Emergence of a new pair-coherent phase in many-body quenches of repulsive bosons

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We investigate the dynamical mode population statistics and associated first- and second-order coherence of an interacting bosonic two-mode model when the pair-exchange coupling is quenched from negative to positive values. It is shown that for moderately rapid second-order transitions, a new pair-coherent phase emerges on the positive coupling side in an excited state, which is not fragmented as the ground-state single-particle density matrix would prescribe it to be.

PACS numbers: 42.50.Lc, 03.75.Gg, 47.70.Nd, 64.70.Tg

The fundamental question whether an interacting system of bosons is a single or fragmented condensate has conventionally been answered in favor of the single Bose-Einstein condensate. This conclusion is gained from highly symmetric (e.g. rotationally invariant) situations, for example in antiferromagnetic spinor condensates or rotating gases. The fragmented condensate states occurring for these symmetrical Hamiltonians are extremely fragile against decay into a coherent state (a single condensate) by small perturbations coupling the single-particle modes, breaking, e.g., rotational symmetry. As a consequence, the fragmented states are also extremely sensitive to small time-dependent perturbations like number fluctuations and generally excitations above the fragmented condensate ground state. Therefore, the instability of fragmentation towards a single condensate was traditionally assumed to be generic. However, a recent result within the two-mode approximation for scalar bosons with general interaction couplings (that is when one moves away from points of high symmetry), has shown that a continuous variety of ground state fragmentation can be obtained in a single trap. This type of fragmentation is, importantly, robust to perturbations coupling on the single-particle level.

In the following, we investigate whether the robustness of continuous fragmentation also persists against rapid changes on the dynamical many-body level, i.e. when interaction couplings rapidly change. Due to their many-body origin which is relying on the (relative) values of the couplings, fragmented states might then be expected to be more fragile. Here, we show that the sensitivity of fragmentation strongly depends on the range covered by a given coupling sweep. For a second-order dynamical quantum phase transition from the coherent to the fragmented phase, the creation of single-trap fragmentation from a coherent state is possible only for very slow sweeps of the coupling of bosonic pair exchange essentially determining the character of the ground state (single versus fragmented condensate). For moderately rapid exponential sweeps, the final degree of fragmentation is suppressed. The single-particle coherence measure $g_1$ (when averaged over time) vanishes after the sweep as well, while an analogously defined pair-coherence measure $g_2$ is macroscopically large. We therefore obtain a new pair-coherent phase which shows no single-particle fragmentation, in contrast to the ground state. The emergence of this phase is due to crossing the singular point of vanishing pair-exchange coupling. On the other hand, for sweeps entirely on the positive exchange-coupling side, no excited-state suppression is obtained even for large sweep rates, and the degree of fragmentation remains close to its ground-state value. We stress that these phenomena cannot occur in the fragmented phase of a conventional double-well with no pair exchange between sites included.

Let us consider the following two-mode Hamiltonian describing the dynamics of particles in an arbitrary trap and for a two-body interaction:

$$\hat{H} = \sum_{i=0,1} \epsilon_i \hat{n}_i + \frac{A_1}{2} \hat{n}_0(\hat{n}_0 - 1) + \frac{A_2}{2} \hat{n}_1(\hat{n}_1 - 1) + \frac{A_3}{2} \left( \hat{a}_0^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_0 + \text{h.c.} \right) + \frac{A_4}{2} \hat{n}_0 \hat{n}_1. $$ (1)

The Hamiltonian may be understood to result from going one step beyond the familiar semiclassical Gross-Pitaevskii theory, i.e., by inserting the field operator decomposition $\Psi = \hat{a}_0 \Psi_0 + \hat{a}_1 \Psi_1 + \cdots$ into the full second-quantized Hamiltonian and truncating the expansion after the first two modes. We thus neglect $O(1)$ fluctuations on top of these (now generally still quantum) modes, which are assumed to be the only modes macroscopically populated with a finite fraction of the number of particles, $N_i = O(N)$. The modes and two-body interactions are inhomogeneous and anisotropic in an independent way, leading to a set of interaction couplings $\{A_i\}$ with essentially arbitrary relative magnitudes and signs. We assume that the modes $\Psi_i$ have been determined, e.g., by the multiorbital mean-field method delineated in ..., and integrated out.

The sign of the pair-exchange coupling constant $A_3$ basically decides upon the classes of many-body ground states which can be obtained from the two-mode model. In contrast to optical lattices with pair-hopping, here both the couplings $A_3$ and $A_4$ have generally equal importance as $A_1$ and $A_2$. The Hamiltonian
then describes, e.g., single-trap fragmentation in harmonically trapped quasi-1D and quasi-2D gases in the weakly confining directions \( 15 \).

In what follows, we assume for simplicity that the single-particle states are degenerate, \( c_0 = c_1 \), so that we can omit the first term in \( 1 \); this does not change our results in any essential way. We employ the following ansatz for the many-body wave function

\[
|\Psi\rangle = \sum_{l=0}^{N} \psi_l(t) \left( \frac{(a^+_0)^{N-l}}{\sqrt{(N-l)!}} (a^+_1)^l \right) |0\rangle \equiv \sum_{l=0}^{N} \psi_l(t) |l\rangle ,
\]

which represents a linear superposition of Fock states \(|N-l,l\rangle \equiv |l\rangle \). We are interested in the time-dependence of the occupation amplitudes \( \psi_l(t) \), which comprise the information on the quantum many-body dynamics. At any instant, \( |\psi_l(t)|^2 \) gives the probability that \( l \) particles are in the second mode and \( N - l \) in the first. Both the amplitude and phase of the \( \psi_l \) will influence the temporal behavior of the first- and second-order coherence functions \( g_1 \) and \( g_2 \), to be described below.

The degree of fragmentation of an interacting many-body system, when maximally two field operator modes are macroscopically occupied, can be defined in an invariant manner from the difference of the (macroscopic) eigenvalues of the single-particle density matrix \( 1,8 \)

\[
\mathcal{F} = 1 - \frac{4}{N^2} \left( N_0 N_1 - |\langle \hat{a}_0^\dagger \hat{a}_1^\dagger \rangle|^2 \right) .
\]

Here, \( N_i = \langle \hat{n}_i \rangle \) are the diagonal elements of the single-particle density matrix, while the first order coherence \( g_1 = \frac{1}{2} \langle \hat{a}_0^\dagger \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_0 \rangle \) contains the real part of the off-diagonal correlator. For a coherent state with relative phase \( \Delta \theta \), \( g_1 = \sqrt{N_0 N_1} \cos(\Delta \theta) \), and \( \mathcal{F} \) vanishes.

We assume that the interaction couplings \( A_l \) are large enough for the system to attain a fragmented state \( 13 \), and that the couplings fulfill the condition \( A_1 + A_2 + 2 |A_3| > 4 > 0 \) \( t \) \( 8 \). To set the stage for the dynamical case and introduce some notions, we first discuss the stationary ground state solution for the \( \psi_l \) amplitudes. Due to structure of the Hamiltonian, even and odd \( l \) sectors decouple from each other for \( A_3 \neq 0 \) (cf. Eq. \( 17 \) below), and one gets a solution of the matrix equations for \( \psi_l \) with a state for even and odd \( l \) separately, \( |\phi\rangle = \sum_{\text{even} l} \phi_l |l\rangle \), \( |\Phi\rangle = \sum_{\text{odd} l} \Phi_l |l\rangle \). These two states are degenerate in the large \( N \) limit. Consequently, any complex choice of \( a \) and \( b \) in the superposition \( |\Psi\rangle = a |\phi\rangle + b |\Phi\rangle \), \( |a|^2 + |b|^2 = 1 \) leads to a ground state at the same energy, with vanishing first-order coherence \( g_1 \) and generally nonvanishing fragmentation \( \mathcal{F} \) on the \( A_3 > 0 \) side. There results, for \( A_3 > 0 \), a purely imaginary (or vanishing) correlator \( \langle \hat{a}_0^\dagger \hat{a}_1^\dagger \rangle = \sum_{\text{odd} l} \omega_l \psi_l^2 \hat{\Phi}_{l+1}^* \)

\[
\simeq 2i |ab| \sin \theta \sum_{\text{odd} l} \omega_l |\Phi_l|^2 ,
\]

with \( \omega_l \equiv \sqrt{(l+1)(N-l)} \) and we defined the relative phase between even and odd sectors \( \theta = \arg(b) - \arg(a) \).

The second line is valid in the continuum approximation of slowly varying occupation amplitudes, \( |\Phi_l| \simeq |\phi_{l \pm 1}| \), and \( \omega_l \simeq \omega_{l \pm 1} \). Hence \( g_1 \), the real part of the above correlator, vanishes in the continuum approximation.

The degree of fragmentation \( 13 \), as a function of \(|a|, |b| \), and the relative phase \( \theta \) between \( a \) and \( b \) (which were assumed to be real in \( 3 \) then evaluates to

\[
\mathcal{F} = 1 - \frac{2}{N^2} \left| ab \right| \sin \left( \theta - \frac{\sigma^2 + 2 \sigma^2}{N^2} \right)^2 + \sigma^2 .
\]

We used the Gaussian ground state distribution of \( |\Phi_l| \simeq |\phi_{l \pm 1}| \simeq \left( \sqrt{\pi / 4 \sigma} \right)^{-1/2} \exp[-(j - \Theta)/(2 \sigma^2)] \) representing a solution in the continuum limit \( 4,8 \). We defined \( j = l - N/2 \), \( \Theta = N/2 - N_0 = N_1 - N/2 \) as the shift from a maximally fragmented state and the distribution width \( \sigma = \sqrt{NR^{3/4}} \) with \( R \{ A_j \} = \frac{\text{max} \{ A_j \}}{\text{max} \{ A_j \} + A_{\text{largest}} - A_{\text{smallest}} \} \) (when \( \Theta \ll N/2 \)). For \( \theta = \pi/2 + \delta \) \( (|\delta| \ll 1) \) and \( |a| = |b| = 1/\sqrt{2} \), the degree of fragmentation is suppressed to \( \mathcal{F} = \sqrt{R} / (\delta^2 / 2 \), while being maximal for a given set \( \{ A_j \} \) at \( \theta = 0 \) \( \mod \pi \). Adding a small \( (\text{e.g.} \Omega = \mathcal{O}(A_1 / N)) \)

Josephson type perturbation

\[
\hat{H}_J = -\frac{\Omega}{2} (\hat{a}_0^\dagger \hat{a}_1^\dagger + \text{h.c.})
\]

on the \( A_3 < 0 \) side, the system is driven to a coherent state with \( a = b \) and \( \mathcal{F} = 0 \). On the \( A_3 > 0 \) side, the ground-state fragmentation is insensitive to \( \Omega \), the correction to \( \mathcal{F} \) being of order \( \Omega^2 / (N A_3^2) \), provided the singular region around \( A_3 = 0 \) is excluded.

We now proceed to the dynamical case, using \( A_1 \equiv 1 \) as unit of energy in the following. We assume an exponential sweep of the form \( A_3(t) = (A_1 - A_f) \exp[-\alpha t] + A_f \) with \( A_1 = A_3(t = 0) \) and \( A_f = A_3(t \to \infty) \), and that all other couplings remain essentially constant during the sweep \( \partial_t A_3 \gg \partial_t A_1, \partial_t A_2, \partial_t A_4 \) \( 16 \). The matrix equations resulting from \( 11 \) and \( 2 \) \( \hbar = 1 \)

\[
i \partial_t \psi_l = \frac{A_3(t)}{2} [d_{l+2} \psi_{l+2} + d_{l-2} \psi_{l-2}] + c r \psi_l - \frac{\Omega}{2} \left[ \omega_l \psi_{l+1} - \omega_{l-1} \psi_{l-1} \right]
\]

are solved numerically, where the coefficients \( c_l = \frac{1}{2} A_1(N - a) \right( N - a - 1 \right) + \frac{3}{2} A_2(l - 1) + \frac{3}{2} A_4(N - l) \) and \( d_l = \sqrt{(l+2)(l+1)(N-l-1)(N-l)} \).

The Josephson parameter \( \Omega \) is only dynamically effective in a small window around \( A_3 = 0 \) according to the ratio \( \Omega / N A_3(t) \) \( \text{cf. the ground state considerations above} \), and its effect is correspondingly small even for slow sweeps across the phase transition at \( A_3 = 0 \); we illustrate this insensitivity by showing additional \( \Omega = 1 \) data in Fig.\( 1 \) (green squares). While for second-order transitions, some small resonance peaks appear for slow sweeps \( \text{cf. Fig.} \ 1(a) \), at sufficiently large values of \( \alpha \), the
is crossed. For a second-order transition (a) $A_1 = A_4 = 1$, $A_2 = 0.5$, $A_3 = A_3(t = 0) = -0.2$, $A_f = A_3(\infty) = 0.4$, $N = 100$, ground state final value of $\mathcal{F}_{\infty} = 0.6$, and for (weakly) first order in (b) they are $A_2 = 0.6$, $N = 200$, $\mathcal{F}_{\infty} = 0.71$, $\Delta F \equiv 1/3$, others identical. The green squares are obtained by adding a perturbation of the form $\mathcal{B}$ with $\Omega = 1$. The inset shows $\mathcal{F}(t)$ for $\alpha = 0.01$; the blue arrow indicates where $A_3 = 0$. Note the different vertical axis origin for (a) and (b).

We have verified that taking $\Omega = 1$ also does not qualitatively alter the other $\Omega = 0$ results to follow.

During the sweep, the relative phase between the even and odd sectors, $\theta \equiv \frac{\pi}{N} \sum_{k=0}^{N/2} \{\operatorname{arg}(\psi_{2k+1}) - \operatorname{arg}(\psi_{2k})\} \forall |\psi_l|^2 > 0$, becomes time dependent. We will see that this has a crucial influence on the final degree of fragmentation $\mathcal{F}$ for sweeps from the coherent $A_3 < 0$ to the fragmented $A_3 > 0$ side. In the latter quantum phase transition, the singular point $A_3 = 0$ is crossed. At this point of vanishing pair-exchange coupling, the matrix problem in $\mathcal{B}$ becomes diagonal in the $|l\rangle$ Fock-space, and thus is easily solved. One Fock state $|l\rangle$ is obtained, with a fragmentation jump $\Delta \mathcal{F} = 1 - |A_1^l + A_3^l|^2$. The transition is therefore generally of first order, with a discontinuous change of fragmentation at $A_3 = 0$. We explore here both the second- and first-order cases of the dynamical quantum phase transition $\mathcal{B}$ when crossing the singular $\psi_l$-distribution point at $A_3 = 0$.

We observe a strong dependence on there being a ground-state fragmentation jump at $A_3 = 0$, i.e. on the transition being second ($\Delta \mathcal{F} = 0$) or first order ($\Delta \mathcal{F} \neq 0$). The final average degree of fragmentation is defined as $\bar{F}(\infty) \equiv \frac{1}{t_2-t_1} \int_{t_1}^{t_2} \mathcal{F}(t') dt'$, where $t_2 \gg t_1$ are two late times well after the phase transition point is crossed. For $\alpha \gg 1/N$, the final degree of fragmentation $\bar{F}(\infty)$ quickly tends to zero in the second-order case (Fig.2(a)). On the other hand, we obtain that $\bar{F}(\infty)$ decays much less rapidly with sweep rate $\alpha$ in the first-order case, cf. Fig.2(b). We show the dependence of $\bar{F}(\infty)$ on $\Delta \mathcal{F}$ in the left plot of Fig.2. For the second-order case (a) in Fig.2 the phase difference between the even and odd $l$ sectors is rapidly driven towards an average value $\bar{\theta} \approx \pi/2$ after crossing $A_3 = 0$ for intermediate values of $\alpha$ (cf. Fig.2). The phase difference of 90 degrees between even and odd $l$ sectors explains the strong suppression of fragmentation in this regime of $\alpha \ll 1$, while for first-order transitions, $\bar{\theta}$ well after the transition is significantly less than $\pi/2$. The reason for this intimate relation between $\bar{F}(\infty)$ and $\bar{\theta}(\infty)$ is that the argument leading to the ground-state result (11) is still approximately valid when the condition $\operatorname{arg}(\psi_l) + \operatorname{arg}(\psi_{l-1}) \approx \pi (\mod 2\pi)$ is fulfilled for most $l$ values, a property which we have verified.

The above behavior for the phase-transition sweep needs to be contrasted with the case $A_3$ strictly positive during the whole sweep, imposing that $A_3 \gg \mathcal{O}(1/N)$. The average degree of fragmentation is not suppressed, even when $\alpha \gg 1$ (and thus larger than the interaction couplings $A_i$). We illustrate this in Fig.3 cf. the fragmentation suppression observed for the quench case displayed in Fig.1. The insensitivity of fragmentation therefore persists for dynamical changes of $A_3$, provided the singular region around $A_3 = 0$ is not traversed.

We now discuss the pair-exchange coherence, measured by the expectation value

$$g_2 \equiv \frac{1}{2} \langle \hat{a}_0^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_0 + \hat{a}_1^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_1 \rangle. \quad (8)$$

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We observe, first of all, that the quantity $g_2$ can be macroscopic, i.e., $g_2 \sim \mathcal{O}(N^2)$, when the many-body state is neither coherent nor fragmented. In the ground state, it can be shown by direct calculation that for either sign of $A_3$, there is pair coherence except right at $A_3 = 0$ (where $g_2$ crosses zero), and that $g_2$ is independent of the weights $a$ and $b$. In particular, we have $g_2 \simeq -N^2/4 + \Omega^2/(8N^2A_3^2) + \sigma^2/2 + \delta^2$ for $A_3 > 0$.

The dynamical behavior of $g_2$ across the sweep, along with that of its single-particle counterpart $g_1$ is shown in Fig. 4. Whereas the degree of fragmentation is suppressed (see also Fig. 3), and the time-averaged value of first-order coherence is zero, an essentially stationary pair condensate emerges, cf. the bottom row of Fig. 3. For a (weakly) first-order transition (in the case shown, $\Delta F = 1/3$), fluctuations become stronger and there is an increasing suppression of pair-coherence for larger $\alpha$.

While on the single-particle coherent side, $g_1 \neq 0$, positive pair-exchange coherence is trivially achieved due to the existence of first-order coherence, on the $A_3 > 0$ side pair-coherence without single-particle fragmentation is the manifestation of a new pair-correlated phase emerging after the sweep. We emphasize that the pair coherence does not result from attraction between bosons, as all $A_i$ are chosen positive on the $A_3 > 0$ side [18].

We have shown that for moderately rapid variations of the pair-exchange coupling from negative to positive values in a second-order quantum phase transition, a new pair-coherent phase is created. In contrast to ground-state expectations, the resulting many-body state is not a single-particle fragmented state, with the microscopic origin that the average phase difference between even and odd sectors of the many-body amplitudes approaches $\pi/2$ after the quench. Rapid temporal changes of the interaction couplings of a many-body system can thus result in an emergent quantum phase with coherence properties strikingly different from those of the adiabatic ground state.

This research was supported by the Brain Korea BK21 program and the NRF of Korea, grant No. 2010-0013103.

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