k = 1, ..., M\}$ and $\{\tilde{\phi}_i, i = 1, ..., M\}$. The action of $\mathbf{U}$ on a single permanent Fock state is then

$$\mathbf{U}|\vec{n}\rangle = \widetilde{|\vec{n}\rangle} \tag{2.12}$$

$$= \prod_{i=1}^{M} \left[(n_i!)^{-\frac{1}{2}} \left(\sum_{k_i=1}^{M} U_{k_i i} \hat{a}_{k_i}^\dagger \right)^{n_i} \right] |vac\rangle. \tag{2.13}$$

To process this result further, it lies at hand to use the multinomial expansion theorem for the multinomials $\left(\sum_{k_i=1}^{M} U_{k_i i} \hat{a}_{k_i}^\dagger\right)^{n_i}$. The resulting expression reads:

$$\widetilde{|\vec{n}\rangle} = \sum_{\substack{\{n_{ij}\} \\ \sum_{j=1}^{M} n_{ij} = n_i}} \frac{\left(\prod_{i=1}^{M} n_i!\right)^{\frac{1}{2}}}{\prod_{i,j=1}^{M} n_{ij}!} \prod_{\kappa=1}^{M} \left[\prod_{j_\kappa=1}^{M} \left(U_{j_\kappa \kappa} \hat{a}_{j_\kappa}^\dagger \right)^{n_{\kappa j_\kappa}} \right] |vac\rangle. \tag{2.14}$$

For convenience, an integer M-by-M matrix n_{ij} was introduced, whose elements fulfill the constraints that the sum of all its columns are equal to the occupations in the original Fock state $|\vec{n}\rangle$, i.e., $\sum_{j=1}^{M} n_{ij} = n_i$. Labeling the row sums of n_{ij} by m_j, i.e., $\sum_{i=1}^{M} n_{ij} = m_j$, one can rewrite the Fock vector on the right-hand side of the above expression as follows:

$$\widetilde{|\vec{n}\rangle} = \sum_{\substack{\{n_{ij}\} \\ \sum_{j=1}^{M} n_{ij} = n_i}} \frac{\left(\prod_{i=1}^{M} n_i!\right)^{\frac{1}{2}}}{\prod_{i,j=1}^{M} n_{ij}!} \left(\prod_{l=1}^{M} m_l! \right)^{\frac{1}{2}} \left(\prod_{k,l=1}^{M} U_{lk} \right)^{n_{kl}} |m_1, ..., m_M\rangle. \tag{2.15}$$

Now, the sum over all the products of the powers $U_{lk}^{n_{kl}}$, for all possible matrices n_{ij}, can be written as a permanent of a specific N-by-N matrix $\mathbf{U}\,[n_1, ..., n_M|m_1, ..., m_M]$. Its entries are taken from the transformation matrix U_{qs} as follows: the row index of U_{qs} appears n_q times and the column index appears m_s times. Furthermore, it is convenient to use the vector notation for the $m_i, i = 1, ..., M$, too, i.e., $|\vec{m}\rangle = |m_1, ..., m_M\rangle$. Consequently, $\mathbf{U}\,[n_1, ..., n_M|m_1, ..., m_M] = \mathbf{U}\left[\vec{n}|\vec{m}\right]$. Finally, denoting with $\mathrm{Per}(\cdot)$ the permanent of a matrix, one arrives at a compact expression,

$$\mathbf{U}|\vec{n}\rangle = \widetilde{|\vec{n}\rangle} = \sum_{\{\vec{m}\}} \prod_{i=1}^{M} \sqrt{m_i! n_i!}\ \ \mathrm{Per}\left(\mathbf{U}\left[\vec{n}|\vec{m}\right]\right)\ \ |\vec{m}\rangle, \tag{2.16}$$

where, the sum runs on all possible distributions of N particles in M orbitals, $\{\vec{m}\}$. It is noteworthy to mention that the unitary transform of a single configuration will have contributions to all possible configurations in the new basis set. It is, therefore, intimately related to the multiconfigurational expansion which will be used frequently later on. Moreover, Eq. (2.16) makes evident the connection between unitary transformations of many-body states of bosons and the computation of permanents and shows, thus, the big complexity of such a transformation [6, 7].

For the sake of completeness and its possible later use, the unitary transformation for multiconfigurational states, i.e., $|\Psi\rangle = \sum_{\{\vec{n}\}} C_{\vec{n}}|\vec{n}\rangle$ is specified here:

$$\mathbf{U}|\Psi\rangle = \mathbf{U}\sum_{\{\vec{n}\}} C_{\vec{n}}|\vec{n}\rangle = \sum_{\{\vec{n}\}} C_{\vec{n}}\mathbf{U}|\vec{n}\rangle. \tag{2.17}$$

The unitary transformation is applied to each configuration, respectively. Now, $\mathbf{U}|\vec{n}\rangle$ can be replaced by Eq. (2.16):

$$\mathbf{U}\sum_{\{\vec{n}\}} C_{\vec{n}}|\vec{n}\rangle = \sum_{\{\vec{n}\}} C_{\vec{n}} \sum_{\{\vec{m}\}} \prod_{i=1}^{M} \sqrt{m_i! n_i!}\ \ \mathrm{Per}\left(\mathbf{U}\left[\vec{n}|\vec{m}\right]\right)\ \ |\vec{m}\rangle. \tag{2.18}$$

A few remarks should be made here. The general unitary transform of a *single* permanent, as specified in Eq. (2.16), contributes to *all other possible* configurations, and it is hence already a quite complicated object. Note that the time-evolution operator $e^{-i\hat{H}t}$ of a given Hamiltonian is a unitary transformation. By writing down the unitary transform in Eq. (2.16) one, thus, arrives at the conclusion that *the only way* to properly account for the time-evolution of a system is by using a multiconfigurational wave function. To continue, it is indicated to define some useful operators and their expectation values.

2.1.1.2 One-Body Operators

In general, a sum of one-body operators $\hat{t}$ in second quantization takes the form

$$T = \sum_i \hat{t}_i = \sum_{i,j} t_{ij} \hat{a}_i^\dagger \hat{a}_j; \tag{2.19}$$

$$\text{where} \quad t_{ij} = \langle i|\hat{t}|j\rangle.$$

Often occurring examples of one-body operators are the occupation number operator,

$$\hat{n}_i = a_i^\dagger a_i; \qquad \hat{n}_i|..., n_i, ...\rangle = n_i|..., n_i, ...\rangle,$$

the particle number operator, $\hat{N} = \sum_i \hat{n}_i$, the kinetic energy $\hat{T}$, or the potential $\hat{V}$.

2.1.1.3 Two-Body Operators

In second quantization the sum of two-body operators $\hat{W} = \frac{1}{2}\sum_{a\neq b} w(\vec{r}_a, \vec{r}_b)$ takes the form

$$\hat{W} = \frac{1}{2} \sum_{i,j,k,l} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l w_{ijkl}; \tag{2.20}$$

$$\text{where} \quad w_{ijkl} = \langle i, j|\hat{w}|k, l\rangle = \int d\vec{r}_a \int d\vec{r}_b \phi_i^*(\vec{r}_a)\phi_j^*(\vec{r}_b) w(\vec{r}_a, \vec{r}_b)\phi_k(\vec{r}_a)\phi_l(\vec{r}_b).$$

An example of this is the two-body interaction occurring in Eq. (2.1) and its simplest form $\hat{w}(\vec{r}_i, \vec{r}_j) = \lambda_0 \delta(\vec{r}_i - \vec{r}_j)$.

2.1.1.4 Field Operators

It is often useful to have operators $\hat{\Psi}(\vec{r}, t)$ $[\hat{\Psi}^\dagger(\vec{r}, t)]$ which create [annihilate] a particle at position $\vec{r}$, i.e., in the state $|\vec{r}\rangle$. These are called field operators and read:

$$\hat{\Psi}^\dagger(\vec{r}) = \sum_i \phi_i^*(\vec{r})\hat{a}_i^\dagger; \qquad \hat{\Psi}(\vec{r}) = \sum_i \phi_i(\vec{r})\hat{a}_i. \tag{2.21}$$

To simplify the reading, the time-dependency of the field operators will be omitted where appropriate. They obey the usual bosonic commutation relations, just like the operators $\hat{a}_i, \hat{a}_j^\dagger$, and can be used to rewrite, among others, the operator for particle density $\hat{n}(\vec{r}) = \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i)$ as $\hat{n}(\vec{r}) = \hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r})$. The Hamiltonian in Eq. (2.2) expressed with field operators results in

$$\hat{H} = \int d\vec{r} \left(\frac{\hbar^2}{2} \nabla \hat{\Psi}^\dagger(\vec{r}) \nabla \hat{\Psi}(\vec{r}) + V(\vec{r}, t) \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}(\vec{r}) \right) + \frac{1}{2} \int d\vec{r} \int d\vec{r}' \hat{W}(\vec{r}, \vec{r}', t) \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}^\dagger(\vec{r}') \hat{\Psi}(\vec{r}) \hat{\Psi}(\vec{r}'). \tag{2.22}$$

For more details, the reader is referred to Ref. [2] and References therein. With this subsection all the necessary second quantization notations and concepts have been introduced. To continue, it is now appropriate to introduce the quantum many-body measures and analysis techniques which are important throughout this work.

2.1.2 Quantities of Interest

The scope of this subsection is to equip the reader with the analysis methods and viewpoint applied throughout this thesis and also place their development in a broader context. Since the prediction of BEC in 1924 (Refs. [8, 9]) some attention was devoted to the quantum mechanical condensation of bosonic particles in the lowest possible single-particle level. In 1956 Penrose and Onsager (Ref. [10]) were concerned with the presence of BEC in superfluid Helium and found a rigorous definition for condensation in quantum systems: a quantum system is condensed, when its reduced one-body density matrix (1-RDM) has a single macroscopic eigenvalue. In recent developments and experiments on BEC it turned out that *fragmentation* (see e.g. Refs. [11–19]) may occur. Fragmentation is defined as the situation where *several* eigenfunctions of the 1-RDM are macroscopically populated. The occurrence of fragmentation is ubiquitous especially in dynamical scenarios.The quantum mechanical description of condensation and fragmentation with the eigenvalues of the 1-RDM is intimately related to Glauber's quantum theory of optical coherence, starting in the 1960s (see Refs. [20–22]). It has been shown, that it is fully equivalent to have complete condensation and full coherence: when the single eigenvalue of the 1-RDM is N then all the normalized correlation functions are constant for all space and time [11, 22]. The systems considered in this thesis are initially confined and coherent systems that are decaying by tunneling through a barrier. Hence, it is instructive to introduce here also some measures which are especially adapted to quantify and assess the dynamics in these processes. The survival or nonescape probability of a decaying many-body quantum system can be defined as an integral either on the one-body density or on the full wave function.

The introduction and definition of the mentioned quantities are done in the following paragraphs. Further quantities, like the so-called particle loss and the principle of *local fragmentation* are deferred to the Appendices A and B (this is due to their complexity and because these quantities have yet to be implemented in the MCTDHB package [23]). Local fragmentation and the expectation values of particle loss operators can in principle be used to improve the detail of the investigation on the many-body mechanism of the tunneling process also locally.

2.1.2.1 Reduced Density Matrices

The p-particle reduced density matrix of a system (p-RDM), $\rho^{(p)}$, is defined by tracing $N-p$ coordinates from the N-particle density , $|\Psi\rangle\langle\Psi|$:

$$\begin{aligned}\rho^{(p)}(\vec{r}_1,...,\vec{r}_p|\vec{r}_1',...,\vec{r}_p';t) &= Tr_{\vec{r}_{p+1}\cdots\vec{r}_N}\left[|\Psi\rangle\langle\Psi|\right] \\ &= \frac{N!}{(N-p)!}\int d\vec{r}_{p+1}\cdots d\vec{r}_N\,\Psi(\vec{r}_1,...,\vec{r}_N,t) \\ &\quad \Psi^*(\vec{r}_1',...,\vec{r}_p',\vec{r}_{p+1},...,\vec{r}_N,t).\end{aligned} \tag{2.23}$$

The second line illustrates the action of the trace operation $Tr[\cdot]$. The 1-RDM plays a special role for the definition of condensation and fragmentation, as well as for the analysis of bosonic systems:

$$\rho^{(1)}(\vec{r}_1|\vec{r}_1';t) = \frac{N!}{(N-1)!}\int d\vec{r}_2\cdots d\vec{r}_N\,\Psi(\vec{r}_1,...,\vec{r}_N,t)\Psi^*(\vec{r}_1',\vec{r}_2,...,\vec{r}_N,t). \tag{2.24}$$

Similar to the above Eq. (2.24), the RDMs can also be obtained in momentum representation. When the starting point is a many-boson wave function specified in momentum space, the RDMs are simply obtained by replacing $\vec{r}$s with $\vec{k}$s in the above Equations (2.23) and (2.24). This holds also for the quantities computed from the RDMs, which are discussed in the next three paragraphs, i.e., the one-body density, natural occupations/orbitals, and normalized correlation functions.

2.1.2.2 The One-Body Density

Probably the most analyzed and the most intuitive quantity to look at in a quantum system is the one-body density. This is simply the diagonal of the 1-RDM of Eq. (2.24):

$$\begin{aligned}\rho(\vec{r},t) &\equiv \rho(\vec{r}_1=\vec{r}|\vec{r}_1'=\vec{r};t) \\ &= \frac{N!}{(N-1)!}\int d\vec{r}_2\cdots d\vec{r}_N\,\Psi(\vec{r},...,\vec{r}_N,t)\Psi^*(\vec{r},\vec{r}_2,...,\vec{r}_N,t).\end{aligned} \tag{2.25}$$

From a probabilistic point of view, it can be interpreted as the probability to find one particle at position $\vec{r}$, while the remaining are *somewhere in space*.

2.1.2.3 Natural Occupation Numbers and Natural Orbitals

One of the key measures to assess the degree of condensation and coherence or, complementarily, fragmentation and incoherence, is the diagonal representation of the 1-RDM in Eq. (2.24):

$$\rho^{(1)}(\vec{r}_1|\vec{r}_1';t) = \sum_{k,q=1}^{M} \rho_{kq}(t)\phi_k^*(\vec{r}_1',t)\phi_q(\vec{r}_1,t)$$
$$= \sum_{i=1}^{M} \rho_i^{(NO)}(t)\phi_i^{*(NO)}(\vec{r}_1',t)\phi_i^{(NO)}(\vec{r}_1,t). \tag{2.26}$$

In first equality the 1-RDM or any arbitrary function is expanded in a suitable basis set $\{\phi_i, i = 1, ..., M\}$. The $\rho_{kq}(t)$ are termed one-body matrix elements. In the second equality, one simply diagonalizes the $\rho_{kq}(t)$ matrix to achieve the simplest possible representation of the 1-RDM. The corresponding basis set, $\{\phi_i^{(NO)}, i = 1, ..., M\}$, is termed natural orbitals and their weights, $\rho_i^{(NO)}(t)$ are termed natural occupations. The $\{\rho_i^{(NO)}(t), i = 1, ..., M\}$ and $\{\phi_i^{(NO)}, i = 1, ..., M\}$ are the eigenvalues and eigenfunctions of the 1-RDM, respectively.

2.1.2.4 Normalized Correlation Functions

The normalized $p-$particle correlation function, $g^{(p)}$, is defined by the relation of the p-RDM, see Eq. (2.23), to the diagonals of the 1-RDM at the p different coordinates (see Refs. [20–22, 24]):

$$g^{(p)}(\vec{r}_1', ..., \vec{r}_p', \vec{r}_1, ..., \vec{r}_p; t) = \frac{\rho^{(p)}(\vec{r}_1, ..., \vec{r}_p|\vec{r}_1', ..., \vec{r}_p'; t)}{\sqrt{\prod_{i=1}^{p} \rho_1(\vec{r}_i|\vec{r}_i; t)\rho_1(\vec{r}_i'|\vec{r}_i'; t)}}. \tag{2.27}$$

Coherence of p-th order is achieved, if $g^{(p)} = 1$ holds. It is straightforward to see that this holds only if the p-RDM is a product of 1-RDMs [20]. This is the case if the 1-RDM can be represented by a single complex-valued function, which, in turn, means that the 1-RDM has a single eigenvalue. Therefore, this 1-RDM corresponds to a fully condensed system. From a probabilistic point of view $g^{(p)}$ measures the degree of statistical dependence of the simultaneous measurement of a set of p coordinates $\vec{r}_1, ..., \vec{r}_p$. If $g^{(p)} = 1$ then the measurement of the p coordinates is statistically independent and, consequently, the positions of the particles are not correlated. In this case it is said that the system is p-th order coherent. Full coherence can only be reached for $p = 1$. In the case of big particle numbers and $p \ll N$, the maximally achievable p-th order coherence is $1 + \mathcal{O}(N^{-1})$ [20, 24]. In the case of $g^{(p)} > 1$ the measurement of the p positions is correlated and in the case of $g^{(p)} < 1$ it is anticorrelated. In this respect, coherence comes with condensation and correlation/anticorrelation comes with fragmentation. Of course, the equivalent p-th order normalized correlation functions can be obtained also in momentum space from the p-RDMs in momentum space.

2.1.2.5 The Nonescape Probability

Tunneling processes occur in potentials that have regions separated by a barrier which is higher than the energy of the considered system. Usually, the initial state is localized on one side of this barrier with a probability almost equal to one. During its time evolution the system is eventually no longer localized on one side of the barrier. There are two ways to measure the survival or nonescape probability of the state in question. One can integrate either the one-body density or the full wave function in the part of space Ω where the state is initially localized. This integration defines the density-related and the wave function-related nonescape probabilities, $P_{not,\rho}(t)$ and $P_{not,\Psi}(t)$, respectively:

$$P_{not,\rho}(t) = \int_{\Omega} \rho(\vec{r}, t) d\vec{r}, \tag{2.28}$$

$$P_{not,\Psi}(t) = \int_{\Omega} \Psi^*(\vec{r}_1, ..., \vec{r}_N)\Psi(\vec{r}_1, ..., \vec{r}_N) d\vec{r}_1 \cdots d\vec{r}_N. \tag{2.29}$$

$P_{not,\rho}(t)$ measures the nonescape probability on the level of single particles, whereas $P_{not,\Psi}(t)$ measures the nonescape probability on the N-particle level. For non-interacting particles, the relation $P_{not,\rho}(t) \propto \sqrt[N]{P_{not,\Psi}(t)}$ is obvious. Additionally, it is reasonable to expect that $P_{not,\Psi}(t)$ is proportional to the autocorrelation function $c(t) = \langle \Psi(t = 0) | \Psi(t) \rangle$. This at least holds in the case of open systems, where $P_{not,\Psi}(t)$ and $c(t)$ are monotonously decreasing functions. One can formulate the nonescape probabilities discussed in this paragraph also in relation to the so-called particle loss operators (see Appendix A).

2.2 Theoretical Methods Employing the Full Many-Boson Hamiltonian

2.2.1 The Time-Dependent Variational Principle

The derivation of the TDGP, BMF, and of the MCTDHB is done by tackling the full many-boson Schrödinger equation with the time-dependent variational principle (TDVP) using different ansatzes. To motivate and place the following introduction to these methods on a solid ground, it is instructive to review briefly the TDVP as given in Ref. [25]. The basic idea is that the action functional $\mathcal{S}$ is minimized by the actual time-evolution taken by the system. Hence,

$$\delta \mathcal{S} \stackrel{!}{=} 0. \tag{2.30}$$

The action $\mathcal{S}$ is the time-integral of the Lagrangian of the considered system described by a set of so-called generalized coordinates. For a quantum mechanical (many-

body) system, having a constant particle number and and a Hermitian operator $i\partial_t$, the Lagrangian takes the form:

$$\mathcal{L}(\Psi(t), \Psi^*(t)) = \langle \Psi(t)|i\partial_t - \hat{H}|\Psi(t)\rangle. \tag{2.31}$$

Consequently, requiring the action to be stationary results in demanding the following expression to vanish:

$$\delta\mathcal{S}\left[\Psi(t), \Psi^*(t)\right] = \delta\int_{t_1}^{t_2} \mathcal{L}(\Psi(t), \Psi^*(t))dt \tag{2.32}$$

$$= \delta\int_{t_1}^{t_2} \langle \Psi(t)|i\partial_t - \hat{H}|\Psi\rangle \stackrel{!}{=} 0. \tag{2.33}$$

It is possible with this machinery to derive the equations of motion for any wisely or unwisely chosen *generalized coordinates* Ψ and Ψ^*. Kramer and Saraceno aptly described this issue in Ref. [25], on p. 6:

> "As is well-known, a variational principle is a blind and dumb procedure that always provides an answer, but it's accuracy depends crucially on the choice of the trial function."

In what follows, the quest for a more and more accurate variational description in terms of improvement of the ansatz for the trial function (wave function) Ψ for many-boson systems is presented and discussed.

2.2.2 The Time-Dependent Gross–Pitaevskii Equation

The main working tool for the description of the physics of ultracold bosons and BEC is the famous and successful time-dependent Gross–Pitaevskii equation (see Refs. [1, 26] and the References therein). Phenomenologically, it was the natural first step taken to understand the quantum physics of the TDSE, Eq. (2.1), with the many-boson Hamiltonian, Eq. (2.2), using the TDVP. The starting point to obtain the TDGP is to use a contact interparticle potential, $\hat{W}(\vec{r}, \vec{r}') = \lambda_0\delta(\vec{r} - \vec{r}')$. In order to cover the phenomenology of BEC, one assumes that all bosons occupy only one quantum mechanical single-particle state. This implies the truncation of the field operator, Eq. (2.21), to a single time-dependent mode function $\Phi(\vec{r}, t)$:

$$\hat{\Psi}(\vec{r}, t) \equiv \Phi(\vec{r}, t)\hat{b}(t). \tag{2.34}$$

From this, the (single) boson creation operator,

$$\hat{b}(t) = \int \Phi^*(\vec{r}, t)\hat{\Psi}(\vec{r}, t)d\vec{r}, \tag{2.35}$$

is defined. As a result, the GP many-boson wave function is a product state,

$$|\Psi(t)\rangle = \frac{1}{\sqrt{N!}}\left(\hat{b}^{\dagger}(t)\right)^{N}|vac\rangle = |N,0,...;t\rangle = \frac{1}{\sqrt{N!}}\prod_{i=1}^{N}\Phi(\vec{r}_i,t). \tag{2.36}$$

The expectation value of $i\,\partial_t - \hat{H}$ then reads

$$\langle\Psi|i\,\partial_t - \hat{H}|\Psi\rangle = -N\int d\vec{r}\{\Phi^*(\vec{r},t)\hat{h}\Phi(\vec{r},t) + \frac{(N-1)}{2}\lambda_0|\Phi(\vec{r},t)|^4\} + \langle\Psi|i\,\partial_t|\Psi\rangle \tag{2.37}$$

Plugging this ansatz, Eq. (2.37), in the action functional, Eq. (2.33), and requiring the latter to be stationary, results in the following Equation:

$$\frac{\delta\mathcal{S}\left[\Phi(\vec{r},t)\right]}{\delta\Phi^*(\vec{r},t)} = 0 \quad \rightarrow \quad i\,\partial_t\Phi(\vec{r},t) = \left[\hat{h} + \lambda_0(N-1)|\Phi(\vec{r},t)|^2\right]\Phi(\vec{r},t). \tag{2.38}$$

Equation (2.38) describes the dynamics of interacting bosons which are *completely condensed* into a single particle state and is referred to as the time-dependent Gross–Pitaevskii equation.

2.2.3 Best Mean-Field

The straightforward generalization of the GP ansatz for the many-boson wave function is simply to allow the bosons to occupy M, instead of one, single particle states. This permits the description of *single-configurational* condensed *or* fragmented quantum states, given that one uses an appropriate number M of single-particle states. Here, *single-configurational* means that a single permanent, cf. Eq. (2.8), is used in the description. This section will sketch the derivation of the equations of motion of the time-dependent multi-orbital mean-field or, in short, *best mean-field* (BMF) as given in [27]. Note that there is also a time-independent version of the best mean-field for condensates, which for brevity is not presented here (see Ref. [28]). The ansatz for the time-dependent best mean-field with M orbitals reads:

$$\Phi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N,t) = \hat{\mathcal{S}}\Big[\underbrace{(\phi_1(\vec{r}_1,t)\phi_1(\vec{r}_2,t)\cdots)}_{n_1\text{ times}}\underbrace{(\phi_2(\vec{r}_{n_1+1},t)\phi_2(\vec{r}_{n_1+2},t)\cdots)}_{n_2\text{ times}}\cdots$$
$$\underbrace{(\phi_M(\vec{r}_{N-n_M+1},t)\phi_M(\vec{r}_{N-n_M+2},t)\cdots)}_{n_M\text{ times}}\Big], \tag{2.39}$$

where $\hat{\mathcal{S}}$ is a symmetrization operator. In the second quantization formalism, the above Eq. (2.39) reads:

$$|\Phi\rangle = |n_1,n_2,...,n_M;t\rangle.$$

As in the previous derivation of the TDGP, the TDVP is used to obtain equations of motion (EOMs) for the variational parameters $\phi_1(\vec{r},t)$, ..., $\phi_M(\vec{r},t)$. Obviously, the TDGP is recovered in the case of $M=1$ in Eq. (2.39). The functional action is given as

$$S=\int dt\left[\langle\Phi|\hat{H}-i\partial_t|\Phi\rangle-\sum_{k=1,j=1}^{M}\mu_{kj}(t)\left[\langle\phi_k|\phi_j\rangle-\delta_{kj}\right]\right], \tag{2.40}$$

where μ_{kj} are Lagrange multipliers to ensure the orthonormality of the time-evolution of the orbitals ϕ_k and ϕ_j. For convenience, the time-dependencies will be omitted in the following where they are not explicitly needed. It is convenient to define:

$$\begin{aligned}
h_{kj} &= \int \phi_k^*(\vec{r})\hat{h}(\vec{r})\phi_j(\vec{r})d\vec{r},\\
(i\partial_t)_{kj} &= \int \phi_k^*(\vec{r})\,(i\partial_t)\,\phi_j(\vec{r})d\vec{r}\\
&= \int \phi_k^*(\vec{r})\dot{\phi}_j(\vec{r})d\vec{r},\\
W_{kjql} &= \int\int \phi_k^*(\vec{r})\phi_j^*(\vec{r}')W(\vec{r}-\vec{r}')\phi_q(\vec{r})\phi_l(\vec{r}')d\vec{r}d\vec{r}',\\
W_{kj[ql]} &= W_{kjql}+W_{kjlq},\\
\hat{J}_l(\vec{r}) &= \int \phi_l^*(\vec{r})W(\vec{r}-\vec{r}')\phi_l(\vec{r}')d\vec{r}',\\
\hat{K}_l(\vec{r}) &= \int \phi_l^*(\vec{r})W(\vec{r}-\vec{r}')\mathcal{P}_{\vec{r}\vec{r}'}\phi_l(\vec{r}')d\vec{r}',\\
\boldsymbol{P} &= \mathbf{1}-\sum_{i=1}^{M}|\phi_i\rangle\langle\phi_i|.
\end{aligned} \tag{2.41}$$

Here, $\mathcal{P}_{\vec{r}\vec{r}'}$ swaps $\vec{r}$ with $\vec{r}'$ in the expression on its right side. By demanding the action to be stationary when varying the parameters in the ansatz, $\{\frac{\delta S}{\delta\phi_j^*(\vec{r},t)}\stackrel{!}{=}0,\ j=1,...,M\}$ one gets (after the elimination of the Lagrange multipliers) the following EOMs for the BMF:

$$\boldsymbol{P}i|\dot{\phi}_k\rangle=\boldsymbol{P}\left[\hat{h}+\lambda_0(n_k-1)\hat{J}_k+\sum_{l\neq k}^{M}\lambda_0 n_l(\hat{J}_l+\hat{K}_l)\right]|\phi_k\rangle. \tag{2.42}$$

These EOMs are a coupled set of non-linear integro-differential equations. The details of their derivation, as well as illustrative numerical examples can be found in Refs. [14, 15, 27–29]. In physical situations that are fully described by a single configuration, i.e., one permanent, the BMF theory is a good approach. Note that any initial set of occupations, n_1, ..., n_M, will remain unchanged by the time-evolution

under Eq. (2.42). This means that the BMF theory lacks the capability of describing processes in which the many-boson system under consideration undergoes fragmentation or condensation, because the occupation numbers, $n_1, n_2, ..., n_M$, cannot change. The MCTDHB circumvents this flaw of the BMF and will be the topic of Sect. 2.2.4

2.2.4 The Multiconfigurational Time-Dependent Hartree Method for Bosons

The natural generalization of the BMF towards a better description of the full Hilbert space of the many-boson system is to consider not only a *single configuration* (see Eqs. (2.39), (2.8)) but, instead, *many configurations*, i.e., all possible configurations that can be formed from a set of M single-particle states. The method thus becomes *multiconfigurational* and, as the time-dependent configurations and derivation come from the Hartree method, its name is the multiconfigurational time-dependent Hartree method for bosons (MCTDHB). There is a wealth of multiconfigurational Hartree theories for mixtures of different species of bosons and fermions, see Refs. [30, 31], with particle conversion and up to three-body interactions. The following introduction considers and sketches only the single-species version as given in Ref. [32, 33] because this version will be amply used, benchmarked with analytical results, and compared with other methods in the field throughout the present work. It is instructive to start from the field operator expanded in the basis of a set of M orthonormal, time-dependent functions (orbitals), $\{\phi_k(\vec{r}, t), k = 1, ..., M\}$:

$$\begin{aligned} \hat{b}_k(t) &= \int \phi_k^*(\vec{r}, t)\hat{\Psi}(\vec{r})d\vec{r}; \qquad k = 1, ..., M, \\ \hat{\Psi}(\vec{r}) &= \sum_k^M \hat{b}_k(t)\phi_k^*(\vec{r}, t). \end{aligned} \tag{2.43}$$

This is the bosonic field operator. The *only* approximation introduced here, is the assumption that the set of M orbitals is sufficient to describe the Hilbert space occupied by the many-boson wave function. Using the $\hat{b}_k(t)$, their commutation relations, $\hat{b}_k(t)\hat{b}_j^\dagger(t) - \hat{b}_j^\dagger(t)\hat{b}_k = \delta_{kj}$, and the abbreviation $\vec{n} = (n_1, n_2, ..., n_M)$, one arrives at the ansatz for the variational derivation of the MCTDHB EOMs:

$$\begin{aligned} |\Psi(t)\rangle &= \sum_{\{\vec{n}\}} C_{\vec{n}}(t)|\vec{n}; t\rangle \\ &= \sum_{\{(n_1,...,n_M)\}} \frac{C_{(n_1,...,n_M)}(t)}{\sqrt{n_1! \cdots n_M!}} \left(\hat{b}_1^\dagger(t)\right)^{n_1} \cdots \left(\hat{b}_M^\dagger(t)\right)^{n_M} |vac\rangle. \end{aligned} \tag{2.44}$$

Here, $|vac\rangle$, stands for the vacuum state with no boson present and the sum runs over all $N_{conf} = \binom{N+M-1}{N}$ possible configurations, $\{(n_1, ..., n_M)\}$, of $N = \sum_{i=1}^{M} n_i$ particles occupying the M orbitals. Note that both, the coefficients $\{C_{\vec{n}}\}$ and the orbitals $\{\phi_k\}$, are *time-dependent* and both will be used as variational parameters for the following derivation of the equations of motion. Introducing Lagrange multipliers, $\mu_{kj}(t)$, ensuring the orthonormality of the orbitals (as in the BMF case, cf. Eq. (2.40)), the action functional takes the form:

$$S\left[\{C_{\vec{n}}(t)\}, \{\phi_k(\vec{r}, t)\}\right] = \int dt \left[\langle \Psi | \hat{H} - i\,\partial_t | \Psi \rangle - \sum_{k,j=1}^{M} \mu_{kj}(t) \left[\langle \phi_k | \phi_j \rangle - \delta_{kj} \right] \right]. \tag{2.45}$$

Now, one demands this action to be stationary when varying *all* the N_{conf} coefficients, i.e., $\frac{\delta S}{\delta C^*_{\vec{n}}(t)} \stackrel{!}{=} 0$ and when varying the M orbitals, i.e., $\frac{\delta S}{\delta \phi^*_k(\vec{r},t)} \stackrel{!}{=} 0$. The details of the derivation and how the elimination of the Lagrange multipliers results in the emergence of projectors, $\hat{\boldsymbol{P}}$, are given in Ref. [33]. The EOMs for the coefficients reads:

$$\boldsymbol{H}(t)\boldsymbol{C}(t) = i\,\partial_t \boldsymbol{C}(t); \qquad \boldsymbol{H}(t) = \{H_{\vec{n}\vec{n}'}(t)\} = \{\langle \vec{n}; t | \hat{H} | \vec{n}'; t \rangle\}. \tag{2.46}$$

Here $\boldsymbol{C}(t)$ collects the coefficients $\{C_{\vec{n}}(t)\}$ in a vector. On the other hand, the EOMs for the orbitals read:

$$\begin{aligned} i\,\partial_t |\phi_j\rangle &= \hat{\boldsymbol{P}} \left[\hat{h} |\phi_j\rangle + \sum_{k,s,q,l=1}^{M} \{\boldsymbol{\rho}(t)\}^{-1}_{jk} \rho_{ksql} \hat{W}_{sl} |\phi_q\rangle \right], \\ \hat{W}_{sl}(\vec{r}, t) &= \int \phi^*_s(\vec{r}', t) \hat{W}(\vec{r} - \vec{r}', t) \phi_l(\vec{r}', t) d\vec{r}', \\ \hat{\boldsymbol{P}} &= 1 - \sum_{i=1}^{M} |\phi_i\rangle\langle\phi_i|. \end{aligned} \tag{2.47}$$

Here $\{\boldsymbol{\rho}\}^{(-1)}$ is the inverse of the reduced one-body matrix elements, the ρ_{ksql} are the matrix elements of the reduced two-body density and the $\hat{W}_{sl}(\vec{r}, t)$ are referred to as *local time-dependent potentials*. The Eqs. (2.46), (2.47) are the core of the MCTDHB and their numerical solution is implemented in a Fortran program package, see Ref. [23], which will be described in Sect. 2.4. It is appropriate to note that the Hilbert space covered by the ansatz of the MCTDHB, Eq. (2.45), is N_{conf} times bigger than the one covered by the TDGP. Yet, one obtains back the TDGP from the MCTDHB for $M = 1$ in the above equations of motion. This could also be deduced already from the field operator, see Eq. (2.43). Extending beyond TDGP, fragmented states (up to M-fold) are described self-consistently by the MCTDHB. The dynamics of fragmentation and condensation processes, which go beyond the realm of the BMF, can be described by MCTDHB because the coefficients of the

permanents which assemble the many-boson wave function are time-dependent. A benchmark of the quality and convergence properties of the MCTDHB approximation is the topic of Chap. 3.

2.3 Theoretical Methods Employing Model Hamiltonians

2.3.1 Bose–Hubbard and Time-Evolved Block Decimation

One of the most frequently used models in the field of ultracold bosons is the so-called Bose–Hubbard (BH) model. To arrive at the BH model Hamiltonian (following Ref. [34]) one assumes a periodic potential, such as $V_0(\vec{x}) = \sum_{j=1}^{3} V_{j0} \sin kx_j$, a so-called optical lattice. Furthermore, one uses the zero-range pseudopotential of Eq. (2.3). Now, a deep potential (large coefficients V_{j0}) is assumed and the field operator $\hat{\Psi}(\vec{x})$ is expanded in a Wannier basis. The Wannier functions $w_k(\vec{x} - \vec{x}_i)$ are linear combinations of Bloch waves which are localized at certain lattice sites $\vec{x}_i$. The final assumption is, that the lattice is deep and the higher Wannier functions $k \geq 2$ do not contribute. The resulting field operator reads

$$\hat{\Psi}(\vec{x}) = \sum_i \hat{b}_i w(\vec{x} - \vec{x}_i). \tag{2.48}$$

The resulting so-called BHH reads:

$$\hat{H} = -J \sum_{\{i,j\}} \hat{b}_i^\dagger \hat{b}_j + \sum_i \epsilon_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1). \tag{2.49}$$

Here, the following abbreviations are used:

$$J = \int d\vec{x} w^*(\vec{x} - \vec{x}_i)\hat{h}(\vec{x})w(\vec{x} - \vec{x}_i); \tag{2.50}$$

$$U = \lambda_0 \int d\vec{x} |w(\vec{x})|^4; \tag{2.51}$$

$$\epsilon_i = \int d\vec{x} V_T(\vec{x}_i)|w(\vec{x} - \vec{x}_i)|^2. \tag{2.52}$$

Here, V_T is some additional external, slowly varying, potential leading to an energy shift, see Ref. [34]. To compute the time-evolution of the BHH an algorithm called time-evolving block decimation (TEBD) is frequently employed. TEBD works for quasi-one-dimensional systems only. Hence, the following discussion of the BHH and TEBD is restricted to one spatial dimension. TEBD relies on the idea, that one achieves a good approximation to a given pure quantum state $|\Psi\rangle$ by rewriting it

as $|\Psi\rangle = \sum_{\alpha=1}^{D} \lambda_\alpha^{[l]} |\Phi_\alpha^{[1\cdots l]}\rangle |\Phi_\alpha^{[(l+1)\cdots N]}\rangle$ and restricting D to some D_ϵ [35]. Here, $|\Phi_\alpha^{[1\cdots l]}\rangle$ and $\lambda_\alpha^{[l]}$ are obtained from a Schmidt decomposition of $|\Psi\rangle$ onto subspaces containing less than the total number of particles, $l < N$ and $l - N < N$. For any l, the entries of $\lambda^{[l]}$ are the decreasingly ordered Schmidt coefficients. The approximated state reads:

$$|\Psi\rangle = \left(\sum_{\alpha=1}^{D_\epsilon} |\lambda_\alpha^{[l]}|^2 \right)^{-\frac{1}{2}} \sum_{\alpha=1}^{D_\epsilon} \lambda_\alpha^{[l]} |\Phi_\alpha^{[1\cdots l]}\rangle |\Phi_\alpha^{[(l+1)\cdots N]}\rangle. \tag{2.53}$$

For further details see Refs. [35, 36] and References therein. For the BHH it is intuitively a good idea to make such an approximation, because there is only a direct nearest-neighbor interaction and it is a reasonable approximation to consider subsystems as uncorrelated, hence, $D_\epsilon \ll D$. This means, that the computation of the time-evolution of a state under the BHH to a quite good accuracy is cheap, depending on the D_ϵ chosen. The great achievements of these intuitive approximations, see Ref. [37] and References therein, have to be contrasted with the examples where they fail [11, 24, 38, 39]. This failure is mostly due to the incapability of the BH model to properly cover the physics of the considered system which involves higher bands or delocalized states. Such a comparison must rely on a many-body method, such as the MCTDHB, which is able to capture the rich physics beyond the BH model.

2.3.2 The Discrete Non-Linear Schrödinger Equation

In principle, the BH model is capable to describe a system of ultracold bosons which are *not* condensed. Yet, one can imagine, that in the mean-field limit it is feasible to describe the state of the system as a coherent product state. In this mean-field limit, the following assumptions are introduced:

$$N \to \infty; \qquad \frac{NU}{J} = const.; \qquad U \to 0.$$

One can derive the resulting discrete nonlinear Schrödinger equation by replacing the creation and annihilation operators $\hat{b}_i, \hat{b}_j^\dagger$ in the BHH, Eq. (2.49), by complex numbers, b_i, b_j^*. The time evolution of these numbers is then defined solely by their canonical equations of motion, cf. Ref. [40]. The result is the so-called discrete nonlinear Schrödinger equation (DNLS) which can be used to find the coherent dynamics within the BH model. It reads:

$$i\dot{b}_i = -J(b_{i+1} + b_{i-1}) + \frac{U\bar{n}}{2}|b_i|^2 b_i; \qquad \bar{n} = N/L. \tag{2.54}$$

Here $\bar{n} = N/L$ is the number of atoms per lattice site. The physical situation where this approximation to the BH model is applicable is deep optical lattices with a very weak interaction. Nevertheless, the authors of Ref. [41] benchmarked the BHH and the DNLS with each other on a tunneling problem with long-range correlations and delocalized states. It is instructive to perform a check on the validity of the predictions of this benchmark, by a comparison to numerically exact solutions of the same problem obtained with the MCTDHB method, see Chap. 4.

2.4 Numerical Methods

This section provides an overview of the numerical methods applied throughout this work. The focus is on introducing the concepts which are needed to achieve the numerical results presented in later chapters, as well as to give an overview of the current implementation and capabilities of the MCTDHB package [23].

2.4.1 The Multiconfigurational Time-Dependent Hartree for Bosons Software Package

The MCTDHB package is a collection of Fortran programs and Bash-scripts. The current organization of the code consists in two programs: the main program which performs the computation, and the analysis program to extract quantities of interest from the results of a computation.

2.4.1.1 Current Implementation

The current implementation of the MCTDHB package is mostly in FORTRAN 90/95. It has two main parts: a hybridly parallel one for solving the TDSE and one to analyze the many-body properties of the solutions. As discussed in Sect. 2.2.4, MCTDHB is simply a reformulation of the TDSE of many-boson systems into two sets of coupled partial differential equations. To solve the two sets, i.e., the coefficient EOMs and the orbital EOMs, numerical solvers for partial differential equations have been implemented. Namely, the coefficient EOMs are solved with a Krylov subspace method: the short iterative Lanczos (SIL) integrator. Various numerical integrators for the orbital EOMs are available: the 16th order Bullirsch–Stoer method, a Runge–Kutta method of 5th/8th order and an Adams–Bashforth–Moulton predictor–corrector integrator (ABM) of $7th$ order are the implicit methods available – they work well in the case that the orbital EOMs are not stiff. For the case of dominating non-linearity, i.e., stiff orbital EOMs, the so-called ZVODE integrator [42], an implementation of a Gear- type second order backwards differentiation formula (BDF) was chosen.

2.4.1.2 Integrators

The scope of this subsection is to introduce the integrators implemented in the current version of the MCTDHB package and provide the peculiarities of it as well as its specifications. The documentation of most of the integrators is available in the Heidelberg multiconfigurational time-dependent Hartree (MCTDH) package documentation and References therein, see Ref. [43]. The focus here is on the integrators either not provided in the MCTDH package, either the ones which rely on a different implementation, namely, the SIL, the ABM and the BDF. For the details on the other numerical integrators the reader is referred to Ref. [44] and the References therein.

2.4.1.3 The Short Iterative Lanczos

To build the Krylov basis which is needed for the SIL algorithm, one has to apply powers of the Hamiltonian $\hat{H}^k$ depending on the order $k+1$ of the method, to the state vector of the coefficients. The action of the Hamiltonian is computationally the most demanding part in the SIL algorithm and therefore the part which is parallelized. This evaluation can be extremely efficiently done according to the scheme described in Ref. [45]. As soon as the basis of the Krylov subspace is constructed, the problem of the computation of the time-evolution of the coefficient vector is reduced to the diagonalization of the SIL matrix, i.e., a $(k+1) \times (k+1)$ matrix, which is done with a LAPACK routine [46]. The advantage of the SIL algorithm is that it is generally very stable when the ground state or a propagation with high accuracy are desired. Yet, in the case of degeneracies or the computation of excited states more advanced numerical techniques are needed, such as the Arnoldi or Davidson methods, see Ref. [43].

2.4.1.4 The Adams–Bashforth–Moulton Predictor–Corrector Integrator

The ABM implementation in the MCTDHB package is in principle identical to the one in the MCTDH package [43], but it is parallelized using OpenMP. The ABM algorithm is a multistep method, which relies on a polynomial extrapolation of the solution of the partial differential equation tackled. The term "predictor-corrector" stands for the error control mechanism on which it relies: if the prediction of the next order is sufficiently close to the actual next order solution the integration step is accepted; it is otherwise rejected and the step size is adjusted dynamically. It turns out that the most time-consuming parts in the ABM algorithm are the evaluations of the right-hand side of the orbital EOMs and the various products of orbital vectors which have to be evaluated. The evaluation of the right-hand side of the orbital EOMs is done by a hybridly parallel scheme outlined in the following subsection. The evaluation of the products of orbital vectors is done in OpenMP parallelized loops inside the ABM routine. For large grids the evaluation time is greatly reduced

by this parallelization, while for small grids the execution time spent in the integrator is negligible.

2.4.1.5 The Gear-type Second Order Backwards Differentiation Formula

In the case of strong interparticle interactions, the set of orbital EOM becomes a stiff set of partial differential equations. For stiff equations the integration schemes mentioned and/or described above become inefficient or even unstable. It was proven that in the case of stiff differential equations an implicit integrator of second order relying on a backwards differentiation formula would globally minimize the introduced error, see Ref. [44]. The essential advantage of this kind of integrator lies in its superior stability which allows for bigger step-sizes as compared to other methods in the case of stiff differential equations. ZVODE from the ODEPACK package, see e.g. [42], is an implementation of the Gear-type second order backwards differentiation scheme and the needed changes for its use in the MCTDHB package were minor. Yet, for the cases of dynamics of strongly interacting bosons, see e.g. Ref. [47], it has proven to be essential.

2.4.1.6 Parallelization

In order to provide most of the numerical results presented in this thesis, the algorithm implemented in the MCTDHB package solving the coupled sets of EOM has to be efficient enough to provide a time-evolution in a reasonable time. The only way to achieve the desired efficiency is to parallelize the algorithm by distributing the computational tasks among several computers in a network. During the development of MCTDHB, all the available platforms were mostly homogeneous clusters, in which several identical computers with multi-core processors are connected by a network of the InfiniBand or Cray Gemini II standard. Hence, the current parallelization is adapted to such platforms. Further parallelization, like the usage of GPU-computing might be of relevance for future developments, but is not part of the current package. The algorithm basically deals with two different sets of equations: a linear one for the coefficients and a non-linear one for the orbitals. Depending on the chosen setup, the overall computational effort can be dominated by the former or the latter, or it might be balanced. For each of the two sets, the solutions of the EOMs is done by integrators which need possibly many evaluations of the complicated right-hand side of the EOMs, Eqs. (2.46), (2.47). The major part of the execution time is hence spent in the evaluation of these right-hand sides. Consequently, the strategy was to parallelize this evaluation, as shown in Fig. 2.1.

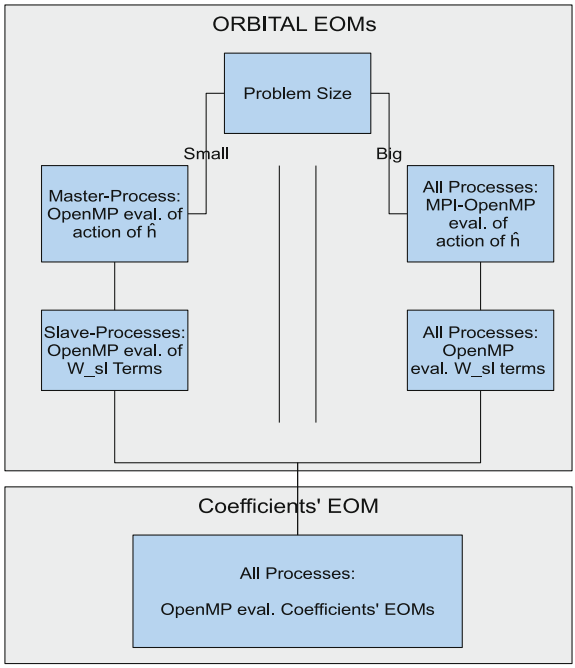

Fig. 2.1 Scheme of the Parallelization of the MCTDHB Main Program

2.4.1.7 The Parallelization of the Orbital EOMs

The parallelization scheme for the orbital EOMs was done by means of a hybrid OpenMP-MPI parallel algorithm and is problem-size adaptive. In the case of rather small problems, i.e., problems with a primitive grid size of less than 1024 functions, the communication time overhead of an MPI-parallel calculation of the one-body Hamiltonian terms was dominating. Hence, it was beneficial not to communicate the needed data and use only OpenMP threads to evaluate the one-body Hamiltonian terms on the master node. The more time consuming evaluation of the two-body Hamiltonian terms is done by distributing the W_{kqsl} terms equally among the slave processes, communicate to them the needed orbital vectors and evaluate the integrals – in principle sums of point wise products of vectors – using OpenMP threads. In the case of larger problems, i.e., problems with a primitive grid size of equal to or more than 1024 functions, the evaluation of the one-body and the two-body Hamiltonian terms is distributed among all MPI-processes and done with OpenMP threads. It is appropriate here to make a remark on the scaling behavior. The number of one-body Hamiltonian terms scales with $\sim M^2$ and the number of two-body terms with $\sim M^4$. Interestingly, so far, no case occurred where the communication overhead actually dominated the benefits of the parallelization scheme implemented. Hence, the more orbitals were taken, the closer to linear the speedup was for both, large and small problem sets. In the current implementation, all the

orbitals are communicated to all the MPI processes. In order to achieve the close-to-linear speedup for problems with fewer orbitals as well as to have it for problems with a *very* large number of orbitals, it would be beneficial to further optimize this communication. This optimization is achievable by determining in the initialization phase of the program which orbitals are needed for the computational tasks assigned to a particular MPI process.

2.4.1.8 The Parallelization of the Coefficient EOMs

The coefficient EOMs are propagated using the SIL algorithm described above. This renders the main part of the computation to be the application of the Hamiltonian $\hat{H}$, and its powers, for the construction of the Krylov subspace basis. The many-body basis employed in MCTDHB consists of the time-dependent Fock states with M modes at maximum. If one represents the Hamiltonian in the basis of the corresponding time-dependent creation and annihilation operators, it can be shown that each and every one-body term corresponds to a re-addressing of one element of the vector of coefficients. Similarly, each and every two-body term corresponds to a re-addressing of, at most, two elements of the vector of coefficients. With the knowledge of this re-addressing-scheme (for details, see Ref. [45]), it is no more necessary to build up a Hamiltonian matrix – the action of the Hamiltonian is available by re-addressing the elements according to the representation of the Hamiltonian in terms of the time-dependent creation and annihilation operators. Most importantly, the re-addressings needed for the $N_{1b} = \frac{M(M+1)}{2}$ one- and $N_{2b} = \frac{N_{1b}(N_{1b}+1)}{2}$ two-body operators are independent of each other. Hence, the parallelization distributes the $N_{1b} + N_{2b}$ needed re-addressings among the number of available MPI processes, where they are done with OpenMP threads. The current implementation of this scheme provides all MPI processes with a full copy of the coefficients, which might be a huge array. Therefore, the necessary communication limits the favorable scaling of this parallelization scheme to a few tens of MPI processes. Of course, this depends on the system architecture and the number of coefficients. A further improvement on this scheme would be, in principle, available by finding a suitable partitioning for the coefficients' vector. Yet, the inter-dependencies of the coefficients encoded in the re-addressing scheme are intricate and render a suitable partitioning complicated.

2.4.1.9 IMEST Algorithm

The interaction matrix evaluation by successive transforms is an efficient way to evaluate the two-body matrix elements for two-particle interaction potentials $\hat{W}(\boldsymbol{y})$, which depend only on the distance $\boldsymbol{y} = |\vec{r} - \vec{r}'|$ between the two interacting particles. The IMEST was invented by Kaspar Sakmann and the derivation here follows the one given in his Ph.D. thesis, see Ref. [48]. It is instructive to first consider the case of time-independent $\hat{W}$. For convenience, the matrix elements of the interaction and the local time-dependent potentials are repeated:

$$
\begin{aligned}
W_{ksql}(t) &= \int\int d\vec{r}' d\vec{r} \phi_k^*(\vec{r},t)\phi_s^*(\vec{r}',t)\hat{W}(\vec{r}-\vec{r}')\phi_q(\vec{r},t)\phi_l(\vec{r},t) \\
&= \int d\vec{r}\phi_k^*(\vec{r},t)\hat{W}_{sl}(\vec{r},t)\phi_q(\vec{r},t), \\
\hat{W}_{sl}(\vec{r},t) &= \int d\vec{r}'\phi_s^*(\vec{r}',t)\hat{W}(\vec{r}-\vec{r}')\phi_l(\vec{r}',t).
\end{aligned} \tag{2.55}
$$

Here, it is worthwhile to note that the evaluation of the $\hat{W}_{sl}$, as well as the evaluation of the W_{ksql}, is only a single integration on $\vec{r}'$ and $\vec{r}$, respectively. Given that the considered interaction $\hat{W}$ depends only on $\vec{r}-\vec{r}'$, one can write its Fourier and inverse Fourier transforms in the following form:

$$
\hat{W}(\vec{r}-\vec{r}') = \frac{1}{\sqrt{2\pi}^D}\int d\vec{k}\tilde{\hat{W}}(\vec{k})e^{i\vec{k}(\vec{r}-\vec{r}')} \tag{2.56}
$$

$$
\tilde{\hat{W}}(\vec{k}) = \frac{1}{\sqrt{2\pi}^D}\int d\mathbf{y}\hat{W}(\mathbf{y})e^{-i\vec{k}\mathbf{y}}. \tag{2.57}
$$

It is now straightforward to insert Eq. (2.56) into the above expression for $\hat{W}_{sl}$. This results in the following expression:

$$
\hat{W}_{sl}(\vec{r},t) = \int d\vec{r}'\phi_s^*(\vec{r}',t)\frac{1}{\sqrt{2\pi}^D}\left[\int d\vec{k}\tilde{\hat{W}}(\vec{k})e^{i\vec{k}(\vec{r}-\vec{r}')}\right]\phi_l(\vec{r}',t). \tag{2.58}
$$

Here, one can split up the exponential, $e^{i\vec{k}(\vec{r}-\vec{r}')} = e^{-i\vec{k}\vec{r}'}\cdot e^{i\vec{k}\vec{r}}$, in order to collect the terms dependent solely on $\vec{r}'$ and $\vec{k}$:

$$
\hat{W}_{sl}(\vec{r},t) = \int d\vec{k}\frac{1}{\sqrt{2\pi}^D}\left[\int d\vec{r}'\phi_s^*(\vec{r}',t)\phi_l(\vec{r}',t)e^{-i\vec{k}\vec{r}'}\right]\tilde{\hat{W}}(\vec{k})e^{i\vec{k}\vec{r}}. \tag{2.59}
$$

The expression in square brackets is the Fourier transform $\tilde{f}_{sl}(\vec{k})$ of the function $f_{sl}(\vec{r}',t) = \phi_s^*(\vec{r}',t)\phi_l(\vec{r}',t)$. Revisiting Equation (2.59), the integration on $\vec{k}$ can be canceled by a Fourier transform and a multiplication by $\sqrt{2\pi}^D$, giving an appealing form to the Fourier transform $\hat{\tilde{W}}_{sl}(\vec{k},t)$ of $\hat{W}_{sl}(\vec{r},t)$:

$$
\begin{aligned}
\hat{\tilde{W}}_{sl}(\vec{k},t) &= \frac{1}{\sqrt{2\pi}^D}\int d\vec{r}\hat{W}_{sl}(\vec{r},t)e^{-i\vec{k}\vec{r}} \\
&= \sqrt{2\pi}^D\tilde{f}_{sl}(\vec{k},t)\tilde{\hat{W}}(\vec{k}).
\end{aligned} \tag{2.60}
$$

Consequently, the local time-dependent potentials, occurring in the right-hand side of the orbital EOMs of the MCTDHB (cf. Eqs. (2.47), (2.46)) are available as the inverse Fourier transform of the above Eq. (2.60):

$$\hat{W}_{sl}(\vec{r},t) = \frac{1}{\sqrt{2\pi}^D} \int d\vec{k}\, \hat{\tilde{W}}_{sl}(\vec{k},t) e^{i\vec{k}\vec{r}}. \tag{2.61}$$

Equations (2.60) and (2.61) are the working equations of the IMEST. The key advantage here is that, for time-independent $\hat{W}(\vec{r},\vec{r}') = \hat{W}(\vec{r}-\vec{r}')$, it is sufficient to evaluate once the Fourier transform of the interaction potential, $\hat{\tilde{W}}(\vec{k})$ and at each time-step the Fourier transform of $f_{sl}(\vec{r},t)$, $\tilde{f}_{sl}(\vec{k},t)$, and the inverse Fourier transform of the $\hat{\tilde{W}}_{sl}(\vec{k},t)$. This is much more efficient than directly evaluating the integrals needed for the matrix elements $W_{ksql}(t)$, especially when it comes to perform computations with a large number of grid points. For details on the implementation and an assessment of the numerical effort, see Ref. [48]. For time-dependent two-body interactions, $\hat{W}(\vec{r},\vec{r}',t) = \hat{W}(\vec{r}-\vec{r}',t)$, like, e.g., the ones presented in Chap. 3, the computational effort increases because the Fourier transform of the interaction potential $\hat{\tilde{W}}$ is now also a function of time, i.e., $\hat{\tilde{W}} = \hat{\tilde{W}}(\vec{k},t)$. Therefore, it has to be evaluated at each time-step. This implies that, at each time-step, three, instead of two, additional Fourier transforms have to be evaluated. Still, the procedure is much more efficient than the direct evaluation of the integrals. The IMEST algorithm, also in its time-dependent form, were crucial for performing the calculations in Chap. 3 and for comparing the results of Chap. 6 with a zero-range potential to computations with a short-range Gaussian potential.

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Tunneling Dynamics in Open Ultracold Bosonic Systems
Numerically Exact Dynamics - Analytical Models - Control Schemes
Lode, A.U.J.
2015, XIX, 139 p. 43 illus. in color., Hardcover
ISBN: 978-3-319-07084-1