Emergence and destruction of macroscopic wave functions

Bettina Gertjerenken and Martin Holthaus
Institut für Physik, Carl von Ossietzky Universität - D-26111 Oldenburg, Germany

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Abstract – The concept of the macroscopic wave function is a key for understanding macroscopic quantum phenomena. The existence of this object reflects a certain order, as it is present in a Bose-Einstein condensate when a single-particle orbital is occupied by a macroscopic number of bosons. We extend these ideas to situations in which a condensate is acted on by an explicitly time-dependent force. While one might assume that such a force would necessarily degrade any pre-existing order, we demonstrate that macroscopic wave functions can persist even under strong forcing. Our definition of the time-dependent order parameter is based on a comparison of the evolution of $N$-particle states on the one hand, and of states with $N - 1$ particles on the other. Our simulations predict the possibility of an almost instantaneous dynamical destruction of a macroscopic wave function under currently accessible experimental conditions.

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Introduction. – Superconductors, superfluids, and atomic Bose-Einstein condensates are described in terms of a macroscopic wave function, a notion originally conceived in London’s theory of superfluidity [1]: Instead of considering the Schrödinger wave function $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; t)$ of a Bose-condensed interacting $N$-particle system, one works with an effective single-particle wave function $\Phi(\mathbf{r}; t)$ which obeys the nonlinear Gross-Pitaevskii equation [2–6]. Experimental justification for the concept of the macroscopic wave function is provided by the observation of Josephson tunneling [7] between two superconductors coupled by a weak link [8]. Moreover, the occurrence of vortices, as observed in a series of landmark experiments with Bose-Einstein condensates [9–11], is a direct consequence of the existence of a macroscopic wave function. Obviously, the reduction of the full $N$-particle dynamics to that of a single-particle wave function requires that the system under consideration is highly ordered. This order is connected to the idea that $\Phi(\mathbf{r}; t)$ represents a macroscopically occupied single-particle orbital, so that the terms “macroscopic wave function” and “order parameter” often are used synonymously [12].

But now new experimental developments are posing new theoretical challenges. There is an increasing tendency to subject Bose-Einstein condensates to strong time-dependent forcing, so as to “engineer” novel systems which may not be accessible without such forcing. For instance, dynamic localization and quasi-energy band engineering has been demonstrated with Bose-Einstein condensates in strongly shaken optical lattices [13,14], and coherent control over the superfluid-to-Mott insulator transition has been achieved [15,16]. Moreover, giant Bloch oscillations have been realized with condensates in tilted, ac-driven optical lattices [17,18]. Still further experiments have demonstrated time-reversal symmetry breaking in shaken triangular lattices [19], and controlled photon-assisted tunneling [20,21]. A particularly ambitious line of this research addresses the realization and usage of tunable artificial gauge fields [22–25] or, phrased more generally, the exploitation of Bose-Einstein condensates in strongly forced optical lattices for quantum simulation purposes [26].

These activities lead to an important question: To what extent is the underlying order degraded if one subjects a macroscopic wave function to strong forcing? It has been emphasized already quite early that the solution to the time-dependent Gross-Pitaevskii equation does not represent a condensate if it becomes chaotic [27]. The obvious conflict between dynamical chaos and the possible existence of an order parameter has inspired further studies especially on $\delta$-kicked condensates, both theoretical and experimental ones [28–31]. But while the nonlinear...
Gross-Pitaevskii equation naturally can produce chaotic solutions in the presence of external forcing, the actual \( N \)-particle system still is described by a linear Schrödinger equation. Hence, while the \( N \)-particle wave functions cannot become chaotic in the sense of nonlinear dynamics, there should nonetheless be a certain quality of the time-dependent \( N \)-particle system which decides whether or not the solution to the Gross-Pitaevskii equation actually qualifies as a macroscopic wave function, and there should be a measure which quantifies the degree of order remaining in a Bose-Einstein condensate under the action of an external force. In this letter we suggest an approach to these issues which does not involve the familiar partitioning of the field operator into a condensate part and a noncondensate part \([32–37]\), but focuses on the evolution of neighboring states in Fock space. This may be seen as similar in spirit to the characterization of the degree of chaos in classical dynamical systems by probing the way initially close trajectories separate in time.

The order parameter. – A key question is how the time-dependent macroscopic wave function, if it exists, is obtained from the full \( N \)-particle state. A guide to the answer can be inferred from the discussion given by Lifshitz and Pitaevskii \([38]\): Let \( |\Psi(t)\rangle_N \) be a time-dependent \( N \)-particle condensate state, and let \( |\tilde{\Psi}(t)\rangle_{N-1} \) be a “like” state of \( N-1 \) particles; then the macroscopic wave function, normalized to unity, should be given by

\[
\Phi(r; t) = \lim_{N \to \infty} N^{-1} \langle \tilde{\Psi}(t)|\hat{\psi}(r)|\Psi(t)\rangle_{N}/\sqrt{N},
\]

where \( \hat{\psi}(r) \) is the bosonic field operator. But this leaves open the question how to quantify the “likeness” of \( |\Psi(t)\rangle_N \) and \( |\tilde{\Psi}(t)\rangle_{N-1} \); if two such states are “like” at one particular moment \( t_0 \), they might not remain so under the influence of time-dependent forcing. Moreover, it seems desirable to get rid of the limit of an infinite particle number, and to study the emergence of a “macroscopic” wave function already when \( N \) is relatively small. With this background, we proceed as summarized by fig. 1: We start from an initially given \( N \)-boson state \( |\Psi(t_0)\rangle_N \), which is not necessarily a pure condensate. Under the influence of some force which does not need to be specified at this point it develops in time into the \( N \)-particle state \( |\Psi(t)\rangle_N \), as determined by the system’s time-evolution operator \( \hat{U}(t, t_0) \). In order to generate suitable \((N-1)\)-particle states for taking the matrix elements suggested by eq. (1), we act with the bosonic annihilation operators \( \hat{\psi}(r) \) on the initial state, and normalize the results, obtaining

\[
|\tilde{\Psi}(r|t_0\rangle_{N-1} = \frac{\hat{\psi}(r)|\Psi(t_0)\rangle_N}{\|\hat{\psi}(r)|\Psi(t_0)\rangle_N\|}.
\]

These subsidiary states likewise evolve in time under the action of the very same evolution operator, giving states \( |\tilde{\Psi}(r|t\rangle_{N-1} \). We then define a function \( \Phi(r; t) \) according to

\[
\sqrt{N}\Phi(r; t) = \langle \tilde{\Psi}(r|t\rangle_{N-1}|\hat{\psi}(r)|\Psi(t)\rangle_N.
\]

Observe the difference to the above tentative prescription (1): We employ not just one single subsidiary \((N-1)\)-particle state, but infinitely many; in principle, there is one state \( |\tilde{\Psi}(r|t\rangle_{N-1} \) associated with each \( r \) considered. Still, \( \Phi(r; t) \) as defined by eq. (3) should qualify as a macroscopic wave function for sufficiently large \( N \), and obey the Gross-Pitaevskii equation, provided the above “likeness” condition is satisfied. This means that the state trajectories evolving from the respective initial states \( |\tilde{\Psi}(r|t_0\rangle_{N-1} \) and \( |\Psi(t_0)\rangle_N \) in Fock space should not diverge from each other too much, in a suitable sense. To bring this intuitive idea into a precise form, we also annihilate a boson from the time-evolved \( N \)-particle state, thus producing

\[
|\tilde{\Psi}(r|t\rangle_{N-1} = \frac{\hat{\psi}(r)|\Psi(t)\rangle_N}{\|\hat{\psi}(r)|\Psi(t)\rangle_N\|} = \frac{\hat{\psi}(r)\hat{U}(t, t_0)|\Psi(t_0)\rangle_N}{\|\hat{\psi}(r)|\Psi(t_0)\rangle_N\|}.
\]

Then the scalar products

\[
R(r; t) = \langle \tilde{\Psi}(r|t\rangle_{N-1}|\tilde{\Psi}(r|t\rangle_{N-1} = \frac{\langle \tilde{\Psi}(r|t\rangle_{N-1}|\hat{\psi}(r)|\tilde{\Psi}(r|t\rangle_{N-1})}{\|\hat{\psi}(r)|\tilde{\Psi}(r|t\rangle_{N-1}\|\|\hat{\psi}(r)|\tilde{\Psi}(r|t\rangle_{N-1}\|}
\]

have a particular significance: If \( R(r; t) = 1 \), the candidate \( \Phi(r; t) \) provided by eq. (3) is a true macroscopic

\[
\begin{align*}
|\Psi(t_0)\rangle_N & \xrightarrow{\hat{U}(t, t_0)} |\Psi(t)\rangle_N \\
\hat{\psi}(r) & \quad |\tilde{\Psi}(r|t\rangle_{N-1} \\
|\tilde{\Psi}(r|t_0\rangle_{N-1} & \xrightarrow{\hat{U}(t, t_0)} |\tilde{\Psi}(r|t\rangle_{N-1} \\
\end{align*}
\]
wave function, obeying the Gross-Pitaevskii equation. In general, the magnitude $|R(r;t)|$, varying between 0 and 1, provides the desired measure of the degree of order of the time-evolving $N$-boson system.

The justification for this statement stems from the observation that the proper macroscopic wave function has to satisfy the requirement

$$N|\Phi(r;t)|^2 = N\langle \Psi(t)|\hat{\psi}^\dagger(r)\hat{\psi}(r)|\Psi(t)\rangle_N,$$  \tag{6}

demanding that its absolute square, multiplied by the particle number $N$, yields the exact $N$-particle density of the system \[38\]. Introducing the projection operators

$$\hat{Q}_t = |\Xi(r;t)|_{N-1}N |\Xi(r;t)|,$$  \tag{7}

we have the obvious identity

$$N\langle \Psi(t)|\hat{\psi}^\dagger(r)\hat{\psi}(r)|\Psi(t)\rangle_N = N\langle \Psi(t)|\hat{\psi}^\dagger(r)\hat{Q}_t\hat{\psi}(r)|\Psi(t)\rangle_N,$$  \tag{8}

Now, if this projector (7) were equal to the projector $\hat{P}_t$ defined by

$$\hat{P}_t = |\Psi(r;t)|_{N-1}N |\Psi(r;t)|,$$  \tag{9}

which, in its turn, would be the case if $|\Xi(r;t)|_{N-1}$ differed from $|\Xi(r;t)|_{N-1}$ by not more than a phase factor, we could deduce

$$N\langle \Psi(t)|\hat{\psi}^\dagger(r)\hat{\psi}(r)|\Psi(t)\rangle_N = N\langle \Psi(t)|\hat{\psi}^\dagger(r)\hat{P}_t\hat{\psi}(r)|\Psi(t)\rangle_N,$$  \tag{10}

from which the desired identity (6) follows immediately, keeping in mind the definition (3).

This reasoning deserves still more scrutiny. Namely, if $|\Xi(r;t)|_{N-1}$ indeed differs from $|\Psi(r;t)|_{N-1}$ merely by a phase factor, then $\hat{\psi}(r)|\Psi(t)\rangle_N$ is proportional to $|\Psi(r;t)|_{N-1}$, wherefrom one is led to the relation

$$\hat{\psi}(r)|\Psi(t)\rangle_N = \sqrt{N}\hat{\Phi}(r;t)|\Psi(r;t)\rangle_N.$$  \tag{11}

This is reminiscent of what defines a condensate: Assuming that the $N$-particle state at some moment $t_0$ corresponds to an $N$-fold occupied single-particle orbital $\phi(r, t_0)$ and thus is a pure condensate state of the form

$$|\Psi_\phi(t_0)\rangle_N = \frac{1}{\sqrt{N!}}\int d^3r \phi(r; t_0) \hat{\psi}^\dagger(r)^N|\text{vac}\rangle,$$  \tag{12}

it obeys the equation

$$\hat{\psi}(r)|\Psi_\phi(t_0)\rangle_N = \sqrt{N}\hat{\phi}(r; t_0)|\Psi_\phi(t_0)\rangle_{N-1}$$  \tag{13}

at that moment $t_0$. Therefore, the condition (11), which (if satisfied) guarantees that the time-dependent order parameter takes on its maximum value $|R(r;t)| = 1$, and thus makes sure that the candidate $\Phi(r;t)$ defined through eq. (3) actually is a macroscopic wave function, generalizes the familiar characterization of a pure condensate expressed by eq. (13) so as to also involve time evolution, and reduces to it when the time $t$ is close to $t_0$. Again adopting the dynamical-systems viewpoint, the projection (5) compares the trajectory of the given $N$-particle state in Fock space to that of subsidiary, neighboring $(N-1)$-particle states. If it does not matter whether one annihilates first and propagates then, or whether one propagates prior to annihilating, the flow in Fock space may be considered as (locally) stiff. Hence, we refer to the magnitude $|R(r;t)|$ as stiffness, with maximum stiffness $|R(r;t)| = 1$ expressing time-preserved coherence in the sense of eq. (11).

Note that the formal employment of subsidiary $(N-1)$-particle states is necessary only to provide a reference for the evolution of the true $N$-boson system: We do not violate particle number conservation, and hence do not involve spontaneous symmetry breaking \[32–34\]. Moreover, an interesting observation can be made here: If the decisive relation (11) is satisfied, then the definition (5) immediately yields

$$R(r;t) = \frac{\Phi(r;t)}{|\Psi(r;t)|},$$  \tag{14}

meaning that the phase of $R(r;t)$ equals that of $\Phi(r;t)$. Read in the reverse direction, this implies that the phase of a macroscopic wave function contains information on the difference of the evolution of “neighboring” $N$- and $(N-1)$-particle states. This is well known in the equilibrium case, when the phase of the solution to the Gross-Pitaevskii equation is determined by the chemical potential, i.e., by the energy required to add one more particle to the system. The present considerations show that the phase retains a similar meaning even in case of nonequilibrium, in which a chemical potential does not exist.

**Numerical simulations.** In order to illustrate some consequences of the concepts developed above, we utilize the model of a bosonic Josephson junction \[34,39\], as described by the Hamiltonian

$$H_0 = -\frac{\hbar\Omega}{2}\left(a_1^\dagger a_2 + a_2^\dagger a_1\right) + \hbar\kappa\left(a_1^\dagger a_1 a_2 a_1 + a_2^\dagger a_2 a_2 a_1\right).$$  \tag{15}

Here the hopping matrix element between the two sites labeled 1 and 2 is given by $\hbar\Omega/2$, so that $\hbar\Omega$ is the single-particle tunneling splitting, while $2\hbar\kappa$ quantifies the repulsion energy of two particles occupying a common site. The bosonic operator $a_j$ annihilates a particle at the $j$-th site; $a_j^\dagger$ is its adjoint creation operator. This system is subjected to a time-dependent bias with carrier frequency $\omega$ and envelope $\hbar\mu(t)$, as specified by

$$H_1(t) = \hbar\mu(t)\sin(\omega t)\left(a_1^\dagger a_1 - a_2^\dagger a_2\right),$$  \tag{16}

the total Hamiltonian then reads

$$H(t) = H_0 + H_1(t).$$  \tag{17}

Even with constant amplitude $\mu(t) = \mu_1$ this model captures nontrivial features of many-body dynamics \[40,41\]; it
is one of the very rare systems which allows one to monitor the emergence of a macroscopic wave function numerically, but without further approximations on the $N$-particle level. For all following simulations we select the ground state $|\Psi(0)\rangle_N$ of the time-independent junction (15) with scaled interaction strength $N\kappa/\Omega = 2.0$ as the initial state. Note that this ground state is no $N$-fold occupied single-particle state in the sense of eq. (12), because the relatively strong interparticle interaction leads to sizeable depletion [42]. The required subsidiary states (2) then are given by

$$|\tilde{\Psi}_j(N-1)\rangle = \frac{a_j|\Psi(0)\rangle_N}{\|a_j|\Psi(0)\rangle_N\|}$$

for $j = 1, 2$. Moreover, we fix the scaled carrier frequency $\omega/\Omega = 1.6$, and consider a Gaussian envelope

$$\mu(t) = \mu_{\text{max}} \exp\left(-t^2/2\sigma^2\right)$$

with width $\sigma/T = 10$, where the time scale is set by $T = 2\pi/\omega$. In fig. 2 we monitor the response of a system with $N = 100$ particles to a pulse with maximum driving strength $\mu_{\text{max}}/\Omega = 0.51$ by plotting the scaled population imbalance

$$\langle J_z(t)\rangle/N = N\langle \Psi(t)|a_1^\dagger a_1 - a_2^\dagger a_2|\Psi(t)\rangle_N/(2N)$$

vs. time. We also show the stiffness $|R_1(t)|$; the corresponding quantity $|R_2(t)|$ obtained for the other site looks practically identical. Although $N = 100$ is not “macroscopically large”, one observes that $|R_1|$ stays close to unity almost until the pulse’s middle, and then decreases in an oscillating manner. Thus, already in this situation there exists a good macroscopic wave function during the entire pulse, indicating that one can subject a macroscopic wave function to strong forcing almost without reducing its order.

Increasing the particle number to $N = 1000$, while keeping $N\kappa/\Omega$ and all other parameters constant, we obtain fig. 3. This is a truly remarkable finding: Although the $N$-particle state undergoes violent changes when adjusting itself to the driving force, the stiffness remains close to its theoretical maximum during the entire pulse, indicating that one can subject a macroscopic wave function to strong forcing almost without reducing its order.

A quite different scenario is depicted in fig. 4. Here we have increased the driving amplitude to $\mu_{\text{max}}/\Omega = 0.55$, and consider both $N = 1000$ (upper panel) and $N = 10000$ (lower panel). While we observe excellent stiffness during the first half of the pulse, with $1 - |R_1(t)|$ apparently scaling with $1/N$, the macroscopic wave function is destroyed suddenly; this sudden destruction cannot be counteracted by an increase of $N$ [42]. We utilize this example also to illustrate one more feature: As long as it exists, the macroscopic wave function should conform to the Gross-Pitaevskii equation. One may still solve that equation even beyond the point of destruction of the macroscopic wave function, but then the solution no longer captures the actual $N$-particle dynamics. This is verified by fig. 5, where we superimpose the $N$-particle imbalance (20) for $N = 1000$ to the prediction made by the Gross-Pitaevskii equation. As long as there is close-to-perfect stiffness, both curves are almost indistinguishable from each other, confirming the accuracy of the Gross-Pitaevskii approach under conditions of time-preserved coherence. But when the macroscopic wave function is destroyed, the Gross-Pitaevskii dynamics become chaotic, losing their connection to the $N$-particle level.
Fig. 4: (Colour on-line) Dynamically induced destruction of macroscopic wave functions. As in fig. 2, but with higher driving amplitude $\mu_{\text{max}}/\Omega = 0.55$, and $N = 1000$ (upper panel) or $N = 10000$ (lower panel). The macroscopic wave function is not destroyed gradually, but quite suddenly; this destruction cannot be prevented by increasing the particle number.

Discussion. – The observations made in this work have both conceptual and experiment-oriented consequences. We have addressed the question why the solution to the time-dependent nonlinear Gross-Pitaevskii equation can provide a good description of a forced condensate only when it behaves in a regular, nonchaotic manner: That distinction between order and chaos should have a counterpart already on the linear $N$-particle level. As one possible characterization of this difference we suggest to monitor the time evolution of “neighboring” trajectories in Fock space of states consisting of $N$ and $N - 1$ particles, respectively. With $N$-particle states being orthogonal to states consisting of one particle less, the required measure of proximity of these states is provided by the projection of the former after annihilation of one particle onto the latter. In this way, one can not only give a more definite meaning to the sketch by Lifshitz and Pitaevskii on how to construct the wave function of the condensate [38], but one also obtains the desired indicator for the quality of this construction: The presence of a time-dependent macroscopic wave function necessarily requires that initially close state trajectories stay close to each other in the course of time. If this condition is satisfied, the unmodified Gross-Pitaevskii equation provides an excellent description of the $N$-particle dynamics; if not, the macroscopic wave function is destroyed [42].

Our matter-of-principle discussion is of little practical help when it comes to computing the instability of a driven Bose-Einstein condensate in experimentally realistic situations, implying that knowledge of the exact $N$-particle state cannot be obtained. In such cases one requires other approaches, such as the second-order number-conserving self-consistent treatment developed by Gardiner and Morgan [35], which has been applied to a toroidally trapped, $\delta$-kicked condensate by Billam et al. [36,37]. One then couples the solution of a generalized Gross-Pitaevskii equation to modified Bogoliubov-de Gennes equations, assuming that the ratio of noncondensate to condensate particle numbers be a small parameter. This approach allows one to assess driven condensate dynamics with experimentally realistic particle numbers [35–37].

Yet, even our idealized model calculations, which are not tied to any small parameter, do convey messages of practical importance. We have shown that a driving force does not necessarily destroy a macroscopic wave function when it is applied smoothly, in the form of forcing pulses with a sufficiently slowly changing envelope. This particular manifestation of the quantum adiabatic principle signals green light for systematic quantum engineering with macroscopic wave functions. The identification
of maximum stiffness, or of time-preserved coherence in the sense of eq. (11), as the salient feature of a time-dependent macroscopic wave function may guide future investigations. Our simulations also illustrate an important fact: The initial N-particle state considered therein, which is the ground state of the model (15), equals a pure condensate state only for vanishing interaction, that is, for $N\kappa/\Omega = 0$ [42], whereas we consider strong interparticle interaction, $N\kappa/\Omega = 2.0$. Nonetheless, maximum stiffness can still be attained to an amazing degree of accuracy, as exemplified in fig. 3. Finally, the observation that substantial degradation of the underlying order parameter may not occur gradually in time, but rather can be connected to certain critical driving strengths, is open to experimental verification. Such experiments do not necessarily require a driven bosonic Josephson junction, but can also be performed in other configurations. For instance, one could subject a Bose-Einstein condensate in a strongly anharmonic trap to a smooth forcing pulse, and perform a time-of-flight measurement of the condensate fraction after the pulse is over. If one repeats this measurement with successively stronger pulses, one should observe a sudden disappearance of the condensate peak at a certain critical maximum driving amplitude.

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