Distinguishing mesoscopic quantum superpositions from statistical mixtures in periodically shaken double wells

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Received 21 October 2011, in final form 13 December 2011

Published 9 January 2012

Abstract

For Bose–Einstein condensates in double wells, \(N\)-particle Rabi-like oscillations often seem to be damped. Far from being a decoherence effect, the apparent damping can indicate the emergence of quantum superpositions in the many-particle quantum dynamics. However, in an experiment it would be difficult to distinguish the apparent damping from decoherence effects. This paper suggests using controlled periodic shaking to quasi-instantaneously switch the sign of an effective Hamiltonian, thus implementing an ‘echo’ technique which distinguishes quantum superpositions from statistical mixtures. The scheme for the effective time reversal is tested by numerically solving the time-dependent \(N\)-particle Schrödinger equation.

Some figures may appear in colour only in the online journal.

Small Bose–Einstein condensates (BECs) of some 1000 [1] or even 100 atoms [2] have been a topic of experimental research for several years. Recently, the investigation of many-particle wavefunctions of BECs in phase space became experimentally feasible [3]. This experimental technique will lead to further investigations of beyond-mean-field (Gross–Pitaevskii) behaviour for small BECs.

For a BEC initially loaded into one of the wells of a double-well potential, the many-particle oscillations often seem to be damped compared to the mean-field behaviour. Figure 1 shows such an apparent damping, which in fact is a collapse which will eventually be followed by at least partial revivals (cf. [4, 5]), for \(N = 100\) particles. This apparent damping coincides with an increase of the fluctuations of the number of particles in each well (figure 1(b)).

In order to numerically calculate the many-particle dynamics, the Hamiltonian in the two-mode approximation [6] is used,

\[
\hat{H}_0 = -J\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1 + \frac{U}{2} \sum_{j=1}^{2} \hat{n}_j (\hat{n}_j - 1),
\]

where \(\hat{c}_j^\dagger\) are the boson creation and annihilation operators on site \(j\), \(\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j\) are the number operators, \(J\) is the hopping matrix element and \(U\) is the on-site interaction energy.

The experimentally measurable [7] population imbalance is useful to quantify the oscillations depicted in figure 1:

\[
\langle z \rangle (\tau) = \frac{\langle n_2 \rangle (\tau) - \langle n_1 \rangle (\tau)}{2N},
\]

where \(\tau\) is the dimensionless time

\[
\tau \equiv \frac{tJ}{\hbar}.
\]

The variance of the population imbalance can be quantified by using the experimentally measurable [7] quantity

\[
F_z \equiv \frac{\langle (\hat{n}_1 - \hat{n}_2)^2 \rangle - \langle \hat{n}_1 - \hat{n}_2 \rangle^2}{N},
\]

with \(0 \leq F_z \leq N\). If all atoms are in the same single-particle state, this can be expressed by using the atomic coherent states [8].

\[
|\theta, \phi\rangle_N = \sum_{n=0}^{N} \left(\begin{array}{c} N \\ n \end{array}\right)^{1/2} \cos^n (\theta/2) \sin^{N-n} (\theta/2) \times e^{i(N-n)\phi} |n, N-n\rangle.
\]
Initially, $N = 100$ atoms are in well 1, the quantum dynamics is given by the Hamiltonian (1) ($NU/J = 0.4$).

The result reads

$$F_z = 4[\cos^2(\theta/2) - \cos^4(\theta/2)]$$

and hence $0 \leq F_z \leq 1$. Thus, while $F_z < 1$ would not be sufficient to distinguish product states, as in equation (5), from ‘spin-squeezed states’ [7], for which $F_z < 1$ is also true, a pure state with $F_z > 1$ has to be in a quantum superposition. For numeric solutions of the Schrödinger equation corresponding to Hamiltonians like the one given in equation (1), one always knows that the system is in a pure state and thus that any state with $F_z > 1$ is a quantum superposition. In an experiment, the situation would be more complicated. The focus of this paper lies on providing a way to distinguish quantum superpositions with $F_z > 1$ from statistical mixtures with $F_z > 1$ via an ‘echo’ technique.

For pure states, equation (4) coincides with quantum Fisher information [9]. Like the spin-squeezed states investigated in [7] (and references therein), quantum superpositions with large fluctuations are also relevant to improve interferometric measurements beyond single-particle limits. A prominent example of a quantum superposition relevant for interferometry is the NOON states [10]

$$|\psi_{\text{NOON}}\rangle = \frac{1}{\sqrt{2}} (|N, 0\rangle + |0, N\rangle),$$

i.e. quantum superpositions of all particles either being in well 1 or well 2; $|n_1, n_2\rangle$ refers to the Fock state with $n_1$ particles in well 1 and $n_2$ particles in well 2. Suggestions on how such states can be obtained for ultracold atoms can be found in [5, 11–17] and references therein. For pure states, $F_z > 1$ indicates that this quantum superposition is relevant for interferometry [9]. However, it remains to be shown that the increased fluctuations are really due to pure states rather than statistical mixtures.

It might sound tempting to use the revivals investigated in [4, 5] to identify pure quantum states. However, while such revivals can be observed, e.g., for two-particle systems [18], the situation for a BEC in a double well is more complicated. In principle, very good revivals of the initial wavefunction should occur as long as the system is described by the Hamiltonian (1). While partial revivals (cf figure 1(c)) can easily be observed, (nearly) perfect revivals might occur for times well beyond experimental timescales—in particular if the experiment is performed under realistic conditions subject to decoherence effects. It is thus not obvious how such an apparent damping might be distinguished experimentally from decoherence effects which would lead to statistical mixtures.

For computer simulations, numerical errors might produce an effective decoherence which would again prevent nearly perfect revivals from occurring at very long timescales.
with (now truly) damped oscillation similar to that shown figure 1. The focus of this paper thus lies on an experimentally realizable ‘echo’ technique to distinguish statistical mixtures from quantum superpositions by using periodic shaking.

Periodic shaking [19] is currently being established experimentally to control tunnelling of BECs [20–25]. For the model (1), periodic shaking can be included via

$$\hat{H} = \hat{H}_0 + K \cos(\omega t) (\hat{n}_2 - \hat{n}_1),$$

where $K$ is the strength of shaking and $\omega$ is its (angular) frequency. For large shaking frequencies and not-too-large interactions, the time-dependent Hamiltonian (8) can be replaced by a time-independent effective Hamiltonian:

$$\hat{H}_{\text{eff}} = - J_{\text{eff}}(\hat{c}_1^\dagger \hat{c}_2^\dagger + \hat{c}_2 \hat{c}_1) + \frac{U}{2} \sum_{j=1}^{2} \hat{n}_j (\hat{n}_j - 1)$$

with

$$J_{\text{eff}} = J \sqrt{J_0(K_0); \quad K_0 = \frac{K}{\hbar \omega}},$$

where $J_0$ is the Bessel function depicted in figure 2(b). Such effective Hamiltonians have been successfully tested experimentally in optical lattices, see, e.g., [20, 26]; negative $J_{\text{eff}}$ have been experimentally investigated in [22, 25]. While numerically it is much easier to investigate the two-site Hamiltonian (9) or its time-dependent counterpart (8), experimentally it might be preferable to realize such models in optical lattices for parameters in which the one-band approximation is good [20, 21]. There are, however, also examples [27, 28] for which two or more Bessel functions are needed to understand the tunnelling dynamics.

In the present situation, the effective description (9) offers the possibility to quasi-instantaneously switch the sign of both the kinetic energy (via shaking, cf figure 2) and the interaction (via a Feshbach resonance [29]). Contrary to special cases where the wavefunction can be changed by quasi-instantaneously changing both the tunnelling term (by switching the shaking amplitude, e.g., between values shown in figure 2(b)) and the sign of the interaction via a Feshbach resonance [29],

$$\dot{H}_{\text{ideal}} \equiv \begin{cases} +\hat{H}_{\text{eff}}(\tau = 0) : \tau < \tau_0 \\ -\hat{H}_{\text{eff}}(\tau = 0) : \tau \geq \tau_0. \end{cases}$$

The corresponding unitary time evolution is given by

$$U(0, \tau) = \begin{cases} \exp\left(-\frac{i\tau \hat{H}_{\text{eff}}(\tau = 0)}{\hbar J}\right) : \tau < \tau_0 \\ \exp\left(\frac{i(\tau - 2\tau_0)\hat{H}_{\text{eff}}(\tau = 0)}{\hbar J}\right) : \tau \geq \tau_0, \end{cases}$$

with perfect return to the initial state at $\tau = 2\tau_0$. However, the turning point $\tau_0$ has to be chosen with care: only by taking $\tau_0$ close to the maximum of the shaking can unwanted excitations be excluded (cf [32–34]). Recent related investigations of the influence of the initial phase of the driving (replacing $\cos(\omega t)$ in the Hamiltonian (8) by $\cos(\omega t + \phi)$) can be found in [35–37].

In the following, the time reversal is demonstrated by numerically solving the full, time-dependent Hamiltonian (8) corresponding to the ideal time-reversal Hamiltonian (11) using the Shampine–Gordon routine [38]. Contrary to time-reversal schemes on the level of the Gross–Pitaevskii equation [39, 40], here time reversal is used to distinguish interesting quantum superpositions from statistical mixtures. Before implementing the time reversal, figure 3 shows the wavefunction for $N = 100$ particles which were initially in one well. After several oscillations, the wavefunction no longer is in a product state. Both the population imbalance and the phase can be measured experimentally [7]; in figure 3, the squared modulus of the scalar product with the atomic coherent states (5) is plotted. The angle $\theta$ corresponds to a population imbalance of

$$\langle \zeta \rangle = \frac{\cos(\theta)}{2}.$$

Ideally, it should be possible to show that the wavefunction of figure 3(a) indeed is a quantum superposition by using the time reversal of equation (11) and then investigating

$$\langle \zeta_{\text{end}} \rangle \equiv \langle \zeta \rangle(2\tau_0).$$
damping is displayed for $\tau \geq \tau_{imbalance}$ as a function of time $\tau = J/\hbar$ for the same parameters as in figure 3(a). (b) Solid line: all other parameters as in panel (a) except for $\tau > \tau_0 = 13.5\pi \simeq 42.41$; $K_0 = 3.8317 J$ and $U = -0.4 J/N$; the revival of the initial state is visible near $\tau \approx 85$. (c) Population imbalance for the same situation as in panel (a) but for much longer timescales. (d) If the switching takes place continuously rather than instantaneously (equation (16)), the revival of the initial state can still be observed (same parameters as for panel (b)) ($\gamma = 0$ corresponds to instantaneous switching; in the limit $\hbar\omega J \to \infty$ the maximum of this curve would be at $\gamma = 0$).

Firstly, there is only one many-particle wavefunction which fulfills

$$\langle z_{\text{end}} \rangle = 1.$$  \hspace{1cm} (15)

Secondly, the unitary evolution of solutions of the Schrödinger equation guarantees that for two different solutions $|\psi_1(2\tau_0)\rangle = U(\tau_0, 2\tau_0)|\psi_1(\tau_0)\rangle$ and $|\psi_2(2\tau_0)\rangle = U(\tau_0, 2\tau_0)|\psi_2(\tau_0)\rangle$, the scalar product would be the same at $\tau = \tau_0$ and at $\tau = 2\tau_0$ (as $U^\dagger U = 1$).

However, the Hamiltonian (11) is a high-frequency approximation, and it has, thus, to be shown that this works for realistic driving frequencies (cf figure 4). Furthermore, although there is only one wavefunction at $\tau = \tau_0$ which exactly leads to the value $\langle z \rangle_{\text{end}} = 1$ at $\tau = 2\tau_0$, other (less interesting) wavefunctions might lead to values close to $\langle z \rangle_{\text{end}} = 1$ (cf figure 5).

Figure 4 shows that the time-reversal dynamics is indeed feasible. On timescales for which there is not even a partial
Figure 5. (a) For the Hamiltonian which leads to the curve in figure 4(b), at \( \tau = \tau_0 \) product states (equations (5) and (17); \( z_0 = \cos(\theta_0) \)) are implemented. Displayed is the two-dimensional projection of \( \langle z_{\text{max}} \rangle/2 \) as a function of both the initial phase and the initial population imbalance. This lies well below the values obtained in figure 4(b), thus indicating that any wavefunction which leads to the values of \( \langle z \rangle_{\text{end}} \) at \( \tau = 2\tau_0 \) comparable to figure 4(b) was indeed a quantum superposition at \( \tau = \tau_0 \). (b) Two-dimensional projection of \( \Delta z \) (equation (19)), which indicates how accurately \( \langle z \rangle_{\text{max}} \) can be determined, shows that \( \langle z \rangle \) (as for figure 4(b)) does not change dramatically on short timescales. Thus, choosing the time of observation is not that crucial. (c) \( F_z \) lead to considerably larger fluctuations than obtained for the curve in figure 4(b) (which goes below the function of both driving amplitudes, normalized by their ideal values—cf figure 2) still lies well above the values shown in panel (a).

In addition to not approaching \( \langle z \rangle_{\text{max}} \) which is analogously defined by equation (19) to calculate

\[
\Delta z = \frac{\langle z_{\text{max}} \rangle - \langle z_{\text{min}} \rangle}{2},
\]

which indicates how accurately \( \langle z \rangle_{\text{max}} \) can be determined. In addition to not approaching \( \langle z \rangle = 1 \), many product states lead to very large fluctuations (figure 5(c)); these fluctuations are particularly large if one compares them with the tiny values of \( F_z(2\tau_0) \equiv 0.4 \) for the curve in figure 4(b). Carefully investigating how the product states

3 In the limit \( \hbar \omega/J \to \infty \), one would even have \( F_z(2\tau_0) = 0 \).
with large contributions to figure 3(a) behave offers an additional route to distinguish quantum superpositions as in figure 3(a) from statistical mixtures. Figure 5(d) shows that the time-reversal scheme is feasible even if the driving amplitudes only approximately meet the ideal values (figure 5(d)). Many of the features displayed in figures 5(a)–(c) could be understood by comparing them to the mean-field behaviour— including the fact that the fluctuations are large for some parameters and low for others (cf [41]). However, the main focus within this paper lies on showing that the return to the initial state displayed in figure 5(a) is much lower than what can be obtained in figure 5(b). In addition, the fluctuations displayed in figure 5(c) are much larger than would be obtained by the time-reversal dynamics displayed in figure 5(b).

To conclude, time reversal via quasi-instantaneously changing the sign of the effective Hamiltonian is experimentally feasible for ultracold atoms in a periodically shaken double well. The change of the sign of the Hamiltonian is achieved by changing both the driving amplitude and the sign of the interaction; a particularly useful initial state is the state with all particles in one well. Numeric investigations show that the revival of the initial state can be used to distinguish damping introduced via decoherence from the apparent damping related to a collapse phenomenon. Even if the revival of the initial state is not perfect, the scheme clearly distinguishes product states from quantum superpositions with potential interferometric applications. While this paper focuses on an experimentally relevant example for which the time-reversal dynamics can distinguish intermediate quantum superpositions from statistical mixtures, a perfect return to the initial state would prove that for all initial states. For general cases (which might include general product states (5)), more precise measurements [3] of both the initial and the final state including both population imbalance and fluctuations as well as measuring the phase distribution will be necessary.

Acknowledgments

I would like to thank S A Gardiner and M Holthaus for their support and T P Billam, B Gertjerenken, E Haller, C Hoffmann, J Hoppenau, A Ridinger, T Sternke and S Trotzky for discussions.

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