Appendix A
Particle Loss Operators

In order to define an operator, whose expectation value defines the υ-particle loss from an N-indistinguishable-particle system it is convenient to first define corresponding projectors employing Heaviside functions. For the sake of simplicity the considerations in this paragraph are restricted to the one-dimensional case. The Heaviside functions readily are the projectors up to a certain position C—in the case of a tunneling problem C is usually the position of the barrier. Yet, it is noteworthy, that it is straightforward to generalize these considerations to projectors also in 2 or 3 dimensions. The one-dimensional projectors read:

$$\Theta_k^- = \Theta(C - x_k) = (1 - \Theta_k^+); \qquad \Theta_k^+ = \Theta(x_k - C). \tag{A.1}$$

In principle, these operators measure the probability density of particle k to be in the interior, $x_k < C$ (Θ_k^-), or the exterior $x_k > C$ (Θ_k^+) parts of space. These operators are the building blocks for the general operators describing the υ-particle loss from an N-particle reservoir, denoted by $\hat{L}_\upsilon^N$. Clearly, the $\hat{L}_\upsilon^N$ will be simple products of the 1D projectors above and it will be possible to exploit the indistinguishability of the particles in the reservoir for their computation. It is instructive to start with the case, where one measures the probability that the whole system survives. This is the probability of all particles remaining in the interior, $x_k < C, \forall k$. Thus one finds

$$\hat{L}_0^N = \prod_{i=1}^{N} \Theta_i^- \tag{A.2}$$

The expectation value of this operator is completely equivalent to the above defined wave function-related nonescape probability $P_{not,\Psi}(t)$, cf. Eq. (2.29), where $\Omega = \{x_i < C, i = 1, ..., N\}$:

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$$\langle\Psi|\hat{L}_0^N|\Psi\rangle = \int \Psi^*(x_1, ..., x_N; t) \prod_{i=1}^{N} \Theta_i^- \Psi(x_1, ..., x_N; t) dx_1 \cdots dx_N \quad \text{(A.3)}$$
$$= \int_{-\infty}^{C} \Psi^*(x_1, ..., x_N; t)\Psi(x_1, ..., x_N; t) dx_1 \cdots dx_N = P_{not,\Psi}(t).$$

In the last equality it is used that the action of $\hat{L}_0^N$ can be simply incorporated by restricting the boundaries for the integration on the different coordinates $x_1, ..., x_N$ to $x_i < C, i = 1, ..., N$. In the case in which all N particles of the N-particle reservoir are lost, one finds analogously:

$$\hat{L}_N^N = \prod_{i=1}^{N} \Theta_i^+. \quad \text{(A.4)}$$

It is instructive to write down the operators for the one- and two particle losses in order to generalize them to an arbitrary number $\upsilon \leq N$.

$$\hat{L}_1^N = \sum_{\kappa=1}^{N} \Theta_\kappa^+ \prod_{\substack{i=1 \\ i\neq\kappa}}^{N} \Theta_i^- = N\Theta_1^+ \prod_{i=2}^{N} \Theta_i^-, \quad \text{(A.5)}$$

$$\hat{L}_2^N = \sum_{\{\kappa,\nu\}} \Theta_\kappa^+ \Theta_\nu^+ \prod_{\substack{i=1 \\ i\neq\kappa \\ i\neq\nu}}^{N} \Theta_i^- = M_2 \Theta_1^+ \Theta_2^+ \prod_{i=3}^{N} \Theta_i^-. \quad \text{(A.6)}$$

Here, the sums are running over all possible configurations of one or two of the N particles being in the exterior and the respective last equality uses the indistinguishability of the considered particles. M_2 denotes the cardinality of the different possibilities to realize a subset of two elements out of N. Clearly, $M_2 = \binom{N}{2}$ and $M_\upsilon = \binom{N}{\upsilon}$. It is now straightforward to write down the υ-of-N-particle loss operator:

$$\hat{L}_\upsilon^N = \sum_{\{j_1,...,j_\upsilon\}} \left[\prod_{\kappa=1}^{\upsilon} \Theta_{j_\kappa}^+\right] \left[\prod_{\substack{i=1 \\ i\notin\{j_1,...,j_\upsilon\}}}^{N} \Theta_i^-\right] \quad \text{(A.7)}$$
$$= \binom{N}{\upsilon} \prod_{\kappa=1}^{\upsilon} \Theta_\kappa^+ \prod_{\xi=\upsilon+1}^{N} \Theta_\xi^-. \quad \text{(A.8)}$$

Here, the last equality uses the indistinguishability of the considered particles. With the expectation value of this operator it is possible to measure the loss of an arbitrary number υ of particles from a reservoir of N by defining an interior and an exterior region. Basically, the particle loss operators are nothing else but projectors on the

Hilbert space of a definite particle number whose coordinates are restricted. For instance, $\hat{L}_1^N$ is a projector on the Hilbert space where one coordinate is restricted to the exterior and all other $N-1$ coordinates are restricted to the interior. Note that, for an N-particle system, these are N-body operators and hence very difficult to evaluate. In practical numerical computations, N-body operators' expectation values require N-dimensional integrals to be evaluated, which is a demanding task.

Appendix B
The Concept of Local Fragmentation

Fragmentation, i.e., the macroscopic (of order $\mathcal{O}(N)$) occupation of more than one natural orbital, is a quantity intimately related to the natural occupations $\rho_i^{(NO)}(t)$, i.e., the eigenvalues of the reduced one-body density matrix $\rho^{(1)}(x_1'|x_1;t)$, cf. Sect. 2.1.2 and Ref. [1]. The 1-RDM is a quantity defined on the whole Hilbert space of the system under consideration as an integral of the wave function. It is a natural question to ask how to assess the fragmentation of a system *locally*, because the full information might not be available in a given experimental setup. From a fundamental theoretical point of view there are two ways of approaching the question. The first idea takes the 1-RDM and applies a projection to a subspace to obtain a new, truncated 1-RDM from which one computes the local natural occupations. The second way to obtain local occupation numbers applies the projection to the subspace on the wave function and computes from the truncated wave function a new 1-RDM on the considered subspace, from which in turn one can obtain local natural occupations. The first is termed 1-RDM-related local natural occupations and the second way is termed wave function-related local natural occupations. The scope of this section is to clarify the properties and the differences of the two approaches.

B.1 The 1-RDM-Related Local Natural Occupations

To define local occupation numbers $\tilde{\rho}_{i,\tau}^{(NO)}$ and local natural orbitals $\tilde{\phi}_{i,\tau}^{(NO)}$ it is a natural approach to simply truncate the 1-RDM by projection to some subspace $\Omega = \{(x_1, ..., x_N)\,|x_j \leq x_{\tau,j},\, j = 1, ..., N\}$ of the entire space $\mathcal{H}$. For the sake of simplicity one-dimensional systems are considered in this subsection. The projector $\hat{P}$ onto Ω is:

$$\hat{P} = \prod_{j=1}^{N} \hat{p}_j = \prod_{j=1}^{N} \Theta(x_{\tau,j} - x_j). \tag{B.1}$$

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Now one applies $\hat{P}$ to the 1-RDM $\rho^{(1)}(x_1|x_1'; t)$:

$$\begin{aligned} \hat{P}\rho^{(1)}(x_1|x_1'; t) &= \hat{p}_1\rho^{(1)}(x_1|x_1'; t) \\ &= \hat{p}_1 N \int dx_2 \cdots dx_N \Psi^*(x_1', x_2, ..., x_N; t)\Psi(x_1, ..., x_N; t). \end{aligned} \tag{B.2}$$

Here, it was firstly used that the 1-RDM is a function of only x_1 and x_1', so only $\hat{p}_1$ acts onto it. Secondly, the definition of $\rho^{(1)}$, see Eq. (2.24), was inserted. Next, one uses the possibility to express the 1-RDM expanded in a basis set ϕ_i, $i = 1, ..., M$, cf. the paragraph on natural orbitals and occupations:

$$\begin{aligned} \hat{p}_1\rho^{(1)}(x_1|x_1'; t) &= \hat{p}_1 \sum_{k,q=1}^{M} \rho_{kq}\phi_i^*(x_1', t)\phi_i(x_1, t) \\ &= \sum_{k,q=1}^{M} \rho_{kq}\hat{p}_1\phi_i^*(x_1', t)\hat{p}_1\phi_i(x_1, t) \\ &\equiv \sum_{k,q=1}^{M} \tilde{\rho}_{kq}\phi_{i,\tau}^*(x_1', t)\phi_{i,\tau}(x_1, t) \\ &\equiv \sum_{i=1}^{M} \tilde{\rho}_{i,\tau}^{(NO)}(t)\tilde{\phi}_{i,\tau}^{*(NO)}(x_1', t)\tilde{\phi}_{i,\tau}^{(NO)}(x_1, t). \end{aligned} \tag{B.3}$$

In the first step one uses the fact that $\hat{p}_1$ only acts on the functions used to expand $\rho^{(1)}$. In the second step, the respective truncated basis $\phi_{i,\tau} = \hat{p}_1\phi_i$, $i = 1, ..., M$ was introduced. In the last step the obtained truncated 1-RDM was diagonalized to obtain a set of truncated occupations, $\tilde{\rho}_{i,\tau}^{(NO)}(t)$, as well as a set of truncated natural orbitals $\tilde{\phi}_{i,\tau}^{(NO)}(x, t)$. Equation (B.3) also are an easy, practical guide for the implementation of this analysis tool.

B.2 The Wave function-Related Local Natural Occupations

In this section the notion of wave function-related local natural occupation numbers is introduced. In order to define local occupation numbers $\rho_{i,\tau}^{(NO)}(t)$ and local natural orbitals $\phi_{i,\tau}^{(NO)}$ starting from the wave function, one first uses the projector $\hat{P}$ defined in the previous subsection to obtain a truncated wave function Ψ_τ. This is done in the following specifically for the case of a multiconfigurational wave function:

$$\begin{aligned}\Psi_\tau(x_1,...,x_N,t) &= \hat{P}\Psi(x_1,...,x_N,t)\\ &= \hat{P}\sum_{\mathbf{n}} C_{\mathbf{n}}(t)|\mathbf{n};\mathbf{t}\rangle\\ &= \sum_{\mathbf{n}} C_{\mathbf{n}}(t)\hat{P}|\mathbf{n};\mathbf{t}\rangle\\ &\equiv \sum_{\mathbf{n}} C_{\mathbf{n}}(t)|\mathbf{n};\mathbf{t}\rangle_\tau.\end{aligned} \tag{B.4}$$

Here, the multiconfigurational ansatz for the wave function is inserted in the second line of the above equation. In this case, the projector $\hat{P}$ acts only on the configurations $|\mathbf{n},\mathbf{t}\rangle$ (third of the above equalities) and this leads to the introduction of new, projected configurations $|\mathbf{n};\mathbf{t}\rangle_\tau = \hat{\mathbf{P}}|\mathbf{n};\mathbf{t}\rangle$. Two things have to be noted here: first, that the new set of configurations is no longer orthogonal (!) and, second, that the projector $\hat{P}$ again only acts on the single particle functions constructing the permanents. In principle one thus relies on the same basis set $\phi_{i,\tau}$, $i = 1,...,M$ as in the previous paragraph. To continue, one constructs a truncated 1-RDM $\rho_\tau(x_1|x_1';t)$ from the truncated wave function Ψ_τ:

$$\begin{aligned}\rho_\tau(x_1|x_1';t) &= N\int dx_2\cdots dx_N\Psi_\tau^*(x_1',x_2,...,x_N)\Psi_\tau(x_1,x_2,...,x_N)\\ &= N\int_\Omega dx_2\cdots dx_N\hat{p}_1\Psi^*(x_1',x_2,...,x_N)\hat{p}_1\Psi(x_1,x_2,...,x_N).\end{aligned} \tag{B.5}$$

Here, the first identity is simply the definition of $\rho^{(1)}$ with Ψ replaced by Ψ_τ and in the second identity the action of the projectors was incorporated as the boundaries of the integration. Of course, as in the previous subsection, also this truncated 1-RDM can be represented in the basis $\phi_{i,\tau}$, $i = 1,...,M$ with weights $\rho'_{kq}(t)$:

$$\begin{aligned}\rho_\tau^{(1)}(x_1|x_1';t) &= \sum_{k,q=1}^{M}\rho'_{kq}\phi^*_{i,\tau}(x_1',t)\phi_{i,\tau}(x_1,t)\\ &\equiv \sum_{i=1}^{M}\rho'^{(NO)}_{i,\tau}(t)\phi^{*(NO)}_{i,\tau}(x_1',t)\phi^{(NO)}_{i,\tau}(x_1,t).\end{aligned} \tag{B.6}$$

Note that $\rho'_{kq}(t) \neq \tilde{\rho}_{kq}(t)$. This is because the space where the wave function is integrated or, in other terms, the applied projectors are different, see Eqs. (B.2) and (B.3), from the case of the truncated $\rho^{(1)}$ in the previous subsection. To assess and understand better the concept of local fragmentation, it is instructive to compare the 1-RDM based approach to the present wave function-based approach directly.

B.3 Comparison of the Wave function- and 1-RDM-Based Approaches

The simplest way to compare two quantities is to simply calculate their difference. For the wave function-based and 1-RDM based local 1-RDMs this is achievable straightforwardly by subtracting Eq. (B.5) from (B.2):

$$\begin{aligned}
\rho'_{1,\tau} - \tilde{\rho}_{1,\tau} &= \hat{p}_1 N \int dx_2 \cdots dx_N \Psi^*(x'_1, x_2, ..., x_N; t)\Psi(x_1, ..., x_N; t) \\
&\quad - N \int_{\Omega} dx_2 \cdots dx_N \hat{p}_1 \Psi^*(x'_1, x_2, ..., x_N) \hat{p}_1 \Psi(x_1, ..., x_N) \\
&= \hat{p}_1 \int_{\mathcal{H}\setminus\Omega} dx_2 \cdots dx_N \Psi^*(x'_1, x_2, ..., x_N)\Psi(x_1, ..., x_N).
\end{aligned} \tag{B.7}$$

A comment on the two approaches from a practical point of view is in order. The computation of the wave function-related local occupations is a numerically demanding task because it relies on N-body operators or quantities. In particular, the evaluation of the integral in Eq. (B.5) demands (unitary) transformations of permanents (see Eqs. (2.16), (2.18)) which constitute a big numerical effort and are not yet implemented in the software developed (see Ref. [2]) and in use throughout this thesis.

Appendix C
Reduced One-Body Density Matrix and Momentum Distribution of a Gross–Pitaevskii Wave Function Composed of Two Plane Waves

This Appendix demonstrates that one can in principle construct coherent quantum product states for $N = 2$ bosons incorporating two momenta.

Assumed GP Orbital:
One assumes a Gaussian $g(x)$ inside the well, $x < x_c$, and 2 plane waves with momenta k_1 and k_2 outside, $x > x_c$, where the Gaussian is 0 (no overlap is assumed).

$$\varphi(x) = g(x) + \theta(x - x_C)\left[e^{ik_1 x} + e^{ik_2 x}\right]. \tag{C.1}$$

Construction of the GP-Wave function:
Eq. (C.1) is used and the normalization is of no significance here and skipped therefore:

$$\begin{aligned}
\Psi_{GP} &= \prod_{i=1}^{N} \varphi(x_i); \qquad N := 2 \\
&= \prod_{i=1}^{2} g(x_i) + \theta(x_i - x_C)\left[e^{ik_1 x_i} + e^{ik_2 x_i}\right] \qquad \text{(C.2)} \\
&= g(x_1)g(x_2) \\
&\quad + \theta_{x_C}\left[e^{ik_1(x_1+x_2)} + e^{i(k_1x_1+k_2x_2)} + e^{i(k_2x_1+k_1x_2)} + e^{i(k_2x_1+k_2x_2)}\right]. \qquad \text{(C.3)}
\end{aligned}$$

Construction of the RDM:

$$\begin{aligned}
\rho^{(1)}(x_1|x_1') &= N\int \Psi^*(x_1', x_2, ..., x_N) \times \Psi(x_1, ..., x_N)dx_2 \cdots dx_N \\
&= 2\int \Psi^*_{GP}(x_1', x_2) \times \Psi_{GP}(x_1, x_2)dx_2 \qquad \text{(C.4)} \\
&= \int \Big\{ (g(x_1))^2\, g(x_1')g(x_2)
\end{aligned}$$

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$$+ \quad \theta_{x_C} \times \left[e^{-ik_1(x_1'+x_2)} + e^{-i(k_1x_1'+k_2x_2)} + e^{-i(k_2x_1'+k_1x_2)} + e^{-i(k_2x_1'+k_2x_2)} \right]$$
$$\times \quad \left[e^{ik_1(x_1+x_2)} + e^{i(k_1x_1+k_2x_2)} + e^{i(k_2x_1+k_1x_2)} + e^{i(k_2x_1+k_2x_2)} \right] \Big\} dx_2, \quad \text{(C.5)}$$

using the abbreviation $\theta_{x_C} := \theta(x_1 - x_C)\theta(x_2 - x_C)$ in the step from Eq. (C.4) to Eq. (C.5). Evaluating the integrand, $I = \Psi^*(x_1, x_1')\Psi(x_1, x_2)$, of Eq. (C.5):

$$\begin{aligned} I = (g(x_1))^2 g(x_1')g(x_2) + \theta_{x_C} \times \\ \Big\{ e^{i(k_1x_2-k_1x_1')} + e^{i(k_2x_2-k_1x_1')} + e^{i(k_2x_1+k_1x_2-k_1(x_1+x_1'))} + e^{i(k_2x_1+k_2x_2-k_1(x_1+x_1'))} \\ + \quad e^{i(k_1x_2-k_2x_1')} + e^{i(k_2x_2-k_2x_1')} + e^{i(k_2x_1+k_1x_2-k_1x_1-k_2x_1')} + e^{i(k_2x_1+k_2x_2-k_1x_1-k_2x_1')} \\ + \quad e^{i(k_1x_1+k_1x_2-k_2x_1-k_1x_1')} + e^{i((k_1-k_2)x_1+k_2x_2-k_1x_1'} + e^{i(k_1x_2-k_1x_1')} + e^{i(k_2x_2-k_1x_1')} \\ + \quad e^{i((k_1-k_2)x_1+k_1x_2-k_2x_1')} + e^{i((k_1-k_2)x_1+k_2x_2-k_2x_1')} + e^{i(k_1x_2-k_2x_1')} + e^{i(k_2(x_2-x_1'))} \Big\}. \end{aligned} \quad \text{(C.6)}$$

Performing the Integration, $\rho^{(1)} = \int I dx_2$, using the abbreviations and assuming the existence of $A = \int \theta_{x_C} e^{i(k_1x_2)} dx_2$ and $B = \int \theta_{x_C} e^{i(k_2x_2)} dx_2$ and $C = \int g(x_2)dx_2$

$$\begin{aligned} \rho^{(1)} \quad &= \int C\,(g(x_1))^2\, g(x_1') + \theta_{x_C} \times \\ &\Big\{ Ae^{-ik_1x_1'} + Be^{ik_1x_1'} + Ae^{i(k_2x_1-k_1(x_1+x_1'))} + Be^{i((k_2-k_1)x_1-k_1x_1')} \\ &+ \quad Ae^{-ik_2x_1'} + Be^{-ik_2x_1'} + Ae^{i((k_2-k_1)x_1-k_2x_1')} + Be^{i((k_2-k_1)x_1-k_2x_1')} \\ &+ \quad Ae^{i((k_1-k_2)x_1-k_1x_1')} + Be^{i((k_1-k_2)x_1-k_1x_1')} + Ae^{-ik_1x_1'} + Be^{-ik_1x_1'} \\ &+ \quad Ae^{i((k_1-k_2)x_1-k_2x_1')} + Be^{i((k_1-k_2)x_1-k_2x_1')} + Ae^{-ik_2x_1'} + e^{-ik_2x_1'} \Big\}. \end{aligned} \quad \text{(C.7)}$$

After simplifications, one obtains:

$$\begin{aligned} \rho^{(1)} = \int C\,(g(x_1))^2\, g(x_1') + \theta_{x_C} \times \\ \Big\{ (2(A+B)) \left(e^{-ik_1x_1'} + e^{-ik_2x_1'} \right) \\ + (A+B) \Big[e^{i((k_2-k_1)x_1-k_1x_1')} + e^{i((k_1-k_2)x_1-k_1x_1')} \\ + e^{i((k_1-k_2)x_1-k_2x_1')} + e^{i((k_2-k_1)x_1-k_2x_1')} \Big] \Big\}. \end{aligned} \quad \text{(C.8)}$$

Calculation of the Momentum Distribution:
By definition the momentum distribution is the Fourier transform of the RDM: $\rho(j) = \int dx_1 dx_1' e^{-ij(x_1-x_1')} \rho^{(1)}(x_1|x_1')$. Using the abbreviations $\aleph(j)$ for the Gaussian-shaped Fourier transforms of the Gaussian $g(x)$ one arrives at:

$$\rho^{(1)}(j) = C\aleph(j) + \int \Big\{\theta_{x_C} \tag{C.9}$$
$$\times 2A\left[e^{-i((k_1-j)x_1'+jx_1)} + e^{-i((k_2-j)x_1'+jx_1)}\right]$$
$$+ 2B\left[e^{-i((k_2-j)x_1'+jx_1)} + e^{-i((k_1-j)x_1'+jx_1)}\right]$$
$$+ (A+B)\left[e^{-i((k_2-k_1)x_1-k_1x_1'-j(x_1-x_1'))} + e^{-i((k_1-k_2)x_1-k_1x_1'-j(x_1-x_1'))}\right]\Big\}dx_2$$
$$= C\aleph(j) + (2A+2B)\left[\delta(j-k_1) + \delta(j-k_2)\right]$$
$$+ (A+B)\left[\delta(j-k_1)\delta(j-(k_2-k_1))\right]$$
$$+ (A+B)\left[\delta(j-k_1)\delta(j-(k_1-k_2))\right] \tag{C.10}$$
$$= C\aleph(j) + (2A+2B)\left[\delta(j-k_1) + \delta(j-k_2)\right]. \tag{C.11}$$

where Eq. (C.11) follows from the fact that $k_2 \neq 0$ in Eq. (C.10).
A comment is in place here: the momentum density and reduced density matrix described above do resemble the ones obtained in exact numerical simulations (cf. Chaps. 6, 7). The key difference is, that the exact solutions do not preserve the coherence whenever there is more than one momentum present. This is caused by the state constructed above being energetically much higher than its prescribed fragmented counterpart (cf. Appendices D, G). States of higher energy are excluded from the dynamics by the TDVP [3].

Appendix D
Derivation of the Reduced One-body Density for a System Tunneling with Two Momenta

The RDM of the $N = 2$ boson system with the wave function constructed in the orbitals given in Eq. (5.24) reads as follows:

$$
\begin{aligned}
\rho^{(1)}(x_1|x_1') &= \int \Psi(x_1, ..., x_N) \times \Psi^*(x_1', x_2, ..., x_N) dx_2 \cdots dx_N \\
&= \int \Psi(x_1, x_2) \times \Psi^*(x_1', x_2) dx_2 \\
&= (C_{\mathbf{n_1}})^2 \int dx_2 \left[e^{-\frac{1}{2}(x_1^2 + (x')_1^2 + 2x_2^2)} + \theta(x - x_c) e^{ik_1(x_1 - x_1')} \right] \\
&\quad + \theta(x - x_c) C_{\mathbf{n_1}} C_{\mathbf{n_2}} \int dx_2 \left[e^{i(k_1(x_1+x_2) - k_1 x_1' - k_2 x_2)} + e^{i(k_1(x_1+x_2) - k_1 x_2 - k_2 x_1')} \right] \\
&\quad + \theta(x - x_c) C_{\mathbf{n_1}} C_{\mathbf{n_2}} \int dx_2 \left[e^{i((k_1 x_1 + k_2 x_2) - k_1(x_1' + x_2))} + e^{i(k_1 x_2 + k_2 x_1 - k_1(x_1' + x_2))} \right] \\
&\quad + \theta(x - x_c)(C_{\mathbf{n_2}})^2 \int dx_2 \left[e^{i(k_1(x_1 - x_1'))} + e^{i(k_2(x_1 - x_1'))} \right] \\
&\quad + \theta(x - x_c)(C_{\mathbf{n_2}})^2 \int dx_2 \left[e^{i(k_1 x_1 - k_1 x_2 + k_2 x_2 - k_2 x_1')} + e^{i(k_1 x_2 + k_2 x_1 - k_1 x_1' - k_2 x_2)} \right] \\
&\quad + \theta(x - x_c)(C_{\mathbf{n_3}})^2 \int dx_2 \left[e^{ik_2(x_1+x_2) - ik_2(x_1'+x_2)} \right] \\
&\quad + \theta(x - x_c) C_{\mathbf{n_3}} C_{\mathbf{n_2}} \int dx_2 \left[e^{-i(k_2(x_1'+x_2)} (e^{i(k_1 x_1 + k_2 x_2)} + e^{i(k_1 x_2 + k_2 x_1)}) \right] \\
&\quad + \theta(x - x_c) C_{\mathbf{n_3}} C_{\mathbf{n_2}} \int dx_2 \left[e^{i(k_2(x_1+x_2)} (e^{-i(k_1 x_1' + k_2 x_2)} + e^{-i(k_1 x_2 + k_2 x_1')}) \right] \\
&\quad + \theta(x - x_c) C_{\mathbf{n_3}} C_{\mathbf{n_1}} \int dx_2 \left[e^{-ik_2(x_2 + x_1')} e^{ik_1(x_1+x_2)} + e^{ik_2(x_2+x_1)} e^{-ik_1(x_1'+x_2)} \right].
\end{aligned}
\tag{D.1}
$$

This equation drastically reduces when one takes the diagonal $x_1 = x_1'$ and uses the addition theorems $\cos^2\left(\frac{\lambda}{2}\right) = \frac{1}{2}(1 + \cos(\lambda))$ and $\cos(\lambda) = \frac{e^{i\lambda} + e^{-i\lambda}}{2}$:

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$$\begin{aligned}
\rho(x_1|x_1) &= (C_{\mathbf{n_1}})^2\left[\sqrt{\pi}e^{-x_1^2}\right] \\
&+ C_{\mathbf{n_1}}C_{\mathbf{n_2}}\theta(x-x_c)\left[4\cos^2(x_1(\frac{k_1-k_2}{2}))\right] \\
&+ (C_{\mathbf{n_2}})^2\theta(x-x_c)\left[4\cos^2(x_1(\frac{k_1-k_2}{2})\right] \\
&+ C_{\mathbf{n_3}}C_{\mathbf{n_2}}\theta(x-x_c)\left[4\cos^2(\frac{(k_1-k_2)}{2}x_1)\right] \\
&+ C_{\mathbf{n_3}}C_{\mathbf{n_1}}\theta(x-x_c)\left[2\cos((k_1-k_2)x_1)\right] \\
&+ \theta(x-x_c)\left[2(C_{\mathbf{n_3}})^2+2(C_{\mathbf{n_2}})^2\right]x_2 \\
&= (C_{\mathbf{n_1}})^2\left[\sqrt{\pi}e^{-x_1^2}\right] \\
&+ \theta(x-x_c)\left[(C_{\mathbf{n_2}})^2+C_{\mathbf{n_3}}C_{\mathbf{n_2}}+C_{\mathbf{n_1}}C_{\mathbf{n_2}}\right]\left[4\cos^2(x_1(\frac{k_1-k_2}{2}))\right] \\
&+ \theta(x-x_c)C_{\mathbf{n_3}}C_{\mathbf{n_1}}2\cos((k_1-k_2)x_1) \\
&+ \theta(x-x_c)\left[2(C_{\mathbf{n_3}})^2+2(C_{\mathbf{n_2}})^2\right]x_2.
\end{aligned} \tag{D.2}$$

As the reduced one body density is a function of x_1 and x_1' the term with x_2 is actually a constant coming from the undefined integral in the x_2 degree of freedom. Thus, $x_2 = \xi = const.$, is furthermore assumed. Thus one gets after introducing the abbreviations $D = (C_{\mathbf{n_1}})^2$; $E = \theta(x-x_c)\left[(C_{\mathbf{n_2}})^2+C_{\mathbf{n_3}}C_{\mathbf{n_2}}+C_{\mathbf{n_1}}C_{\mathbf{n_2}}\right]$; $G = \theta(x-x_c)\left[2(C_{\mathbf{n_3}})^2+2(C_{\mathbf{n_2}})^2\right]\xi$ and $F = \theta(x-x_c)C_{\mathbf{n_3}}C_{\mathbf{n_1}}$:

$$\begin{aligned}
\rho(x_1|x_1) = D&\left[\sqrt{\pi}e^{-x_1^2}\right] \\
&+ 4E\left[\cos^2(x_1(\frac{k_1-k_2}{2}))\right] \\
&+ 2F\cos((k_1-k_2)x_1) \\
&+ G.
\end{aligned} \tag{D.3}$$

Appendix E
Derivation of the Diagonal of the Reduced Two-body Density for a System Tunneling with Two Momenta

The two-body density of the $N = 2$ boson system with the wave function constructed from the orbitals given in Eq. (5.24) reads as follows:

$$\begin{aligned}\rho^{(2)}(x_1, x_2|x_1, x_2; t) &= \int \Psi(x_1, ..., x_N)\Psi^*(x_1, ..., x_N)dx_3 \cdots dx_N \\ &= \Psi(x_1, x_2)\Psi^*(x_1, x_2) \\ &= (C_{\mathbf{n_1}})^2 \left[e^{-(x_1^2+x_2^2)}\right] \\ &\quad + \theta(x-x_c)(C_{\mathbf{n_1}}\frac{C_{\mathbf{n_2}}}{\sqrt{2}})\left[e^{i(k_1-k_2)x_1} + e^{i(k_2-k_1)x_1} + e^{i(k_1-k_2)x_2} + e^{i(k_2-k_1)x_2}\right] \\ &\quad + \theta(x-x_c)(C_{\mathbf{n_3}})^2\left[e^{i[(k_1-k_2)x_1+(k_2-k_1)x_2]} + e^{i[(k_1-k_2)x_2+(k_2-k_1)x_1]}\right].\end{aligned} \tag{E.1}$$

The indices $\mathbf{n_1}, \mathbf{n_2}, \mathbf{n_3}$ refer to the configurations $|2, 0\rangle$, $|1, 1\rangle$, $|0, 2\rangle$, respectively. Introducing the abbreviations $A = (C_{\mathbf{n_1}})^2$; $B =; \theta(x - x_c)(C_{\mathbf{n_1}}\frac{C_{\mathbf{n_2}}}{\sqrt{2}})$ and $C = \theta(x - x_c)(C_{\mathbf{n_3}})^2$ and using the relation $\cos(\lambda) = \frac{e^{i\lambda}+e^{-i\lambda}}{2}$ one arrives at the following:

$$\begin{aligned}\rho^{(2)}(x_1, x_2|x_1, x_2; t) \quad &= A\left[e^{-(x_1^2+x_2^2)}\right] \\ &\quad + B\left[2\left(\cos((k_1-k_2)x_1) + \cos((k_1-k_2)x_2)\right)\right] \\ &\quad + C\left[2\cos((k_1-k_2)x_1)\cos((k_1-k_2)x_2)\right].\end{aligned} \tag{E.2}$$

The second row of the equation above can be transformed to a single factor via the relation $\cos(\lambda) + \cos(\lambda') = \cos(\frac{\lambda+\lambda'}{2}) \cdot \cos(\frac{\lambda-\lambda'}{2})$ times the coefficient B: if one further assumes real coefficients the diagonal of $\rho^{(2)}$ reads as follows:

$$\begin{aligned}\rho^{(2)}(x_1, x_2|x_1, x_2; t) &= A\left[e^{-(x_1^2+x_2^2)}\right] \\ &\quad + B\left[4\left(\cos((k_1-k_2)\frac{(x_1+x_2)}{2})\cos((k_1-k_2)\frac{(x_1-x_2)}{2})\right)\right] \\ &\quad + C\left[2\cos((k_1-k_2)x_1)\cos((k_1-k_2)x_2)\right].\end{aligned} \tag{E.3}$$

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Appendix F
Derivation of the Diagonal of the Second Order Correlation Function for a System Tunneling with Two Momenta

The construction of $|g^{(2)}(x_1, x_2|x_1, x_2, t)|^2$ (definition see Sect. 2.1.2) for the wave function constructed from the orbitals in Eq. (5.24) is presented in the following. As in the previous Appendix E, the indices $\mathbf{n_1}, \mathbf{n_2}, \mathbf{n_3}$ refer to the configurations $|2, 0\rangle, |1, 1\rangle, |0, 2\rangle$, respectively. Using the abbreviations $\alpha = x_1(\frac{(k_1-k_2)}{2})$; $\beta = x_2(\frac{(k_1-k_2)}{2})$; $A = (C_{\mathbf{n_1}})^2$; $B =; \theta(x - x_c)(C_{\mathbf{n_1}} \frac{C_{\mathbf{n_2}}}{\sqrt{2}})$; $C = \theta(x - x_c)(C_{\mathbf{n_3}})^2$; $D = (C_{\mathbf{n_1}})^2$; $E = \theta(x - x_c)\left[(C_{\mathbf{n_2}})^2 + C_{\mathbf{n_3}} C_{\mathbf{n_2}} + C_{\mathbf{n_1}} C_{\mathbf{n_2}}\right]$ and $F = \theta(x - x_c) C_{\mathbf{n_3}} C_{\mathbf{n_1}}$ and defining straightforwardly:

$$\begin{aligned}
g^{(2)}(x_1, x_2|x_1, x_2) &= \frac{\rho^{(2)}(x_1, x_2|x_1, x_2)}{\sqrt{\rho^{(1)}(x_1|x_1)\rho(1)(x_2|x_2)}} \\
|g^{(2)}(x_1, x_2|x_1, x_2)|^2 &\equiv \frac{\mu}{\nu}.
\end{aligned}$$

One finds the following for μ and ν:

$$\begin{aligned}
\mu \quad &= A^2 e^{-(2x_1^2+2x_2^2)} + \theta(x - x_c)[A^2 + 2AB\,(\cos(\alpha) + \cos(\beta)) \\
&+ (\cos(\alpha)\cos(\beta))\left[AC + 4BC(\cos(\alpha) + \cos(\beta)) + 4C^2(\cos(\alpha)\cos(\beta))\right] \\
&+ 16B^2\cos^2(\alpha + \beta)\cos^2(\alpha - \beta)],
\end{aligned} \tag{F.1}$$

and

$$\begin{aligned}
\nu = D^2 e^{-(x_1^2+x_2^2)} &+ \theta(x - x_c)[E^2 + 4EF(\cos^2(\alpha) + \cos^2(\beta)) \\
&+ 16F^2(\cos^2(\alpha)\cos^2(\beta))].
\end{aligned} \tag{F.2}$$

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Appendix G
Densities of a Model with Delocalized Orbitals and Two Momenta

The scope of this appendix is to derive the resulting densities $\rho^{(1)}$ and $\rho(2)$ with the ansatz for the orbitals given in Eq. (5.26), where one assumes the interior $\mu(x)$ part to be a Gaussian. This assumption yields the orbitals:

$$\phi_1(x) = e^{-\frac{x^2}{2}} \cdot e^{ik_1 x} \quad ; \quad \phi_2(x) = e^{-\frac{x^2}{2}} \cdot e^{ik_2 x}. \tag{G.1}$$

Furthermore, the description is restricted here to $N = 2$ bosons. In this case the possible permanents contributing to the full wave function are $|2, 0\rangle$, $|1, 1\rangle$, and $|0, 2\rangle$. Explicitly, they read:

$$\begin{aligned}
|2, 0\rangle &= e^{ikx - \frac{x^2}{2} + ik_1 y - \frac{y^2}{2}} \\
|1, 1\rangle &= e^{ik_1 x - \frac{x^2}{2} + ik_2 y - \frac{y^2}{2}} + e^{ik_2 x - \frac{x^2}{2} + ik_1 y - \frac{y^2}{2}} \\
|0, 2\rangle &= e^{ik_2 x - \frac{x^2}{2} + ik_2 y - \frac{y^2}{2}}.
\end{aligned} \tag{G.2}$$

From this basis, it is straightforward to form a multiconfigurational wave function. The above orbitals and permanents are not normalized, but one can just assume that the normalization is absorbed in the coefficients, u, v, w, of the multiconfigurational expansion:

$$\begin{aligned}
|\Psi\rangle &= u|2, 0\rangle + v|1, 1\rangle + w|0, 2\rangle \\
&= e^{-\frac{x^2}{2} - \frac{y^2}{2}} \left(e^{ik_1(x+y)} u + e^{i(k_1 x + k_2 y)} v + e^{i(k_2 x + k_1 y)} v + e^{ik_2(x+y)} w \right).
\end{aligned} \tag{G.3}$$

Having at hands the wave function one can write down the two-body density $\rho^{(2)}(x, y)$:

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$$\rho^{(2)}(x,y) = Tr_{x_3\cdots x_N}\left[|\Psi\rangle\langle\Psi|\right] = \Psi^*(x,y)\Psi(x,y)$$
$$= e^{-x^2-y^2}\Big(u^2+2v^2+w^2$$
$$+2v(v\cos[(k_2-k_1)(x-y)]$$
$$+(u+w)(\cos[(k_2-k_1)x]+\cos[(k_2-k_1)y]))$$
$$+2uw\cos[(k_2-k_1)(x+y)]\Big)\,. \tag{G.4}$$

In the derivation the same addition theorems for trigonometric functions as in Appendix E were used. It is interesting to note that the oscillatory pattern is identical to the one presented in Appendix E. It remains to evaluate the reduced one-body density $\rho^{(1)}$:

$$\rho^{(1)}(x,y) = Tr_{x_2,\cdots,x_N}|\Psi\rangle\langle\Psi|$$
$$= \int dx_2\Psi^*(y,x2)\Psi(x,x_2)$$
$$= \Bigg[\frac{1}{2}e^{-ik_2x-ik_1x-\frac{x^2}{2}-\frac{y^2}{2}}\sqrt{\pi}$$
$$\times\left(e^{i(k_2x+ky)}\left(u^2+v^2\right)+e^{ik_2(x+y)}v(u+w)\right.$$
$$\left.+e^{ik_1(x+y)}v(u+w)+e^{i(k_1x+k_2y)}\left(v^2+w^2\right)\right)$$
$$\times Erf[x_2]+\frac{1}{2}e^{\frac{1}{4}\left(-k_2^2-k_1^2+2k_2(k_1-2ix)-4ik_1x-2\left(x^2+y^2\right)\right)}$$
$$\times\sqrt{\pi}\left(\left(e^{ik_1y}u+e^{ik_2y}v\right)\left(e^{ik_2x}v+e^{ik_1x}w\right)\right.$$
$$\times Erf\left[\frac{1}{2}(ik_2-ik_1+2x_2)\right]$$
$$+\left(e^{ik_2x}u+e^{ik_1x}v\right)\left(e^{ik_1y}v+e^{ik_2y}w\right)$$
$$\left.\times\ Erf\left[\frac{1}{2}(-ik_2+ik_1+2x_2)\right]\right)\Bigg]_{-\infty}^{\infty}. \tag{G.5}$$

When finally taking the limits in the above expression the terms dependent on x_2 and the error functions Erf disappear:

$$\rho^{(1)}(x,y) = e^{\frac{1}{4}\left(-k_2^2-k_1^2-4i(k_2+k_1)x-2\left(x^2+y^2\right)\right)}$$
$$\times\sqrt{\pi}\Big(2e^{\frac{k_2k_1}{2}+ik_2x+ik_1y}uv+e^{\frac{1}{4}\left(k_2^2+4ik_2x+k_1(k_1+4iy)\right)}$$
$$\times\left(u^2+v^2\right)+2e^{\frac{k_2k_1}{2}+ik_2x+ik_2y}vw+e^{\frac{1}{4}\left(k_2^2+k_1^2+4ij(x+y)\right)}v(u+w)$$
$$+e^{\frac{1}{4}\left(k_2^2+k_1(k+4i(x+y))\right)}v(u+w)+e^{\frac{1}{2}k(k_2+2i(x+y))}\left(v^2+uw\right)$$

$$+ e^{\frac{1}{2}k_2(k_1+2i(x+y))}\left(v^2 + uw\right) + e^{\frac{1}{4}\left(k_2^2+k_1(k_1+4ix)+4ik_2y\right)}\left(v^2 + w^2\right)\Big). \tag{G.6}$$

This concludes the analytical exposition of this appendix. It has been verified that the numerical diagonalization of the above one-body density matrix reproduces the natural occupation numbers $\rho_{1/2}^{(NO)}$ of the exact solutions of the $N = 2$ boson dynamics if values of coefficients in MCTDHB calculations are taken for the coefficients u, v, w.

Appendix H
Author's Works and Awards

Publications:

- *Numerically exact quantum dynamics of bosons with time-dependent interactions of harmonic type*,
  A.U.J. Lode, K. Sakmann, O.E. Alon, L.S. Cederbaum, and A.I. Streltsov, Phys. Rev. A **86**, 063606 (2012).
- *How an interacting many-body system tunnels through a potential barrier to open space*,
  A.U.J. Lode, A.I. Streltsov, K. Sakmann, O.E. Alon, and L.S. Cederbaum, Proc. Natl. Acad. Sci. USA **109**, 13521 (2012).
- *Wave chaos as signature for depletion of a Bose–Einstein condensate,*
  I. Březinová, A.U.J. Lode, A.I. Streltsov, O.E. Alon, L.S. Cederbaum, and J. Burgdörfer, Phys. Rev. A **86**, 013630 (2012).
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- *Mechanism of Tunneling in Interacting Open Ultracold Few-Boson Systems*,
  A.U.J. Lode, A.I. Streltsov, O.E. Alon, and L.S. Cederbaum, arXiv:1005.0093 [cond-mat.quant-gas] (2010).
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  A.U.J. Lode, A.I. Streltsov, O.E. Alon, H.-D. Meyer, and L.S. Cederbaum, J. Phys. B: At. Mol. Opt. Phys. **42**, 044018 (2009); see also: *Corrigendum*, J. Phys. B: At. Mol. Opt. Phys. **43**, 029802 (2010).
- *Excitation spectra of many-body systems by linear response: General theory and applications to trapped condensates*,
  J. Grond, A.I. Streltsov, A.U.J. Lode, O.E. Alon, and L.S. Cederbaum, Phys. Rev. A **88**, 023606 (2013).
- *Numerically-Exact Schrödinger Dynamics of Closed and Open Many- Boson Systems with the MCTDHB Package*,

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

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- *Elastic scattering of a Bose–Einstein condensate at a potential landscape*, I. Březinová, A. U. J. Lode, A.I. Streltsov, L.S. Cederbaum, O.E. Alon, L.A. Collins, B.I. Schneider, and J. Burgdörfer, Journal of Physics: Conference Series, ICPEAC Proceedings (2013).
- *Controlling the Velocities and Number of Emitted Particles in the Tunneling to Open Space Dynamics*, A.U.J. Lode, S. Klaiman, O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, arXiv:1309.4253 [quant-ph], Phys. Rev. A **89**, 053620 (2014).
- *What to do with targeted IL-2.*
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Software:

- *The Recursive Multiconfigurational time-dependent Hartree for Bosons package*, http://r-mctdhb.org; http://schroedinger.org; http://ultracold.org, A.U.J. Lode, and M.C. Tsatsos (2013).
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- *The Open Multiconfigurational time-dependent Hartree for Bosons package*, Version 2.3, Heidelberg, http://tc.uni-hd.de/mctdhb/OpenMCTDHB.html, K. Sakmann, A.U.J. Lode, A.I. Streltsov, O.E. Alon, and L.S. Cederbaum (2013).

Awards and Scholarships:

- Ph.D. Scholarship of the International Graduiertenkolleg 710, Complex Processes: Modeling, Simulation and Optimization, 2008.
- Dr. Sophie-Bernthsen award of the University of Heidelberg, 2011.
- Minerva Short Term Research Grant, 2012.

Contributions:

- *Mechanism of the Decay by Tunneling Dynamics in Interacting Open Ultracold Few-Boson Systems*,
Hybrid Quantum Systems, Heidelberg (2010).
- *Tunneling Dynamics in Open Ultracold Bosonic Systems*,
Finite-Temperature Non-Equilibrium Superfluid Systems, Heidelberg (2011).
- *Insights on the Many-Body Physics of Tunneling from Numerically Exact Solutions of the Time-Dependent Schrödinger Equation for Ultracold Bosons*,
Seminar at the Technion, Haifa (2012);
Quantum Technologies Conference, Warsaw (2012).
- *Numerically-Exact Schrödinger Dynamics of Closed and Open Many- Boson Systems with the MCTDHB Package*,
16th HLRS Review workshop, Stuttgart (2013).

- *How tunneling of interacting bosons to open space works and how to control it*, Quantum Optics and Statistics Group, Freiburg (2013);
  Condensed Matter Theory and Quantum Computing Group, Basel (2013);
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