Quantum dynamics of an atomic Bose-Einstein condensate

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ABSTRACT
We consider the quantum dynamics of a neutral atom Bose-Einstein condensate in a double-well potential, including hard-sphere particle interactions. Using a mean-field factorisation we show that the coherent oscillations due to tunnelling are suppressed when the number of atoms exceeds a critical value. An exact quantum solution, in a two-mode approximation, shows that the mean-field solution is modulated by a quantum collapse and revival sequence. Chaotic dynamics results when the potential is modulated.

Keywords: BEC, tunnelling, chaos

1. INTRODUCTION
The recent experimental observation of Bose-Einstein condensation (BEC) in dilute systems of trapped neutral atoms opens a new context for studying the quantum mechanics of mesoscopic systems. In particular, atomic BECs can be expected to display a variety of quantum interference phenomena, and Javanainen and Grossmann and Holthaus have previously suggested the possibility of condensate tunnelling between two adjacent atomic traps. This tunnelling, resulting in oscillatory exchange of the atoms between the traps, is analogous to the Josephson effect for neutral atoms, in which the exchange results from the phase difference between the macroscopic wave functions for the two traps.

We consider the case of an atomic BEC formed in a double-well potential with well separated minima, where each potential well represents an atomic trap. Using the mean-field factorisation assumption, together with a two-mode approximation, we find an analytic solution to the Gross-Pitaevskii equation including hard-sphere interactions. If the condensate is initially localised in one well, it can oscillate between the wells by quantum tunnelling. However, due to the nonlinearity arising from particle interactions, this oscillation is suppressed when the number of atoms in the condensate exceeds a critical value. We also calculate the full quantum dynamics and show that the oscillations arising in the mean field approximation are modulated by a collapse and revival sequence. The time for a complete collapse and revival depends very strongly on the number of particles in the condensate, becoming longer as the particle number is increased.

The many-body Hamiltonian may be written in terms of annihilation and creation operators \( c_i, c_i^\dagger \) which annihilate and create particles in Gaussian single particle states. These states are the ground states of the harmonic approximation to the potential around each minima. Within this two-mode approximation the many body Hamiltonian may be written

\[
\hat{H} = \frac{\hbar \Omega}{2} (c_1^\dagger c_2 + c_2^\dagger c_1) + \hbar \kappa \left( (c_1^\dagger)^2 c_1^2 + (c_2^\dagger)^2 c_2^2 \right),
\]

where \( \kappa = U_0/2hV_{eff} \), and \( V_{eff}^{-1} \) is the effective mode volume of each well, and where \( U_0 = 4\pi \hbar^2 a/m \) measures the strength of the two-body interaction, and \( a \) is the s-wave scattering length. We have retained only self-phase modulation arising from self-interaction within each well since the cross-interaction terms should be consistently
neglected in the two-mode approximation. The term proportional to $\Omega$ represents quantum tunnelling between the two wells at the single particle tunnelling rate $\Omega$.

The Hamiltonian (1) has the form of that for the discrete self-trapping equation, and has previously been studied in the context of the quantum dimer,11 as a model for anharmonic oscillations in small molecules, and also in the context of the nonlinear optical directional coupler.12 Here we explore the consequences of this model for atomic BEC in a double-well potential.

### 2. SEMICLASSICAL DYNAMICS

Before proceeding to the full quantum analysis of the Hamiltonian (1), we first consider the mean-field approximation. For this we employ the Hartree approximation13 for a fixed number of atoms $N$, and write the atomic state vector as

$$|\Psi_N(t)\rangle = \frac{1}{\sqrt{N!}} \left[ \int d^3 r \phi_N(r, t) \psi^*(r, 0) \right]^N |0\rangle,$$

where $|0\rangle$ is the vacuum. The self-consistent nonlinear Schrödinger equation or Gross-Pitaevskii equation for the condensate wave function $\phi_N(r, t)$ follows from the Schrödinger equation $i\hbar \frac{\partial \phi_N}{\partial t} = H(0)|\Psi_N(t)\rangle$, and is given by

$$i\hbar \frac{\partial \phi_N}{\partial t} = \left[ \frac{\hbar^2}{2m} \nabla^2 + V(r) + NU_0|\phi_N|^2 \right] \phi_N.$$  

For a particular choice of the global potential $V(r)$, Eq. (3) can be solved numerically for a given initial condition. In the two-mode approximation we use the local modes described above and write

$$\phi_N(r, t) = e^{-iE_0t/\hbar} [b_1(t)u_1(r) + b_2(t)u_2(r)].$$

Then, to first-order in $\epsilon$ we obtain the coupled-mode equations

$$\frac{db_j}{dt} = -\frac{i\Omega}{2} b_{3-j} - 2i\kappa N|b_j|^2 b_j,$$  

The number of atoms in the $j^{th}$ well is given by

$$N_j(t) = \langle \Psi_N(t)|c_j^\dagger c_j|\Psi_N(t)\rangle = N|b_j(t)|^2,$$

and this provides the link between the coupled-mode amplitudes and the expectation values of the quantum problem.

The coupled-mode Eqs. (5) have an exact solution.9 For the case that all $N$ atoms are initially localised in well 1, $N_1(0) = N|b_1(0)|^2 = N$, the number of atoms in well 1 varies in time as

$$N_1(t) = \frac{N}{2} \left[ 1 + cn(\Omega t|N^2/N_0^2) \right],$$

with $N_1(t) + N_2(t) = N$. Here $cn(\phi|m)$ is a Jacobi elliptic function, and $N_c$ is the critical number of atoms given by

$$N_c = \frac{\Omega}{\kappa}.$$  

For $N < N_c$ this solution exhibits complete and periodic oscillations between the two condensates with a period $K(N^2/N_0^2)$ which depends on the number of atoms, where $K(m)$ is a complete elliptic integral of the first kind. For $N << N_c$, $cn$ becomes cos, and the oscillations are precisely those in the Josephson effect.6 As the number of atoms is increased the oscillation period increases, until at $N = N_c$ the period is infinite. This marks a bifurcation in the nonlinear system and at this point the system asymptotically evolves to equal number of atoms $N/2$ in each well. For $N > N_c$ the period of oscillation reduces again but the exchange between the wells is no longer complete. That is, the coherent tunnelling oscillations are inhibited at high numbers of atoms, and this is the analogue of the self-trapping transition for the double-well BEC.

The choice of initial conditions depends on the condensate state. In a typical case one might expect that there would be equal numbers of atoms in each of the wells, and thus the many-body ground state would reflect the fundamental
Mean-field solutions for the occupation difference \( \langle S_x \rangle = \frac{1}{2} (|b_2|^2 - |b_1|^2) \) versus time in units of the inverse tunnelling period. The solid line is for \( \kappa N/\Omega = 0.9 \), and the dashed line is for \( \kappa N/\Omega = 2 \), the critical value being for \( \kappa N/\Omega = 1 \).

Figure 1.

Symmetry of the potential. This would mean that the quantity \( (|b_2|^2 - |b_1|^2) \) would initially be zero. However as the total number of atoms is conserved we have, \( 1 = (|b_2|^2 + |b_1|^2) \), we must have

\[
b_1 b_2 = \frac{1}{2} e^{-i\theta}
\]

(9)

where \( \theta \) is the phase difference between the phases of \( b_1 \) and \( b_2 \) respectively. The condensate may thus be regarded as having a phase. According to the usual argument of spontaneous symmetry breaking\(^{15,16}\) this phase is random and if averaged would give a zero value to the phase dependent term in the ensemble.

To investigate the consequences of spontaneous symmetry breaking for the semiclassical dynamics, it will be convenient to define the three real variables \( S_x, S_y, S_z \) by

\[
S_x = \frac{1}{2} (|b_2|^2 - |b_1|^2)
\]

(10)

\[
S_y = -\frac{i}{2} (b_1^* b_2 - c.c)
\]

(11)

\[
S_z = \frac{1}{2} (b_1^* b_2 + c.c)
\]

(12)

In section 3 we will show that \( S_y \) is the mean momentum of the condensate, while \( S_z \) is the atomic number difference between the two single-particle energy eigenstates of the double well system. If \( S_x = 0 \) we must have \( S_y = \frac{1}{2} \sin \theta \) and \( S_z = \frac{1}{2} \cos \theta \). If the mean momentum of the condensate is initially zero, \( \theta = 0 \) and \( S_z(0) = 0.5 \). Such an initial condition is a stationary point of the dynamics, as is easily seen if we write the equations of motion in terms of the real variables define above;

\[
\dot{S}_x = -\Omega S_y
\]

(13)

\[
\dot{S}_y = \Omega S_x - 4\kappa N S_x S_z
\]

(14)

\[
\dot{S}_z = 4\kappa N S_x S_y
\]

(15)

These equations indicate a linear precession around the \( S_z \) axis at rate \( \Omega \), and a nonlinear precession around the \( S_x \) axis at a rate \( 4\kappa N S_z \). It is easily seen that \( S_x^2 + S_y^2 + S_z^2 = 1/4 \) is a constant of the motion, which corresponds to conservation of particle number.

In Fig. 1 we show the mean-field solutions for the quantity \( \langle S_x \rangle = \frac{1}{2} (|b_2|^2 - |b_1|^2) \) which represents the occupation difference of the two wells: The solid line is for \( \kappa N/\Omega = 0.9 \), and complete oscillations between the wells is observed (we scale time in units of the tunnelling period so that \( \Omega = 1 \) in all the figures). In contrast, the dashed curve is for \( \kappa N/\Omega = 2 \), and the coherent oscillations are no longer complete. This corresponds to the discrete trapping identified in reference\(^9\).

We now determine the response of the condensate to periodic driving. If the barrier height of the double well potential is modulated periodically in time, then for small modulation we can describe the dynamics of the condensate.
Figure 2.
Phase-space stroboscopic portrait of the semiclassical response of the condensate for modulation strength \( \epsilon = 0.8 \), with \( \alpha = 1.0 \) and \( \omega_D = 1.37\Omega \).

by allowing the single particle tunneling frequency to become time dependent,

\[
\Omega(t) = \Omega(1 + \epsilon \cos \omega_D t)
\]

(16)

It is no longer possible to obtain an analytic solution, indeed we expect such a periodically driven nonlinear system to exhibit a transition to chaos. It is then more appropriate to view the dynamics at the period of the driving frequency. We first define the stereographic projection of the variables \( x = S_x, y = S_y, z = S_z \) through the real (a) and imaginary (b) parts of the complex variable \( \nu \) where

\[
\nu = \frac{x + iy}{0.5 + z}
\]

(17)

The scaled parameter \( \alpha = 4\kappa N/\Omega \) is used to quantify the relative strength of the nonlinearity.

In figure 2 we plot the stroboscopic phase-space, that is \( a \) versus \( b \) at periods of the driving frequency. We have taken \( \alpha = 1 \) so as to be near a separatrix in the undriven dynamics. The phase-space clearly shows regions of regular and chaotic dynamics. We thus conclude that the nonlinear response of the condensate can become chaotic in the presence of strong driving.

3. QUANTUM DYNAMICS

Within the two-level approximation we can obtain an exact solution to the full quantum problem in order to assess the effect of quantum fluctuations on the predictions of the Gross-Pitaevskii equation. The total number operator \( \hat{N} = c_1^\dagger c_1 + c_2^\dagger c_2 \), is a constant of motion and thus we set it equal to the total number of atoms \( N \). We now define three operators, which obey SU(2) commutation relations, by

\[
\hat{J}_x = \frac{1}{2}(c_1^\dagger c_2 - c_2^\dagger c_1),
\]

(18)

\[
\hat{J}_y = \frac{1}{2}(c_1^\dagger c_2 + c_2^\dagger c_1),
\]

(19)

\[
\hat{J}_z = \frac{i}{2}(c_1^\dagger c_2 - c_2^\dagger c_1).
\]

(20)

The Casimir invariant is easily seen to be

\[
\hat{J}^2 = \frac{\hat{N}}{2} \left( \frac{\hat{N}}{2} + 1 \right)
\]

(21)

This is analogous to an angular momentum model with total angular momentum given by \( j = N/2 \).

The operator \( \hat{J}_z \) corresponds to the particle occupation number difference between the single-particle energy eigenstates. For example the maximal weight eigenstate \( |j, j\rangle \) corresponds to all the particles occupying the highest
single particle energy eigenstate, \( \psi_2(x) \). The operator \( \hat{J}_z \) gives the particle number difference between the localised states \( \{ u_1, u_2 \} \) of each well. In fact, for the one dimensional case, the position operator in the field representation is
\[
\hat{x} \rightarrow \frac{2q_0}{N} \hat{j}_z
\] (22)
Thus the maximal and minimal weight eigenstates of \( \hat{J}_z \) correspond to the localisation of all the particles in one well or the other. The interpretation of \( \hat{J}_y \) is crucial for an understanding of tunnelling. In one dimension, the field representation of the single particle momentum operator \( i\hbar \frac{\partial}{\partial x} \) is
\[
\hat{p} \rightarrow -\frac{\hbar \Omega}{g_0 \omega_0} \hat{j}_y
\] (23)
Thus the operator \( \hat{J}_y \) represents the condensate momentum.

The two-mode Hamiltonian (1) may be written,
\[
\hat{H} = \hbar \Omega \hat{J}_z + 2\hbar \kappa \hat{J}_z^2,
\] (24)
where we neglected constant energy shifts which depend on the total number \( N \). This Hamiltonian describes linear precession around the \( z \)-axis at the tunnelling frequency and a nonlinear precession around the \( z \)-axis at a rate determined by the value of \( z \) component of angular momentum. It is interesting to note that Eq. (24) looks similar to the nonlinear top models considered by Haake.\(^{17}\) This Hamiltonian is symmetric under rotations of \( \pi \) about the \( z \) axis. Such a transformation corresponds to \( \hat{J}_z \rightarrow -\hat{J}_z \) which in view of the interpretation of \( \hat{J}_z \) discussed above corresponds to the parity symmetry of the double well potential. Thus all eigenstates belong to one of two parity classes corresponding to the two eigenvalues of this transformation.

The semiclassical solution suggests that for \( N \) small the first term in Eq(24) dominates, in which case the energy eigenstates are close to the \( N + 1 \) eigenstates of \( \hat{J}_z \). The condensate state will be near the minimum weight state \( |j, -j \rangle \). This state is of course just the single particle ground state of the double well potential, and thus the density function of the condensate will be symmetric as expected. In this case the dynamics is dominated by a precession around the \( z \)-axis. If the system then starts with broken symmetry so that
\[
\langle \hat{J}_y \rangle = N S_y \neq 0,
\] (25)
(which corresponds to a non-zero momentum state), precession around the \( z \)-axis will cause \( \langle \hat{J}_z \rangle \) to oscillate at frequency \( \Omega \). This means that the condensate accumulates first in one well then the other at a frequency determined by the single-particle tunnelling frequency \( \Omega \). This is analogous to the general case for superfluidity when spontaneous symmetry breaking gives the condensate a phase and a non-zero momentum.\(^{15}\)

On the other hand for large \( N \) we expect the system to be dominated by the second nonlinear term in the Hamiltonian. This suggests that the eigenstates of the Hamiltonian are close to the eigenstates of \( \hat{J}_z^2 \). The ground state, and thus the condensate state, is close to the zero weight state \( |j, 0 \rangle \), with all other states being doubly degenerate. Note that this state corresponds to an equal number of particles in each of the localised states in each well and thus will also have a symmetric density function. Some results on the spectrum of this model were presented in reference\(^{11}\)

In figures 3,4 we calculate the eigenvalues of the Hamiltonian for different values \( \Omega/\kappa \) and total particle number \( N \). In figure 3 the ratio is large and the low lying part of the spectrum is dominated by the eigenstates of \( \hat{J}_z \), with a characteristic linear increase with the integer labelling the sequence of eigenstates. As the ratio of \( \Omega/\kappa \) increases figure, 4, the doubly degenerate eigenstates of \( \hat{J}_z^2 \) begin to dominate and the energies increase quadratically with the integer labelling the eigenstates.

The most natural set of states which exhibit spontaneous broken symmetry for this system are the angular momentum coherent states\(^{18}\) defined in terms of the \( \hat{J}_z \) eigenstates by
\[
|\alpha\rangle = \sum_{m=-j}^{j} \binom{2j}{m+j}^{1/2} \frac{\alpha^{m+j}}{1 + |\alpha|^2 j} |j, m\rangle
\] (26)
with $\alpha = e^{-i\phi} \tan \theta/2$. For these states we have that $\langle J_x \rangle = \frac{N}{2} \sin \theta \cos \phi$, $\langle J_y \rangle = \frac{N}{2} \sin \theta \sin \phi$, and $\langle J_z \rangle = \frac{N}{2} \cos \theta$. These states have a binomial, rather than Poisson, distribution of particle number over the two single particle energy eigenstates of the potential. These states were recently by used by Wong et al.\textsuperscript{19} to test aspects of spontaneous broken symmetry As previously for a condensate of zero momentum we would have $\theta = 0$.

We now determine the quantum dynamics of this model and contrast the results with the semiclassical results. The Heisenberg equations of motion are

$$\frac{d\hat{S}_x}{dt} = -\Omega \hat{S}_y,$$

$$\frac{d\hat{S}_y}{dt} = \Omega \hat{S}_x - 2\kappa N(\hat{S}_z \hat{S}_x + \hat{S}_x \hat{S}_z),$$

$$\frac{d\hat{S}_z}{dt} = 2\kappa N(\hat{S}_y \hat{S}_x + \hat{S}_x \hat{S}_y),$$

where we have defined the scaled, or intensive, many-body operators by $\hat{S}_\alpha = \hat{J}_\alpha / N$. If we now consider the equations of motion for the mean values and factorise all product averages, we can define an equivalent mean-field model. The resulting equations are equivalent to Eqs. (5) with the identification $\langle S_x \rangle = \frac{1}{2}(\langle b_2 \rangle^2 - \langle b_1 \rangle^2)$, $\langle S_y \rangle = -\frac{1}{2}(\langle b_1^* b_2 - b_2^* b_1 \rangle)$, $\langle S_z \rangle = \frac{1}{2}(\langle b_1^* b_2 + b_1 b_2^* \rangle)$.

To obtain the quantum dynamics, we represent the two-mode Hamiltonian Eq. (24) in the eigenbasis of $J_x$, and expand the states in the same basis. The time evolution can then be found by integrating the Schrödinger equation in this basis. In Figs. 4 and 5 we plot the mean value $\langle J_x(t)/N \rangle = S_x$ for the initial state $|j, -j\rangle_x$, corresponding to a state localised in one well, and equivalent to that used for the mean-field solutions shown in Fig. 1.

We take two cases, $N = 100, N = 400$, with $\kappa N$ above and below the critical or threshold case with $\kappa N = \Omega$. For convenience we normalise the time in units of the single-particle tunnelling period so that in these units $\Omega = 1$. 

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{figure3.png}
\caption{A plot of the energy spectrum in the two-mode approximation with $\Omega/\kappa = 50$ and $N = 100$.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{figure4.png}
\caption{A plot of the energy spectrum in the two-mode approximation with $\Omega/\kappa = 1$ and $N = 100$.}
\end{figure}
In Fig. 5 we plot the mean value of $S_x$ versus time for an initial state $|j,-j\rangle$, for the case $\kappa = 0.9$. For short times the quantum and mean-field dynamics are similar, with the same oscillation frequency. However, the oscillations of the quantum mean decay due to the intrinsic quantum fluctuations in the initial condition. That is, although the total particle number is fixed the number of atoms in each individual well are not and must be considered fluctuating quantities. More interesting, however, is the revival of the oscillation that occurs at later times. This is entirely due to the discrete spectrum of the many-body Hamiltonian. The revival is rather irregular in the below threshold case in Fig. 5 when compared with the above threshold case, Fig. 6. In both cases increasing the number of atoms $N$ while keeping $\kappa N$ fixed, increases the collapse and revival time. Thus, it is clear that the mean-field factorisation approximation will be valid for sufficiently long time scales if $N$ is large enough.

To observe this result it would be necessary to prepare the condensate in a maximal eigenstate of $\hat{J}_x$, that is, entirely localised in one well or the other. To observe the collapse and revival one would need to monitor the initially unoccupied well. This could be done using off-resonant light scattering, which is dependent on the particle density, so long as the probe laser could be focussed down to distinguish a single well.

The single-particle tunnelling frequency will depend on the details of how the double well is constructed. In fact in the MIT experiment something like a double well was formed by using an off-resonant optical dipole force to perturb a magnetic-rf trap. Suppose that the harmonic frequency at the bottom of the trap were of the order of 1kHz. In the case of sodium this results in $\Delta = 1.4 \times 10^{-12}$ m$^2$. In the MIT experiment, $U_0$ is approximately $1.8 \times 10^{-50}$ Jm$^3$. This gives a value for $\kappa = 53$ s$^{-1}$. The maximum value of $\Omega$ is 37% of the harmonic frequency at the bottom of the wells. If this harmonic frequency is 1kHz, then the critical number of atoms is $N_c \approx 7$, a rather small number. Thus in a realistic experiment it is likely that the single particle tunnelling will be strongly suppressed by the atomic interactions. Furthermore it is known that quantum tunnelling is very sensitive to noise, being rapidly suppressed for even small noise sources. For example small fluctuations in the potential can cause the bottoms of the double wells to fluctuate in energy. This will tend to cause localisation of the condensate in one well or the other. However due to the considerable isolation of atomic condensates from their environments we expect that this problem will be not as serious for these systems as it has been for other many particle tunnelling systems such as Josephson tunnelling.
ACKNOWLEDGEMENTS

We wish to thank R.J. Glauber.

REFERENCES