A Layman’s guide to the Multiconfigurational Time-Dependent Hartree Method for Bosons

Lecture notes

based on


Software: http://ultracold.org

by

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1 Introduction

1.1 Background

The idea that bosons, particles obeying Bose-Einstein statistics, can all condense into their very ground state was first proposed by S. Bose and A. Einstein back in 1924. It was not, however, until 1995 that the Bose-Einstein condensation was realized in dilute gases of ultracold alkali bosons by three independent research groups (Ketterle at MIT, Cornell and Wieman at JILA both with repulsive systems and Hulet at Rice working with attractive ones). Using some elaborate laser and magnetic evaporative cooling techniques the dilute vapours were cooled down to a less than a millionth of a Kelvin degree, temperature that is necessary for the manifestation of the condensation. Since then, the field of ultracold atoms has seen galloping experimental and theoretical developments. Interacting gases at ultralow temperatures \( T \) (close to absolute zero) allow for an unprecedented amount of experimental control and offer thus new possibilities. The external confinement (trap) of the atoms as well as their interparticle interaction can be controlled almost at will. This is now routinely done by adjusting the configuration of lasers and applied magnetic fields in the laboratory. Most strikingly, properties of the gas as its topology and dimensionality can be manipulated. Hence, ultracold atoms serve as a quantum simulator for other many-body physics, for instance solid state systems or crystals whose Hamiltonian does not offer the same flexibility.

In the case of atomic Bose-Einstein condensates (BECs), the Hamiltonian \( \hat{\mathcal{H}} \) as well as the governing equation, the time-dependent Schrödinger equation are known. This implies that an exact theoretical study is possible, at least in principle. The problem that arises when trying to obtain the solution of the time-dependent many-body Schrödinger equation (TDSE) lies in the complexity of the solution \( \Psi \). Generally, the wavefunction depends on the coordinates of all \( N \) particles and the time \( t \). For instance, imagine that we want to represent in the computer the wavefunction \( \Psi \) of \( N = 10 \) particles. Using 10 grid points for each coordinate the problem would require the storage of \( 10^{10} \) complex numbers; and that for a single one point in time. At double precision and 16 bytes per number, this translates already to a data volume of 160GB! Storing a single time-series of, for instance, 1000 time-steps would take 160TB; space that already exceeds the storage capacity of many of the present-day computing centres! This demonstrates the impossibility of storing and computing the solution \( \Psi \) of the TDSE with standard (brute force) expansions in time-independent basis sets. Hence, a clever approach to represent the high-dimensional and time-dependent many-body state of a system is a must when trying to solve the TDSE.

1.2 Theoretical Approaches

From a theoretical point of view, two main approaches are conventionally undertaken to describe the many-body physics of bosons. The first, main line is to find simpler effective many-body Hamiltonians that can be either adapted to a specific situation and can be solved exactly or are amenable to a numerical treatment (for instance the Bose-Hubbard Hamiltonian for bosonic atoms in optical lattices). The second kind of approach treats the full many-body Hamiltonian \( \hat{\mathcal{H}} \) but makes an approximation on the state \( \Psi \) of the system. The present discussion concerns the second kind of approach and focuses on three different ansatzes of increasing generality and complexity. With these three ansatzes, motivated by three distinct quantum many-body phenomena, the problem is treated variationally.
i) **Condensation** means that all particles occupy the same single-particle state and this situation is well described by the most famous and widespread of these approximations: a mean-field approach that assumes that the solution $\Psi$ can be written as a product of a single particle state $\Psi(\vec{r}_1, ..., \vec{r}_N; t) \equiv \phi(\vec{r}_1; t) \cdots \phi(\vec{r}_N; t)$. The variational treatment of this ansatz results in the time-dependent Gross-Pitaevskii (TDGP) that describes systems that are condensed at all time.

ii) **Fragmentation** means that the particles in $\Psi$ macroscopically occupy several single particle states and is built up by taking a symmetrized product of several single particle states $\Psi = \hat{S} \phi_1(\vec{r}_1; t) \phi_2(\vec{r}_2; t) \cdots \phi_N(\vec{r}_N; t)$ as an ansatz for the variational derivation. The derivation yields the time-dependent multi-orbital mean-field (TDMF) equations that describe systems which are fragmented at all times – the particle numbers in the different fragments remain unchanged by the time-evolution.

iii) **The transition between condensation and fragmentation** necessitates a description that accounts for both coherent and fragmented many-body configurations, i.e., fragments which have time-dependent occupations. This can be formulated in a multiconfigurational ansatz that is a sum of all possible different configurations $|\vec{n}; t\rangle$ of $N$ particles in $M$ orbitals weighted by complex, time-dependent coefficients, $\Psi = \sum_{\{\vec{n}\}} C_{\vec{n}} |\vec{n}; t\rangle$. This ansatz yields the equations of motion of the multiconfigurational time-dependent Hartree method for bosons (MCTDHB). With the MCTDHB theory it is possible for the first time to obtain descriptions of many-body physics of ultracold atoms which go beyond mean-field and are even, in principle, exact. Since the above models i)–iii) build upon each other, it is instructive to introduce them in steps of increasing complexity. The next paragraph illustrates the three models and regimes of many-body physics i)–iii) in the case of an interacting system in a symmetric double well potential.

### 1.3 Example: Interacting Ultracold Atoms in a Double Well

Interacting particles in a symmetric one-dimensional double well potential feature all three many-body features, condensation, fragmentation, as well as the transition between condensation and fragmentation. The double well used here is a parabolic trap with a Gaussian barrier in the center. Let’s introduce a parameter $\lambda$ that stands for the strength of the interaction in the system. In ultracold atoms this parameter is related to the s-wave scattering length. For brevity, the time-dependence of some quantities is omitted in this subsection.

**Condensation:**

For weak and no interactions $\lambda \sim 0$, the many-body wavefunction in a double-well is indeed found to be condensed. Despite the spatial separation of the barrier, all particles occupy the same single-particle state $\phi(\vec{r})$, see Figure 1 for a plot. In the case of condensation, the many-body wavefunction is well described by the Gross-Pitaevskii equation (TDGP). This equation describes the dynamics of a one-dimensional gas of bosons in a double well potential.

**Figure 1: Condensation in a double well potential:** For no or very weak interactions, $\lambda \sim 0$, all particles occupy the same single-particle state despite the barrier which separates them. The red solid line shows the density of the delocalized single particle state $\phi(\vec{r})$ and the blue dashed line is the double well potential.
body wavefunction is indeed a product of \( N \) identical single-particle functions or orbitals \( \phi(\vec{r}) \),

\[
\Psi_{GP}(\vec{r}_1 \cdots \vec{r}_N) = \mathcal{N} \prod_{i=1}^{N} \phi(\vec{r}_i),
\]

where \( \mathcal{N} \) is some normalization. It is interesting to note here that such a quantum state is always fully coherent over all space and time.

**Fragmentation:**

For larger interactions, \( \lambda = \mathcal{O}(1) \), the many-body wavefunction in a double-well fragments into left-localized and right localized single-particle states or orbitals. Fragmentation occurs, because it is energetically favourable for the system to fragment and it would actually cost energy to overcome the repulsion and make it coherent. Two or more orbitals \( \phi_k(\vec{r}) \), \( k = 1, 2, \ldots \) are necessary to capture the wavefunction qualitatively. See Figure 2 for a plot.

![Figure 2: Fragmentation in a double well potential:](image)

In the case of two-fold fragmentation, the many-body wavefunction may be represented as a symmetrized product of two single-particle states

\[
\Psi_{TDMF}(\vec{r}_1, \ldots, \vec{r}_N) = \mathcal{N} \hat{S} \left[ \prod_{i=1}^{\frac{N}{2}} \phi_1(\vec{r}_i) \prod_{k=\frac{N}{2}+1}^{N} \phi_2(\vec{r}_k) \right] = \mathcal{N} \left| \frac{N}{2}, \frac{N}{2} \right>,
\]

where \( \mathcal{N} \) is some normalization and \( \hat{S} \) is a symmetrization operator that sums up the expression to its right exchanging the particle coordinates to obtain a state of bosonic symmetry, which reads \( |\frac{N}{2}, \frac{N}{2}\rangle \) in occupation number or second quantized representation. Of course, an even number of particles was assumed. Such a state can no longer be considered as coherent, since the wavefunction is a (potentially) huge sum of orbital products.

It is important to note that the one-body density \( \rho(\vec{r}) = \frac{N}{2} |\phi_1(\vec{r})|^2 + \frac{N}{2} |\phi_2(\vec{r})|^2 \) may be very similar to the condensed case (cf. Figure 1); thus, one needs to look at other quantities, such as for example the phase relation between the left and the right well, to detect the fragmentation of the system. If the phase of the left and right well is fixed then a perfect interference should occur, whereas a lack of phase relation in the fragmented case would result in a bad contrast of the interference of the left and right well atoms’ wavefunction.

**Transition from Condensation to Fragmentation:**

Consider the situation of significant interactions where we transform the potential of the system smoothly from a parabolic to a double-well potential, see Figure 3. The ground state at
the chosen interaction is condensed in the parabolic trap but fragmented in the double well potential. Even if the change of potential would be adiabatic, the description of the state $\Psi$ during this change needed to incorporate many configurations ranging from the initial one $|N,0\rangle$ to the final one $|\frac{N}{2},\frac{N}{2}\rangle$.

Figure 3: Transition from condensation to fragmentation: For significant interactions $\lambda$, the state in a single well trap remains mostly condensed as shown in the left panel. All the particles reside in a single orbital. Yet, the many-body ground state in the double well is fully fragmented (right panel). Half of the particles occupy the right-localized orbital $\phi_1(\vec{r})$ (red solid line) while the other half of the particles occupies the left-localized orbital $\phi_2(\vec{r})$ (red dashed line). Considering an adiabatic transformation of the parabolic trap to the double well trap would necessitate the occupation of many different mean-field configurations.

When one considers an adiabatic change from the initial potential with a density $\rho(\vec{r}, t = 0) = N|\phi_1(\vec{r}; t = 0)|^2$ to the final potential with density $\rho(\vec{r}, t = t_f) = N|\phi_2(\vec{r}; t = t_f)|^2$, it becomes evident that the density must gradually evolve from merely being defined by $\phi_1(\vec{r}; t)$ to being equally defined by $\phi_2(\vec{r}; t)$. To capture such a transition from a condensed to a fragmented state, it is necessary to allow the occupations of $\phi_1(\vec{r}; t)$ and $\phi_2(\vec{r}; t)$, $n_1(t)$ and $n_2(t)$, to be time-dependent. A straightforward way to capture this time-dependence of occupations, is to setup the ansatz to incorporate all possible configurations $n_i = |i, N - i\rangle$; $i = 0, ..., N$.

A wavefunction ansatz that contains all configurations can be formed by a superimposing symmetrized products of two orbitals $\phi_1(\vec{r}; t), \phi_2(\vec{r}; t)$ weighted with complex coefficients $C_i(t); i = 0, ..., N$ that are time-dependent:

$$
\Psi_{MB}(\vec{r}_1, ..., \vec{r}_N; t) = \left( C_0(t) \prod_{i=1}^{N} \phi_1(\vec{r}_i; t) \right) + C_1(t) \hat{S} \left[ \prod_{i=1}^{N-1} \phi_1(\vec{r}_i; t) \right] \phi_2(\vec{r}_N; t) + C_2(t) \hat{S} \left[ \prod_{i=1}^{N-2} \phi_1(\vec{r}_i; t) \right] \left( \prod_{i=0}^{1} \phi_2(\vec{r}_{N-i}; t) \right) + ...
$$

Here, the symmetrization operator was again used to “convert” products of different orbitals to fully symmetric configurations $|n_1, n_2; t\rangle \equiv |n; t\rangle$. Each of the $N + 1$ configurations is weighted by a coefficient $C_{\vec{n}}(t)$ that is time-dependent. For the normalization, $\sum_{\{\vec{n}\}} C_{\vec{n}}(t)^* C_{\vec{n}}(t) = 1$ must hold. Using these conventions to express equation (4), one arrives at the more compact form

$$
|\Psi_{MB}; t\rangle = \sum_{\{\vec{n}\}} C_{\vec{n}}(t)|\vec{n}; t\rangle.
$$
This ansatz is capable of describing any configuration or linear combination of configurations of $N$ bosons in $M = 2$ time-dependent orbitals and hence can capture the transition from a coherent to a fragmented state. It is the basic form of the ansatz that is used for the derivation of the MCTDHB equations of motion with the variational principle. The coefficients and time-dependent orbitals are used as independent variational parameters.

**Time-dependent variational principle:**

The scheme to obtain equations of motion for variational parameters (functions or scalars) is a 3-step procedure.

1. The ansatz is written down. The ansatz contains a set of variational parameters that are to be determined such that the action is minimized at all times. The ansatzes we want to treat are the above $\Psi_{GP}$, $\Psi_{TDMF}$ and $\Psi_{MB}$. The variational parameters in $\Psi_{GP}$ and $\Psi_{TDMF}$ are the orbitals $\phi_k(\vec{r}; t)$ only, whereas $\Psi_{MB}$ contains orbitals $\phi_k(\vec{r}; t)$ and coefficients $C_{\vec{n}}(t)$.

2. Formulate the action of the system $S = \int dt L = \int dt \langle \Psi | \hat{H} - i \partial_t | \Psi \rangle$ and add in the constraints (orthogonality, normalization, ...) that the variational parameters need to fulfil using Lagrange multipliers.

3. Perform the variational calculation, i.e., demand the stationarity of the action when varying the variational parameters: $\delta S \equiv 0 = \int dt \langle \delta \Psi | \hat{H} - i \partial_t | \Psi \rangle$.

With the definition of the ansatz and the formulation of the above procedure, all the necessary ingredients to derive variational equations of motion for the many-body dynamics of quantum systems are at hand.

## 2 Derivation of the Time-Dependent Gross-Pitaevskii Equation

This section variationally derives the equation of motion for a many-body wavefunction that is a product of a single quantum mechanical state, which results in the time-dependent Gross-Pitaevskii equation. The Hamiltonian contains one-body parts $\hat{h}$ and two-body interaction $\hat{W}$,

$$\hat{H} = \sum_{i=1}^{N} \hat{h}_i(\vec{r}_i) + \lambda_0 \sum_{i<j=1}^{N} \hat{W}(\vec{r}_i - \vec{r}_j),$$

where $\hat{h}_i$ contains the potential $V(\vec{r}_i)$ and kinetic energy $-\frac{1}{2} \partial_{\vec{r}_i}^2$ of the $i$-th boson and $\hat{W}(\vec{r} - \vec{r}')$ is the interparticle interaction of two bosons at $\vec{r}$ and $\vec{r}'$. To start the derivation, we write down the ansatz for the the coherent state,

$$\Psi_{GP}(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N; t) = \prod_{i=1}^{N} \phi(\vec{r}_i; t),$$

where all particles occupy the same single state $\phi(\vec{r}; t)$. The action of the system reads

$$S_{GP} = \int \langle \Psi_{GP} | \hat{H} - i \partial_t | \Psi_{GP} \rangle - \mu(t) \left[ \langle \Phi | \Phi \rangle - 1 \right],$$
To eliminate the orbital throughout time from this equation. To achieve this, we multiply equation 11 by the same result. Next, we perform the variation of the action with respect to \( \phi \). Here, we used in the second step, equation 10 that the integration for all coordinates gives the same result. Next, we perform the variation of the action with respect to \( \phi^*(\vec{r}; t) \),

\[
\frac{\delta S[\phi^*(\vec{r}; t)]}{\delta \phi^*(\vec{r}; t)} = 0 \tag{11}
\]

\[
\Rightarrow N \hat{h}(\vec{r}) \phi(\vec{r}; t) + \lambda_0 N(N-1) \int d\vec{r}^\prime \phi^*(\vec{r}^\prime; t) \hat{W}(\vec{r} - \vec{r}^\prime) \phi(\vec{r}^\prime; t) - \mu(t) \phi(\vec{r}; t) = N i \partial_t \phi(\vec{r}; t).
\]

It remains to eliminate the Lagrange multiplier \( \mu(t) \) which ensures the normalization of the orbital throughout time from this equation. To achieve this, we multiply equation 11 by \( \phi^*(\vec{r}; t) \) and integrate over \( d\vec{r}^\prime \). Further, we define the time-dependent local interaction potential, \( \hat{W}(\vec{r}; t) = \int d\vec{r}^\prime \left[ \phi^*(\vec{r}^\prime; t) \hat{W}(\vec{r} - \vec{r}^\prime) \phi(\vec{r}^\prime; t) \right] \). Finally, the Lagrange multiplier \( \mu(t) \) reads:

\[
\mu(t) = N \int d\vec{r}^\prime \phi^*(\vec{r}^\prime; t) \left[ \hat{h}(\vec{r}) - i \partial_t + \lambda_0 (N-1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}). \tag{12}
\]

To eliminate \( \mu(t) \) from equation 11 we reinsert equation 12 into it and obtain:

\[
N \left[ \hat{h}(\vec{r}) - i \partial_t + \lambda_0 (N-1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}) - N \int d\vec{r}^\prime \phi^*(\vec{r}^\prime; t) \left[ \hat{h}(\vec{r}) - i \partial_t + \lambda_0 (N-1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}) = 0 \tag{13}
\]

Here, we rearranged the term \( i \partial_t \phi(\vec{r}; t) \) in order to motivate the introduction of the projection operator,

\[
\hat{P} = 1 - \phi(\vec{r}; t) \int d\vec{r}^\prime \phi^*(\vec{r}^\prime; t). \tag{14}
\]

From equation 12 and 13 we notice the relation

\[
\begin{aligned}
&= \left( 1 - \phi(\vec{r}; t) \int d\vec{r}^\prime \phi^*(\vec{r}^\prime; t) \right) \left[ \hat{h}(\vec{r}) - i \partial_t + \lambda_0 (N-1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}; t) \\
&= \left[ \hat{h}(\vec{r}) - i \partial_t + \lambda_0 (N-1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}; t) \frac{\mu(t)}{N} \phi(\vec{r}; t) \tag{15}
\end{aligned}
\]

Hence, the projector \( \hat{P} \) can be factored out from equation 11 to give:

\[
\hat{P} \left[ \hat{h}(\vec{r}) + \lambda_0 (N-1) \hat{W}(\vec{r}; t) - i \partial_t \right] \phi(\vec{r}; t) = 0. \tag{16}
\]
Interestingly, the elimination of the Lagrange multiplier $\mu(t)$ lead to the emergence of the projection operator $\hat{P}$, which ensures the normalization of the state $\phi(\vec{r}; t)$. 

Reordering equation \[16\] finally gives the first form of the time-dependent Gross-Pitaevskii (TDGP) equation,

$$\hat{P}i\partial_t\phi(\vec{r}; t) = \hat{P} \left[ \hat{h}(\vec{r}) + \lambda_0 (N - 1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}; t). \quad (17)$$

To get to the commonly employed version of the TDGP, we choose the relation $\int \phi^*(\vec{r}; t) i\partial_t \phi(\vec{r}; t) \equiv 0$. It directly yields $\hat{P}i\partial_t\phi(\vec{r}; t) = i\partial_t\phi(\vec{r}; t)$. We are allowed to make this choice, because it merely corresponds to the phase assignment $\phi(\vec{r}; t) \rightarrow \exp\{i/N \int \mu(t) \, dt\} \phi(\vec{r}; t)$. We obtain:

$$i\partial_t\phi(\vec{r}; t) = \hat{P} \left[ \hat{h}(\vec{r}) + \lambda_0 (N - 1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}; t). \quad (18)$$

If we further set $\hat{W}(\vec{r} - \vec{r}') \equiv \delta(\vec{r} - \vec{r}')$, we get

$$i\partial_t\phi(\vec{r}; t) = \hat{P} \left[ \hat{h}(\vec{r}) + \lambda_0 (N - 1)|\phi(\vec{r}; t)|^2 \right] \phi(\vec{r}; t). \quad (19)$$

It is interesting to note that one could omit the projection operator $\hat{P}$ in the above equation to get the standard TDGP

$$i\partial_t\phi(\vec{r}; t) = \left[ \hat{h}(\vec{r}) + \lambda_0 (N - 1) \hat{W}(\vec{r}; t) \right] \phi(\vec{r}; t). \quad (20)$$

This representation can be derived by making the phase assignment $\phi(\vec{r}; t) \rightarrow \exp\{i/N \int \mu(t) \, dt\} \phi(\vec{r}; t)$ in equation \[11\]. This phase assignment merges the Lagrange multiplier $\mu(t)$ into the orbital $\phi(\vec{r}; t)$. The above equations \[17\],\[18\],\[19\],\[20\] constitute the main result of this section. Although the elimination of the projection operator is possible, it’s not desireable in practical numerical computations, because it maintains the orthonormality of the temporal change $i\partial_t\phi(\vec{r}; t)$ with respect to $\phi(\vec{r}; t)$ and this makes the propagation of the TDGP more stable and accurate at a lower computational cost.

We obtained a time-dependent mean-field equation which describes the dynamics of a condensate, the TDGP. This is the answer we would expect from a variational calculation with an ansatz that is designed for the situation of all particles occupying the same state. The TDGP is probably the most commonly used model to describe ultracold atoms, but it is limited to the physical situation where all particles are condensed and it cannot capture the exciting physics that emerge due to the correlations between particles in a many-body system. To account for the basic features of such correlations, like the occurrence of fragmentation a more elaborate method that allows several single-particle states to be occupied, will be derived in the next section.

**Related Literature**


3 Derivation of the Time-Dependent Multi-Orbital Mean-Field

To arrive at equations of motion for a generally fragmented state of \( N \) particles that sit in \( M \) different fragments or orbitals \( \phi_1(r; t), \ldots, \phi_M(r; t) \), we proceed following the same procedure as previously for the derivation TDGP equation. First, the ansatz for a general fragmented \( M \)-orbital state is stated, second, the action is formulated, also adding the Lagrange multipliers corresponding to the required orthogonality constraints on the orbitals. Last, the variation of the action with respect to all the time-dependent single-particle functions \( \phi_i(r; t) \), were introduced and \( |\text{vac}\rangle \) denotes the vacuum state with no particles. The action of the system with the Lagrange multipliers that ensure the orthonormality of the orbitals \( \phi_j; j = 1, \ldots, M \) reads:

\[
S_{TDMF} = \int dt \left[ \langle \Psi_{TDMF} | \hat{H} - i \partial_t | \Psi_{TDMF} \rangle - \left( \sum_{k,j=1}^{M} \mu_{kj}(t)(|\langle \phi_k | \phi_j \rangle - \delta_{kj}|) \right) \right].
\]

To proceed, we first evaluate the expectation value of the first integrand \( \langle \Psi_{TDMF} | \hat{H} - i \partial_t | \Psi_{TDMF} \rangle \) we introduce the matrix elements of the one-body and two-body operators \( \hat{h} \) and \( \hat{W} \):

\[
h_{jk} = \langle \phi_j | \hat{h} | \phi_k \rangle \tag{25}
\]

\[
(i \partial_t)_{ij} = \langle \phi_i | i \partial_t | \phi_j \rangle \tag{26}
\]

\[
W_{ijkl} = \int d\vec{r} \int d\vec{r}' \phi_i^*(\vec{r}; t) \phi_j^*(\vec{r}'; t) \hat{W}(\vec{r}; \vec{r}') \phi_k(\vec{r}; t) \phi_l(\vec{r}; t). \tag{27}
\]

With these matrix elements, Eqs. (27), (25) and the creation operators in Eq. (23), the Hamiltonian can be cast into second quantized form,

\[
\hat{H} = \sum_{kq} h_{kq} b_k^\dagger b_q + \frac{\lambda_0}{2} \sum_{ksql} W_{ksql} b_s^\dagger b_k^\dagger b_l b_q. \tag{28}
\]

Since we consider a single configuration \( |\vec{n}; t\rangle \), only terms in \( \hat{H} \) which do not change any of the occupation numbers \( n_i; i = 1, \ldots, M \) have to be taken into account and one obtains

\[
\langle \Psi_{TDMF} | \hat{H} - i \partial_t | \Psi_{TDMF} \rangle = \sum_k n_k h_{kk} - \sum_k n_k (i \partial_t)_{kk} + \frac{\lambda_0}{2} \sum_{k=1}^{M} n_k (n_k - 1) W_{kkkk} + \frac{\lambda_0}{2} \sum_{l \neq k} \sum_{kl} [n_k n_l (W_{klkl} + W_{klkl})] = \sum_k n_k \left[ h_{kk} - (i \partial_t)_{kk} + \frac{\lambda_0}{2} (n_k - 1) W_{kkkk} + \frac{\lambda_0}{2} \sum_{l \neq k} [n_l (W_{klkl} + W_{klkl})] \right]. \tag{29}
\]
Note that also non-diagonal matrix elements of the interaction operator, which involve contributions of two distinct orbitals are contributing to this expression – in other theories, like for instance the Bose-Hubbard Hamiltonian, these contributions are neglected. With expression (29) it is now straightforward to evaluate the variational derivative of the action $S_{TDMF}$:

$$\frac{\delta S[\phi_j^*(\vec{r}; t), \ldots, \phi_M^*(\vec{r}; t)]}{\delta \phi_k^*(\vec{r}; t), k = 1, \ldots, M} = 0$$  \hspace{1cm} (30)

$$\sum_j\mu_{kj}|\phi_j\rangle = n_k\hat{h}|\phi_k\rangle - n_k (i\partial_t)|\phi_k\rangle + \lambda_0 n_k (n_k - 1) W_{kk}|\phi_k\rangle + n_k \sum_{l\neq k} \lambda_0 n_l \left(W_{ll} + \tilde{W}_{ll}\right)|\phi_k\rangle$$

$$\sum_j\mu_{kj}|\phi_j\rangle = n_k \left[\hat{h} - (i\partial_t) + \lambda_0 (n_k - 1) W_{kk} + \sum_{l\neq k} \lambda_0 n_l \left(W_{ll} + \tilde{W}_{ll}\right)\right]|\phi_k\rangle,$$

Here we made use of the local interaction potentials,

$$W_{ij}(\vec{r}; t) = \int d\vec{r}' \phi_i^*(\vec{r}'; t)\hat{W}(\vec{r}, \vec{r}'; t)|\phi_j\rangle = \int d\vec{r}' \phi_i^*(\vec{r}'; t)W(\vec{r}' - \vec{r})\pi_\rho \phi_j(\vec{r}'; t).$$  \hspace{1cm} (31)

The operator $\pi_\rho$ permutes the dependencies on $\vec{r}$ and $\vec{r}'$ of the two orbitals to its right. To eliminate the Lagrange multipliers $\mu_{kj}(t)$ in the equations of motion of the multi-orbital mean-field (30), we first project with $|\phi_j\rangle$ from the left in the third line of (30) and divide by $n_k$ to get

$$\frac{\mu_{kj}(t)}{n_k} = [h_{jk} - (i\partial_t)_{jk} + \lambda_0 (n_k - 1) W_{jkkk} + \sum_{l\neq k} \lambda_0 n_l (W_{jllk} + W_{jkl})].$$  \hspace{1cm} (32)

Equipped with this equation, one notices the relation

$$\left[\hat{h} - (i\partial_t) + \lambda_0 (n_k - 1) W_{kk} + \sum_{l\neq k} \lambda_0 n_l \left(W_{ll} + \tilde{W}_{ll}\right)\right]|\phi_k\rangle - \sum_{j=1}^M \frac{\mu_{kj}(t)}{n_k}|\phi_j\rangle$$

$$= \hat{P} \left[\hat{h} - (i\partial_t) + \lambda_0 (n_k - 1) W_{kk} + \sum_{l\neq k} \lambda_0 n_l \left(W_{ll} + \tilde{W}_{ll}\right)\right]|\phi_k\rangle;$$

$$\hat{P} = 1 - \sum_k |\phi_k\rangle\langle\phi_k|.$$  \hspace{1cm} (33)

As in the case of TDGP, the elimination of the Lagrange multipliers again manifests in the emergence of a projector $\hat{P}$. Reinserting the relation (33) into the variation (30) and bringing the time-derivative to the right-hand side, we finally obtain the equations of motion of the TDMF:

$$\hat{P}i\partial_t|\phi_k\rangle = \hat{P} \left[\hat{h} + \lambda_0 (n_k - 1) W_{kk} + \sum_{l\neq k} \lambda_0 n_l \left(W_{ll} + \tilde{W}_{ll}\right)\right]|\phi_k\rangle.$$  \hspace{1cm} (35)

Up to the diagonal part of the local interaction potential, $W_{kk}$, this set of equations resembles the nonlinear form of the TDGP [compare equation (17)]. The terms proportional off-diagonal to the off-diagonal interaction matrix elements $W_{ll}, W_{lk}$, however are not present in the TDGP. These terms couple the time-evolution of the different orbitals with each other and make the set of coupled equations that is involved to solve than just the TDGP. Similarly to the case of the TDGP, we proceed by eliminating the projector on the left-hand side of (35) by imposing the constraints that any orbital’s time-evolution is orthogonal to the orbital, i.e. $\langle i\partial_t|\phi_k\rangle \equiv 0$. This constraint corresponds to assigning a time-dependent phase

$$\phi_k(\vec{r}; t) \rightarrow \phi_k(\vec{r}; t) \exp \left[i \int dt \langle \partial_t|\phi_k\rangle \right] \Rightarrow \hat{P}i\partial_t|\phi_k\rangle = i\partial_t|\phi_k\rangle.$$  \hspace{1cm} (36)
The right hand side of this equation holds because the off-diagonal elements of the time-derivative, \((i\partial_t)_{jk}\), are 0 for all \(j \neq k\), because the corresponding operators \(b_j^\dagger b_k\) would change the occupations \(|\vec{n};t\rangle\). The equations of motion then become:

\[
i\partial_t|\phi_k\rangle = \hat{P}\left[\hat{h} + \lambda_0 (n_k - 1) W_{kk} + \sum_{l \neq k} \lambda_0 n_l \left(\hat{W}_{kl} + \hat{\hat{W}}_{kl}\right)\right]|\phi_k\rangle.
\]

For the sake of completeness, let’s specify the case of contact interactions, \(\lambda_0 \hat{W}(\vec{r},\vec{r}') = \lambda_0 \delta(\vec{r} - \vec{r}')\):

\[
i\partial_t|\phi_k\rangle = \hat{P}\left[\hat{h} + \lambda_0 (n_k - 1) W_{kk} + \sum_{l \neq k} 2\lambda_0 n_l |\phi_l\rangle^2 |\phi_k\rangle\right].
\]

Here, we used that \(W_{ll} = \int d\vec{r}' \phi^* (\vec{r}'; t) \delta(\vec{r} - \vec{r}') \phi_l (\vec{r}'; t) = |\phi_l (\vec{r}; t)|^2\) and

\[
\hat{W}_{kl} \phi_k (\vec{r}; t) = \int d\vec{r}' \phi^* (\vec{r}'; t) \delta(\vec{r} - \vec{r}') \pi_{\vec{r}} \phi_l (\vec{r}; t) \phi_k (\vec{r}; t) = |\phi_l (\vec{r}; t)|^2 \phi_k (\vec{r}).
\]

This concludes the present exposition of the TDMF equations of motion. Some comments are in place, here. The TDMF can describe the time-evolution of a generally fragmented condensate under the assumption that the occupations \(\vec{n}\) do not change with time. It’s interesting to note that the off-diagonal Lagrange multipliers cannot generally be included in the orbitals and hence it’s not possible to remove the projector from equation (37). The projector \(\hat{P}\) on the right-hand side of equations (35), (37), and (38) ensures explicitly the orthonormality of the set \(\phi_k (\vec{r}; t)\) with respect to its time-derivative on the left-hand side and makes the numerical solution stable even for long propagation times. Next, in order to cover also systems which have occupations that vary with time, like for instance systems that undergo a transition from condensation to fragmentation dynamically, the MCTDHB will be introduced and discussed.

**Related Literature**

4 Derivation of MCTDHB

In this section, the equations of motion are derived for a general ansatz which is a sum of all possible distinct configurations of \( N \) particles in \( M \) orbitals. The theory is therefore called multiconfigurational. Each of the configurations is of the same principle nature as the time-dependent multiorbital mean-field ansatz (22) which was treated previous section, but has different occupations. Once the ansatz is stated, the action will be formulated with Lagrange multipliers for the orthonormality of the orbitals. The variation of the action with respect to both coefficients and orbitals gives the equations of motion of MCTDHB. Two sets are obtained: the first set for the time-evolution of the coefficients is a linear system whereas the second set for the orbitals is nonlinear and integro-differential. Both sets are coupled via matrix elements.

The ansatz for a general many-body state reads

\[
|\Psi_{MB}\rangle = \sum_{\vec{n}} C_{\vec{n}} |\vec{n}; t\rangle. \tag{40}
\]

This sum is indexed by the vector \( \vec{n} = (n_1, n_2, \ldots, n_M)^T \), i.e., the configurations \( |\vec{n}; t\rangle \) are just identical to \( |\Psi_{TDMF}\rangle \) in equation (22). Importantly, the coefficients \( C_{\vec{n}}(t) \) allow a change in the system’s many-body state from condensation to fragmentation. Using the second quantized representation introduced previously,

\[
|\vec{n}; t\rangle = |n_1, \ldots, n_M; t\rangle = \frac{1}{\sqrt{\prod_{i=1}^{M} n_i!}} \left( b_{1}^{\dagger}(t) \right)^{n_1} \cdots \left( b_{M}^{\dagger}(t) \right)^{n_M} |\text{vac}\rangle,
\]

one can rewrite the MCTDHB ansatz (40)

\[
|\Psi_{MB}\rangle = \sum_{\{n_1, \ldots, n_M\}} \frac{C_{n_1, \ldots, n_M}(t)}{\sqrt{\prod_{i=1}^{M} n_i!}} \left( b_{1}^{\dagger}(t) \right)^{n_1} \cdots \left( b_{M}^{\dagger}(t) \right)^{n_M} |\text{vac}\rangle. \tag{41}
\]

It is important to note here that both previously discussed theories, the TDGP and TDMF are contained in this ansatz as special cases. TDGP is equivalent to the situation where a single configuration for which \( n_k = N \) for a certain \( k \in 1, \ldots, M \) is contributing. Hence, only a single coefficient, \( C_{0, \ldots, 0, n_k, 0, \ldots}(t) \) is nonzero. TDMF corresponds to a case where a single configuration \( \vec{n}' = (n'_1, n'_2, \ldots, n'_M)^T \) is contributing, i.e., all but the coefficient \( C_{\vec{n}'} \) are zero. Furthermore, it is important that (40) spans the full \( N \)-body Hilbert space in the limit \( M \to \infty \) and is, at least in principle, an exact description of an \( N \)-body state. The operators \( b_{k}^{\dagger}(t) \) are defined as follows:

\[
b_{k}^{\dagger}(t) = \int d\vec{r} \phi_{k}^{\dagger}(\vec{r}; t) \hat{\Psi}^{\dagger}(\vec{r}; t); k = 1, \ldots, M; \quad \hat{\Psi}^{\dagger}(\vec{r}; t) = \sum_{k} b_{k}^{\dagger}(t) \phi_{k}(\vec{r}; t).
\]

As done previously in the case of the TDMF, we restate the Hamiltonian using the creation and anihilation operators and the matrix elements of the one- and two-body operators [cf. (28)]:

\[
\hat{H} = \sum_{kq} h_{kq} b_{k}^{\dagger} b_{q} + \frac{1}{2} \sum_{kqsl} W_{kqsl} b_{k}^{\dagger} b_{l}^{\dagger} b_{q} b_{l}.
\tag{42}
\]

In contrast to the TDMF case, equation (28), we absorb the interparticle interaction strength \( \lambda_0 \) into the interparticle interaction potential \( W(\vec{r}; \vec{r}') \) (see below). The standard functional action with the ansatz (40) is

\[
S_{MCTDHB} = \int dt \left\{ \langle \Psi_{MB} | \hat{H} - i \partial_t | \Psi_{MB} \rangle - \sum_{k} \mu_{kj}(t) \left[ |\langle \phi_{k} | \phi_{j} \rangle - \delta_{kj} \right] \right\}. \tag{43}
\]
Here, the Lagrange multipliers take care of the orthonormality of the orbitals throughout their time-evolution. As a first step to compute the variation of \((43)\) with respect to the coefficients, we compute the expectation value of \(\hat{H} - i\partial_t\):

\[
\langle \Psi_{MB} \left| \hat{H} - i\partial_t \right| \Psi_{MB} \rangle = \sum_{\vec{n}} C_{\vec{n}}^{*} \left[ \sum_{\vec{n}'} \langle \vec{n}; t \left| \hat{H} - i\partial_t \right| \vec{n}'; t \rangle C_{\vec{n}'} - i\partial_t C_{\vec{n}} \right].
\]  

Equipped with this equation, one readily can demand the stationarity of the action \((43)\) when the coefficients \(C_{\vec{n}}(t)\) are varied:

\[
\frac{\delta S}{\delta \{C_{\vec{n}}(t)\}} = 0 \implies \sum_{\vec{n}'} \langle \vec{n}; t \left| \hat{H} - i\partial_t \right| \vec{n}'; t \rangle C_{\vec{n}'} = i\partial_t C_{\vec{n}}.
\]  

To arrive at an appealing form of this linear equation for the coefficients, we define the time-dependent matrix \(H(t)\) with the elements

\[
H_{\vec{n}\vec{n}'}(t) = \langle \vec{n}; t \left| \hat{H} - i\partial_t \right| \vec{n}'; t \rangle C_{\vec{n}'} (46)
\]

and collect the coefficients in the vector \(C(t)\). We arrive at the matrix equation

\[
H(t) C(t) = i\partial_t C(t),
\]  

which is the first main set of equations of motion of the MCTDHB method. The total dimension of the vector \(#\{C(t)\} = N_{\text{Conf}} = (N+M-1)^2\). The number \(N_{\text{Conf}}\) can be seen as the size of the Hilbert space treated in relation to the TDGP or TDMF methods which both use a single configuration, only. Next, to derive the equation of motion for the set of orbitals \(\{\phi_k(\vec{r}; t); k = 1, \ldots, M\}\), it is instructive to define the matrix elements of the reduced one- and two-body matrices:

\[
\rho_{kq} = \langle \Psi_{MB} | b_k^* b_q | \Psi_{MB} \rangle \]  
\[
\rho_{ksql} = \langle \Psi_{MB} | b_k^* b_q b_s b_l | \Psi_{MB} \rangle .
\]  

It is instructive to verify that these matrix elements are functions of the coefficients, only. For instance, \(\rho_{kk}(t) = \sum_{\vec{n}} C_{\vec{n}}^{*} C_{\vec{n}}(t)n_k\) and \(\rho_{kq}(t) = \sum_{\vec{n}} C_{\vec{n}}^{*} C_{\vec{n}}(t)\sqrt{n_k(n_q + 1)}\) for \(k \neq q\). Note, that in the present case all the operators are making a contributions, i.e., for the case that a boson is transferred from one orbital to another, different configurations are making up the matrix elements. For brevity, the explicit form of the two-body matrix elements \((49)\) is deferred to appendix A. Further, we remind the matrix elements of the one-body Hamiltonian \(\hat{h}\), the time-derivative \(i\partial_t\) and the interparticle interaction \(\hat{W}\) [see also equations \((26)\), \((25)\), \((27)\)],

\[
h_{jk} = \langle \phi_j | \hat{h} | \phi_k \rangle
\]

\[
(i\partial_t)_{ij} = \langle \phi_i | i\partial_t | \phi_j \rangle
\]

\[
W_{ijkl} = \int d\vec{r} \int d\vec{r}' \phi_i^*(\vec{r}; t)\phi_j^*(\vec{r}'; t)\hat{W}(\vec{r}; \vec{r}')\phi_k(\vec{r}'; t)\phi_l(\vec{r}; t).
\]

Now it is straightforward to compute the expectation value of the operator \(\hat{H} - i\partial_t\) with the ansatz of equation \((40)\),

\[
\langle \Psi_{MB} \left| \hat{H} - i\partial_t \right| \Psi_{MB} \rangle = \sum_{k,q=1}^{M} \rho_{kq} h_{kq} - \rho_{kq} \langle i\partial_t | \rangle_{kq} + \frac{1}{2} \sum_{k,s,q,l=1}^{M} \rho_{ksql} W_{ksql} - i\sum_{\vec{n}} C_{\vec{n}}^{*} (t) \partial_t C_{\vec{n}}(t).
\]  

\[
(50)
\]
The variation of the action $S_{MCTDHB}$ with respect to the orbitals $\phi_k(\vec{r}; t)$ is demanded to be stationary:

$$
\frac{\delta S}{\delta \{\phi_k(t)\}_{k=1}^M} = 0
$$

$$
\Rightarrow \sum_{q=1}^M \left( \rho_{kq} \left[ \hat{h} - i\partial_t \right] \right) |\phi_q\rangle + \left( \sum_{s,q,l=1}^M \rho_{ksql} \hat{W}_{sl} \right) |\phi_q\rangle - \sum_{j=1}^M \mu_{kj}(t) |\phi_j\rangle = 0.
$$

(51)

Note, that use of the time-dependent potential $\hat{W}_{sl}$ was made [cf. equation (31)]. Next, we eliminate the Lagrange multipliers from this equation. When we multiply equation (51) from the left by $\langle \phi_j |$, we obtain:

$$
\mu_{kj}(t) = \sum_{q=1}^M \left[ \rho_{kq} [h_{jq} - (i\partial_t)_{jq}] + \sum_{s,l=1}^M \rho_{ksql} W_{jsql} \right],
$$

(52)

noticing the identities,

$$
\sum_{q=1}^M \left( \rho_{kq} \left[ \hat{h} - i\partial_t \right] \right) |\phi_q\rangle + \left( \sum_{s,q,l=1}^M \rho_{ksql} \hat{W}_{sl} \right) |\phi_q\rangle - \sum_{j'=1}^M \mu_{kj'}(t) |\phi_{j'}\rangle = \left( 1 - \sum_{j'=1}^M |\phi_{j'}\rangle \langle \phi_{j'} | \right) \left( \sum_{q=1}^M \left( \rho_{kq} \left[ \hat{h} - i\partial_t \right] \right) |\phi_q\rangle + \left( \sum_{s,q,l=1}^M \rho_{ksql} \hat{W}_{sl} \right) |\phi_q\rangle \right).
$$

(53)

one obtains the equations of motion of the orbitals,

$$
\hat{P} \sum_{q=1}^M \rho_{kq} i\partial_t |\phi_q\rangle = \hat{P} \left[ \sum_{q=1}^M \rho_{kq} \left[ \hat{h} \right] |\phi_q\rangle + \sum_{s,q,l=1}^M \rho_{ksql} \hat{W}_{sl} |\phi_q\rangle \right]; \quad \hat{P} = 1 - \sum_{k=1}^M |\phi_k\rangle \langle \phi_k |.
$$

(54)

To simplify, we multiply by the inverse of the matrix elements of the reduced one-body density, $\{ \rho(t) \}_{jk}^{(-1)}$ and sum on the $k$-index, such that the $\rho_{kq}$ are eliminated from the left-hand side and the one-body parts of the right-hand side in the above equation:

$$
\hat{P} i\partial_t |\phi_j\rangle = \hat{P} \left[ \hat{h} |\phi_j\rangle + \sum_{s,q,l=1}^M \{ \rho(t) \}_{jk}^{(-1)} \rho_{ksql} \hat{W}_{sl} |\phi_q\rangle \right];
$$

(55)

The projection operator on the left-hand side of the equations of motion of the orbitals can be eliminated by demanding the constraints

$$
\langle \phi_k | i\partial_t |\phi_q\rangle = 0 \quad \forall k, q = 1, ..., M.
$$

For a proof, that this choice of constraints corresponds to a unitary transformation on the set of orbitals and does not alter the Hilbert space described by this set, see appendix B. With these constraints, also the coefficients’ equation of motion simplify – the matrix elements of the Hamiltonian with the configuration now read [compare equation (46)]

$$
\hat{\mathcal{H}}_{n\bar{n'}} = \langle \bar{n}; t|\hat{\mathcal{H}}|n\rangle; n, \bar{n}',
$$

(56)

i.e., the time-derivative from equation (46) is dropped. Together, the equations of motion of the MCTDHB ansatz take on the final, appealing form

$$
i\partial_t |\phi_j\rangle = \hat{P} \left[ \hat{h} |\phi_j\rangle + \sum_{s,q,l=1}^M \{ \rho(t) \}_{jk}^{(-1)} \rho_{ksql} \hat{W}_{sl} |\phi_q\rangle \right]; \quad \hat{P} = 1 - \sum_{k'=1}^M |\phi_{k'}\rangle \langle \phi_{k'} |,
$$

(57)

$$
\mathcal{H}(t)C(t) = i\partial_t C(t).
$$

(58)
In almost all cases there is no analytical solution to these equations and to the time-dependent many-boson Schrödinger equation in general. Nevertheless, one can solve the TDSE numerically exactly using a numerical solution of the above equations for the following reasons: the ansatz used for the derivation of MCTDHB is formally exact and our derivation used the variational principle. When one finds the convergence of the above equations with respect to the number of used variational parameters, one is guaranteed that the obtained solution is also a solution of the TDSE. This has also been proven in a convergence study with an interacting time-dependent and exactly solvable many-body model as well as for few-boson systems in the fermionization limit.

It is important to notice, that equations (57) and (58) contain the TDGP and the TDMF approaches in a self-consistent way – if the TDGP or the TDMF is indeed applicable to a problem, the solutions provided by MCTDHB will be identical to them. Since the number of variational parameters is controlled in the MCTDHB approach by the number of used orbitals $M$, one can read the error of a computation from the smallest occupation of an orbital. Usually, the term numerically exact is invoked if the least occupation is smaller than $N \times 10^{-4}$.

The numerical solution of equations (57) and (58) has to happen simultaneously since they are coupled. The integration follows a seven-step integration scheme that dynamically adapts the time-step according to the error tolerance demanded. This scheme is implemented in the recursive MCTDHB software package (R-MCTDHB) and documented in the literature appended below. How the obtained many-body dynamics can be analyzed, will be part of the next lecture.

**Related Literature**

5 Quantities of interest from a many-body point of view

This section is dedicated to how to analyse the dynamics of many-body systems. Generally, having solved the time-dependent many-body Schrödinger equation provides us with a many-body wavefunction \( \Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N; t) \) which is high-dimensional and potentially complicated object. In order to measure the ongoing many-body physics one needs to define simpler and more intuitive quantities that provide information on the state of the system. The definitions of such quantities is given in the following section and afterwards the example of a many-boson system tunneling to open space is discussed.

5.1 Definitions

The standard measure for the state of the system is the one-body density \( \rho(\vec{r}; t) \) of the system,

\[
\rho(\vec{r}; t) = \int d\vec{r}_2 d\vec{r}_3 \cdots d\vec{r}_N \Psi^*(\vec{r}, \vec{r}_2, ..., \vec{r}_N; t) \Psi(\vec{r}, \vec{r}_2, ..., \vec{r}_N; t).
\]  (59)

This defines the probability to measure a particle at \( \vec{r} \) at time \( t \) while the information on all other particles is ignored, i.e., their coordinates traced out by integration (i.e. measuring them everywhere). \( \rho(\vec{r}; t) \) is the diagonal of the reduced one-body density matrix (1-RDM) \( \rho^{(1)} \) of the system,

\[
\rho^{(1)}(\vec{r}_1'|\vec{r}_1; t) = N \int d\vec{r}_2 d\vec{r}_3 \cdots d\vec{r}_N \Psi^*(\vec{r}_1', \vec{r}_2, ..., \vec{r}_N; t) \Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N; t).
\]  (60)

The 1-RDM is a trace of all but one particle from the full density operator \( |\Psi\rangle \langle \Psi| \). One can represent \( \rho^{(1)}(\vec{r}_1'|\vec{r}_1; t) \) in a basis representation,

\[
\rho^{(1)}(\vec{r}_1'|\vec{r}_1; t) = \sum_{k} \rho_{kq} \phi^*_k(\vec{r}_1'; t) \phi_q(\vec{r}_1; t) = \sum_{k} \rho^{(NO)}_{k}(t) \phi^*_k(t) \phi_k(t).
\]  (61)

In the last equation we diagonalized the matrix elements \( \rho_{kq} \) to get the time-dependent natural occupations \( \rho^{(NO)}_{k}(t) \) and natural orbitals \( \phi^{(NO)}(t) \). It’s noteworthy that the natural orbitals are a unique basis; the natural representation necessitates only a minimal effort to store and compute the reduced one-body density matrix. From the natural orbital occupations one can learn how many one-particle states are (macroscopically) occupied and contribute to the dynamics of the system. Condensation or fragmentation of a system is thus related to the natural occupations of the system: if only a single occupation \( \rho^{(NO)}_{k}(t) \) is macroscopical, then only a single orbital determines all the many-body features and the wavefunction is a product of this orbital and is referred to as condensed state – if, on the other hand, several occupations \( \rho^{(NO)}_{k}(t) \) are macroscopical, then the wavefunction \( |\Psi\rangle \) is dependent on multiple single-particle states and is referred to as a fragmented state. In other words, the degree of condensation of a system is defined by how well its many-body wavefunction can be represented as a product of a single complex valued function. The best quantity to quantify this property is the normalized one-body correlation function,

\[
g^{(1)}(\vec{r}_1'|\vec{r}_1; t) = \frac{\rho^{(1)}(\vec{r}_1'|\vec{r}_1; t)}{\sqrt{\rho(\vec{r}_1'; t) \rho(\vec{r}_1; t)}}.
\]  (62)

When only a single state is contributing to the many-body state at positions \( \vec{r}_1' \) and \( \vec{r}_1 \) then one finds \( |g^{(1)}(\vec{r}_1'|\vec{r}_1;)|^2 = 1 \). A state for which \( |g^{(1)}|^2 = 1 \) holds for all positions is also referred to as first-order coherent. Interestingly, one can hence find out with \( g^{(1)} \) where the first-order coherence is lost and this probably allows to make conclusions on the many-body mechanism
that lies behind. It’s interesting to note here, that one can of course analyze equivalently momentum space representations of the density \( \rho(\vec{r}; t) \), 1-RDM \( \rho^{(1)}(\vec{r}_1; t) \), or \( g^{(1)}(\vec{r}_1^1; t) \) by computing the Fourier transform \( \phi^{(NO)}(\vec{k}; t) \) of the respective natural orbitals and constructing \( \rho^{(1)} \) using the natural occupations \( \rho^{(NO)}_i(t) \):

\[
\rho^{(1)}(\vec{k}_1|\vec{k}_1'; t) = \sum_k \rho_k^{(NO)}(t) \phi_k^{*}(\vec{k}; t) \phi_k^{(NO)}(\vec{k}_1'; t).
\]

Analogously, the momentum space correlation function can be defined as \( g^{(1)}(\vec{k}_1|\vec{k}_1'; t) = \frac{\rho^{(1)}(\vec{k}_1|\vec{k}_1'; t)}{\sqrt{\rho^{(1)}(\vec{k}_1; t)\rho(\vec{k}_1'; t)}} \).

This function can be used to judge at which momenta the first-order coherence of the system is lost. In the same manner as the 1-RDM and the first order correlation function \( g^{(1)} \) the two-body reduced density matrix (2-RDM), \( \rho^{(2)} \) and normalized second-order correlation function \( g^{(2)} \) can be defined (for the general definition of the \( p \)-RDM and \( g^{(p)} \), see appendix C). The 2-RDM \( \rho^{(2)} \) and its diagonal are given by

\[
\rho^{(2)}(\vec{r}_1', \vec{r}_2'|\vec{r}_1, \vec{r}_2; t) = N(N-1) \int d\vec{r}_3d\vec{r}_4 \cdots d\vec{r}_N \Psi^*(\vec{r}_1', \vec{r}_2', \vec{r}_3, ..., \vec{r}_N; t)\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N; t); \quad (64)
\]

\[
\rho^{(2)}(\vec{r}_1, \vec{r}_2; t) \equiv \rho^{(2)}(\vec{r}_1 = \vec{r}_1', \vec{r}_2 = \vec{r}_2'|\vec{r}_1, \vec{r}_2; t).
\]

This quantity measures to the probability to find two particles simultaneously at positions \( \vec{r}_1 \) and \( \vec{r}_2 \) at time \( t \). Using the same strategy as in the case of \( \rho^{(1)} \) to represent functions in a basis, we can represent also \( \rho^{(2)} \) in a basis of single-particle states:

\[
\rho^{(2)}(\vec{r}_1', \vec{r}_2'|\vec{r}_1, \vec{r}_2; t) = \sum_{k,s,q,l} \rho_{ksql} \phi_k^*(\vec{r}_1; t)\phi_s^*(\vec{r}_2; t)\phi_q(\vec{r}_1; t)\phi_l(\vec{r}_2; t); \quad (65)
\]

The momentum space representations are identical to the above, but the single particle functions \( \{\phi_k(\vec{r}; t)\} \) are replaced by their Fourier transforms \( \{\tilde{\phi}_k(\vec{k}; t)\} \). The diagonal the two-body correlation function \( g^{(2)}(\vec{r}_1 = \vec{r}_1', \vec{r}_2 = \vec{r}_2'|\vec{r}_1, \vec{r}_2; t) = g^{(2)}(\vec{r}_1, \vec{r}_2; t) \) relates \( \rho^{(2)} \) to \( \rho^{(1)} \):

\[
g^{(2)}(\vec{r}_1, \vec{r}_2; t) = \frac{\rho^{(2)}(\vec{r}_1, \vec{r}_2; t)}{\rho(\vec{r}_1; t)\rho(\vec{r}_2; t)}. \quad (66)
\]

Intuitively, the diagonal of \( g^{(2)} \) measures how much the simultaneous measurement of two particles at \( \vec{r}_1 \) and \( \vec{r}_2 \) differs from the separate measurement of two particles at \( \vec{r}_1 \) and \( \vec{r}_2 \). From a stochastic point of view, the diagonal of \( g^{(2)} \) measures the (in-)dependence of the measurement of particles at \( \vec{r}_1 \) and \( \vec{r}_2 \). The case \( g^{(2)}(\vec{r}_1, \vec{r}_2; t) < 1 \) is referred to as anti-bunching and the case \( g^{(2)}(\vec{r}_1, \vec{r}_2; t) > 1 \) is termed bunching. Full 2-nd order or two-particle coherence is the achieved for \( g^{(2)}(\vec{r}_1, \vec{r}_2; t) = 1 \) – that is, when the measurements of any two particles at any positions \( \vec{r}_1, \vec{r}_2 \) are stochastically independent.

### 5.2 Analysis example: Many-body tunneling to open space

In this section the measures to quantify the dynamics of many-body systems which were introduced in the previous subsection are analyzed in the example of many-body tunneling to open space dynamics. We investigate systems of \( N = 2, 4, 101 \) particles with a contact interparticle interaction in one spatial dimension and an interparticle interaction strength of \( \lambda = \lambda_0(N - 1) = 0.3 \). To model the tunneling to open space process, we first prepare the eigenstate of an interacting system in a parabolic trap \( V(x; t \leq 0) \). Subsequently, the trap is
**Figure 4: Protocol of the tunneling process.** An initial density $\rho(x, t < 0)$ (blue line) is prepared as the groundstate of the interacting system in a parabolic trap $V(x, t < 0)$ (dashed black line). The trap is transformed to the open shape $V(x, t \geq 0)$ (black line), which allows the system to tunnel to open space. Figure reprinted from PNAS 109, 13521 (2012). See this article for the detailed form of the potential.

Transformed to a shape $V(x; t > 0)$ which allows for tunneling through a potential barrier to open space. See Fig. 4 for a plot of $V(x; t \leq 0)$ and $V(x; t > 0)$. The time-evolution of the density can best be quantified by investigating the real-space and momentum space nonescape probabilities $P^x_{not}$ and $P^k_{not}$. In real-space $P^x_{not}(t)$ is simply the integral

$$P^x_{not}(t) = \int_0^C dx \rho(x; t),$$

where $C$ denotes the position of the maximum of the barrier. Complementarily, $P^k_{not}$ measures by a least-squares fit, how much of the momentum space density $\rho(k; t)$ has a Gaussian shape $\rho^\text{Gauss}(k; t)$:

$$P^k_{not}(t) = \int dk \rho^\text{Gauss}(k; t).$$

For a plot, see Figure 5. Since the two descriptions using $P^x_{not}(t)$ and $P^k_{not}(t)$, respectively, do coincide, it’s natural to consider the Hilbert space of the system split into an exterior and an interior part and to attribute the part of the momentum density $\rho(k; t)$ which is not of Gaussian shape to the exterior part of the wavefunction, i.e., $\rho^\text{exterior}(k; t) = \rho(k; t) - \rho^\text{Gauss}(k; t)$ [cf. equation (68)]. To proceed, let us have a look at the exterior part of the momentum distribution.

**Figure 5: Many-body tunneling to open space is a fundamentally exponential decay process.** To confirm that the fraction of atoms remaining in the trap decays exponentially with time, we depict the density related nonescape probabilities $P^x_{not}(t)$ in real and $P^k_{not}(t)$ in momentum space, indicated by the respective solid green and red lines. Interestingly, the rate of the decay does not depend much on the particle number $N$. All quantities shown are dimensionless. Figure reprinted from PNAS 109, 13521 (2012).
Figure 6: The peak structures in the momentum distributions characterize the physics of many-body tunneling to open space. The total momentum distributions \( \rho(k, t) \) for \( N = 101 \) (top center) and their peak structures for \( N = 2, N = 4, N = 101 \), and the respective Gross-Pitaevskii solutions, at times \( t_1 < t_2 < t_3 < t_4 \). The broad Gaussian-shaped backgrounds correspond to the bosons remaining in the trap, the sharp peaks with positive momenta can be associated with the emitted bosons. For \( N = 2 \) we find two peaks in panel i), for \( N = 4 \) we find three peaks and an emerging fourth peak at longer times, in panel ii). In panel iv) we find three washed out peaks for \( N = 101 \). The corresponding GP dynamics reveals only a single peak for all times in iii). The arrows in the plots mark the momenta obtained from the model consideration (see PNAS 109, 13521 (2012) for details). All quantities shown are dimensionless. Figure reprinted from PNAS 109, 13521 (2012).
Figure 7: Monitoring the coherence of the system. **Left:** The first order correlation functions in momentum space $|g^{(1)}(k'k; t)|^2$ for $N = 101$ are plotted at $t = 0, 400, 600, 700$. At $t = 0$ the system is totally coherent, i.e., $|g^{(1)}|^2 = 1$. At times $t > 0$, the system remains coherent everywhere in $k$-space apart from the region around $k = 1$, where we find peaks in the momentum distributions. The loss of coherence, $|g^{(1)}|^2 \approx 0$ only in these regions allows us to conclude that the source (trapped) bosons remain coherent at all times while the emitted ones are incoherent. **Right:** The time evolution of the first few natural occupation numbers $\rho_{NO}^{(N)}(t)$ for $N = 2$, $N = 4$, and $N = 101$ bosons. The coherence in the systems is gradually lost with time. The systems fragment because more and more natural orbitals become populated. All quantities shown are dimensionless. Figure reprinted from PNAS 109, 13521 (2012).

(Strikingly, the exterior momentum densities are in a narrow window of momenta and show a distinct peak structure: two peaks for $N = 2$ bosons, three and an emerging fourth peak for $N = 4$ particles, and a washed out, broad peak for $N = 101$ bosons. Conversely, the TDGP prediction shows only a single peak. The difference between the mean-field and the MCTDHB prediction is a signature of many-body effects, such as for instance fragmentation and it is hence tempting to make the conclusion that each of the peaks corresponds to a particle in a separate single-particle state travelling at a certain momentum. In fact, such a model consideration allows one to accurately predict the emission momenta of the particles (see black arrows in Figure 6 and PNAS 109, 13521 (2012) for details of the model). To get deeper insight in the many-body physics that cause the departure of the process from the mean-field description, it is instructive to analyze the natural occupations $\rho_{NO}^{(N)}(t)$ and the first-order correlation function $|g^{(1)}|^2$, see Figure 7. As anticipated from the discrepancies in $\rho(k; t)$ of the MCTDHB and TDGP descriptions, one indeed finds that the first-order coherence of the system is lost and fragmentation gradually develops throughout the tunneling to open space process. From $g^{(1)}(k'k; t)$ in the left panel of Figure 7 and the momentum distributions in Figure 6 we can even deduce the mechanism of the loss of coherence; loss of coherence, $|g^{(1)}|^2 \approx 0$, is occurring precisely at the positions in $k$-space where the peaks in $\rho(k; t)$ are appearing. For the particles at rest, i.e., with $k \leq 1$, $|g^{(1)}|^2 \approx 1$ holds and coherence is maintained. Therefore, the particles which are travelling in open space are losing their coherence both among each other and with the source. This, after enough particles have been ejected from the coherent source, leads to the gradual emergence of fragmentation. With this finding, we conclude the exposition of the quantities of interest, for further details, see PNAS 109, 13521 (2012) and Phys. Rev. A 89, 053620 (2014).
Related Literature


A Matrix elements of the reduced two-body density matrix

This appendix collects the matrix elements of the reduced two-body density matrix, \( \rho_{ksql} = \langle \Psi | b \dagger_k b \dagger_q b_l | \Psi \rangle \). We use here a shorthand notation for configurations \( \vec{n}_{ab} \) where one particle from the \( a \)-th orbital is removed and then added to the \( b \)-th orbital. Similarly, \( \vec{n}_{cd}^{ab} \) is a configuration where two particles are removed from the \( a \)-th and \( b \)-th orbitals and then added to the \( c \)-th and \( d \)-th orbital, respectively.

\[
\begin{align*}
\rho_{kkek} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k \left( n_k^2 - n_k \right), \\
\rho_{ksks} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k n_k n_s, \\
\rho_{kkqk} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k \sqrt{(n_k - 1)n_k(n_q + 1)(n_q + 2)}, \\
\rho_{kkll} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k (n_k - 1)\sqrt{n_k(n_l + 1)}, \\
\rho_{kssk} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k n_s \sqrt{n_k(n_s + 1)}, \\
\rho_{kkql} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k \sqrt{(n_k - 1)n_k(n_q + 1)(n_l + 1)}, \\
\rho_{ksqq} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k \sqrt{n_k n_s(n_q + 1)(n_q + 2)}, \\
\rho_{kssl} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k n_s \sqrt{n_k(n_l + 1)}, \\
\rho_{ksql} &= \sum_{\vec{n}} C_{\vec{n}}^k C_{\vec{n}}^k \sqrt{n_k n_s(n_q + 1)(n_l + 1)}. 
\end{align*}
\] (69)

B Orbital constraints

This appendix proves that the Hilbert subspace remains unchanged by demanding the orthogonality of the orbitals with respect to their temporal changes. Let’s define the matrix of overlaps of the orbitals and time derivatives \( i\partial_t \) of orbitals,

\[
D_{kq}(t) = i\langle \phi_k | i\partial_t | \phi_q \rangle. 
\] (70)

This matrix is Hermitian. Let’s assume the existence of a unitary transformation which transforms the orbitals as follows

\[
\tilde{\phi}_q = \sum_{k=1}^M U_{kq}(t) \phi_k(t), 
\] (71)

such that the transformed set now fulfills

\[
\tilde{D}_{kq} = i\langle \tilde{\phi}_k(t) | i\partial_t | \tilde{\phi}_q(t) \rangle = 0. 
\] (72)

To show that the unitary transform \( U \) exists, we compute the time derivative \( i\partial_t \tilde{\phi}_q \):

\[
i\partial_t \tilde{\phi}_q = \sum_{k=1}^M \left[ (i\partial_t U_{kq}(t)) \phi_k(t) + U_{kq}(t)(i\partial_t \phi_k(t)) \right]. 
\] (73)
Now we substitute this time derivative \( \frac{\partial}{\partial t} \) back into the definition of the constraints \( D_{kq}(t) = 0 \) and obtain

\[
\left[ \sum_{s=1}^{M} U_{sk}(t) \langle \phi_s(t) \rangle \right] \left[ \sum_{k=1}^{M} \left[ (i\partial_t U_{kq}(t)) |\phi_k(t)\rangle + U_{kq}(t)(i\partial_t |\phi_k(t)\rangle) \right] \right] = 0. \tag{74}
\]

Solving for the time-derivative of \( U \), we obtain,

\[
i\partial_t U_{sq}(t) = -\sum_{k=1}^{M} D_{sk}(t) U_{kq}(t). \tag{75}\]

This equation can be integrated and yields

\[
U(t) = \exp \left( i \int_0^t D(t') dt' \right) U(t = 0). \tag{76}\]

Since \( D \) is Hermitian, it remains to show that \( U(t = 0) \) is unitary and unique. To see this, we use the diagonal representation of \( D(t) \),

\[
D(t) = T^\dagger(t) d(t) T(t), \tag{77}\]

where \( d(t) \) is diagonal and contains the eigenvalues of \( D(t) \) on the diagonal. Using the equality \( e^{T^\dagger(t) d(t) T(t)} = T^\dagger(t) e^{d(t) T(t)} \) and taking the limit \( \lim_{\tau \to 0} \) in (76), we find:

\[
U(\tau) = T(0) \exp \left[ i \tau d(0) \right], \tag{78}\]

which shows that \( U \) is indeed a unitary matrix and therefore,

\[
\tilde{\phi}_q(\tau) = \sum_{k=1}^{M} U_{kq}(\tau) \phi_k(\tau) \quad \Rightarrow \quad \tilde{D}_{kq}(\tau) = 0. \tag{79}\]

So, by constructing \( U \) we have shown that the constraints \( \tilde{D} \) can be fulfilled using a unitary transform that does not alter the Hilbert subspace spanned by the set \( \phi_k \).

### C General definition of \( p \)-particle reduced densites and \( p \)-particle correlation

The \( p \)-particle reduced density (p-RDM) is the trace of all but \( p \) particles from the \( N \)-body density operator:

\[
\rho^{(p)}(\vec{r}_1',...,\vec{r}_p'|\vec{r}_1,...,\vec{r}_p; t) = \frac{N!}{(N-p)!} \int d\vec{r}_{p+1} \cdots d\vec{r}_N \Psi^*(\vec{r}_1',...,\vec{r}_p',\vec{r}_{p+1},...,\vec{r}_N; t) \Psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N; t). \tag{80}\]

From the p-RDM it is straightforward to compute a measure of the \( p \)-th order coherence, namely, the \( p \)-particle normalized correlation function \( g^{(p)} \), by normalizing \( \rho^{(p)} \) with the respective diagonals of \( \rho^{(1)} \):

\[
g^{(p)}(\vec{r}_1',...,\vec{r}_p') = \frac{\rho^{(p)}(\vec{r}_1',...,\vec{r}_p'|\vec{r}_1,...,\vec{r}_p; t)}{\sqrt{\prod_{i=1}^{p'} \rho(\vec{r}_i'; t) \rho(\vec{r}_i; t)}}. \tag{81}\]