Images of a Bose-Einstein condensate at finite temperature *

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A condensate initially prepared at finite temperature evolves under external time-dependent perturbation into a time-dependent mixed state. In these notes I use number-conserving time-dependent Bogoliubov theory to derive probability distribution for different outcomes of density measurement on the time-dependent excited state.

I. INTRODUCTION

Quantum measurements on Bose-condensed systems can give quite unexpected results. For example, in the classic paper by Javanainen and Yoo [1] a density measurement on a Fock state $|N/2, N/2\rangle$ with $N$ particles equally divided between two counter-propagating plane waves $e^{\pm ix}$ reveals an interference pattern $\rho(x|\varphi) \sim \cos^2(x - \varphi)$ with a phase $\varphi$ chosen randomly in every realization of the experiment. The Fock state has a uniform single particle density distribution, but its measurement unexpectedly reveals interference between the two counter-propagating condensates. The Fock state is a quantum superposition over $N$-particle condensates with different relative phases $\varphi$ in their wave functions [2], $|N/2, N/2\rangle \sim \int d\varphi \ |N : e^{+i(x-\varphi)} + e^{-i(x-\varphi)}\rangle$, but every single realization of the experiment reveals such a density distribution as if the state before the density measurement were one of the condensates $|N : e^{+i(x-\varphi)} + e^{-i(x-\varphi)}\rangle$ with a randomly chosen phase $\varphi$. This effect is best explained [2] when the density measurement, which is a destructive measurement of all particle positions at the same time, is replaced by an equivalent sequential measurement of one position after another. With an increasing number $n$ of measured positions a quantum state of the remaining $N-n$ particles gradually “collapses” from the initial uniform superposition over all phases to a state with a more and more localized phase $\varphi$. For a large $N$ a measurement of only a small fraction $n/N \ll 1$ of all particles practically collapses the state of remaining $N-n$ particles to a condensate with definite phase $\varphi$.

A lesson from this instructive example [1,2] is that quantum measurement on an $N$-particle state with highly occupied single particle modes “collapses” the state to a definite condensate with a definite condensate wave function $\phi(x)$. The question is: what is the probability distribution for different measurement outcomes $\phi(x)$? As the set of condensates is not an orthonormal basis this is not a trivial question.

In Ref. [6] we derived this probability distribution in the framework of the time-dependent Bogoliubov theory at zero temperature. At zero temperature a condensate initially prepared in its $N$-particle ground state evolves under external time-dependent perturbation into a time-dependent excited state. The excited state is a time-dependent Bogoliubov vacuum i.e. at any time $t$ there exists a complete set of quasiparticle annihilation operators for which the excited state is a vacuum. In Ref. [6] it was shown that the time-dependent vacuum has a simple diagonal structure which directly leads to a compact gaussian probability distribution for different condensate wave functions $\phi(x)$. As the case of zero temperature is covered in Ref. [6], in these notes I describe the general case of finite temperature when the initial state is a condensate in equilibrium with a thermal cloud of atoms. I derive gaussian probability distribution for $\phi(x)$ at any time $t$ when the external perturbation drives the initial thermal state into an excited mixed state.

II. N-CONSERVING BOGOLIUBOV THEORY

Number conserving Bogoliubov theory [7] is a quadratic approximation to the second quantized Hamiltonian (in trap units)

$$
\hat{H} = \int dx \left[ \frac{1}{2} \partial_x \hat{\psi} \partial_x \hat{\psi}^\dagger + \frac{1}{2} x^2 \hat{\psi} \hat{\psi}^\dagger + V(t, x) \hat{\psi} \hat{\psi}^\dagger + \frac{1}{2} g \hat{\psi} \hat{\psi}^\dagger \hat{\psi} \hat{\psi}^\dagger \right].
$$

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Here $\hat{\Psi}(x)$ is the bosonic annihilation operator, $V(t,x)$ is the external perturbation potential, and $g$ is strength of contact interaction between atoms. Here and in the following I will use one-dimensional notation but all equations can be generalized by the simple replacement $x \rightarrow \vec{x}$. The annihilation operator is split into condensate and non-condensate part
\[
\hat{\Psi}(x) = \hat{a}_0 \phi_0(x) + \delta\hat{\psi}(x).
\] (2)

It is assumed that most atoms occupy the condensate mode $\phi_0(x)$. Equation (2) is substituted to the Hamiltonian (1) and then the Hamiltonian is expanded in powers of the fluctuation operator $\delta\hat{\psi}$, see Ref. [7].

Many experiments on dilute atomic condensates can be clearly divided in two steps: as a first step a condensate is prepared in its ground state and then in the second step an external potential $V(t,x)$ is applied to manipulate with the condensate wave function. Generic examples are phase imprinting of dark solitons [5], atomic interferometry [3], or generation of shock waves in Bose-Einstein condensates [4]. At finite temperature the initial state before the manipulation is a thermal state including thermal excitations above the $N$-particle ground state. The initial condensate wave function $\phi_0$ solves the stationary Gross-Pitaevskii equation
\[
\mu\phi_0 = -\frac{1}{2}\partial_x^2 \phi_0 + \frac{1}{2}x^2 \phi_0 + g|\phi_0|^2 \phi_0.
\] (3)

In Bogoliubov approximation the ground state is Bogoliubov vacuum $|0_b\rangle$ which can be written as a gaussian superposition over condensates [8]
\[
|0_b\rangle = \int d^2b e^{-\frac{1}{4}\sum_{m=1}^M b_m^* b_m} \left| N : \phi_0(x) + \frac{1}{\sqrt{N}} \sum_{m=1}^M b_m u_m(x) + b_m^* v_m(x) \right|.
\] (4)

Here the state $|N : \phi\rangle$ is a condensate of $N$ atoms in the normalized condensate wave function $\frac{\phi}{\sqrt{|\phi|}}$. The Bogoliubov modes $u_m$ and $v_m$ are eigenmodes of the stationary Bogoliubov-de Gennes equations
\[
\omega_m u_m = -\frac{1}{2}\partial_x^2 u_m + \frac{1}{2}x^2 u_m + 2g|\phi_0|^2 u_m + g\phi_0^2 v_m ,
\]
\[-\omega_m v_m = -\frac{1}{2}\partial_x^2 v_m + \frac{1}{2}x^2 v_m + 2g|\phi_0|^2 v_m + g (\phi_0^*)^2 u_m .
\] (5)

Numerical solution of these equations gives a finite number of modes $M$. At finite temperature the initial state is a thermal state $\hat{\rho}(0)$ with thermal quasiparticle excitations. The thermal state is also a gaussian state [8]
\[
\hat{\rho}(0) = \int d^2b_L \int d^2b_R e^{-\frac{1}{4}\sum_{m=1}^M b_m^* b_m + b_L^* b_R + b_R^* e^{-\beta\omega} b_R} \left| N : \phi_0(x) + \frac{1}{\sqrt{N}} \sum_{m=1}^M b_{L,m} u_m(x) + b_{L,m}^* v_m(x) \right|.
\] (6)

Here $b_{L,m}^* b_L = \sum_{m=1}^M b_{L,m}^* b_{L,m}$ and $b_{L,m}^* e^{-\beta\omega} b_R = \sum_{m=1}^M b_{L,m}^* e^{-\beta\omega} b_{R,m}$.

In Bogoliubov theory the initial thermal state evolves under external perturbation $V(t,x)$ into an excited state $\hat{\rho}(t)$ which has the same form as the initial $\hat{\rho}(0)$ in Eq.(6) but with time-dependent Bogoliubov modes $u_m(t,x)$ and $v_m(t,x)$ which solve time-dependent Bogoliubov-de Gennes equations
\[
i\partial_t u_m = -\frac{1}{2}\partial_x^2 u_m + \frac{1}{2}x^2 u_m + 2g|\phi_0|^2 u_m + g\phi_0^2 v_m ,
\]
\[-i\partial_t v_m = -\frac{1}{2}\partial_x^2 v_m + \frac{1}{2}x^2 v_m + 2g|\phi_0|^2 v_m + g (\phi_0^*)^2 u_m.
\] (7)

with initial conditions being the eigenmodes of the stationary BdG equations (5). The time-dependent condensate wave function $\phi_0(t,x)$ solves the time-dependent Gross-Pitaevskii equation
\[
i\partial_t \phi_0 = -\frac{1}{2}\partial_x^2 \phi_0 + \frac{1}{2}x^2 \phi_0 + g|\phi_0|^2 \phi_0 .
\] (8)
III. PROBABILITY DISTRIBUTION FOR OUTCOMES

As mentioned before, density measurement is “collapsing” N-particle state to a Bose-Einstein condensate. The aim of the measurement theory is to provide probability distribution for different condensate wave functions $\phi$. In the present context of Bogoliubov theory it is convenient to split possible condensate wave functions into the condensate part and the non-condensate part: $\phi = \phi_0 + \sqrt{\lambda} \delta \phi$. The aim is to find gaussian probability distribution for $\delta \phi$ in the gaussian state $\hat{\rho}(t)$. Ideally the gaussian distribution would be fully determined by the following equalities between second order correlators of the gaussian $\delta \phi(x)$ and second order correlators of the field operators:

$$\overline{\delta \phi^*(x) \delta \phi(y)} = \frac{2}{2} \langle \hat{\delta \phi}^*(x) \hat{\delta \phi}(y) \rangle = \sum_{m,n} n_m u^*_m(x) u_m(y) + (1 + n_m) v^*_m(x) v_m(y) , \quad (9)$$

$$\overline{\delta \phi(x) \delta \phi^*(y)} = \frac{2}{2} \langle \hat{\delta \phi}(x) \hat{\delta \phi}^*(y) \rangle = \sum_{m,n} n_m v^*_m(x) v_m(y) + (1 + n_m) u_m(x) u^*_m(y) , \quad (10)$$

$$\overline{\delta \phi(x) \delta \phi(y)} = \frac{2}{2} \langle \hat{\delta \phi}(x) \hat{\delta \phi}(y) \rangle = \sum_{m,n} n_m v^*_m(x) u_m(y) + (1 + n_m) u_m(x) v^*_m(y) , \quad (11)$$

$$\overline{\delta \phi^*(x) \delta \phi^*(y)} = \frac{2}{2} \langle \hat{\delta \phi}^*(x) \hat{\delta \phi}^*(y) \rangle = \sum_{m,n} n_m u^*_m(x) v_m(y) + (1 + n_m) v_m(x) u^*_m(y) . \quad (12)$$

Here the most right hand sides follow from the Bogoliubov theory $[7]$. $n_m = (e^{\beta\omega_m} - 1)^{-1}$ is average number of thermally excited Bogoliubov quasiparticles in the initial state. Unfortunately, because of the non-zero commutator $[\delta \phi(x), \delta \phi^*(y)] = \delta(x - y) - \phi_0^*(x) \phi_0(y)$, the first two conditions cannot be satisfied simultaneously. I replace them with the condition

$$\overline{\delta \phi^*(x) \delta \phi(y)} = \left(\overline{\delta \phi(x) \delta \phi^*(y)}\right)^* = \frac{1}{2} \langle \delta \phi^*(x) \delta \phi(y) + \delta \phi(y) \delta \phi^*(x) \rangle . \quad (13)$$

It is convenient to expand the fluctuation as

$$\delta \phi(x|z) = \sum_{\alpha=1}^{\infty} \phi_{\alpha}(x) \quad (14)$$

in the orthonormal basis of the eigenmodes $\phi_{\alpha}$ of the reduced single particle density matrix

$$\langle \delta \phi^*(x) \delta \phi(y) \rangle = \sum_{\alpha=1}^{M} \delta N_{\alpha} \phi_{\alpha}^*(x) \phi_{\alpha}(y) . \quad (15)$$

Here the left hand side is given by Eq.(9). The right hand side is obtained after diagonalization of the hermitean operator on the left. The real eigenvalues $\delta N_{\alpha}$ are average occupation numbers of the corresponding non-condensate modes $\phi_{\alpha}$. The correlators (12) after the semiclassical approximation (13) determine the matrix of correlators of the complex gaussian random variables $z_{\alpha}$:

$$\begin{pmatrix}
\frac{\langle z_{\alpha} z_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle} & \frac{\langle z_{\alpha} \gamma_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle} \\
\frac{\langle \gamma_{\alpha} z_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle} & \frac{\langle \gamma_{\alpha} \gamma_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle}
\end{pmatrix} = \begin{pmatrix}
D_{\alpha\beta} & C_{\alpha\beta} \\
C_{\alpha\beta}^* & D_{\alpha\beta}^*
\end{pmatrix} . \quad (16)$$

Here the $M \times M$ matrices on the right hand side are

$$D_{\alpha\beta} = \frac{1}{2} \left( U_{\alpha m}^* n_m U_{\beta m} + V_{\alpha m}^* (1 + n_m) V_{\beta m} + U_{\alpha m} (1 + n_m) U_{\beta m}^* + V_{\alpha m} n_m V_{\beta m}^* \right) , \quad (17)$$

$$C_{\alpha\beta} = U_{\alpha m}^* n_m V_{\beta m} + V_{\alpha m}^* (1 + n_m) U_{\beta m} , \quad (18)$$

with the matrix elements $U_{\alpha m} = \langle \phi_{\alpha}|u_m\rangle$ and $V_{\alpha m} = \langle \phi_{\alpha}|v_m\rangle$. Replacing $z_{\alpha}$'s with real coordinates, $z_{\alpha} = x_{\alpha} + iy_{\alpha}$, we get a real symmetric matrix of correlators

$$\begin{pmatrix}
\frac{\langle x_{\alpha} x_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle} & \frac{\langle x_{\alpha} y_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle} \\
\frac{\langle y_{\alpha} x_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle} & \frac{\langle y_{\alpha} y_{\beta} \rangle}{\langle \delta \phi^*(x) \delta \phi(y) \rangle}
\end{pmatrix} = \frac{1}{2} \begin{pmatrix}
\operatorname{Re} D_{\alpha\beta} + \operatorname{Re} C_{\alpha\beta} & \operatorname{Im} C_{\alpha\beta} \\
\operatorname{Im} C_{\alpha\beta} & \operatorname{Re} D_{\alpha\beta} - \operatorname{Re} C_{\alpha\beta}
\end{pmatrix} . \quad (19)$$

and a condition that $\operatorname{Im} D_{\alpha\beta} = 0$ - a good test of the correctness of the calculations. Diagonalization of the correlation matrix (19) gives eigenvalues $\lambda_s \geq 0$ with $s = 1, \ldots, 2M$. Corresponding eigenvectors are columns of an orthogonal matrix $O$. The eigenvectors define convenient parametrization of the gaussian fluctuation as
\[
\delta \phi(x) = \sum_{\alpha=1}^{M} z_\alpha \phi_\alpha(x) = \sum_{\alpha=1}^{M} \phi_\alpha(x) \sum_{s=1}^{2M} (O_{\alpha,s} + iO_{M+\alpha,s}) q_s \equiv \sum_{s=1}^{2M} \Phi_s(x) q_s
\]  

(20)

with independent real gaussian random variables \(q_s\) of zero mean and variances \(\overline{q_s^2} = \lambda_s\). However, this is not the end of the story yet.

As a result of the semiclassical approximation in Eq.(13) averages like e.g. average density of depletion \(\overline{\delta \phi^*(x) \delta \phi(x)}\) are divergent because there is infinite number of unoccupied modes \(\phi_\alpha(x)\), every one of them contributing to this depletion density a term \(\frac{1}{2} \delta \phi^*(x) \delta \phi(x)\). In stochastic averages like \(\overline{\delta \phi^*(x) \delta \phi(x)}\) average occupation numbers of modes \(\phi_\alpha(x)\) seem to be \(\delta N_\alpha + \frac{1}{2}\) instead of the correct \(\delta N_\alpha\). This artifact of the semiclassical approximation can be corrected by introducing to Eq.(20) of regularization factors:

\[
\delta \phi(x)|_{\text{reg}} = \sum_{\alpha=1}^{M} z_\alpha \left( \frac{\delta N_\alpha}{\delta N_\alpha + \frac{1}{2}} \right)^{1/2} \phi_\alpha(x) = \sum_{\alpha=1}^{M} \left( \frac{\delta N_\alpha}{\delta N_\alpha + \frac{1}{2}} \right)^{1/2} \phi_\alpha(x) \sum_{s=1}^{2M} (O_{\alpha,s} + iO_{M+\alpha,s}) q_s \equiv \sum_{s=1}^{2M} \Phi_s(x) q_s
\]  

(21)

As expected in semiclassical approximation, the regularizing factors \(\left( \frac{\delta N_\alpha}{\delta N_\alpha + \frac{1}{2}} \right)^{1/2}\) are approximately 1 for the highly occupied modes with \(\delta N_\alpha \gg 1\) which dominate in the density distribution, but at the same time they remove the divergence coming from the infinity of unoccupied modes. The wave functions \(\Phi_s(x)\) are in general neither normalized nor orthogonal, except in the quantum limit of zero temperature, see the proof in Ref. [6].

IV. CONCLUSION

In conclusion, a recipe to simulate density measurement on the time-dependent excited thermal state has the following steps:

• Solve stationary Gross-Pitaevskii and Bogoliubov-de Gennes equations (3,5) to provide initial conditions for \(\phi_0(t,x), u_m(t,x)\) and \(v_m(t,x)\), and the initial quasiparticle frequencies \(\omega_m\).

• Solve time-dependent Gross-Pitaevskii and Bogoliubov-de Gennes equations (8,7) with respect to \(\phi_0(t,x), u_m(t,x)\) and \(v_m(t,x)\).

• Diagonalize the reduced single particle matrix (15) to get its non-condensate eigenmodes \(\phi_\alpha\) with their average occupation numbers \(\delta N_\alpha\).

• Build the matrices \(D_{\alpha \beta}\) and \(C_{\alpha \beta}\) in Eqs.(17,18), and then the real symmetric correlation matrix in Eq.(19).

• Diagonalize the correlation matrix in Eq.(19) to get its real eigenvalues \(\lambda_s\) and corresponding eigenvectors \(O_{\alpha,s}\).

• Build the regularized modes \(\Phi_s\) according to their definition implicit in Eq.(21):

\[
\Phi_s(x) = \sum_{\alpha=1}^{M} \left( \frac{\delta N_\alpha}{\delta N_\alpha + \frac{1}{2}} \right)^{1/2} \phi_\alpha(x) (O_{\alpha,s} + iO_{M+\alpha,s})
\]  

(22)

• Choose independent real random variables \(q_s\)'s from their gaussian distributions of zero mean and variance \(\overline{q_s^2} = \lambda_s\), and then combine the chosen \(q\)'s into condensate density

\[
\rho(x|q) = \overline{\sqrt{\sum_{s=1}^{2M} q_s \Phi_s(x)}}^2.
\]  

(23)

The \(\rho(x|q)\) defines a family of all possible density measurement outcomes with a gaussian probability distribution for different \(q\)'s.

In the limit of zero temperature this general recipe coincides with the recipe derived by different methods in Ref. [6]. At zero temperature the wave functions become \(\Phi_s(x) \sim \phi_\alpha(x)\) for \(\alpha = 1, \ldots, M\) and zero otherwise (here the \(\sim\) means equality up to a phase factor). Corresponding variances are \(\overline{q_s^2} = \delta N_\alpha\).
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