Limit of Spin Squeezing in Finite Temperature Bose-Einstein Condensates

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Atomic clocks based on cold alkali atoms in two hyperfine states \(a\) and \(b\) are widely used as frequency standards. When atoms in uncorrelated quantum states are used, the clock precision is limited by the so-called projection noise, resulting from the quantum nature of the collective spin \(S\), i.e., the sum of the effective spin 1/2 of each atom. This limit is actually already reached in most precise clocks \([1]\). Spin squeezing \([2]\) amounts to creating quantum correlations among the atoms so as to increase the precision of the atomic clock beyond this standard quantum limit. The relative improvement on the variance of the measured frequency \(\Delta \omega_{ab}^2\) defines the spin squeezing parameter \(\xi^2\). In atomic ensembles was first obtained by quantum non-demolition measurements \([4, 5]\). Recently a significant amount of spin squeezing \((\text{e.g.} 6 \text{ or } 8 \text{ dB})\) has been achieved using atoms in a resonant optical cavity \([6]\) or exploiting atomic interactions in bimodal Bose-Einstein condensates \([7, 8]\). The ultimate limits of the different paths to spin squeezing are still an open question. We determine here the influence of the non-condensed fraction for spin squeezing schemes using Bose-Einstein condensates \([8-10]\).

A central issue is the scaling of the squeezing for large atom numbers. Most studies are based on a two-mode description \([2]\). In this case the squeezing parameter optimized over time \(\xi^2_{\text{best}}\) tends to zero (infinite metrology gain) for \(N \to \infty\) as \(\xi^2_{\text{best}} \sim N^{-2/3}\). The first analysis of squeezing at finite temperature \([11]\) used a large \(N\) expansion in a Bogoliubov-like approach and could not predict any deviation of spin squeezing from the two-mode model. Here, using fully non-perturbative semi-classical field simulations and a powerful formulation of Bogoliubov theory in terms of the time dependent condensate phase operator \([12]\), we find on the contrary a dramatic effect of the multimode nature of the field: For a spatially homogeneous system in the thermodynamic limit, the two-mode scaling \(\xi^2_{\text{best}} \sim N^{-2/3}\) turns out to be completely irrelevant, and the spin squeezing has a finite optimal value that we determine analytically.

The physical problem that we face is the dynamical evolution of a finite temperature Bose condensed gas after a pulse \(\pi/2\) that puts each atom in a coherent superposition of two internal states \(a\) and \(b\). This produces a non-equilibrium state that has a non-trivial evolution due to the atomic interactions inside each internal state. For simplicity, it is assumed that there is no cross-interaction between \(a\) and \(b\) atoms.

**Semi-classical field simulations** - In Fig. 1 we compare the two-mode theory with semi-classical field simulations at finite temperature in a trap. The gas is initially in state \(a\) at thermal equilibrium. In that state, we assume that thermal fluctuations dominate over quantum fluctuations and we use a classical field description \([13, 14]\) with an energy cut-off at \(k_B T\). The initial field \(\psi^{(0)}_h\) is then randomly samples the thermal equilibrium classical field distribution for the canonical ensemble at temperature \(T\). For the initially empty state \(b\), inspired by the truncated Wigner approach \([17, 18]\) we represent the vacuum by a classical field \(\psi^{(0)}_h\) having in each mode independent Gaussian complex fluctuations of zero mean and variance \(1/2\). A sudden \(\pi/2\) pulse mixes the initial fields \(\psi^{(0)}_a\) and \(\psi^{(0)}_b\) so that, at time \(t = 0^+\), i.e. just after the pulse:

\[
\psi_{a,b}(0^+) = \frac{1}{\sqrt{2}} [\psi^{(0)}_{a,b} + \psi^{(0)}_{b,a}].
\]
At later times, each field evolves independently according to the non-linear Schrödinger equation
\[ i\hbar \partial_t \psi_{a,b} = \left[ -\frac{\hbar^2 \Delta}{2m} + \frac{g}{2} |\psi_{a,b}(r,t)|^2 + g \psi_{a,b}(r,t) \right] \psi_{a,b}. \] (2)

This corresponds to a harmonically trapped gas with same oscillation frequency \( \omega \) and same coupling constant \( g = 4\pi \hbar^2 a/m \) for the two internal states, where \( a \) is the s-wave scattering length. As shown in Fig.1, the squeezing is created dynamically by the interactions. However, even for a moderate non-condensed fraction \( \langle N_{\text{nc}} \rangle/N = 0.09 \), the best \( \xi^2 \) in the multimode theory is larger by more than one order of magnitude than in the two-mode theory.

In order to isolate the effect of the non-condensed fraction from other dynamical effects taking place in the trapped system, as for example the spatial dynamics of the condensate wave function \( |\psi_a| \) and \( |\psi_b| \), and we generalize the results to the case of a quantum trapped system, as for example the spatial dynamics of the condensate phase at \( t \rightarrow \infty \).

Our strategy is to perform a double expansion of (\( S_z^2 \)) in the thermodynamic limit and to order one in the non-condensed fraction \( \langle N_{\text{nc}} \rangle/N \). In this framework, we can approximate (\( S_z(t) \)) in the denominator of (17) by its value at \( t = 0^+ \) so that
\[ \xi^2 \simeq \frac{4}{N} \Delta S_{z,\text{min}}^2. \] (14)

We sketch the main steps. In the Bogoliubov limit, the condensate phases at \( t > 0 \) obey
\[ \theta_a - \theta_b = (\theta_a - \theta_b)(0^+) - \frac{pg}{V} t [\langle N_a \rangle - \langle N_b \rangle] + O(1/N). \] (15)

As a first step, we perform semi-classical field simulations for different temperatures and increasing system sizes [21]. The result (not shown) is that \( \xi_{\text{best}}^2 \) converges to a finite value at the thermodynamic limit: \( N \rightarrow \infty \), \( V \rightarrow \infty \), \( p, g, T \) = constant, where \( \rho = N/V \) is the total density. Five independent parameters are in the model, \( h/m, g \) or \( a, k_B T/N \) and \( V \). From dimensional analysis, \( \xi_{\text{best}}^2 \) is a function of the three independent dimensionless quantities that one can form, \( N, \sqrt{\rho a^3} \), and \( k_B T/\rho g \). The existence of a thermodynamic limit then implies
\[ \xi_{\text{best}}^2 = \frac{f(\sqrt{\rho a^3}, k_B T/\rho g)}{T}. \] (8)

As a second step, we performed simulations increasing the density in the weakly interacting limit \( \rho \rightarrow \infty \), \( g \rightarrow 0 \) with \( T, \rho g \) = constant. We find that, for a given \( k_B T/\rho g, \xi_{\text{best}}^2 \) then scales as \( 1/\rho \propto \sqrt{\rho a^3} \). This implies:
\[ \xi_{\text{best}}^2/\sqrt{\rho a^3} = F(k_B T/\rho g). \] (9)

In Fig.2 we show the universal behavior (9). The circles and the squares correspond to two different values of \( \sqrt{\rho a^3} \) in simulations.

Semi-classical field analytics - We now develop an analytical theory to explain these results. We split the fields after the pulse as \( \psi_a = \frac{\rho a}{V} + \psi_{a,\perp} \) and similarly for \( \psi_b \). We introduce the modulus and phase conjugate variables for the condensate modes
\[ a_0 = e^{i\theta_a} \sqrt{N_{a,0}} \quad \text{and} \quad b_0 = e^{i\theta_b} \sqrt{N_{b,0}}. \] (10)

and we introduce number conserving non-condensed fields \( a_k \) and \( b_k \) [22] that we expand over Bogoliubov modes with amplitudes \( c_{ak} \) and \( \bar{c}_{ak} \) respectively [23];
\[ \Lambda_a(e^{i\theta_a} \psi_{a,\perp}) = \sum_{k \neq 0} (U_k c_{ak} + V_k \bar{c}_{ak}) e^{i\theta_k} \] (11)

\[ U_k + V_k = (\frac{E_k}{E_k + \rho g})^{1/4} \quad \text{and} \quad E_k = \frac{\hbar^2 k^2}{2m}. \] (12)

The spin raising component \( S_+ = S_x + iS_y \) is given by
\[ S_+ = e^{-i(\theta_a - \theta_b)} \left( \sqrt{N_{a,0}N_{b,0}} + \sum_k d^3r \Lambda_k^\dagger \Lambda_k \right). \] (13)

Our strategy is to perform a double expansion of (\( S_z^2 \)). We will need terms up to \( \sim N \) in the thermodynamic limit and up to order one in the non-condensed fraction \( \langle N_{\text{nc}} \rangle/N \). In this framework, we can approximate (\( S_z(t) \)) in the denominator of (17) by its value at \( t = 0^+ \) so that
\[ \xi^2 \simeq \frac{4}{N} \Delta S_{z,\text{min}}^2. \] (14)
S is the multimode part of the relative phase derivative that is absent in the two-mode theory. In thermodynamic limit $\theta_a - \theta_b \sim 1/\sqrt{N}$ and it is sufficient to expand the exponential in \(\xi^2\) to second order. In the moduls of \(S_+\) we expand:

$$\sqrt{N_\text{tot}N_\text{tot}} \simeq \frac{N_{\text{tot}}}{2} - \frac{1}{2} \int d^3r \left( |\Lambda_a|^2 + |\Lambda_b|^2 \right) \quad \text{(18)}$$

with \(N_{\text{tot}} = N + \sum_k |b_k^{(0)}|^2\) is the total atom number in the semi-classical field picture.

**Best squeezing** - For the calculation of the best squeezing, one looks at the asymptotic behavior of \(\xi^2\) for $t \to \infty$. One finds:

$$\xi^2(t) = \xi^2_{\text{best}} \left( H_{\text{tot}} \right)^2 \left[ 1 + O \left( \frac{N_{\text{tot}}}{N} \right) \right] + O \left( \frac{1}{N} \right) \quad \text{(19)}$$

with the best squeezing

$$\xi^2_{\text{best}} = \langle S^2 \rangle / N \quad \text{(20)}$$

which remarkably only involves the multimode part \(17\) of the phase difference. An explicit calculation gives

$$\xi^2_{\text{best}} = \frac{1}{2\rho} \int \frac{d^3k}{(2\pi)^3} \left[ s_k n_k^{(0)} \left( \frac{s_k^{(0)}}{s_k^*} \right)^2 + \left( \frac{s_k^*}{s_k^{(0)}} \right)^2 \right] \quad \text{(21)}$$

(solid line in Fig.2). In \(21\), $s_k = U_k + V_k$ given in \(12\), and $s_k^{(0)}$ is the equivalent quantity before the pulse obtained by replacing $\rho g$ with $2\rho g$ in \(12\). $n_k^{(0)} = k_B T / \epsilon_k^{(0)}$ are the equilibrium occupation numbers of Bogoliubov modes before the pulse with $\epsilon_k^{(0)} = |E_k + 2\rho g|^{1/2}$.

**Squeezing time** - From \(19\), the best squeezing is reached in an infinite time, which is a limitation of the analytical approach. However, the numerical squeezing curve as a function of time is indeed quite flat around its minimum, so that it suffices in practice to determine the “close to best” squeezing time $t_\eta$ defined as 

$$\xi^2(t_\eta) = (1 + \eta)\xi^2_{\text{best}}$$

where $\eta > 0$. Then, according to \(19\), $t_\eta$ is finite and given by

$$\frac{pg}{\hbar} t_\eta = \frac{1}{\sqrt{\eta\xi^2_{\text{best}}}} \quad \text{(22)}$$

The “close to best” squeezing time $t_\eta$ for $\eta = 0.2$ is shown in Fig.3 and compared to simulations.

A last important issue is that of thermalization, neglected in Bogoliubov theory and in our analytical treatment, but fully included in the semi-classical field simulations. Indeed it is possible to reach $\xi^2 = (1 + \eta)\xi^2_{\text{best}}$ with $\xi^2_{\text{best}}$ given by \(21\) only if $t_\eta$ given by \(22\) is shorter than the thermalization time

$$t_\eta < t_{\text{therm}} \quad \text{(23)}$$

In Fig.4 we show the squeezing parameter $\xi^2$ and contrast \(S_x\) across the thermalization process that brings the system back to equilibrium after the pulse. For the squeezing, we compare the simulation with (i) the full Bogoliubov theory (without the analytic expansions) that we implement numerically for a finite size system and (ii) a Bogoliubov ergodic model \(12\) where the amplitudes $c_k, \bar{c}_k$ in \(\langle N_a, E_a \rangle \) sample microcanonical distributions with number of particles and the energy \(\langle N_a, E_a \rangle \) fixed to a random value set by the pulse. Note that the simulation agrees with the Bogoliubov model at short times (included the “close to best” squeezing time) and then converges towards the ergodic model. We extract a thermalization time $t_{\text{therm}}$ from the contrast. As thermalization occurs the excited modes dephase and

$$\langle S_x \rangle = \text{Re} \left( \sum_k b_k^* a_k \right) \sim \text{Re} \left( b_0^* a_0 \right) \quad \text{(24)}$$
At zero temperature we get

\[ \xi(0) \approx 2.1 \times 10^{-5} \]

This value is very low, in particular below the limit given by particle losses. Asymptotically for \( k_B T \gg \rho g \), \( \xi_{\text{best}} \) identifies with the initial non-condensed fraction. An interesting result is that at any temperature the initial non-condensed fraction is larger than \( \xi_{\text{best}} \), see these two quantities in the inset of Fig. 2. Already for \( k_B T / \rho g = 2 \), \( \xi_{\text{best}} \) and \( \langle N_{\text{nc}} \rangle / N \) are within a factor three. A similar conclusion seems to hold in a trap, see Fig. 1.

In conclusion we have shown that a realistic description of the limits of spin squeezing in interacting Bose-Einstein condensates has to be multimode: The best achievable spin squeezing \( \xi_{\text{best}}^2 \) admits a finite limit for \( N \to \infty \) at fixed density and interaction strength, contrarily to the vanishing prediction of the two-mode model. We find that \( \xi_{\text{best}}^2 \) is the product of \( \sqrt{\rho a^3} \) and of a universal function of \( k_B T / \rho g \) that we calculated analytically, and is bounded from above by the initial non-condensed fraction. Our analytical treatment is restricted to evolution times smaller than the thermalization time, but this is enough to access \( \xi_{\text{best}}^2 \) as we showed by semi-classical field simulations (that include thermalization) over a wide range of parameters.

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\[ \xi_{\text{best}}^2 = \int \frac{d^3k}{(2\pi)^3} \frac{s_k^4}{2\rho} \left[ \langle n_k^{(0)} \rangle + \frac{1}{2} \left( \frac{\xi_{\text{best}}^2}{s_k^2} + \frac{s_k^4}{(s_k^{(0)})^2} \right) - 1 \right] \]

At zero temperature we get

\[ \xi_{\text{best}}^2 T=0 = \sqrt{\frac{8}{\pi}} \left[ \frac{19}{6} \sqrt{2} - \frac{3}{2} \ln(\sqrt{2} + 1) - \pi \right] \approx 0.2344 \]

In practice \( \rho a^3 < 10^{-6} \) in present squeezing experiments so that \( \xi_{\text{best}}^2 \) predicts \( \xi_{\text{best}}^2 T=0 \approx 2.1 \times 10^{-5} \). This value is very low, in particular below the limit given by particle losses. Asymptotically for \( k_B T \gg \rho g \), \( \xi_{\text{best}}^2 \) identifies with the initial non-condensed fraction. An interesting result is that at any temperature the initial non-condensed fraction is larger than \( \xi_{\text{best}}^2 \), see these two quantities in the inset of Fig. 2. Already for \( k_B T / \rho g = 2 \), \( \xi_{\text{best}}^2 \) and \( \langle N_{\text{nc}} \rangle / N \) are within a factor three. A similar conclusion seems to hold in a trap, see Fig. 1.

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