Coherence of an Interacting Bose Gas: from a Single to a Double Well

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The low energy properties of a trapped boson gas split by a potential barrier are determined over the whole range of barrier heights. We derive a self-consistent two-mode model which reduces, for large $N$, to a Bogoliubov model for low barriers and to a Josephson model for any (asymmetric) double well potential, with explicitly calculated tunneling and pair interaction parameters. We compare the numerical results to analytical results that precisely specify the role of number squeezing and finite temperatures in the loss of coherence.

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A Bose-Einstein condensate (BEC) of ultracold atoms in a double well potential is a model system for the study of matter wave coherence for atom interferometry [1–4], and tunneling and entanglement [5, 6] in many-body systems. Its equivalence with a Josephson junction of two superconductors separated by a tunneling barrier was demonstrated experimentally and theoretically [7–9]. As long as the two parts of the boson gas are well connected and the temperature is very low, most of the atoms occupy a single spatial mode with a well-defined phase, satisfying the Gross-Pitaevskii equation (GPE) [10], while excitations and higher temperature effects are described by a single-particle Hamiltonian, $\hat{\psi}$ is the field operator, $g = 4\pi\hbar^2a/m$ is the interaction constant, $a$ is the s-wave scattering length and $m$ is the particle mass. We expand the field operator in terms of a finite set of orthogonal spatial modes $\phi_j(r)$, $\hat{\psi} = \sum \phi_j \hat{a}_j$, with $\hat{a}_j$ being bosonic annihilation operators. The Hamiltonian then be written as

$$\hat{H} = \sum_{ij} \epsilon_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{ijkl} U_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l,$$

with $\epsilon_{ij} = \langle \phi_i | \hat{H}_0 | \phi_j \rangle$ and $U_{ijkl} = g \int d^3r \ \phi_i^* \phi_j^* \phi_k \phi_l$. Equations of motion for the spatial modes $\phi_i$ may be obtained by multiplying the Heisenberg equations of motion for the field operator, $i\hbar \partial\phi_i/\partial t = [\hat{H}, \phi_i]$ by $\hat{a}_i^\dagger$ from the left and taking the expectation value. Then, using $i\hbar \partial \phi_i/\partial t = \mathcal{P} \left[ H_0 \phi_i + g \sum_{jklm} (\rho^{-1})_{im} \rho_{mklj} \phi_k^* \phi_l \phi_j \right]$.

Here $\mathcal{P} = 1 - \sum_n \phi_n \langle \phi_n |$ is an operator projecting onto the function subspace which is not spanned by the finite set $\{\phi_j\}$ and $\rho_{ij} = \langle \hat{a}_i^\dagger \hat{a}_j \rangle$ and $\rho_{mklj} = \langle \hat{a}_m^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_j \rangle$ are the single-particle and the two-particle reduced density matrices, which should be determined self-consistently with the solution for the mode functions. Equation (2), which was previously obtained using a variational principle [17, 18], is automatically satisfied if $\{\phi_j\}$ are a complete set, since then $\mathcal{P} = 0$; if only a single mode is
Consider a system of $N$ particles which can occupy either mode $\phi_L$ or $\phi_R$. We define $\hat{n} \equiv \hat{a}_L^\dagger \hat{a}_L$ as the number operator for particles in the left mode $\phi_L$, with eigenstates $|n\rangle$ having $n$ particles in the left mode and $N-n$ in the right mode. A general state of the system may be written as $\sum_n c_n |n\rangle$, with $\sum_n |c_n|^2 = 1$. We define the phase operator as $e^{i\hat{\phi}} \equiv \sum_{n=0}^{N-1} (|n\rangle + |0\rangle\langle N|)$, that has eigenstates $|\hat{\phi}\rangle \equiv \sum_n e^{-i\varphi_n} |n\rangle$ and eigenvalues $\varphi_n = 2\pi k/N$ with integer $k$. It can be shown that when the extreme states $|0\rangle$ and $|N\rangle$ in which all the particles occupy either the left or right modes are not significantly populated, the phase and the number operators satisfy conjugate commutation relations, $[\hat{\varphi}, \hat{n}] = i$, similar to position and momentum. When $N$ and $n$ are large, $a_L^\dagger a_R \approx \sqrt{n(N-n)} e^{i\hat{\phi}}$, and, after neglecting constant terms, Hamiltonian (1) goes to,

$$\hat{H} \approx (\epsilon_L - \epsilon_R)\hat{n} - U\hat{n}(N-\hat{n}) - 2J\sqrt{\hat{n}(N-\hat{n})} \cos \hat{\varphi} + 2U_{LRLR}\hat{n}(N-\hat{n})\cos(\hat{\varphi} - 2\cos\hat{\varphi}) \cos \varphi, \quad (5)$$

where $U \equiv (U_L + U_R - 2U_{LRLR})/2$, $\epsilon_i \equiv \epsilon_{\text{left}} + U_i(N-1)/2$, and $U_i \equiv U_{\text{int}}$. The tunneling rate $J$ is approximately

$$J = -\int d^2r \hat{\psi}_L^\dagger (r) \left[ \hat{H}_0 + g(\hat{n}(r)) \right] \phi_R(r). \quad (6)$$

Here $|\hat{n}(r)\rangle \equiv |\hat{\psi}_L^\dagger (r) \hat{\psi}(r)\rangle$ is the particle density, $\hat{\psi}(r) \approx \sqrt{n} \phi_L(r) + \sqrt{N-n} \phi_R(r) e^{i\hat{\phi}}$, and $g(\hat{n})$ is the mean-field potential, which should be self-consistently calculated with the solution of the Hamiltonian. We expand the Hamiltonian (5) around the values of $n = n_0$ and $\varphi = 0$ that minimize the energy ($\hat{H}$), and find that the last term in (5) contributes only fourth order corrections or higher in $\hat{\varphi}$. This term is also negligible when the overlap between $\phi_L$ and $\phi_R$ is small and $U_{LRLR} \to 0$. One can then approximate $\hat{H}$ by the Josephson hamiltonian

$$\hat{H}_J = \hat{U}(\hat{n} - n_0)^2 + JN\eta(1 - \cos \hat{\varphi}), \quad (7)$$

where $\eta \equiv 2\sqrt{n_0(N-n_0)/N}$ ($\eta = 1$ for the symmetric case where $n_0 = N/2$) and $\hat{U} = U + 2J/N\eta^3$.

To gain a physical picture of the transition from a single well coherent gas into a two-mode gas separated into two wells, we solved Eqs. (1) and (2) for a model system reduced to one dimension, using potential and interaction parameters of the same order as those used in experiments reported in Refs. [9, 19] with $^{87}$Rb atoms. We compare these results to analytical predictions of the Bogoliubov and Josephson models above. We use an asymmetric potential $V(x) = \frac{1}{2}m\omega_0^2(x-x_0)^2 + V_0 e^{-x^2/\sigma^2}$ where the harmonic part has a frequency $\omega = 2\pi \times 224$ Hz, shift $x_0 = -0.2$, and Gaussian barrier width $\sqrt{2}\sigma = 5\mu m$ with a varying peak energy $V_0$. For the atom-atom interaction we use $g_{1D}N = 2.36 \times 10^{-36}$ J m, such that the mean-field interaction potential (and hence the form of the spatial modes) is similar for varying particle numbers. In Fig. 1(a) we show the tunneling rate $J$ (for
interaction energy

FIG. 1. (color online) (a) Tunneling rate $J$ and scaled pair interaction energy $U/N$ as a function of barrier height $V_0$ for an asymmetric 1D double-well potential with $N = 1000$ atoms. Our result [Eq. (6)] (solid red curve with squares at the computed points) is compared to the semiclassical results of Zapata et al. [13] using GPE, and the expression of Pitaevskii et al. [14] using the modes $\phi_L$ and $\phi_R$ calculated here. Inset: $V(x)$ and the mode functions for a given $V_0$. (b) Energy $E_{ex}$ of the lowest excitation and (c) number uncertainty $\Delta n$ of the boson gas. The numerical solutions of Eq. (1) (solid curves) are compared to the analytic quadratic approximation to the Josephson Hamiltonian ("q"), excitations of the two-mode Bogoliubov model ["B", Eq. (3)] and the Bogoliubov-de Gennes calculation ["BdG"].

$N = 1000$) calculated from Eq. (6) as a function of $V_0$. We compare this result with a semiclassical calculation based on Eq. (9) of Ref. [13] with the atomic density $\rho$ from a GPE solution, and with the expression $J = (\hbar^2/m) [\phi_L \partial \phi_R / \partial x - \phi_R \partial \phi_L / \partial x]_{x=0}$ [14]. The parameter $J$ drops exponentially with barrier height over the whole tunneling regime ($V_0 > 3$ KHz), while the pair interaction parameter $U$ is approximately constant.

The ground state properties following from the Hamiltonian (7) are determined by the relative magnitude of the pair interaction parameter $U$, which tends to reduce number uncertainty and the tunneling term, which tends to reduce phase uncertainty and hence increase number uncertainty. In the region where $J N \eta > U$ [to the left of the intersection between $J$ and $U/N$ in Fig. 1(a)] the number uncertainty, $\Delta n^2 \equiv \sum_n |c_n|^2 (n - \bar{n})^2$, is wide enough so that $\Delta \varphi \ll 1$ and the $1 - \cos \varphi$ may be approximated by $\varphi^2/2$ in (7). The Hamiltonian then has a harmonic oscillator form, and the ground state and lowest excitations may be approximated by

\[ e^{(k)}_n = \frac{H_k (\frac{n-m}{\sigma})}{(\pi \sigma^2)^{1/4}} e^{-\frac{(n-m)^2}{2 \sigma^2}}, \quad \sigma = \left( \frac{J N \eta}{2U} \right)^{1/4}, \quad (8) \]

where $H_k(x)$ is the $k$th order Hermite polynomial and $\sigma/\sqrt{2}$ is the number uncertainty $\Delta n$ of the ground state. These eigenstates have energies $E_k = E_{ex}(k + \frac{1}{2})$ with $E_{ex} = (2JN\eta U)^{1/2}$, number variance $\langle \Delta n^2 \rangle_k = \sigma^2 (k + \frac{1}{2})$, and phase variance $\langle \Delta \varphi^2 \rangle_k = \sigma^2 (k + \frac{1}{2})$. In the weak interaction limit, $U \ll J/N$, Eq. (8) approximates a coherent state with $c_n = (\frac{n}{\sqrt{N}})^{1/2} \sin^2(\theta/2) \cos^{N-n}(\theta/2)$ and $\eta = \sin \theta$. Number squeezing is characterized by the ratio $\xi \equiv \Delta n/\Delta n_{U=0} = (2J/NU\eta^3)^{1/4}$ between the number uncertainties of a general ground state in (8) and the Poissonian width $\Delta n_{U=0} = \sqrt{N\eta^2}$. The coherent state.

In the strong tunneling regime, transformation of Hamiltonian (5) into the condensate-excitation representation using a rotation angle $\theta \approx \arcsin \eta$, neglecting terms of order 3 or higher in $\tilde{a}_c$, and $\tilde{a}_c^\dagger$, yields the Bogoliubov Hamiltonian (3) with $A = \frac{1}{2}U N \eta^2 + 2J/\eta$ and $B = \frac{1}{2}U N \eta^2$. Hence, the magnitude of the quasi-particle factor $v$ represents the amount of number squeezing, with $v = \frac{1}{2}(1/\xi - \xi)$.

The properties of the system are illustrated in Figs. 1(b) and (c) for different particle numbers and temperatures. As the barrier height $V_0$ grows, number squeezing becomes stronger and the excitation energy $E_{ex}$ drops to the point where $J < U/N$. In this “Fock regime”, $\Delta n < 1$ and $E_{ex} \rightarrow U[2(n_0 + n_0) - 1]$, where $n_0 + n_0$ is the closest integer greater than or equal to $n_0$ and the quadratic approximation in (7) breaks down. Good agreement is found between excitation energies obtained from the full calculation in the strong tuneling regime to the analytic results of the Josephson and Bogoliubov models. However, solutions of the Bogoliubov-de Gennes equations [11] which are not restricted to one excitation mode yield lower excitation energies. As the barrier height grows and $E_{ex}$ drops, the single real-particle excitation mode $\phi_e$ becomes dominant, hence the quasi-particle functions $u(r)$ and $v(r)$ become more similar to $\phi_e(r)$ and the two-mode predictions are more accurate.
The coherence of a split Bose gas, given by the correlation function \( g^{(1)}(r, r') = \langle \psi(r) \psi(r') \rangle / \sqrt{n(r)n(r')} \) with \( r \) and \( r' \) on opposite sides of the barrier, determines the repeatability of interference fringes when the potential is dropped and the two parts begin to overlap. If the modes \( \phi_L, \phi_R \) are well separated, it may be approximated by
\[
C \approx \langle e^{i\phi_2} \rangle_T \approx e^{-\frac{1}{2} \langle \Delta \phi^2 \rangle_T} = e^{-\frac{1}{2\sigma^2} [n_{ex}(T)+1/2]},
\]
where \( n_{ex}(T) = (e^{-E_{ex}/k_BT} - 1)^{-1} \) is the mean number of excitations. The term proportional to \( n_{ex} \) in the exponent of (9) is the finite temperature contribution to the dephasing, while the second term \( 1/4\sigma^2 \) is the contribution of ground-state number squeezing to dephasing. In the regime where the Bogoliubov model is suitable, loss of coherence is equivalent to the population of real particle excitations, as
\[
C \approx 1 - 2n_c/N\eta^2,
\]
where \( n_c \approx \langle b\dagger b \rangle = |v|^2 + n_{ex}(u^2 + |v|^2) \) again includes the effect of ground state squeezing and thermal population of excitations.

Figure 2 compares the analytical expression (9) for the coherence to the full calculation of \( g^{(1)}(x, x') \) with \( x \) and \( x' \) in the middle of the left and right wells, respectively. It demonstrates that the analytical expressions are valid for low temperatures and large \( N \). The cusp in Fig. 2(b) and 1(c) results when \( n_0 \) is close to a half integer.

In summary, we developed a two-mode theory for a Bose gas in a double well that is well-suited to all barrier heights. At low barrier heights and relatively weak interactions, only one mode is macroscopically occupied, hence results using the GPE agree with our two-mode theory. Comparison of the full numerical results to analytical solutions for the Josephson model with explicitly calculated parameters, shows good agreement for large \( N \). Comparison of the excitation energies computed with our theory and with a Bogoliubov-de Gennes model, which is not restricted to two-modes, shows good agreement at medium barrier heights, but only qualitative agreement for low barriers. Our approach will enable development of models for calculating and understanding the steady-state and the time-dependent properties of many-body systems with disconnected potentials and arbitrarily large number of particles.

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