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

Sven Krönke[1,*] and Peter Schmelcher[1,2,†]

[1]*Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany*
[2]*The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany*

(Received 30 January 2015; published 24 August 2015)

The relationship between natural orbitals, one-body coherences, and two-body correlations is explored for bosonic many-body systems of definite 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 nonlocal 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-fluctuation-induced decay of dark solitons.

DOI: 10.1103/PhysRevA.92.023631 PACS number(s): 03.75.Lm, 67.85.Bc, 67.85.De

I. INTRODUCTION

In an ideal Bose-Einstein condensate, all bosons occupy the same single-particle state $\phi_0(\mathbf{r})$, whose density can directly be inferred from an absorption image measurement of the reduced one-body density $\rho_1(\mathbf{r})$ [1]. Yet in a nonideal world, interactions between the atoms not only affect the shape of the condensate wave function $\phi_0(\mathbf{r})$ but also bring more single-particle orbitals into play, even at zero temperature, such that $\rho_1(\mathbf{r})$ equals an incoherent superposition of their densities in general. Theoretically, the many-body state can be characterized by the natural orbitals (NOs) $\phi_i(\mathbf{r})$ [2], i.e., eigenvectors of the reduced one-body density operator $\hat{\rho}_1$ and their populations, i.e., the corresponding eigenvalues: Given a sufficiently large weight, the NO of the largest population is identified with the condensate wave function and quantum depletion manifests itself in the population of other NOs [3]. As a matter of fact, correlation effects can be traced back to both the spatial shapes and the occupation-number distribution of the NOs, allowing a microscopic understanding of various phenomena. Examples of such phenomena are the Mott-insulating phase, where, e.g., an intra-well Tonks-Girardeau transition for a filling factor of 2 can be understood in the NO framework [4,5]; the quantum-fluctuation-induced decay of dark solitons [6–9], where a NO of particular shape is dominantly responsible for the soliton contrast reduction in the reduced one-body density; and fragmented condensates [10–13], which are defined as many-body states with two or more macroscopically occupied NOs. While there are proposals for the detection of fragmentation and its degree [14,15], the one-body density $\rho_1(\mathbf{r})$ has, to the best of our knowledge, not yet been unraveled into the contributions $|\phi_i(\mathbf{r})|^2$ 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 $\rho_1(\mathbf{r},\mathbf{r}')$ 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 $\rho_1(\mathbf{r},\mathbf{r}')$ can be extracted experimentally from the contrast of interfering slices coupled out of a trapped Bose gas [18–20] or homodyning in uniform systems, where one generates copies of one's system by Bragg pulses and lets them interfere [21,22]. Furthermore, there are theoretical proposals for the $\rho_1(\mathbf{r},\mathbf{r}')$ reconstruction based on Raman-pulse sequences [23], variable time-of-flight (TOF) measurements [24], heterodyning with an auxiliary Bose-Einstein condensate [25], or the Jaynes principle of maximum entropy [26]. Yet due to its nonlocal character, it is notoriously difficult to infer $\rho_1(\mathbf{r},\mathbf{r}')$ experimentally, in particular for nonuniform systems.

Rather than aiming at a completely general reconstruction scheme for the NOs, we focus here on bosonic many-body systems of definite parity with two occupied NOs. Assuming only two occupied orbitals constitutes the simplest, natural extension for bosons beyond the mean-field approximation and is physically justified in various situations. For this class of systems, we derive an experimentally accessible reconstruction recipe in which density-fluctuation measurements play a decisive role, and also gain insights into the 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 nonlocal 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 importance of our results as well as their validity when further NOs are slightly populated, we apply our analytical methodology to the analysis of numerical *ab initio* data of the quantum-fluctuation-induced decay of dark solitons obtained by the multiconfiguration time-dependent Hartree method for bosons (MCTDHB) [27–29] and address also the impact of finite experimental resolution.

This work is organized as follows: First, the setup is introduced in Sec. II. Thereafter, we discuss the NO decomposition of the reduced two-body density in Sec. III A, which forms the basis for the reconstruction of the odd- and even-parity NO densities as well as for the characterization of the spatial structure of two-body correlations in Secs. III B, III C, and III D, respectively. Finally, we apply our insights to

*skroenke@physnet.uni-hamburg.de
†pschmelc@physnet.uni-hamburg.de

decaying dark solitons in Sec. III E and conclude with Sec. IV.

II. SETUP

In the following, we consider a system of N bosons which are energetically or dynamically restricted to occupying only two single-particle states of opposite parity, $\hat{\pi}|\phi_i\rangle = (-1)^i|\phi_i\rangle$, $i = 0,1$. 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 definite N-body parity, $\bigotimes_{r=1}^{N}\hat{\pi}_r|\Psi\rangle = \Pi|\Psi\rangle$, $\Pi \in \{-1,1\}$ with $\hat{\pi}_r$ acting on the rth atom, as it is the case for a nondegenerate ground state of a parity-symmetric many-body Hamiltonian, e.g., of a bosonic Josephson junction [30]. For this class of systems, the many-body state is of the form

$$|\Psi\rangle = \sum_{k=0}^{K} A_k|n_0(k),N - n_0(k)\rangle, \tag{1}$$

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 $n_0(K) \leqslant N$. 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, $\Delta = \overline{n}_0/N$, where $\overline{(\ldots)}$ denotes the average with respect to the number-state probability distribution $|A_k|^2$. Thus, the quantum depletion equals $\min\{\Delta,1 - \Delta\}$ and the reduced one-body density is given by the incoherent superposition

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

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 Δ without knowledge about the full density matrix $\rho_1(x,x')$. As a consequence of the NO parities, one finds $|\phi_{0/1}(x)|^2 \propto \rho_1(x) \pm \rho_1(x,-x)$ and $\Delta = [1 + \int dx\, \rho_1(x,-x)]/2 = [1 + \mathrm{tr}(\hat{\pi}\hat{\rho}_1)]/2$, which links Δ 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.

III. RESULTS

A. NO decomposition of the two-body density

Since two-body correlations will indeed provide us an alternative pathway to the reconstruction of the NO densities, we investigate here how the structure of the many-body wave function (1) manifests itself in absorption image noise correlations. The latter have theoretically been proven to give valuable physical insights in particular for low-dimensional systems [31–36] and are measurable both after TOF and *in situ* nowadays [37–48]. For this purpose, we derive the two-body density $\rho_2(x_1,x_2) \equiv \langle\hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2)\hat{\psi}(x_2)\hat{\psi}(x_1)\rangle/[N(N-1)]$, where $\hat{\psi}(x)$ denotes the bosonic field operator:

$$\rho_2(x_1,x_2) = 2\mathrm{Re}[\alpha\,\phi_{11}(x_1,x_2)\phi_{00}^*(x_1,x_2)] + \beta|\phi_{00}(x_1,x_2)|^2 + 2\gamma|\phi_{01}(x_1,x_2)|^2 + \delta|\phi_{11}(x_1,x_2)|^2, \tag{3}$$

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 α, which is a function of the coherences $A_{k+1}^*A_k$ between the respective number states, by virtue of the parity symmetry. The second coefficient is related to the second moment of the number-state distribution $|A_k|^2$ via $\beta = [\overline{n_0^2} - \overline{n}_0]/[N(N-1)]$ 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 $g_2(x_1,x_2) \equiv \rho_2(x_1,x_2)/[\rho_1(x_1)\rho_1(x_2)]$ [49,50] at the symmetry center

$$g_2(0,0) = \frac{\beta}{\Delta^2} = \frac{N}{N-1}\left(1 + \frac{\mathrm{var}(n_0) - \overline{n}_0}{\overline{n}_0^2}\right), \tag{4}$$

where $\mathrm{var}(n_0) = \overline{n_0^2} - \overline{n}_0^2$. By measuring the central density and its fluctuations, one can in principle deduce $g_2(0,0)$ and, thereby, characterize the number-state distribution in the categories Poissonian, sub-Poissonian, and super-Poissonian. Similarly, a measurement of the nth-order correlation function $g_n(x_1 = 0,\ldots,x_n = 0)$ gives insights into the nth moment of the number-state distribution (see, e.g., the experiment in [51] 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 nonlocal two-body correlations. Regarding the impact of an unavoidably given finite experimental resolution, we refer to the discussion at the end of Sec. III E.

B. Density reconstruction of odd NO

In order to eliminate the term proportional to α in Eq. (3), we make use of $\phi_1(0) = 0$ and consider the nonlocal two-body correlations $g_2(x,0) = [\beta|\phi_0(x)|^2 + \gamma|\phi_1(x)|^2]/[\Delta\rho_1(x)]$. After substituting the density of the even NO $|\phi_0(x)|^2$ via Eq. (2) and employing Eq. (4), we obtain

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

which holds[1] for nontrivial 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 nonlocal 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 $|\phi_1(x)|^2$ in terms of the measurable densities $\rho_1(x)$ and

[1]In the limit $g_2(0,0) \to 1$, the right-hand side of Eq. (5) tends to $|\phi_1(x)|^2$ such that no information about the NO is gained. This fact is also reflected by $g_2(0,0) = 1$ implying $g_2(x,0) = 1$ (see Sec. III D).

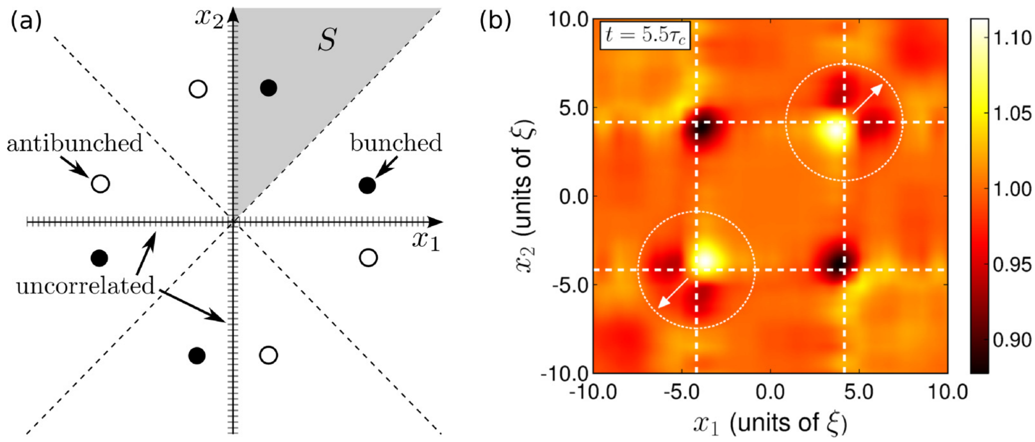

FIG. 1. (Color online) (a) Structure of two-body correlations for the case $g_2(0,0) = 1$. (b) $g_2(x_1,x_2)$ at $t = 5.5\tau_c$ for a density-engineered initial state of $N = 100$ bosons with $\gamma = 0.04$ in a one-dimensional box of length $L = 20\xi$ (obtained by (ML-)MCTDHB simulations). The dashed lines indicate the positions of two counterpropagating gray solitons and the arrows point into their directions of motion. The circles indicate the characteristic correlation pattern observed for a single gray soliton in [9]. Strength of two-body correlations at the symmetry center: $g_2(0,0) \approx 1.003$.

$\rho_2(x,0)$. In particular, this simple reconstruction recipe does not require to measuring 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 [52] and, for not too strong interactions, most of the bosons occupy the NO of even parity. Thus, Eq. (5) gives experimental access to the density of the orbital whose population is responsible for quantum depletion. Besides, the positive semidefiniteness of $|\phi_1(x)|^2$ and $\rho_1(x)$ implies that (anti)bunching at the symmetry center yields $g_2(0,0)$ as an upper (lower) bound for the nonlocal correlation $g_2(x,0)$.

C. Density reconstruction of even NO

Due to the presence of the unknown Δ in Eq. (2), 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 Eq. (5) the possible candidates for $|\phi_0(x)|^2$ can be restricted to a one-parametric family,[2]

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

where $\Delta \in (0,1)$. Thus, a theoretical estimate for Δ by means of, e.g., number-conserving Bogoliubov theory [53–57] would allow the unique determination of the density of the even NO. In order to obtain a measurement protocol for Δ as an alternative, we inspect the first-order coherences $g_1(x,-x) \equiv \rho_1(x,-x)/\sqrt{\rho_1(x)\rho_1(-x)}$ [49,50]. Substituting $|\phi_{0/1}(x)|^2$ by Eqs. (6) and (5), 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 convenient position x^* with $g_2(x^*,0) \neq g_2(0,0)$ is sufficient for determining Δ. In the case when we have only experimental access to the modulus of $g_1(x,-x)$ but not to its sign, we may extract $\Delta = \Delta_\pm(x)$ for both signs, i.e., $\pm|g_1(x,-x)|$, from Eq. (7) for all x of finite density with $g_2(x,0) \neq g_2(0,0)$. One easily verifies $\Delta_+(x) \geqslant \Delta_-(x)$ and, in many situations, the local sign of $g_1(x,-x)$ can then be fixed by requiring Δ not to depend on x. Knowing Δ and an estimate for N, we may also infer var(n_0) from (4). 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 $g_2(x,0)$.

D. 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 $(x_1, \pm x_2)$, 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. First, the g_2 function is fully determined by its values in the sector $S = \{(x_1,x_2)|0 \leqslant x_1 \leqslant x_2\}$ [see Fig. 1(a) for an illustration]. Second, local bunching (antibunching) structures $g_2(x_1,x_2) > 1$ $[g_2(x_1,x_2) < 1]$ for $x_1 \approx x_2$ translate into nonlocal antibunching (bunching) structures of the same magnitude at $(x_1,-x_2)$. Third, pairs of atoms are uncorrelated on the $x_{1/2}$ axis, i.e., $g_2(x,0) = g_2(0,x) = 1$.

(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

[2]In the $g_2(0,0) \to 1$ limit, this equation becomes equivalent to Eq. (2) such that no information is gained.

with the many-body wave function (1):

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

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

E. Applications

Dark solitons, being well known for their stability within the mean-field approximation (see [58] and references therein), suffer from a quantum-fluctuation-induced decay due to an incoherent scattering of atoms from the soliton orbital into an orbital localized at the soliton position; see, e.g., Refs. [6–9]. Due to the increasing population of this orbital, the depth of the characteristic minimum in the reduced one-body density is reduced; i.e., the soliton contrast decreases on average over many absorption image measurements. 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 $\hat{H} = \sum_i \hat{p}_i^2/2 + \sqrt{\gamma}\sum_{i<j}\delta(\hat{x}_i - \hat{x}_j)$ in a unit system based on the chemical potential $\mu_0 = gN/L$, the healing length $\xi = \hbar/\sqrt{m\mu_0}$, and the correlation time $\tau_c = \hbar/\mu_0$, where $\gamma = mgL/(\hbar^2 N)$ denotes the Lieb-Liniger parameter.

Both for finding the initial state and for the subsequent propagation in the following two scenarios, we employ our recently developed multilayer multiconfiguration time-dependent Hartree method for bosons (ML-MCTDHB) [28,29], which reduces to the pioneering MCTDHB method [27] if applied to a single species in one spatial dimension as in the considered cases. This method is based on an expansion of the total many-body wave function with respect to bosonic number states with an underlying time-dependent, dynamically optimized single-particle basis of M states. All conceivable number-state configurations for the given M single-particle states are taken into account. Being based on a variational principle, the MCTDHB equations provide us with a variationally optimized solution to the time-dependent many-body Schrödinger equation. By incrementing M, we found in both scenarios discussed below that convergence is ensured on the considered time scale if $M = 4$ (see [9]). A NO analysis of the full numerical data reveals that two NOs contribute with significant weight while the probability of finding an atom in one of the other two NOs does not exceed 0.023 for the time scales of Figs. 1(b) and 2.

First, we start with the ground state of $N = 100$ atoms in the box with an additional Gaussian barrier $V(x) = h\exp[-x^2/(2w^2)]$, $h = 60\mu_0$, and $w \approx 0.07\xi$ so that we engineer a pronounced density notch at $x = 0$. Having switched off the barrier, we let the interacting many-body system evolve in the box potential. In the course of time, the single density minimum splits into a pair of counterpropagating gray solitons, which are slowly decaying due to quantum fluctuations [9]. We have shown that a single gray soliton is accompanied by highly localized two-body correlations in the vicinity of the instantaneous soliton position resulting in a bunching of atoms in the soliton flank opposite to its direction of movement [see the circles in Fig. 1(b)]. Yet the g_2 function of two counterpropagating gray solitons turns out to be more than the sum of the local correlation patterns of the individual gray solitons; additional nonlocal correlations occur between the two solitons [Fig. 1(b) and Ref. [9]]. Observing numerically that $|g_2(0,0) - 1| \ll 1$, we may now understand these nonlocal correlations as a generic property of parity-symmetric systems with essentially two occupied NOs: With x_R (x_L) denoting the position of the soliton moving to the right (left), our above results imply $g_2(x_R - \epsilon, x_L + \epsilon) \approx 2 - g_2(x_R - \epsilon, x_R - \epsilon)$ such that bunching in the back of a single soliton ($\epsilon > 0$) translates into antibunching of approximately the same magnitude for finding an atom each in the back of each soliton.

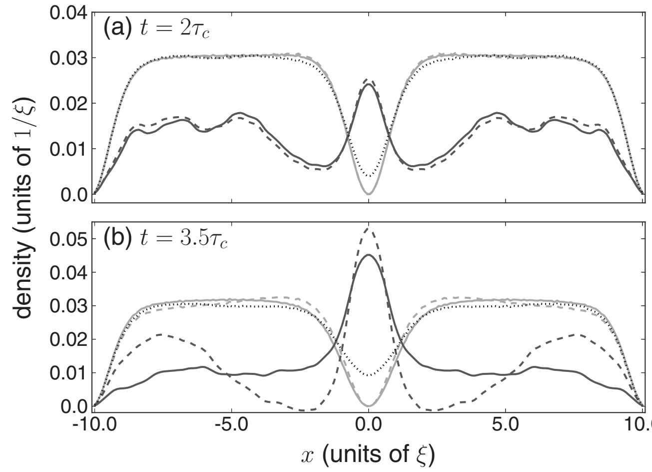

FIG. 2. One-body density and density of the two most dominant NOs at times (a) $t = 2\tau_c$ and (b) $t = 3.5\tau_c$ for a many-body system initially featuring a black soliton centered at $x = 0$. All parameters are as in Fig. 1(b). Dotted line: $\rho_1(x)$. Solid lines: Exact NO densities $|\phi_0(x)|^2$ (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.

Second, in order to realize a situation with significant deviations of $g_2(0,0)$ from unity, we additionally imprint a relative phase of π between the two half spaces at $t = 0$ [6–9]. Thereby, a black soliton is initialized at $x = 0$. As time evolves, the density minimum becomes filled up by incoherently scattered atoms inducing strong bunching correlations at the symmetry center. Figure 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 $|\phi_0(x)|^2$, 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: Due to the phase-imprinting scheme, we expect most of the atoms to reside in an odd NO. Finding numerically $\Delta_-(x) < 1/2 < \Delta_+(x)$, we thus take the negative sign of $g_1(x,-x)$ and estimate Δ by averaging $\Delta_-(x)$ over some interval. As a result, we can fairly well reconstruct $|\phi_0(x)|^2$ according to Eq. (6) for not too long times [Fig. 2(a)]. Thus, our scheme can be used to experimentally verify the microscopic decay mechanism of a black-soliton contrast in the reduced one-body density via a NO being localized at the position of the soliton, given that thermal excitations are sufficiently suppressed as achievable in today's experiments [59]. At longer times [$t \gtrsim 3\tau_c$, see Fig. 2(b)], i.e., when the assumption of only two occupied orbitals becomes less valid, however, the reconstructed $|\phi_0(x)|^2$ deviates much more from the full numerical results compared to the reconstruction of $|\phi_1(x)|^2$.

The reconstruction formulas (5) and (6) have been derived under the assumption of perfect experimental resolution. To test the robustness of the reconstruction recipe against finite resolution, we have (i) embedded our numerical simulation results for the considered purely one-dimensional model into three-dimensional coordinate space by assuming all atoms to reside in the ground state of the transverse harmonic oscillator and (ii) convoluted the one- and two-body densities with a Gaussian point-spread function of variable width σ. These coarse-grained quantities have then been inserted in the reconstruction formulas (5) and (6). We have found that the NO densities and thereby the decay mechanism of the soliton contrast in the reduced one-body density can be reconstructed as long as $\sigma \lesssim \xi/4$, which was to be expected (plots not shown). This requirement on the optical resolution is demanding, of course, but not out of reach since the healing length could be raised above the resolution limit by a Feshbach resonance, for example. For such values of σ, the reconstructed $|\phi_0(x)|^2$ density happens to be sufficiently robust against errors in the depletion Δ, for which we assumed a relative uncertainty of 20%. Finally, we remark that not $\rho_2(x_1,x_2)$ but density-density correlations $\langle[\hat{\psi}^\dagger(x_1)\hat{\psi}(x_1) - N\rho_1(x_1)][\hat{\psi}^\dagger(x_2)\hat{\psi}(x_2) - N\rho_1(x_2)]\rangle$ are measured in experiments. Due to the canonical commutation relations for bosonic field operators, however, these two quantities essentially differ by an autocorrelation peak $\propto \delta(x_1 - x_2)$, which becomes smooth when convoluted with a point-spread function and whose contribution is suppressed as $1/N$ for large particle numbers.

IV. 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 discussed dark-soliton example, our results should be applicable to many other systems such as Bose gases in a double-well potential [30], fragmenting bright solitons [12,13], or symmetrically colliding fragments in a harmonic trap [15,60]. If the central density turns out to be vanishing or 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.

ACKNOWLEDGMENTS

We thank T. Schumm, H. Moritz, J. Simonet, and L. Cao for fruitful discussions as well as J. Knörzer and J. Stockhofe for helpful comments on the manuscript. S.K. gratefully acknowledges a scholarship by the Studienstiftung des deutschen Volkes. P.S. gratefully acknowledges financial support by the Deutsche Forschungsgemeinschaft in the framework of the SFB 925 "Light induced dynamics and control of correlated quantum systems".

[1] C. J. Pethick and H. Smith, *Bose-Einstein Condensates in Dilute Gases*, 2nd ed. (Cambridge University, New York, 2008).
[2] P.-O. Löwdin, Phys. Rev. **97**, 1474 (1955).
[3] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).
[4] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Rev. Lett. **95**, 030405 (2005).
[5] I. Brouzos, S. Zöllner, and P. Schmelcher, Phys. Rev. A **81**, 053613 (2010).
[6] J. Dziarmaga and K. Sacha, Phys. Rev. A **66**, 043620 (2002).
[7] R. V. Mishmash and L. D. Carr, Phys. Rev. Lett. **103**, 140403 (2009).
[8] D. Delande and K. Sacha, Phys. Rev. Lett. **112**, 040402 (2014).
[9] S. Krönke and P. Schmelcher, Phys. Rev. A **91**, 053614 (2015).
[10] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Lett. A **347**, 88 (2005).
[11] K. Sakmann, A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. A **78**, 023615 (2008).
[12] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. **100**, 130401 (2008).
[13] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. **106**, 240401 (2011).
[14] M.-K. Kang and U. R. Fischer, Phys. Rev. Lett. **113**, 140404 (2014).
[15] O. I. Streltsova and A. I. Streltsov, arXiv:1412.4049.
[16] M. Paris and J. Řeháček (eds.), *Quantum State Estimation*, volume 649 of Lecture Notes in Physics (Springer, Berlin, Heidelberg, 2004).
[17] A. Lvovsky and M. Raymer, Rev. Mod. Phys. **81**, 299 (2009).
[18] I. Bloch, T. W. Hänsch, and T. Esslinger, Nature **403**, 166 (2000).
[19] S. Ritter, A. Öttl, T. Donner, T. Bourdel, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **98**, 090402 (2007).
[20] T. Donner, S. Ritter, T. Bourdel, A. Öttl, M. Köhl, and T. Esslinger, Science **315**, 1556 (2007).
[21] E. W. Hagley, L. Deng, M. Kozuma, M. Trippenbach, Y. B. Band, M. Edwards, M. Doery, P. S. Julienne, K. Helmerson, S. L. Rolston, and W. D. Phillips, Phys. Rev. Lett. **83**, 3112 (1999).

[22] N. Navon, A. L. Gaunt, R. P. Smith, and Z. Hadzibabic, Science **347**, 167 (2015).
[23] L.-M. Duan, Phys. Rev. Lett. **96**, 103201 (2006).
[24] W. Zhang and L.-M. Duan, Phys. Rev. A **80**, 063614 (2009).
[25] Q. Niu, I. Carusotto, and A. B. Kuklov, Phys. Rev. A **73**, 053604 (2006).
[26] A. S. Mouritzen and K. Mølmer, Phys. Rev. A **71**, 033602 (2005).
[27] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Rev. A **77**, 033613 (2008).
[28] S. Krönke, L. Cao, O. Vendrell, and P. Schmelcher, New J. Phys. **15**, 063018 (2013).
[29] L. Cao, S. Krönke, O. Vendrell, and P. Schmelcher, J. Chem. Phys. **139**, 134103 (2013).
[30] R. Gati and M. K. Oberthaler, J. Phys. B **40**, R61 (2007).
[31] E. Altman, E. Demler, and M. D. Lukin, Phys. Rev. A **70**, 013603 (2004).
[32] A. G. Sykes, D. M. Gangardt, M. J. Davis, K. Viering, M. G. Raizen, and K. V. Kheruntsyan, Phys. Rev. Lett. **100**, 160406 (2008).
[33] L. Mathey, E. Altman, and A. Vishwanath, Phys. Rev. Lett. **100**, 240401 (2008).
[34] L. Mathey, A. Vishwanath, and E. Altman, Phys. Rev. A **79**, 013609 (2009).
[35] A. Imambekov, I. E. Mazets, D. S. Petrov, V. Gritsev, S. Manz, S. Hofferberth, T. Schumm, E. Demler, and J. Schmiedmayer, Phys. Rev. A **80**, 033604 (2009).
[36] V. P. Singh and L. Mathey, Phys. Rev. A **89**, 053612 (2014).
[37] S. Fölling, F. Gerbier, A. Widera, O. Mandel, T. Gericke, and I. Bloch, Nature **434**, 481 (2005).
[38] M. Schellekens, R. Hoppeler, A. Perrin, J. V. Gomes, D. Boiron, A. Aspect, and C. I. Westbrook, Science **310**, 648 (2005).
[39] S. Manz, R. Bücker, T. Betz, Ch. Koller, S. Hofferberth, I. E. Mazets, A. Imambekov, E. Demler, A. Perrin, J. Schmiedmayer, and T. Schumm, Phys. Rev. A **81**, 031610 (2010).
[40] Chen-Lung Hung, Xibo Zhang, Li-Chung Ha, Shih-Kuang Tung, Nathan Gemelke, and Cheng Chin, New J. Phys. **13**, 075019 (2011).
[41] M. Endres, M. Cheneau, T. Fukuhara, C. Weitenberg, P. Schauß, C. Gross, L. Mazza, M. C. Bañuls, L. Pollet, I. Bloch, and S. Kuhr, Science **334**, 200 (2011).
[42] M. Cheneau, P. Barmettler, D. Poletti, M. Endres, P. Schauß, T. Fukuhara, C. Gross, I. Bloch, C. Kollath, and S. Kuhr, Nature **481**, 484 (2012).
[43] M. Endres, M. Cheneau, T. Fukuhara, C. Weitenberg, P. Schauß, C. Gross, L. Mazza, M. C. Bañuls, L. Pollet, I. Bloch, and S. Kuhr, Appl. Phys. B **113**, 27 (2013).
[44] T. Jacqmin, J. Armijo, T. Berrada, K. V. Kheruntsyan, and I. Bouchoule, Phys. Rev. Lett. **106**, 230405 (2011).
[45] J. Armijo, T. Jacqmin, K. Kheruntsyan, and I. Bouchoule, Phys. Rev. A **83**, 021605 (2011).
[46] J. Armijo, Phys. Rev. Lett. **108**, 225306 (2012).
[47] A. Perrin, R. Bücker, S. Manz, T. Betz, C. Koller, T. Plisson, T. Schumm, and J. Schmiedmayer, Nature Phys. **8**, 195 (2012).
[48] S. Fölling, *Quantum Gas Experiments, Exploring Many-Body States* (World Scientific, Singapore, 2014).
[49] R. J. Glauber, Phys. Rev. **130**, 2529 (1963).
[50] M. Naraschewski and R. J. Glauber, Phys. Rev. A **59**, 4595 (1999).
[51] J. Armijo, T. Jacqmin, K. V. Kheruntsyan, and I. Bouchoule, Phys. Rev. Lett. **105**, 230402 (2010).
[52] R. P. Feynman, *Statistical Mechanics: A Set of Lectures. Frontiers in Physics* (Benjamin Cummings, San Francisco, 1972).
[53] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959).
[54] C. W. Gardiner, Phys. Rev. A **56**, 1414 (1997).
[55] M. D. Girardeau, Phys. Rev. A **58**, 775 (1998).
[56] Y. Castin and R. Dum, Phys. Rev. A **57**, 3008 (1998).
[57] J. Dziarmaga and K. Sacha, Phys. Rev. A **67**, 033608 (2003).
[58] D. J. Frantzeskakis, J. Phys. A **43**, 213001 (2010).
[59] D. M. Weld, P. Medley, H. Miyake, D. Hucul, D. E. Pritchard, and W. Ketterle, Phys. Rev. Lett. **103**, 245301 (2009).
[60] K. Sakmann and M. Kasevich, arXiv:1501.03224.