Collapses and Revivals of Bose-Einstein Condensates Formed in Small Atomic Samples

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The macroscopic wave function for atomic samples composed of a few thousand particles is shown to exhibit collapses and revivals on a few seconds time scale, while Bose-Einstein condensation remains in the form of off-diagonal long-range order in the one-particle reduced density matrix. A recently proposed measurement scheme which is sensitive to Bose-broken gauge symmetry, and hence to the macroscopic wave function, could be used to detect the collapses and revivals experimentally. [S0031-9007(96)01005-8]

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The recent spectacular observations of Bose-Einstein condensation (BEC) in atomic vapors [1-3] open up new avenues of research into the generation and manipulation of coherent atomic beams. Among these possibilities are nonlinear atom optics and development of an atom laser. Future progress in these areas provides impetus for striving toward higher atomic densities. For the condensates reported so far, the number of atoms ranges between 10^3 and 10^5 , small in comparison to the typical number of atoms $N = 10^{20}$ in liquid helium experiments. This suggests that the small samples involved in current atomic experiments may cause deviations from the behavior predicted for macroscopic systems.

Atomic BEC experiments also present the opportunity to further our understanding of BEC since they are weakly interacting Bose gases and are therefore amenable to more detailed theoretical analysis than strongly interacting Bose liquids, such as helium. In particular, following Penrose and Onsager [4], the condition for BEC is that the one-particle reduced density matrix $\rho_1(\mathbf{r}, \mathbf{r}', t) = \langle \hat{\psi}^{\dagger}(\mathbf{r}, t) \hat{\psi}(\mathbf{r}', t) \rangle$ does not vanish for large separation. Here $\hat{\psi}(\mathbf{r}, t)$ and $\hat{\psi}^{\dagger}(\mathbf{r}, t)$ are the Heisenberg picture field operators which annihilate and create atoms at position \mathbf{r} , and $\langle \cdots \rangle$ signifies a broken symmetry average [5,6]. More specifically, the contribution to the one-particle reduced density matrix representing the off-diagonal long-range order (ODLRO) [7] of the condensate is written in the factorized form

$$\rho_1(\mathbf{r}, \mathbf{r}', t) = \Phi^*(\mathbf{r}, t)\Phi(\mathbf{r}', t).$$
(1)

The conventional choice is $\Phi(\mathbf{r}, t) = \langle \hat{\psi}(\mathbf{r}, t) \rangle$, with $\langle \hat{\psi}(\mathbf{r}, t) \rangle$ the macroscopic wave function [8,9], which then acts as an order parameter for the Bose-condensed system [10]. The appearance of a complex order parameter with an arbitrary but fixed phase signals that the U(1) gauge invariance of the underlying Hamiltonian, associated with particle number conservation, is broken spontaneously in the condensation process, and this underlies the concept of Bose-broken gauge symmetry, according to which

the many-body ground state need not display the full symmetry of the Hamiltonian (see, for example, the article by Leggett in Ref. [11]). Discussions of the order parameter are typically restricted to the thermodynamic limit where the number of particles (atoms) tends to infinity while the density is held fixed [10,12]. In general, however, the macroscopic wave function need not act as an order parameter. For example, for an ideal Bose gas the macroscopic wave function vanishes (see the article by Stoof in Ref. [11]), and Stoof [13] has shown that $\langle \hat{\psi}(\mathbf{r}, t) \rangle$ cannot act as an order parameter for a weakly interacting bulk Bose gas with negative scattering length due to its inherent instability.

In this Letter we investigate the macroscopic wave function for BEC in small atomic samples, and its role as an order parameter. If the grand canonical ensemble is used then the macroscopic wave function vanishes as this ensemble corresponds to a density operator which is diagonal when basis states involving fixed numbers of particles are used [10]. This is the case for measurements on the condensate which are performed over long times such that true thermal equilibrium is established [5]. However, for measurement times short compared to relaxation times, quantum coherences associated with the condensate remain intact [5,14]. Here we employ a wave packet composed of states of a fixed number of particles N in the condensate, with expansion coefficients $a_N = |a_N| e^{i\zeta_N}$, hence retaining quantum coherence. The present description of BEC, due to Barnett et al. [14], is therefore different from the conventional η ensemble which employs a wave packet of states corresponding to a different total number of particles, condensate plus noncondensate, and is generally only applicable in the thermodynamic limit [5]. A coherent state with $a_N = \overline{N}^{N/2} e^{iN\eta} e^{-\overline{N}/2} / \sqrt{N!}$ suggests itself, but the states associated with BEC do not generally possess such complete phase coherence [15]. Nevertheless, a pure state description of the condensate may be rendered plausible as follows: Below the Einstein condensation temperature, the many-body ground state of

the system becomes macroscopically occupied, yielding a condensate which should be considered an open quantum system in contact via many-body interactions with the environment or resevoir composed of the noncondensate atoms. It is known from the work of Zurek et al. [16] and Gallis [17] that for a system, in their case a harmonic oscillator, in interaction with an environment certain pure states show considerable stability against loss of quantum coherence, and that in the weak coupling limit the pure states of maximal stability are the coherent states. Thus, the quantum coherence of the condensate may be reasonably represented by a pure state, though perhaps not precisely a coherent state since weak coupling may not hold. This argument does not depend on the size of the system, except that the noncondensate atoms may be viewed as a resevoir, and the conclusions therefore apply even for small condensates far removed from the thermodynamic limit. Here we use the wave packet description to calculate the macroscopic wave function in small atomic samples, and find that it exhibits collapses and revivals in time reminiscent of those which occur in the Jaynes-Cummings model of quantum optics [18]. During the collapse $\langle \hat{\psi}(\mathbf{r}, t) \rangle \rightarrow 0$, so that it cannot be identified as an order parameter for the system.

First we consider the standard treatment of the condensate in a Bose gas [12]. At zero temperature, and for a weakly interacting gas, the particles may be assumed to be predominantly in the condensate. The normalized condensate wave function is then $\psi_N(\mathbf{r}, t) =$ $N^{-1/2}\langle N - 1|\hat{\psi}(\mathbf{r}, t)|N\rangle$, where $|N\rangle$ is a state with N particles in the condensate. The self-consistent nonlinear Schrödinger equation for the condensate wave function is the Gross-Pitaevskii equation [12] generalized to include the isotropic magneto-optical harmonic trap [19,20]. We are interested in the ground state solution of this equation for which we set $\psi_N(\mathbf{r}, t) = \exp(-i\mu_N t/\hbar)\phi_N(\mathbf{r})$, giving the stationary Gross-Pitaevskii equation:

$$\mu_N \phi_N = \left[-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega_t^2 r^2 + N U_0 |\phi_N|^2 \right] \phi_N,$$
(2)

where *m* is the atomic mass, ω_t is the angular frequency of the trap, and $U_0 = 4\pi\hbar^2 a/m$ measures the strength of the two-body interaction, *a* being the *s*-wave scattering length. Here we consider a repulsive interaction so that a > 0. The parameter μ_N is given by $\mu_N = d\mathcal{E}_N/dN$, where \mathcal{E}_N is the expectation value of the energy for *N* particles in the state ϕ_N . By a slight extension of the usual terminology, μ_N will be called the chemical potential of the *N*-particle condensate.

Edwards and Burnett [19], and Ruprecht *et al.* [20] have solved Eq. (2) numerically to obtain both the condensate wave functions and the chemical potentials μ_N as functions of *N* (see also Baym and Pethick [21]). We do not require the full details here, but the main features are that the chemical potential and the spatial extent of the condensate wave function both increase with *N* due to the

repulsive two-body interaction. For low particle number the nonlinear term in Eq. (2) may be neglected, and the characteristic volume of the condensate is $V_t = 4\pi r_t^3/3$, with $r_t = (\hbar/2m\omega_t)^{1/2}$ the spatial scale of the linear harmonic oscillator. For large particle number the characteristic spatial scale r_N of the condensate may be approximated as the minimum of the effective potential $U(r_N) = m\omega_t^2 r_N^2/2 + 3NU_0/4\pi r_N^3$, where we replaced $|\phi_N|^2 = 3/4\pi r_N^3$ in the nonlinear term of Eq. (2), giving $r_N = (9U_0 N / 4\pi m \omega_t^2)^{1/5} \approx 2(N / N_{\min})^{1/5} r_t$, and $N_{\min} = r_t/a$. This formula applies only for $N > N_{\min}$; otherwise, $r_N < r_t$, which is impossible for a repulsive interaction. Thus, the condensate volume is given ap- $V_N \approx 8V_t (N/N_{\rm min})^{3/5}$ atomic density is proximately by and the corresponding $n \approx$ $(1/8) (N_{\rm min}/V_t) (N/N_{\rm min})^{2/5}.$ These approximations are valid if the characteristic length scale or co-herence length $r_{\rm coh} = (8\pi an)^{-1/2}$ [12] is less than the condensate size. Taking numbers representative of an experiment with rubidium-87 atoms [1], $m = 1.44 \times 10^{-25}$ kg, a = 10 nm, $\omega_t = 80\pi$ rad s⁻¹, $r_t = 1.2 \ \mu\text{m}$, and N = 2000, yields $N_{\min} = 120$, $V_N \approx 43V_t$, $n \approx 6.4 \times 10^{12} \text{ cm}^{-3}$, $r_{\text{coh}} = 0.8 \ \mu\text{m}$, and $r_N = 4.2 \ \mu m$, so that the approximations are valid.

The definition of the condensate wave function given above is rigorous in the thermodynamic limit [12]. To investigate the case of a small condensate, say a few thousand atoms, we employ the wave packet description of the condensate, and further assume that the particle number distribution $|a_N|^2$ is sharply peaked with variance ΔN around a mean particle number $\overline{N} > N_{\min}$. As a concrete example, we take a Poissonian distribution for which $\Delta N = \overline{N}^{1/2}$. which is reasonable since the number distribution $|a_N|^2$ of the condensate should be approximately that of a coherent state, though the phases ζ_N may not be so correlated. Then, we require the chemical potential μ_N in a range $\Delta N \ll \overline{N}$ around the mean number \overline{N} . Therefore, the leading order solution of Eq. (2) is obtained for $N = \overline{N}$, giving $\phi_N^{(0)}(\mathbf{r}) = \phi_{\overline{N}}(\mathbf{r})$ and $\mu_N^{(0)} = \mu_{\overline{N}}$, and we treat the remaining term $U_0(N-\overline{N})|\phi_N|^2\phi_N$ as a perturbation. This assumes that $\phi_{\overline{N}}(\mathbf{r})$ is a stable solution of the Gross-Pitaevskii equation, which is the case for a positive scattering length [20]; otherwise, small changes in the particle number N can lead to large changes in $\phi_N(\mathbf{r})$. Then to first order in perturbation theory

$$\phi_N(\mathbf{r}) = \phi_{\overline{N}}(\mathbf{r}), \qquad \mu_N = \mu_{\overline{N}} + \mu'_{\overline{N}}(N - \overline{N}), \quad (3)$$

where $\mu'_{\overline{N}} = U_0 \Gamma_{\overline{N}} / V_t$ and $\Gamma_{\overline{N}} = V_t \int d^3 \mathbf{r} |\phi_{\overline{N}}(\mathbf{r})|^4$. The dimensionless parameter $\Gamma_{\overline{N}}$ can be calculated numerically, but physically it is like the ratio of the linear trap volume to the condensate volume, $V_t / V_{\overline{N}}$, so that $\Gamma_{\overline{N}} \approx (N_{\min}/\overline{N})^{3/5}$. Gathering these results together, we find [21]

$$\mu_{\overline{N}}' \approx \hbar \omega_t \left(\frac{\pi a}{r_t}\right) \left(\frac{N_{\min}}{\overline{N}}\right)^{3/5}.$$
 (4)

For this perturbative calculation $\phi_N(\mathbf{r})$ is fixed and evaluated at $N = \overline{N}$, and the important ingredient is the

dispersion of the chemical potential μ_N with *N* around \overline{N} in Eq. (3). For large mean particle number, $\mu'_{\overline{N}}$ tends to zero so that the dependence on particle number vanishes. These basic features are borne out in the numerical calculations of Ruprecht *et al.*, who observed that the slope of the chemical potential versus nonlinear constant (proportional to particle number) decreases with increasing particle number (see Fig. 2 of [Ref. 20]).

We are now equipped to construct the wave packet for the condensate state vector alluded to above, which we write as

$$|\Psi(t)\rangle = \sum_{N} a_{N} e^{-iN\mu_{N}t/\hbar} (N!)^{-1/2} (\hat{b}^{\dagger})^{N} |0\rangle, \quad (5)$$

where the exponential contains the term $N\mu_N$ since there are N particles each of chemical potential μ_N , the operator $\hat{b}^{\dagger} = \int d^3 \mathbf{r} \phi_{\overline{N}}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}, 0)$ creates particles with distribution $\phi_{\overline{N}}(\mathbf{r})$ [10], with $[\hat{b}, \hat{b}^{\dagger}] = 1$, and $|0\rangle$ is the vacuum state. The approximations employed in Eq. (5) are tantamount to the Hartree approximation. The field annihilation operator can now be written in a mode expansion as $\hat{\psi}(\mathbf{r}, 0) = \hat{b} \phi_N(\mathbf{r}) + \tilde{\psi}(\mathbf{r}, 0)$, where by construction the first term acts on the condensate state vector, whereas the second term accounts for the noncondensate atoms (the environment). Using the state vector (5) we obtain the one-particle reduced density matrix representing the condensate

$$\rho_{1}(\mathbf{r}, \mathbf{r}', t) = \langle \Psi(t) | \hat{b}^{\dagger} \hat{b} | \Psi(t) \rangle \phi_{\overline{N}}^{*}(\mathbf{r}) \phi_{\overline{N}}(\mathbf{r}')$$
$$= \overline{N} \phi_{\overline{N}}^{*}(\mathbf{r}) \phi_{\overline{N}}(\mathbf{r}'), \qquad (6)$$

and the condensate wave function

$$\langle \hat{\psi}(\mathbf{r},t) \rangle = \langle \Psi(t) | \hat{b} | \Psi(t) \rangle \phi_{\overline{N}}(\mathbf{r})$$

= $\overline{N}^{1/2} \phi_{\overline{N}}(\mathbf{r}) e^{-i\mu t/\hbar} \mathcal{F}_{\overline{N}}(t) ,$ (7)

where

$$\mathcal{F}_{\overline{N}}(t) = \sum_{N} \sqrt{\frac{N}{\overline{N}}} a_{N-1}^* a_N \{ \cos[2\mu_{\overline{N}}'(N-\overline{N})t/\hbar] - i \sin[2\mu_{\overline{N}}'(N-\overline{N})t/\hbar] \}, \qquad (8)$$

and $\mu = \mu_{\overline{N}} + \overline{N}\mu'_{\overline{N}}$ is the net chemical potential of the condensate. The one-particle reduced density matrix (6) is of the same form as Eq. (1) with $\Phi(\mathbf{r}, t) \propto \overline{N}^{1/2}\phi_{\overline{N}}(\mathbf{r}, t)$, so that our wave packet yields ODLRO and hence BEC. This conclusion holds for any mean particle number, as long as the mean field approximations employed are valid. Here the ODLRO extends over separations $|\mathbf{r} - \mathbf{r}'| \approx r_{\overline{N}}$, the spatial scale of the condensate. In the experiments the one-particle reduced density matrix is not measured, but rather the momentum space (velocity) distribution is obtained by releasing the atoms from the trap, letting them fall under gravity, and imaging them. The momentum spread will then be $\Delta K \approx 2\pi/r_{\overline{N}}$, so that the ODLRO is transferred to a sharp spike in the imaged atomic distribution [1–3].

Turning now to the macroscopic wave function (7), we see that the factor $\mathcal{F}_{\overline{N}}(t)$ takes the form of a weighted

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sum of trigonometric functions with different frequencies. Such sums are well known from the Jaynes-Cummings model of quantum optics, which describes the interaction between a single-mode radiation field and a two-level atom, and give rise to the phenomenon of collapses and revivals [18], and the same is expected here. Collapse and revivals also appear in the relative phase between two superfluids or superconductors [22]. Directly from the form of Eq. (8) we see that $\mathcal{F}_{\overline{N}}(t)$ is periodic in time with period $T_{\overline{N}} = \pi \hbar / \mu'_{\overline{N}}$, and the revivals occur with this period. The revivals result from the fact that the sum in Eq. (8) is over the discrete particle number, so that they are a direct result of the granularity of matter. The collapses depend on the choice of the number distribution $|a_N|^2$. For our purposes we need only the variance ΔN in particle number and the assumption that the phases are correlated enough that $\mathcal{F}_{\overline{N}}(0)$ does not vanish exactly. Then $\mathcal{F}_{\overline{N}}(t)$ is periodic and has a maximum in magnitude at $t = t_{max}$. At this time the net phases for each N are such that they add most constructively in the sum in Eq. (8). As time increases these phase relations will initially be lost, thus producing collapse of the magnitude of the $\mathcal{F}_{\overline{N}}(t) \to 0$, until the system revives at $t = t_{\text{max}} + T_{\overline{N}}$. The collapse time t_{coll} may be estimated by looking at the spread of frequencies present in the wave packet for particle numbers between $N = \overline{N} \pm \Delta N/2$, which yields $\Delta \Omega = 2\mu'_{\overline{N}}\Delta N/\hbar$, and $t_{\rm coll} \approx 2\pi/\Delta\Omega$. Gathering our results together for the collapse and revival times, we have

$$T_{\overline{N}} \approx \frac{1}{\omega_t} \left(\frac{r_t}{a}\right) \left(\frac{\overline{N}}{N_{\min}}\right)^{3/5}, \qquad t_{\text{coll}} \approx \frac{T_{\overline{N}}}{\Delta N}.$$
 (9)

The collapse phenomenon actually occurs under far more general conditions than reflected by the approximations used here, the essential ingredient being dispersion of the chemical potential μ_N over the particle number variance ΔN . Landau damping of plasma oscillations in an electron plasma is another example of decay of a coherent state. In contrast, the exactly periodic revivals arise from the linear dependence of μ_N on $(N - \overline{N})$ employed in Eq. (3). If higher-order corrections are retained, the revivals are no longer perfectly periodic, and diminish with increasing time. We also note that according to Eq. (6) the single-particle reduced density matrix is insensitive to the collapse and revivals of the macroscopic wave function, which is then also the case for the atomic BEC experiments [1–3].

The thermodynamic limit of these results must be taken with care. In particular, in order to maintain a constant density as the mean particle number is increased, it is necessary to concomitantly increase the linear trap size as $r_t \propto \overline{N}^{1/6}$. Then $T_{\overline{N}} \propto \overline{N}$ and $t_{\text{coll}} \propto \overline{N}^{1/2}$, so that collapse and revivals become irrelevant. In addition, we find that $\mathcal{F}_{\overline{N}}(0) \rightarrow e^{i\eta}$ by the following argument: The approximate uncertainty relation $\Delta N \Delta \eta \approx 1$ holds for the number and phase fluctuations of the condensate. Then, as $\Delta N = \overline{N}^{1/2} \rightarrow \infty$ we have $\Delta \eta \rightarrow 0$, which is the case for a coherent state with phases $\zeta_N = N\eta$. Thus, in the thermodynamic limit the quantum state of the condensate approaches a coherent state for which we find $\mathcal{F}_{\overline{N}}(0) = e^{i\eta}$. We then have $\Phi(\mathbf{r}, t) = \langle \hat{\psi}(\mathbf{r}, t) \rangle = e^{i\eta} \overline{N}^{1/2} \phi_{\overline{N}}(\mathbf{r}) e^{-i\mu t/\hbar}$, and this is precisely the limit in which the macroscopic wave function acts as an order parameter [12].

Turning now to the atomic BEC experiments, if we take the parameter values for the rubidium-87 atoms quoted earlier ($\overline{N} = 2000$) and $\Delta N = 44.7$ as a representative value for the variance, we find for the revival time $T_{\overline{N}} =$ 2.6 s, and the collapse time $t_{coll} = 58$ ms. Thus, even given that our estimates of these times may be off by an order of magnitude, the collapse time is still well within the 15 s condensate lifetime quoted for the rubidium-87 experiment [1]. This means that although BEC is evident in these experiments in the form of ODLRO and nonzero $\Phi(\mathbf{r}, t)$, the condensate wave function $\langle \hat{\psi}(\mathbf{r}, t) \rangle$ exhibits collapses and revivals. Thus, the main result of this work is that there are significant finite-size corrections which invalidate the identification of the macroscopic wave function as an order parameter, at least during the collapse phases. We stress that this conclusion follows even for the best case scenario adopted here in which the Bose condensed system can be described by a pure quantum state. The collapse of the macroscopic wave function can be avoided by increasing the trap size so that $t_{coll} \gg T_0$, where T_0 is the relevant macroscopic time scale. Assuming the finite-trap values used above and taking $T_0 = 15$ s as the condensate lifetime, the thermodynamic-limit scaling laws yield $\overline{N} \gg 1.3 \times 10^8$, $r_t \gg 8 \ \mu m$ for a properly macroscopic trap. These are large numbers by current standards for traps.

In conclusion, we have shown that the condensate wave function in small atomic samples exhibits collapse and revivals in time while the BEC is maintained in the form of ODLRO. To detect the collapses and revivals experimentally, a scheme is required which is sensitive to the macroscopic wave function directly, and this does not seem to be the case for the coherent light scattering methods previously discussed [23-25]. However, Imamoğlu and Kennedy [26] have recently proposed light scattering schemes involving two independent condensates coupled by a common excited state. These schemes rely on the fact that when one condensate is driven optically the light scattered from the other condensate has a nonzero value of the electric field and a phase proportional to the relative phase of the two condensates. By driving both wells and adjusting the phase difference of the fields, the scattering can be suppressed via quantum interference, and this in turn determines the phase difference between the two condensates. The scattering is therefore sensitive to Bosebroken gauge symmetry. In addition, the light scattering rate is proportional to the magnitude of the macroscopic wave function, so these schemes could be used to detect the collapses and revivals experimentally.

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