Two-body correlations and natural orbital tomography in ultracold bosonic systems of well-defined parity

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The relationship between natural orbitals, one-body coherences and two-body correlations is explored for bosonic many-body systems of well-defined parity with two occupied single-particle states. We show that the strength of local two-body correlations at the parity-symmetry center characterizes the number state distribution and controls the structure of non-local two-body correlations. A recipe for the experimental reconstruction of the natural orbital densities and quantum depletion is derived. These insights into the structure of the many-body wave-function are applied to the predicted quantum-fluctuations induced decay of dark solitons.

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Introduction.— In an ideal Bose-Einstein condensate, all bosons occupy the same single-particle state $\phi_0(r)$, whose density can directly be inferred from an absorption image measurement of the reduced one-body density $\rho_1(r)$ [1]. Yet in a non-ideal world, not only do interactions between the atoms affect the shape of the condensate wave-function $\phi_0(r)$ but also bring more single-particle orbitals into play, even at zero temperature, such that $\rho_1(r)$ equals an incoherent superposition of their densities in general. Theoretically, the many-body state can be characterized by the natural orbitals (NOs) $\phi_i(r)$ [2], i.e. eigenvectors of the reduced one-body density operator $\rho_1$, and their populations, i.e. the corresponding eigenvalues: Given a sufficiently large weight, the NO of largest population is identified with the condensate wave-function and quantum depletion manifests itself in the population of other NOs [2]. As a matter of fact, correlation effects can be traced back to both the occupation number distribution of the NOs and their spatial shape, allowing for a microscopic understanding of e.g. the Mott-insulating phase [4], quantum-fluctuations induced decay of dark solitons [27], fragmented condensates [10–12] and entanglement of macroscopic objects such as bright solitons [13]. While there are proposals for the detection of fragmentation and its degree [14, 15], the one-body density $\rho_1(r)$ has, to the best of our knowledge, not yet been unraveled into the contributions $|\phi_i(r)|^2$ of the individual NOs by means of a measurement protocol.

In principle, the NOs can be obtained from a tomographic reconstruction of the reduced one-body density matrix $\rho_1(r, r')$ and diagonalization. Such quantum state tomography is a well established technique for qubit systems and quantized light fields [16, 17]. For interacting ensembles of ultracold atoms, information about the off-diagonal elements $\rho_1(r, r')$ can be extracted experimentally from interfering slices coupled out a trapped Bose gas [18, 20] or homodyning in uniform systems [21, 22] and there are further theoretical proposals for the $\rho_1(r, r')$ reconstruction [23, 24]. Yet due to its non-local character, it is notoriously difficult to infer $\rho_1(r, r')$ experimentally, in particular for non-uniform systems.

Rather than aiming at a completely general reconstruction scheme for the NOs, we focus here on bosonic many-body systems of well-defined parity with two occupied single-particle states. Assuming only two occupied orbitals constitutes the simplest, natural extension for bosons beyond the mean-field approximation and is physically justified in various situations. Further, we derive an experimentally accessible reconstruction recipe, in which density-fluctuation measurements play a decisive role, and also gain insights into generic properties of two-body correlations. In particular, we show how the character of the number state distribution function, the NO densities, the structure of two-body correlations and the relationship between one-body coherences and non-local two-body correlations crucially depend on the strength of two-body correlations at the parity-symmetry center. All these relations are derived exactly from the structure of the many-body wave-function. In order to show the validity and importance of our results, we apply our analytical methodology to the analysis of numerical ab-initio data of the quantum-fluctuations induced decay of dark solitons obtained by the Multi-Layer Multi-Configuration Time-Dependent Hartree Method for Bosons (ML-MCTDHB) [27, 28].

Setup.— In the following, we consider a system of $N$ bosons which are energetically or dynamically restricted to occupy only two single-particle states of opposite parity, $\hat{\pi}\ket{\phi_i} = (-1)^i\ket{\phi_i}$, $i = 0, 1$. Here, $\hat{\pi}$ denotes the single-particle parity operator which inverts either all coordinates or only $x$. For simplicity, we suppress the $y, z$ arguments in the position representation and remark that our results are valid for one-, two- and three-dimensional...
quantum gases. The \( N \)-body state is assumed to possess a well-defined \( N \)-body parity, \( \otimes_{r=1}^{N} \hat{\pi}_r | \Psi \rangle = \Pi | \Psi \rangle \), \( \Pi \in \{-1, 1\} \) with \( \hat{\pi}_r \) acting on the \( r \)-th atom, as it is the case for a non-degenerate ground state of a parity-symmetric many-body Hamiltonian e.g. of a bosonic Josephson junction \[33\]. For this class of systems, the many-body state is of the form

\[
| \Psi \rangle = \sum_{k=0}^{K} A_k | n_0(k), N - n_0(k) \rangle,
\]

where \( | n_0, n_1 \rangle \) denotes a number state with \( n_i \) bosons in \( | \phi_i \rangle \). In the cases of \( N \) even and \( \Pi = 1 \) or \( N \) odd and \( \Pi = -1 \), the correct parity is ensured by \( n_0(k) = 2k \). Otherwise, \( n_0(k) = 2k + 1 \) has to be chosen. In all cases, \( K \) denotes the largest integer with \( n_0(K) \leq N \). By tracing out \( N - 1 \) bosons, one obtains for the reduced one-body density operator \( \hat{\rho}_1 = \Delta | \phi_0 \rangle \langle \phi_0 | + (1 - \Delta) | \phi_1 \rangle \langle \phi_1 | \) so that the NOs are given by \( | \phi_i \rangle \). Here, we have introduced the average fraction of bosons in the even orbital, \( \Delta = \frac{n_0}{N} \), where \((...)\) denotes the average w.r.t the number state probability distribution \( | A_k \rangle \). Thus, the quantum depletion equals \( \min(1, 1 - \Delta) \) and the reduced one-body density is given by the incoherent superposition

\[
\rho_1(x) \equiv \langle x | \hat{\rho}_1 | x \rangle = \Delta | \phi_0(x) \rangle \langle \phi_0(x) | + (1 - \Delta) | \phi_1(x) \rangle \langle \phi_1(x) |. \tag{2}
\]

By measuring \( \rho_1(x) \) and the real-valued off-diagonal elements \( \rho_1(x, -x) \equiv \langle x | \hat{\rho}_1 | -x \rangle \) for all \( x \), one could in principle reconstruct the NO densities and \( \Delta \) without knowledge about the full density matrix \( \rho_1(x, x') \). As a consequence of the NO parities, one finds \( | \phi_{0/1}(x) \rangle^2 \propto \rho_1(x) \pm \rho_1(-x, -x) \) and \( \Delta = [1 + \int dx \rho_1(x, -x)] / [1 + \text{tr}(\hat{\pi}_1)] / 2 \), which links \( \Delta \) to the average single-particle parity. The drawback of this scheme, however, lies in the fact that it requires precise knowledge about \( \rho_1(x, -x) \) for all \( x \), which is a challenging quantity to measure.

**NO decomposition of the two-body density.**—Since two-body correlations will indeed provide us an alternative pathway to the NO reconstruction, we investigate here how the structure of the many-body wavefunction \[41\] manifests itself in absorption image noise correlations. The latter have theoretically been proven to give valuable physical insights in particular for low-dimensional systems \[31,32\] and are measurable both after ToF and in situ nowadays \[37,47\]. For this purpose, we derive the two-body density \( \rho_2(x_1, x_2) \equiv \langle x_1 \rangle x_2 \rangle \psi_2(x_1) \psi_2(x_2) \psi_2(x_1) / \langle N(N - 1) \rangle \rangle \), where \( \psi(x) \) denotes the bosonic field operator:

\[
\rho_2(x_1, x_2) = 2 \Re \left( \alpha | \phi_1(x_1, x_2) \rangle \phi_0^* (x_1, x_2) \right) + \beta | \phi_0(x_1, x_2) \rangle^2 + 2 \gamma | \phi_1(x_1, x_2) \rangle^2 + \delta | \phi_1(x_1, x_2) \rangle^2, \tag{3}
\]

with \( \phi_{ij}(x_1, x_2) \) abbreviating the normalized symmetrization of the Hartree product \( \phi_i(x_1) \phi_j(x_2) \). In the following derivation, we will eliminate the off-diagonal term with the coefficient \( \alpha \), which is a function of the coherences \( A_k^* A_{k+1}^* \) between the respective number states, by virtue of the parity symmetry. The second coefficient \( \beta \) is related to the second moment of the number state distribution \( | A_k |^2 \) via \( \beta = \frac{|n_0^2 - n_0|}{|N(N - 1)|} \) and determines the remaining coefficients \( \gamma = \Delta - \beta \) and \( \delta = 1 + \beta - 2 \Delta \).

Assuming a finite central density, \( \rho_1(0) > 0 \), we calculate the two-body correlation function \( g_2(x_1, x_2) \equiv \rho_2(x_1, x_2) / | \rho_1(x_1) \rho_1(x_2) | \) \[48,49\] at the symmetry center

\[
g_2(0, 0) = \frac{\beta}{\Delta^2} = \frac{N}{N - 1} \left( 1 + \frac{\text{var}(n_0) - n_0}{n_0^2} \right) \tag{4},
\]

where \( \text{var}(n_0) = n_0^2 - n_0^2 \). By measuring the central density and its fluctuations, one can deduce \( g_2(0, 0) \) and, thereby, characterize the number state distribution in the categories Poissonian, sub- and super-Poissonian. Similarly, a measurement of the \( n \)-th order correlation function \( g_n(x_1 = 0, ..., x_n = 0) \) gives insights into the \( n \)-th moment of the number state distribution (cf. e.g. the experiment \[50\] for \( n = 3 \)). As we will show, the strength of two-body correlations at the symmetry center constitutes a key parameter, which controls both the reconstruction of the NO densities and the relationship between local and non-local two-body correlations.

**Reconstruction of odd NO.**—In order to eliminate the term proportional to \( \alpha \) in \[41\], we make use of \( \phi_1(0) = 0 \) and consider the non-local two-body correlations \( g_2(x, 0) = [\beta] | \phi_0(x) \rangle^2 + \gamma | \phi_1(x) \rangle^2 / | \Delta \rho_1(x) | \rangle \rangle \). After substituting the density of the even NO \( | \phi_0(x) \rangle^2 \) via \[42\] and employing \[41\], we obtain

\[
| \phi_1(x) \rangle^2 = \frac{g_2(0, 0) - g_2(x, 0)}{g_2(0, 0) - 1} \rho_1(x), \tag{5}
\]

which holds for non-trivial two-body correlations at the symmetry center, i.e. \( g_2(0, 0) \neq 1 \). Under this condition, we have thus shown that the density of the odd NO is proportional to the total reduced one-body density spatially modulated by the strength of non-local two-body correlations between the symmetry center and the position \( x \) of interest. This relationship constitutes a key result of this work since it provides an explicit reconstruction scheme for the microscopic quantity \( | \phi_1(x) \rangle^2 \) in terms of the measurable densities \( \rho_1(x) \) and \( \rho_2(x, 0) \). In particular, this simple reconstruction recipe does not require to measure the off-diagonal elements \( \rho_1(x, -x) \). For the ground state of a parity symmetric Hamiltonian with short-range interactions, the many-body parity turns out to be even \[51\] and, for not too strong interactions, most of the bosons occupy the NO of even parity. Thus, \[51\] gives experimental access to the density of the orbital causing quantum depletion. Besides, the positive semi-definiteness of \( | \phi_1(x) \rangle^2 \) and \( \rho_1(x) \) implies that (anti-)bunching at the symmetry center yields \( g_2(0, 0) \).
as an upper (lower) bound for the non-local correlation $g_2(x,0)$.

Reconstruction of even NO.— Due to the presence of the unknown $\Delta$ in \[52\], density and density-fluctuation measurements can only be employed to relate the NO density difference $|\phi_0(x)|^2 - |\phi_1(x)|^2$ at different points in space, $x = x_1/2$, but not to extract $|\phi_0(x)|^2$ itself. Nevertheless, using \[54\] the possible candidates for $|\phi_0(x)|^2$ can be restricted to a one-parametric family,

$$\frac{|\phi_0(x)|^2}{\rho_1(x)} = \left(1 + \left(1 - \frac{1}{\Delta}\right)\frac{g_2(0,0) - g_2(x,0)}{g_2(0,0) - 1}\right), \quad (6)$$

where $\Delta \in (0, 1)$. Thus, a theoretical estimate for $\Delta$ by means of e.g. number-conserving Bogoliubov theory \[52\] would allow for uniquely determining the density of the even NO. In order to obtain a measurement protocol for $\Delta$ as an alternative, we assume, for a second, to have access to the first-order coherences $g_1(x, -x) = \rho_1(x, -x)/\sqrt{\rho_1(x)\rho_1(-x)}$ \[48\] \[49\]. Substituting $|\phi_0/1(x)|^2$ by \[52\] and \[54\], respectively, in $\rho_1(x, -x)$, we arrive at

$$g_1(x, -x) = 1 - 2(1 - \Delta)\frac{g_2(0,0) - g_2(x,0)}{g_2(0,0) - 1}. \quad (7)$$

Thus, the additional knowledge of $g_1(x^*, -x^*)$ for some position $x^*$ with $g_2(x^*, 0) \neq g_2(0, 0)$ is sufficient for determining $\Delta$. If we have only experimental access to the modulus of $g_1(x, -x)$ but not to its sign, we may extract $\Delta = \Delta_+ (x)$ for both signs, i.e. $\pm g_1(x, -x)$, from \[7\] for all $x$ of finite density with $g_2(x, 0) \neq g_2(0, 0)$. One easily verifies $\Delta_+(x) \geq \Delta_-(x)$ and, in many situations, the local sign of $g_1(x, -x)$ can then be fixed by requiring $\Delta$ not to depend on $x$. Knowing $\Delta$ and an estimate for $N$, we may also infer $\text{var}(n_0)$ from \[1\]. Finally, Eq. \[7\] gives the conceptual insight that the average fraction of bosons in the even NO mediates a relationship between the first order coherences $g_1(x, -x)$ and two-body correlations $g_2(x, 0)$.

Spatial structure of two-body correlations.— While the two-body correlation function features a particle exchange and a two-body parity symmetry, it does not remain invariant under a parity operation acting on one atom only. By inspecting $\rho_2(x_1, x_2) + \rho_2(x_1, -x_2) - 2\rho_1(x_1)\rho_1(x_2)$, i.e. essentially the sum of density-density correlations at $(x_1, x_2)$, the parities of the NOs can be employed to eliminate the off-diagonal term $\propto \alpha$ such that a relationship between $g_2(x_1, x_2)$ and $g_2(x_1, -x_2)$ can be established. Here, we have to distinguish two cases: (i) In the absence of two-body correlations at the symmetry center, i.e. $g_2(0, 0) = 1$, we obtain the relation $g_2(x_1, x_2) + g_2(x_1, -x_2) = 2$, which has three important consequences. Firstly, the $g_2$ function is fully determined by its values in the sector $S = \{x_1, x_2\}$ (for a illustration). Secondly, local bunching (anti-bunching) structures $g_2(x_1, x_2) > 1$ ($g_2(x_1, x_2) < 1$) for $x_1 \approx x_2$ translate into non-local anti-turning (bunching) structures of the same magnitude at $(x_1, -x_2)$. Thirdly, pairs of atoms are uncorrelated on the $x_1/2$ axis, i.e. $g_2(0, x) = g_2(0, -x) = 1$. (ii) In the presence of two-body correlations at the symmetry center, we may employ the reconstruction formula \[5\] to obtain the following functional equation, which has to be fulfilled for every $g_2$ with $g_2(0, 0) \neq 1$ in order to be compatible with the many-body wave function \[1\],

$$g_2(x_1, x_2) + g_2(x_1, -x_2) = 2\left(1 + \frac{f(x_1)f(x_2)}{g_2(0,0) - 1}\right), \quad (8)$$

with $f(x) \equiv g_2(x, 0) - 1$. This restriction on the functional form of $g_2$ may be used experimentally for testing the validity of the two-orbital approximation.

Applications.— Dark solitons, being well-known for their stability within the mean-field approximation (see \[57\] and references therein), suffer from a quantum-fluctuations induced decay due to an incoherent scattering of atoms from the soliton orbital into an orbital localized at the soliton position such that the characteristic density minimum is filled up with these atoms, e.g. \[6\]. Since this decay process can qualitatively be understood within a two-orbital approximation, dark solitons constitute a straightforward example for testing the validity of the above insights in situations when further orbitals participate with, however, minor weight. In the following, we consider $N$ bosons of mass $m$ in a one-dimensional box potential of length $L$ with a contact interaction strength $g$. This system is governed by the Hamiltonian $H = \sum_i \frac{p_i^2}{2} + \sqrt{\hbar \gamma} \sum_{i<j} \delta(x_i - x_j)$ in a unit system based on the chemical potential $\mu_0 = gN/L$, the healing length $\xi = \hbar/\mu_0$ and the correlation time $\tau_c = \hbar/\mu_0$, where $\gamma = mgL/(\hbar^2N)$ denotes the Lieb-Liniger parameter.

Firstly, we start with the ground state of the
by incoherently scattered atoms inducing strong bunching correlations at the symmetry center. Fig. 2 clearly shows that the density of the dominant NO of odd parity, $|\phi_1(x)|^2$, features the characteristic density notch of a black soliton and can be reliably reconstructed by the scheme \(5\) at times when the soliton contrast in the full density $\rho_1(x)$ has been reduced. For longer times, the reconstructed $|\phi_1(x)|^2$ deviates slightly more from the full numerical results since the third and fourth dominant NO have gained more population. The reconstruction of $|\phi_2(x)|^2$, i.e. the NO mostly responsible for the soliton decay and strong two-body correlations, turns out to be more sensitive to the slight population of these NO.

Conclusions. — We have shown how physical knowledge about the structure of the many-body wave-function can be employed for deriving generic properties of two-body correlations and an experimentally relevant reconstruction scheme for the NO densities. In addition to the presented dark soliton example, our results should be applicable to many other systems such as Bose gases in a double-well potential \(13\) or symmetrically colliding fragments in a harmonic trap \(15\). If the central density turns out to be too small such that $g_2(0,0)$ becomes effectively ill-defined, the whole analysis has to be carried out in momentum space via long ToF measurements. We hope that our work stimulates the interest in NO reconstruction schemes such that these microscopic quantities become experimentally accessible for a broad class of systems.

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Figure 2. One-body density and density of the two most dominant NOs at times $t = 2\tau_c$ (a) and $t = 3.5\tau_c$ (b) for a many-body system initially featuring a black soliton centered at $x = 0$. All parameters are as in fig. 1 (b). Dotted line: Exact NO densities $|\phi_0(x)|^2$ (black) and $|\phi_1(x)|^2$ (gray, reduced by factor 2). All these curves are obtained from ML-MCTDHB ab-initio simulations. Dashed lines: Corresponding reconstructions of the NO densities. Estimated $\Delta \approx 0.079, 0.088$ for (a), (b), respectively. Exact values: $\Delta \approx 0.073, 0.098$. Two-body correlations at the symmetry center: $g_2(0,0) \approx 2.699, 2.013$.
