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Quantum Phase Diffusion of a Bose-Einstein Condensate

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We discuss the quantum properties of the Bose-Einstein condensate of a dilute gas of atoms in a trap. We show that the phase of the condensate undergoes quantum diffusion which can be detected in far off-resonant light scattering experiments. [S0031-9007(96)01469-X]

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Recent observations of the Bose-Einstein condensation (BEC) in systems of trapped alkali atoms [1–3] have triggered enormous interest in the properties of such condensates. These properties can be well described by the mean field Bogoliubov-Hartree (BH) approach [4–6], where the condensate *wave function* fulfills a nonlinear Schrödinger equation (NLSE) [7], whereas elementary excitation (quasiparticle) wave functions fulfill a set of coupled Schrödinger-like equations. Several versions of the BH approach have been discussed in the literature [8–12], but, as pointed out recently by Griffin [13], only some of them are physically sound and gapless in the limit of a large trap (i.e., they are in accord with the Hugenholtz-Pines theorem [14]). Among those there are the “Bogoliubov” approximation [11], which is valid at temperature $T = 0$ and leads to a closed NLSE, and the self-consistent “Popov” approximation [15], valid at finite temperatures.

So far the discussion of the BH approach has mainly concentrated on the condensate wave function and the spectrum of quasiparticle excitations [16,17]. The quantum properties of the condensate have not been thoroughly discussed in the context of recent experiments. Even the most complete presentation of this problem by Blaizot and Ripka [18] limits the discussion to specific examples of homogeneous systems. In this Letter we study the quantum fluctuations of the condensate, in particular, its phase diffusion. This problem is important for three main reasons: (a) In the standard BH approach

(c.f. [11]) one associates the annihilation (creation) operator of the condensate with the condensate wave function $\psi_0(\vec{r})[\psi_0^*(\vec{r})]$. We shall demonstrate that such an approach needs to be revised. (b) The phase of the condensate is a fundamental concept in the theory of U(1) symmetry breaking for interacting Bose gases [19]. The quantum state of an interacting condensate is conventionally assumed to be a *coherent* state with a fixed phase and a nonvanishing mean of the atomic field operators. Javanainen pointed out recently that the phase correlations will also be detected if two condensates are in U(1) symmetric states, e.g., Fock states [20]. Macroscopic populations of such states are sufficient to induce phase correlations independent of the fact whether the gas is interacting or not. This is analogous to laser theory where the density matrix of a lasing system (describing an average over ensemble of measurements) is U(1) symmetric, whereas in a single quantum measurement a fixed phase is selected, and the system exhibits then phase correlations as if it was from the very beginning in a state with broken phase symmetry [21]. We follow this analogy further, and show that the phase of interacting condensate undergoes necessarily quantum diffusion, since having a fixed phase is inconsistent with atom number conservation at $T = 0$ [22]. (c) At finite T the number of condensed atoms N_0 may fluctuate, and the phase diffusion is reduced. (d) The phase diffusion can be measured, for instance, with elastic off-resonant light scattering.

We start with the second quantized Hamiltonian

$$\mathcal{H} = \int d\vec{r} \hat{\Psi}^\dagger(\vec{r}) \left[-\frac{\hbar^2}{2M} \nabla^2 + V_t(\vec{r}) - \mu \right] \hat{\Psi}(\vec{r}) + \frac{u_0}{2} \int d\vec{r} \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}(\vec{r}) \hat{\Psi}(\vec{r}), \quad (1)$$

where $u_0 = 4\pi\hbar^2 a_{sc}/M$ [23], a_{sc} is the scattering length of the interatomic potential, $\hat{\Psi}(\vec{r})$ [$\hat{\Psi}^\dagger(\vec{r})$] is the atomic annihilation (creation) operator, M the atomic mass, and $V_t(\vec{r})$ the trap potential. The chemical potential μ assures the conservation of the average number of atoms $\hat{N} = \int d\vec{r} \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}(\vec{r})$.

Our discussion is based on the ‘‘Bogoliubov’’ approximation, which is the simplest gapless approximation that describes reasonably well both the condensate and its excitations at $T = 0$. We set

$$\hat{\Psi}(\vec{r}) = \sqrt{N} \psi_0(\vec{r}) + \delta\hat{\Psi}(\vec{r}), \quad (2)$$

where the c -number condensate wave function $\psi_0(\vec{r})$ is normalized as $\int d\vec{r} |\psi_0(\vec{r})|^2 = 1$. $\delta\hat{\Psi}(\vec{r})$ is the quantum fluctuations part that fulfills the same standard bosonic commutation relations as $\hat{\Psi}(\vec{r})$. We assume the $\psi_0(\vec{r})$ to be real. We substitute now (2) into Eq. (1) and neglect both 3rd and 4th order terms in fluctuations. The linear terms vanish provided $\psi_0(\vec{r})$ is the lowest energy (μ) solution of the NLSE

$$[\mathcal{L} + u_0\rho(\vec{r})]\psi_0(\vec{r}) = 0, \quad (3)$$

with $\mathcal{L} \equiv (\hbar^2/2M)\nabla^2 + V_t(\vec{r}) - \mu$, and $\rho(\vec{r}) = N \times \psi_0^2(\vec{r})$. The Hamiltonian becomes then a bilinear form of $\delta\hat{\Psi}(\vec{r})$ and $\delta\hat{\Psi}^\dagger(\vec{r})$, and can be transformed to a canonical form by introducing quasiparticle annihilation operators

$$g_k = \int d\vec{r} [U_k(\vec{r})\delta\hat{\Psi}(\vec{r}) + V_k(\vec{r})\delta\hat{\Psi}^\dagger(\vec{r})] \quad (4)$$

and g_k^\dagger . They fulfill bosonic commutation relations, $[g_k, g_{k'}^\dagger] = \delta_{kk'}$, $[g_k, g_{k'}] = 0$, which lead to the standard *biorthonormality* conditions [11] for $U_k(\vec{r})$ and $V_k(\vec{r})$.

For the moment, we suppose that the Hamiltonian will take a canonical form

$$\mathcal{H} \longrightarrow \sum_{k=0}^{\infty} \hbar\omega_k g_k^\dagger g_k, \quad (5)$$

such that $[g_k, \mathcal{H}] = \hbar\omega_k g_k$. The latter equation then gives

$$\begin{aligned} [\mathcal{L} + 2u_0\rho(\vec{r})]U_k(\vec{r}) - u_0\rho(\vec{r})V_k(\vec{r}) &= \hbar\omega_k U_k(\vec{r}), \\ [\mathcal{L} + 2u_0\rho(\vec{r})]V_k(\vec{r}) - u_0\rho(\vec{r})U_k(\vec{r}) &= -\hbar\omega_k V_k(\vec{r}), \end{aligned} \quad (6)$$

We observe that the solutions of the above equations exhibit a time-reversal symmetry; i.e., if a pair (U_k, V_k) is a solution with ω_k , then the pair (V_k^*, U_k^*) is the solution for $-\omega_k$. Time-reversal symmetry assures that $g_k \neq g_k^\dagger$ if $\omega_k \neq 0$. It is easy to check that Eqs. (6) have

a unique solution $U_0(\vec{r}) = V_0^*(\vec{r}) \propto \psi_0(\vec{r})$ with $\omega_0 = 0$. This is a Goldstone mode resulting from the $U(1)$ symmetry breaking. It is the very existence of this zero mode that assures the gaplessness of the ‘‘Bogoliubov’’ approximation. It is easy to check that the operator

$$\hat{P} = \int d\vec{r} \psi_0(\vec{r}) [\delta\hat{\Psi}(\vec{r}) + \delta\hat{\Psi}^\dagger(\vec{r})] \quad (7)$$

commutes with the Hamiltonian and is itself *Hermitian*, and as such cannot be associated with either annihilation, or creation operator of the condensate mode. It should rather be associated with a *collective motion without restoring force*, and interpreted as a ‘‘momentum’’ operator of the condensate mode [18]. We note that \hat{P} commutes with all g_k, g_k^\dagger for $k \neq 0$, i.e., $\int d\vec{r} \psi_0(\vec{r}) [U_k(\vec{r}) - V_k(\vec{r})] = 0$ for $k \neq 0$.

We immediately observe that our initial assumption (5) is inconsistent. The Hamiltonian must be a bilinear form and must commute with \hat{P} , therefore its correct canonical form is

$$\mathcal{H} = \alpha \hat{P}^2/2 + \sum_{k \neq 0} \hbar\omega_k g_k^\dagger g_k, \quad (8)$$

with the coefficient α to be determined. We can introduce a ‘‘position’’ operator canonically conjugated to \hat{P} as

$$\hat{Q} = i \int d\vec{r} \Phi_0(\vec{r}) [\delta\hat{\Psi}(\vec{r}) - \delta\hat{\Psi}^\dagger(\vec{r})], \quad (9)$$

which has to fulfill $[\hat{Q}, \hat{P}] = i$, $[Q, g_k] = 0$ (for $k \neq 0$) by definition, and $[\hat{Q}, \mathcal{H}] = i\alpha\hat{P}$ because of (8). These commutation relations imply that

$$2 \int d\vec{r} \Phi_0(\vec{r}) \psi_0(\vec{r}) = 1,$$

$$\int d\vec{r} \Phi_0(\vec{r}) [U_k(\vec{r}) + V_k(\vec{r})] = 0, \quad (10)$$

for $k \neq 0$, and

$$[\mathcal{L} + 3u_0\rho(\vec{r})]\Phi_0(\vec{r}) = \alpha\psi_0(\vec{r}), \quad (11)$$

which has a unique solution since the operator $\mathcal{L} + 3u_0\rho(\vec{r})$ is positive definite, presented in Fig. 1.

Having defined the ‘‘momentum’’ and ‘‘position’’ operators of the condensate mode, we can introduce the corresponding annihilation operator $g_0 = (\hat{P} - i\hat{Q})/\sqrt{2}$ and the appropriate zero mode functions $U_0(\vec{r}), V_0(\vec{r}) = [\psi_0(\vec{r}) \pm \Phi_0(\vec{r})]/\sqrt{2}$. Only if these functions are taken into account the set of pairs (U_k, V_k) does become complete

$$\begin{aligned} \sum_{k=0}^{\infty} [U_k(\vec{r})U_k^*(\vec{r}') - V_k(\vec{r})V_k^*(\vec{r}')] &= \delta(\vec{r} - \vec{r}'), \\ \sum_{k=0}^{\infty} [U_k(\vec{r})V_k^*(\vec{r}') - V_k(\vec{r})U_k^*(\vec{r}')] &= 0, \end{aligned} \quad (12)$$

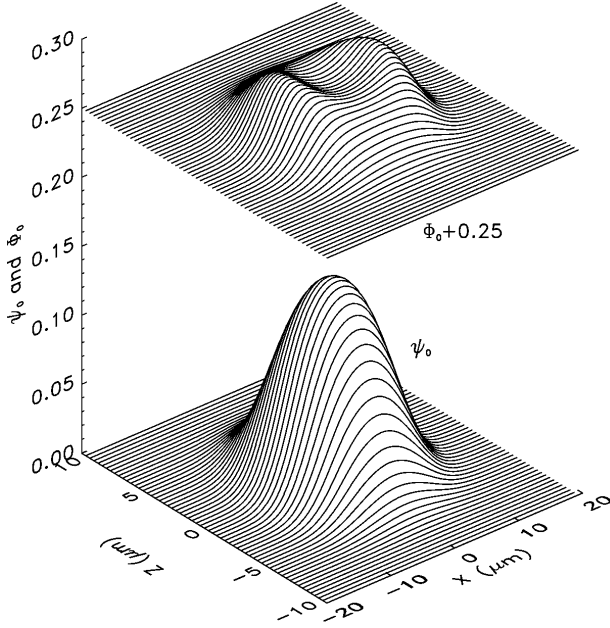


FIG. 1. The wave functions $\psi_0(\vec{r})$ and $\Phi_0(\vec{r})$ for the JILA TOP trap [1]: $N = 2000$, $a_{sc} = 5.2$ (nm), trap frequencies $(\omega_x : \omega_y : \omega_z) = (1 : 1 : 8^{1/2})$ (10 Hz). Our theory gives $\mu = 1.769(\hbar\omega_x)$ and $\alpha = 1.129(\hbar\omega_x)$.

whereas the biorthonormality conditions are valid for any k, k' including zero [11]. The total atomic field (2) can be expanded as

$$\hat{\Psi}(\vec{r}) = \sum_{k=0}^{\infty} [U_k(\vec{r})g_k - V_k^*(\vec{r})g_k^\dagger]. \quad (13)$$

Note that the mean value of $\hat{\Psi}(\vec{r})$ is $\sqrt{N}\psi_0(\vec{r})$ as it should, if and only if the system is in the coherent state $|\sqrt{N}\rangle$ of all the operators $g_k|\sqrt{N}\rangle = z_k|\sqrt{N}\rangle$ that $z_k = z_k^*$, and $z_k = \sqrt{N} \int d\vec{r}' \psi_0(\vec{r}') [U_k(\vec{r}') + V_k(\vec{r}')]$. Note that since $V_k(\vec{r})$ becomes very small as k grows [17], only the low excited states contribute to the coherent part of the atomic field [24].

We can solve Eqs. (3), (10), and (11) using a Thomas-Fermi approximation [5,25], i.e., neglecting the kinetic energy terms. For a 3D isotropic harmonic trap $V_t(\vec{r}) = M\omega_t^2 r^2/2$ yields $\psi_0(\vec{r}) = [15(r_0^2 - r^2)/8\pi \times r_0^5]^{1/2}$, $\Phi_0(\vec{r}) = 3/[8\pi r_0^3 \psi_0(\vec{r})]$ for $r \leq r_0$ and zero otherwise, $\alpha = 3Nu_0/4\pi r_0^3$ with $r_0 = (15Nu_0/4\pi M\omega_t^2)^{1/5}$ and $\mu = M\omega_t^2 r_0^2/2$. Quite generally, α is proportional to the condensate peak density, and in a 3D harmonic trap grows with N as $N^{2/5}$.

Even though the Hamiltonian (8) is bounded from below, it does not possess a stationary ground state. In general, the ground state should not contain any excitation for $k > 0$, but it cannot have $\langle \hat{P}^2 \rangle = 0$, since then the Heisenberg relation would imply that $\langle \hat{Q}^2 \rangle \rightarrow \infty$, and the linearization approximation would cease to be valid. We can only trust the solution provided the total number of excitations $N_{ex} = \int d\vec{r} \langle \delta\hat{\Psi}^\dagger(\vec{r})\delta\hat{\Psi}(\vec{r}) \rangle$

is not much greater than unity, which is the same as saying that the total number of atoms $\int d\vec{r} \langle [\sqrt{N}\psi_0(\vec{r}) + \delta\hat{\Psi}^\dagger(\vec{r})][\sqrt{N}\psi_0(\vec{r}) + \delta\hat{\Psi}(\vec{r})] \rangle \approx N$. The zero temperature state of (8) should have $\langle \hat{P}^2 \rangle < 2\hbar\omega_1/\alpha \approx O(N^{-2/5})$, since otherwise the excitation of the modes with $k \neq 0$ would be energetically favorable. On the other hand, evidently $\langle \hat{P}^2 \rangle > O(N^{-1})$, since otherwise $\langle \hat{Q}^2 \rangle$ becomes at least of the order of N . Moreover, any state with a fixed $\langle \hat{P}^2 \rangle = \sigma^2$ (such as minimal uncertainty squeezed state [26]) is not stationary, since (provided $\langle \hat{P} \rangle = \langle \hat{Q} \rangle = 0$) it exhibits necessarily a quantum diffusion

$$\langle \hat{Q}^2(t) \rangle = 1/4\sigma^2 + \alpha^2\sigma^2 t^2. \quad (14)$$

Since N_{ex} contains a contribution proportional to $\langle \hat{Q}^2(t) \rangle$, Eq. (14) implies that our linearization approximation is valid only for a finite duration. The value of σ^2 is determined by the very process of condensation, and for the extremal case $\sigma^2 = 2\hbar\omega_1/\alpha$, $\langle \hat{Q}^2(t) \rangle$ remains minimal $\approx O(N^{2/5})$ for $\omega_1 t \approx 1$.

What is the solution of this apparent paradox? The laser theory and quantum optics give a hint again. The linearized solution with a broken U(1) symmetry cannot be strictly valid due to the condensate phase diffusion. Similar to the case of a laser, the stationary density matrix is U(1) symmetric, and corresponds to an ‘‘amplitude’’ squeezed state [26]. An elegant way to describe it would employ quasiprobability distributions (such as Glauber’s P , Q , or Wigner’s W functionals). Within such an approach the stationary quasiprobability functionals are always U(1) symmetric, and the phase correlations and diffusion exhibit themselves as in [20] only on the level of higher order correlation functions [27]. An alternative approach to rescue the linearized theory is to reinterpret it in terms of the phase operator of the condensate. To this aim we rewrite the atomic field operators in the form

$$\begin{aligned} \hat{\Psi}(\vec{r}, t) &= \sqrt{N}\psi_0(\vec{r}') - i\psi_0(\vec{r})\hat{Q}(t) + \dots \\ &\approx [\sqrt{N}\psi_0(\vec{r}) + \dots] \exp[-i\hat{Q}(t)/\sqrt{N}]. \end{aligned} \quad (15)$$

With such an ansatz the mean number of atoms is practically conserved, and the variance of \hat{P} may be of order of unity.

The immediate consequence of (15) is that the two-time correlation function (TTCF) $\langle \hat{\Psi}^\dagger(\vec{r}, t + \tau)\hat{\Psi}(\vec{r}, t) \rangle$ decays with τ ; the decay has the form $\exp(-\alpha^2\tau^2/2N)$ if $\langle \hat{P}^2 \rangle = 1$, and if the ‘‘momentum’’ fluctuations are Gaussian. Such decay can be deduced from the standard ‘‘macroscopic’’ theory of BEC, where the condensate wave function behaves as $\sqrt{\rho(\vec{r})} \exp[-i\mu(N)t]$, and the TTCF collapses as $\exp[-N(\partial\mu/\partial N)^2\tau^2/2]$ due to the Poissonian fluctuations of N in the grand canonical ensemble [28]. Indeed, $N(\partial\mu/\partial N)^2 = \alpha^2/N$ for $T = 0$. However, it is easy to repeat our calculation using the ‘‘Popov’’ approximation [13] valid for $T \neq 0$ [i.e., replacing $\rho(\vec{r})$ by $\rho_0(\vec{r}) + 2\delta\rho(\vec{r})$ in Eq. (3),

$\rho(\vec{r})$ by $\rho_0(\vec{r}) + \delta\rho(\vec{r})$ in the diagonal, and $\rho(\vec{r})$ by $\rho_0(\vec{r})$ in the off-diagonal terms in Eqs. (6) with $\rho_0(\vec{r}) = N_0|\psi_0(\vec{r})|^2$, $\delta\rho(\vec{r}) = \langle \delta\hat{\Psi}^\dagger(\vec{r})\delta\hat{\Psi}(\vec{r}) \rangle$. It is then elementary to show that in Thomas-Fermi limit r_0 becomes $r_0(T) = r_0(0)[2 - f(T)]^{1/5}$, where $f(T) = N_0(T)/N$ is the condensate fraction. The phase diffusion rate becomes then $\alpha(T)/\sqrt{N_0(T)} = 3u_0\sqrt{N_0(T)}/4\pi[r_0(T)]^3 = \sqrt{Nf(T)}[\partial\mu(N,T)/\partial N]/[2 - f(T)]$. This expression shows that for $T \neq 0$ the diffusion is only partially related to conservation of N , and the nonconservation of N_0 reduces significantly its rate.

The phase diffusion can be detected, for instance, by measuring the beat note between the two interfering condensates [21]. It can also be measured in coherent light scattering. The coherently scattered field is determined by the mean value of the atomic dipole operator $\langle \hat{d}(\vec{r}, t) \rangle \propto \langle \hat{\Psi}^\dagger(\vec{r}, t)\hat{\Psi}_e(\vec{r}, t) \rangle$, where $\hat{\Psi}_e(\vec{r}, t)$ is the annihilation operator for excited atoms. In the presence of a laser field of the Rabi frequency Ω_L and photon frequency

ω_L , $\hat{\Psi}_r(\vec{r}, t)$ fulfills the quantum Langevin equation

$$\begin{aligned} d\hat{\Psi}_e(\vec{r}, t)/dt = & -(i\omega_e + \gamma + \gamma_d)\hat{\Psi}_e(\vec{r}, t) \\ & - i\hat{\Psi}(\vec{r}, t)\mathcal{E}_{\text{vac}}(\vec{r}, t) - i(\Omega_L/2) \\ & \times \exp(-i\omega_L t)\hat{\Psi}(\vec{r}, t), \end{aligned} \quad (16)$$

where ω_e and 2γ are the energy and natural linewidth of the excited state, whereas $\mathcal{E}_{\text{vac}}(\vec{r}, t)$ is the quantum noise term describing vacuum fluctuations of the electromagnetic field [26]. Equation (16) is derived using the Markov-Born approximation, and neglecting the resonant dipole-dipole interactions between the excited and ground state atoms. It is thus valid only for a dilute BEC. The (complex) rate γ_d accounts for free evolution of the excited wave packet, i.e., its energy shift due to the photon recoil, and its spreading rate. Such approximation works amazingly well in the considered regime of parameters [29]. In the case of weak field scattering, we solve Eq. (16) perturbatively with respect to Ω_L and $\mathcal{E}_{\text{vac}}(\vec{r}, t)$, and using Eq. (15) we obtain at $T = 0$

$$\begin{aligned} \lim_{t \rightarrow \infty} \langle \hat{d}(\vec{r}, t) \rangle & \propto \lim_{t \rightarrow \infty} \int_0^t dt' e^{-(i\omega_e + \gamma)(t-t') - i\omega_L t'} \langle \hat{\Psi}^\dagger(\vec{r}, t)\hat{\Psi}(\vec{r}, t') \rangle \\ & \simeq \left\langle \frac{N|\psi_0(\vec{r})|^2 e^{-i\omega_L t}}{\gamma + \gamma_d + i(\omega_e - \omega_L) + i\alpha/2N - i\alpha\hat{P}/\sqrt{N}} \right\rangle. \end{aligned} \quad (17)$$

The quantum noise term in Eq. (16) does not affect the mean value of the dipole operator, while the spectrum of the elastic scattering is given by the square modulus of the right-hand side of Eq. (17). The phase diffusion causes a shift of the spectrum $\propto \alpha/N$, whereas the fluctuations of \hat{P} cause a broadening $\propto \alpha/\sqrt{N}$. Both effects vanish when $N \rightarrow \infty$: the shift as $N^{-3/5}$, and the broadening as $N^{-1/10}$, provided $\langle \hat{P}^2 \rangle \simeq O(1)$. For finite $N \simeq$ few hundred thousands the latter of these effects is small (of the order of a few ω_L), but should be *detectable*, at least if the condensation occurs in a tight trap, such as a far-off resonance dipole trap, or an optoelectric trap.

Summarizing, we have shown that the standard approach of associating the condensate wave function with the zero mode annihilation operator has to be revised to include the proper description of its quantum fluctuations. The present approach associates the condensate wave function with the condensate ‘‘momentum’’ operator. In effect, the Hamiltonian of quasiparticle excitations contains a term proportional to the square of this ‘‘momentum’’ operator. The condensate is time dependent and exhibits quantum phase diffusion. We have derived analytic expressions for the phase diffusion constant α at low T . The effects of the phase diffusion are measurable in off-resonant elastic light scattering.

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