Quantum dynamics of a binary mixture of BECs in a double-well potential: a Holstein–Primakoff approach

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Abstract
We study the quantum dynamics of a binary mixture of Bose–Einstein condensates (BECs) in a double-well potential starting from a two-mode Bose–Hubbard Hamiltonian. Focussing on the regime where the number of atoms is very large, a mapping onto an SU(2) spin problem together with a Holstein–Primakoff transformation is performed. The quantum evolution of the number difference of bosons between the two wells is investigated for different initial conditions, which range from the case of a small imbalance between the two wells to a coherent spin state. The results show an instability towards a phase separation above a critical positive value of the interspecies interaction while the system evolves towards a coherent tunnelling regime for negative interspecies interactions. A comparison with a semiclassical approach is discussed together with some implications on the experimental realization of phase separation with cold atoms.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Bose–Einstein condensates (BECs) of dilute, weakly interacting gases offer a unique possibility for exploring many-body dynamics, the role of quantum fluctuations and in general macroscopic quantum coherence phenomena [1], thanks to a wide tunability of the interaction parameters. Indeed several experimental strategies can be devised in order to pursue this task, which range from the direct control via magnetic Feshbach resonance techniques [2] to the transverse confinement in a quasi-one-dimensional system [3] as a way to increase the inter-atomic interaction. Finally, the introduction of an optical lattice whose depth can be tuned allows one to decrease the kinetic term in the Hamiltonian. Within the tight binding approximation such systems are described by the Bose–Hubbard Hamiltonian, whose parameters are the hopping frequency $E_J$ between nearest-neighbour lattice sites, the onsite interaction strength $E_c$ and the total number of atoms $N$. When the ratio $E_cN/E_J$ exceeds unity, a quantum phase transition from a superfluid to a Mott insulator [4] takes place and the system enters a quantum regime characterized by strong correlations. The simplest Hamiltonian of this kind that one can devise is the Bose–Hubbard dimer [5], which describes the physics of two weakly coupled condensates. It can be mapped onto an SU(2) spin problem and is deeply related to the physics of Josephson junctions [1, 6, 7]. Furthermore, if the mean field approximation is considered, one obtains the Gross–Pitaevskii theory which gives rise to a variety of phenomena, ranging from Josephson oscillations [8] to macroscopic quantum self-trapping (MQST) [9] and ac and dc Josephson-like effect [10], all experimentally observed in the last decade [11–13].

More recently, after the experimental realization of two-species BECs [14–16], the theoretical analysis on weakly
coupled condensates has been successfully extended to a binary mixture of BECs in a double-well potential [17–22]. The semiclassical regime in which the fluctuations around the mean values are small has been deeply investigated and found to be described by two coupled Gross–Pitaevskii equations. By means of a two-mode approximation such equations can be cast in the form of four coupled nonlinear ordinary differential equations for the population imbalance and the relative phase of each species. The solution results in a richer tunnelling dynamics [23]. In particular, two different MQST states with broken symmetry have been found [20], where the two species localize in the two different wells giving rise to a phase separation or coexist in the same well respectively. Indeed, upon a variation of some parameters or initial conditions, the phase-separated MQST states evolve towards a symmetry-restoring phase where the two components swap places between the two wells, so avoiding each other. Furthermore, the coherent dynamics of a two-species BEC in a double well has been analysed as well focusing on the case where the two species are two hyperfine states of the same alkali metal [24].

In a recent paper [25], we studied the quantum behaviour of a binary mixture of BECs in a double-well potential starting from a two-mode Bose–Hubbard Hamiltonian. We analysed in detail the small tunnelling amplitude regime where number fluctuations are suppressed and a Mott-insulator behaviour is established. Within this regime we performed a perturbative calculation up to second order in the tunnelling amplitude and found the stationary states. In order to carry out analytical calculations, we focused on the symmetric case of equal nonlinear interaction and equal tunnelling amplitude of the two species. Furthermore, we restricted our focus to the case in which the two species are equally populated and imposed the condition of equal population imbalance of the species $a$ and $b$ between the two wells. Then, the dynamics of the junction was investigated in correspondence of a completely localized initial state. In order to avoid the above restrictions on the parameters range, here we focus on the two-mode Bose–Hubbard Hamiltonian describing the two-species BEC ($a$ and $b$) in a double well when $N_a, N_b \gg 1$ and perform a mapping onto an $SU(2)$ spin problem together with a Holstein–Primakoff transformation [26, 27]. As a result we obtain a Hamiltonian of two decoupled quantum harmonic oscillators, similar to that of [28], whose stationary states are readily found. The quantum evolution of the number difference of bosons between the two wells is investigated in detail in correspondence of a variety of initial conditions, which range from an initial state with small imbalance between the two species to a coherent spin state. The whole parameter space is explored by tuning the population, the tunnelling amplitude and the nonlinear interaction for each species as well as the interspecies interaction in a wide range, from a symmetric to a strongly asymmetric case. Finally a detailed comparison with a semiclassical approach is given. Let us note that Holstein–Primakoff transformation makes the system exactly solvable in the weakly interacting regime of interest in this work and that simplifies the study of the tunnelling dynamics as well as the phase separation phenomenon. This is the main advantage of the approach chosen.

The paper is organized as follows. In section 2, we introduce the model Hamiltonian that we study within the two-mode approximation. A Holstein–Primakoff transformation is performed and the semiclassical limit is taken followed by a decoupling of the bosonic degrees of freedom for each species. As a result, the Hamiltonian can be rephrased in terms of two independent harmonic oscillators, whose stationary states are derived in section 3. In section 4, the quantum dynamics of the system is discussed in relation to two different initial conditions: the small imbalance between the two wells and the coherent states. A wide range of values of interspecies interaction is explored and the crossover to an unstable regime with phase separation is found. In section 5, the classical equations of motion are derived and a comparison with the quantum counterpart is carried out. Finally some conclusions and perspectives of this work are briefly outlined.

2. The model

A binary mixture of BECs [18, 20] loaded in a double-well potential is described by the Hamiltonian $H = H_a + H_b + H_{ab}$ where

$$H_i = \int d\vec{r} \left( -\frac{\hbar^2}{2m_i} \nabla^2 \psi_i + \psi_i^* V_i(\vec{r}) \psi_i \right) + \frac{g_{ii}}{2} \int d\vec{r} \psi_i^* \psi_j \psi_i \psi_j, \quad i = a, b \tag{1}$$

$$H_{ab} = g_{ab} \int d\vec{r} \psi_a^* \psi_b \psi_a \psi_b. \tag{2}$$

Here $g_{ii} = \frac{\sqrt{\hbar \alpha_{ii}}}{\sqrt{m_i}}$ is the intraspecies coupling constants, with $m_i$ the atomic mass and $\alpha_{ii}$ the $s$-wave scattering lengths; $g_{ab} = \frac{\sqrt{\hbar \alpha_{ab}}}{\sqrt{m_a m_b}}$ is the interspecies coupling constant, with $m_{ab} = \frac{m_a m_b}{m_a + m_b}$ is the reduced mass; $V_i(\vec{r})$ is the double-well trapping potential and, in the following, we assume $V_a(\vec{r}) = V_b(\vec{r}) = V(\vec{r}); \psi_i^*(\vec{r}), \psi_i(\vec{r}), i = a, b$ are the bosonic creation and annihilation operators for the two species, which satisfy the commutation rules

$$[\psi_i(\vec{r}), \psi_j(\vec{r}')] = [\psi_i^*(\vec{r}), \psi_j^*(\vec{r}')] = 0,$$  \tag{3}

$$[\psi_i(\vec{r}), \psi_j^*(\vec{r}') \psi^*_i(\vec{r}') \psi_j(\vec{r}')] = \delta_{ij} \delta(\vec{r} - \vec{r}'), \quad i, j = a, b, \tag{4}$$

and the normalization conditions

$$\int d\vec{r} |\psi_i(\vec{r})|^2 = N_i, \quad i = a, b, \tag{5}$$

$N_i, i = a, b$, being the number of atoms of species $a$ and $b$, respectively. The total number of atoms of the mixture is $N = N_a + N_b$.

A weak link between the two wells produces a small energy splitting between the mean-field ground state and the first excited state of the double-well potential which allows the dimension of the Hilbert space of the initial many-body problem to be reduced. Indeed for low energy excitations and low temperatures it is possible to consider only two such states and neglect the contribution from the higher ones, the so-called two-mode approximation [9, 29, 30]. In this approximation, the Hamiltonian (1) can be written in terms of
the annihilation operators, \( a_i = \frac{1}{\sqrt{2}}(a_i^+ - a_i) \), \( a_R = \frac{1}{\sqrt{2}}(a_R^+ - a_R) \) and \( b_L = \frac{1}{\sqrt{2}}(b_L^+ + b_L) \), \( b_R = \frac{1}{\sqrt{2}}(b_R^+ - b_R) \) and the corresponding creation operators, where \( a_i, a_R, b_L, b_R \) are the annihilation operators of a particle in the ground and in the first excited state.

When introducing the angular momentum operators:

\[
\begin{align*}
J^a &= \frac{1}{\sqrt{2}}(a^+_R a_L + a^+_L a_R), \\
J^b &= \frac{i}{\sqrt{2}}(a^+_R a_L - a^+_L a_R), \\
J^c &= \frac{1}{2}(b^+_R b_L - b^+_L b_R), \\
J^d &= \frac{1}{2}(b^+_R b_L + b^+_L b_R),
\end{align*}
\]

(6)

where the operators \( J^a, J^b, J^c, J^d \) obey the usual angular momentum algebra together with the relation

\[
(J^a)^2 = \frac{N_a}{N} \left( \frac{N_a}{N} + 1 \right), \quad (J^b)^2 = \frac{N_b}{N} \left( \frac{N_b}{N} + 1 \right),
\]

(7)

the Hamiltonian of the double-species Bose–Josephson junction can be written in the form

\[
H = \frac{1}{2} \Lambda_a (J^a)^2 - K_a J^a + C_a (J^a)^2 + \frac{1}{2} \Lambda_b (J^b)^2 - K_b J^b + C_b (J^b)^2 + \Lambda_{ab} J^a J^b - D_{ab} J^a J^b.
\]

(8)

where \( \Lambda_a, \Lambda_b \) are the tunnelling amplitudes between the two wells, \( K_a, K_b, C_a, C_b, D_{ab} \) describe intraspecies interactions, respectively, while the terms \( \Lambda_{ab} \) and \( D_{ab} \) describe two-particle processes [25]. The form (8) was previously discussed in the classical limit in [20], where it was shown to lead to equations of motion equivalent to the Gross–Pitaevskii equations. For \( \Lambda_{ab} = D_{ab} = 0 \) in equation (8), the Hamiltonian reduces to a sum of two Lipkin–Meshkov–Glick (LMG) model [31, 32] Hamiltonians, one for each species. For \( \Lambda_{ab} \neq 0 \) or \( D_{ab} \neq 0 \), the two LMG models are coupled. Within the experimental parameter range, it is possible to show that \( C_i \ll \Lambda_i, K_i, i = a, b, \) and \( D_{ab} \ll \Lambda_{ab} [6, 20, 25] \), and then in the following we put \( C_a = C_b = 0 \) and \( D_{ab} = 0 \), which corresponds to neglecting the spatial overlap integrals between the localized modes in the two wells. In this way the binary mixture of BECs within two-mode approximation maps to a two-Ising-spin model in a transverse magnetic field, whose Hamiltonian is

\[
H = \frac{1}{2} \Lambda_a (J^a)^2 - K_a J^a + \frac{1}{2} \Lambda_b (J^b)^2 - K_b J^b + \Lambda_{ab} J^a J^b.
\]

(9)

Let us now make the rotation

\[
J^J \rightarrow -J^{\pm}, \quad i = a, b.
\]

(10)

To proceed we perform the Holstein–Primakoff transformation [26–28] in order to map the angular momentum operators into bosonic ones and focus on the regime with a large number of atoms \( N_a, N_b \gg 1 \) and weak scattering strengths \( K_{ab} \gg \Lambda_a, \Lambda_b, \Lambda_{ab} \):

\[
\begin{align*}
J^a &= J^a - \frac{a^a}{2}, \\
J^b &= J^b - \frac{b^b}{2}, \\
J^c &= \sqrt{2} J^c - \frac{a^a b^b}{2}, \\
J^d &= \sqrt{2} J^d - \frac{a^a b^b}{2},
\end{align*}
\]

(11)

where \( J^a = J^a \pm i J^c, i = a, b, J^J = N_a/2 i = a, b, \) thus leading to the Hamiltonian

\[
H = \frac{\Lambda_a}{8} (2 J^a (J^a + 1) - 2 (J^a - a^a)^2 + \sqrt{2} J^a - a^a) (2 J^a - a^a) a^a + \frac{1}{2} \Lambda_b (J^b)^2 + (2 J^a - b^b) (2 J^b - b^b) a^a + \frac{1}{2} \Lambda_{ab} (J^a J^b - D_{ab} J^a J^b)
\]

(12)

Here \( a \) and \( b \) are boson annihilation operators for each species. In this representation, the operators \( e^{i \sigma J^a} \) are equal to \( e^{i \sigma (J^a - v \nu)} \) and their action is simply \( \nu \rightarrow -\nu \). For \( \Lambda_{ab} = 0 \), the Hilbert space of (12) thus breaks into four different sectors, according to the parity of \( a^a + b^b \), while the condition \( \Lambda_{ab} \neq 0 \) breaks it into two different sectors depending on the parity of \( a^a + b^b \). The physical Hilbert space is restricted to \( 0 \leq a^a \leq N_a \) and \( 0 \leq b^b \leq N_b \).

Since we consider a large number of atoms, we have \( J^a, J^b \gg 1 \), while the condition \( K_{ab} \gg \Lambda_a, \Lambda_b, \Lambda_{ab} \) implies \( \langle a^a \rangle \ll 2 J^a \) and \( \langle b^b \rangle \ll 2 J^b \). Under these assumptions one can use the linearized Holstein–Primakoff transformation [26] (i.e., \( J^J = J^J - s^s, J^J = \sqrt{2} J^J s, J^J = s^s \sqrt{2} J^J \) with \( s = a, b \) and derive the effective Hamiltonian

\[
H = \Lambda_a J^a \left( \frac{a + a^a}{2} \right) \left( \frac{a + a^a}{2} \right) + \Lambda_b J^b \left( \frac{b + b^b}{2} \right) \left( \frac{b + b^b}{2} \right) + \frac{1}{2} \Lambda_{ab} \sqrt{2} J^a \left( \frac{a + a^a}{2} \right) \left( \frac{b + b^b}{2} \right) - \frac{1}{2} \Lambda_{ab} \sqrt{2} J^b \left( \frac{b + b^b}{2} \right) \left( \frac{a + a^a}{2} \right) + \Lambda_{ab} \sqrt{2} J^a J^b + K_{ab} a^a b^b.
\]

(13)

In order to decouple the degrees of freedom of each bosonic species, let us introduce the following harmonic oscillator coordinates and momenta, \( q_i, p_i, i = a, b \):

\[
\begin{align*}
q_a &= \frac{1}{\sqrt{2}} (a + a^a), \\
q_b &= \frac{1}{\sqrt{2}} (b + b^b), \\
p_a &= -i \frac{1}{\sqrt{2}} (a - a^a), \\
p_b &= -i \frac{1}{\sqrt{2}} (b - b^b).
\end{align*}
\]

(14)
which satisfy the usual commutation rules \([q_i, p_j] = i\delta_{ij},\) \(i, j = a, b\). Then, by defining

\[
Q_a = \frac{q_a}{\sqrt{\Lambda_a}}, \quad Q_b = \frac{q_b}{\sqrt{\Lambda_b}},
\]

\[
P_a = \frac{p_a}{\sqrt{\Lambda_a}}, \quad P_b = \frac{p_b}{\sqrt{\Lambda_b}},
\]

(15)



where \([Q_a, P_b] = i\delta_{ab}, i, j = a, b\) and by dropping constant terms, equation (13) can be written in a matrix form as [28]

\[
\hat{H}_{2BJJ} \simeq \frac{1}{2} \{\tilde{Q}^T \tilde{\omega}^2 \tilde{Q} + \tilde{P}^T \tilde{P}\},
\]

where

\[
\tilde{\omega}^2 = \left(\frac{\omega_a^2}{\omega_{ab}^2} \omega_{bb}^2 \right)
\]

and \(\tilde{Q}^T = (Q_a, Q_b), \tilde{P}^T = (P_a, P_b)\) (the symbol \(\tilde{\cdot}\) stands for the transpose); \(\omega_a^2 = \Lambda_a J_a^2 K_a^2\), and \(\omega_{ab} = \sqrt{\Lambda_a J_a^2 K_a K_b}\).

A straightforward diagonalization gives the Hamiltonian

\[
H_{2BJJ} \simeq \frac{1}{2} \{\omega_a^2 Q_a^2 + \omega_b^2 Q_b^2 + \omega_{ab}^2 P_a^2 + P_b^2\},
\]

(18)

where, defining \(\Delta_{ab} = \sqrt{\left(\omega_a^2 - \omega_b^2\right)^2 + 4\omega_{ab}^2}\),

\[
\omega_a^2 = \frac{\omega_a^2 + \omega_b^2 - \Delta_{ab}}{2}, \quad \omega_b^2 = \frac{\omega_a^2 + \omega_b^2 + \Delta_{ab}}{2},
\]

(19)

\[
Q_1 = \frac{2\omega_{ab} Q_b - \left[\left(\omega_a^2 - \omega_b^2\right) + \Delta_{ab}\right] Q_a}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_a^2 - \omega_b^2\right) + \Delta_{ab}\right]^2}},
\]

\[
Q_2 = \frac{2\omega_{ab} Q_b - \left[\left(\omega_a^2 - \omega_b^2\right) - \Delta_{ab}\right] Q_a}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_a^2 - \omega_b^2\right) - \Delta_{ab}\right]^2}},
\]

(20)

\[
P_1 = \frac{2\omega_{ab} P_b - \left[\left(\omega_a^2 - \omega_b^2\right) + \Delta_{ab}\right] P_a}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_a^2 - \omega_b^2\right) + \Delta_{ab}\right]^2}},
\]

\[
P_2 = \frac{2\omega_{ab} P_b - \left[\left(\omega_a^2 - \omega_b^2\right) - \Delta_{ab}\right] P_a}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_a^2 - \omega_b^2\right) - \Delta_{ab}\right]^2}}.
\]

(21)

The operators \(Q_1, P_1\) and \(Q_2, P_2\) can be viewed as position and momentum operators of two distinct fictitious particles, associated with modes 1 and 2, i.e. the Hamiltonian (18) is that of two harmonic oscillators.

The eigenvalues \(\omega_{1,2}\) up to order \(K^2\) obtained within the Holstein–Primakoff approach coincide with the zero-mode frequencies of small amplitude oscillations obtained by the semiclassical approach based on the Gross–Pitaevskii equations for the two condensate wavefunctions in [18] (see equation (26) and in [20] (see the equation at the beginning of section IV) for the case of equally populated species. When \(\omega_1^2\) vanishes, a phase separation takes place, resulting in a MQST state.

Indeed, from equations (19), the stability condition is

\[
|\Lambda_{ab}| < \sqrt{\left(\Lambda_a + \frac{K_a}{J_a}\right) \left(\Lambda_b + \frac{K_b}{J_b}\right)} = \Lambda_{ab}^0,
\]

(22)

where \(\Lambda_{ab}^0\) is the critical value of the interspecies interaction which sets the onset of the phase separation regime. Such a condition agrees with the one given in [20] (see equation (10) in section IV) and reduces to

\[
|\Lambda_{ab}| < \sqrt{\Lambda_a \Lambda_b},
\]

(23)

when the limit \(J^a, J^b \to \infty\) is taken.

In the symmetric case \(\Lambda_a = \Lambda_b = \Lambda, K_a = K_b = K, N_a = N_b = \frac{\Lambda}{2}\) we get \(\omega_a^2 = \omega_b^2 = \omega^2\) where \(\omega^2 = \frac{\Lambda}{2}K + K^3\), and \(\omega_{ab} = \frac{\Lambda}{4}K^2\). As a consequence, \(\Lambda_{ab} = 2\omega_{ab}\) and the eigenvalues (19) simplify as

\[
\omega_a^2 = \omega^2 - \omega_{ab}, \quad \omega_b^2 = \omega^2 + \omega_{ab},
\]

(24)

which results in the stability condition

\[
|\Lambda_{ab}| < \Lambda + 2K^3 = \Lambda^0_{ab}.
\]

(25)

In the following sections, we will derive the analytical expressions for the stationary states and discuss the corresponding quantum dynamics of the system.

3. Stationary states

Since the Hamiltonian (18) is that of two independent particles \(H = H_1 + H_2\), the corresponding Hilbert space is simply given by the tensor product \(E_1 \otimes E_2 \equiv E_1 \otimes E_2\) and we can find a basis of eigenvectors for \(H_{2BJJ}\) in the following form: \(|\psi_i\rangle = |\psi_i^1\rangle|\psi_i^2\rangle\), where \(|\psi_i^1\rangle\) and \(|\psi_i^2\rangle\) are eigenvectors of \(H_1\) and \(H_2\) within \(E_1\) and \(E_2\). Since \(H_1\) and \(H_2\) are simply harmonic oscillator Hamiltonians, we could define two pairs of creation and annihilation operators, one for each mode, as follows:

\[
a_i^+ = \frac{1}{\sqrt{2}} \left[\sqrt{\frac{\omega_i}{\hbar}} Q_i - i\frac{P_i}{\sqrt{\omega_i}}\right],
\]

(26)

\[
a_i = \frac{1}{\sqrt{2}} \left[\sqrt{\frac{\omega_i}{\hbar}} Q_i + i\frac{P_i}{\sqrt{\omega_i}}\right],
\]

(27)

with \(i = 1, 2\). Now, if we define the ground states of \(H_1\) and \(H_2\) as \(|\psi_0^1\rangle\) and \(|\psi_0^2\rangle\), we easily obtain eigenvalues and eigenvectors within these two subspaces as

\[
E_n^1 = \left(n + \frac{1}{2}\right)\hbar \omega_1, \quad |\psi_n^1\rangle = \frac{1}{\sqrt{n!}}(a_1^+)^n |\psi_0^1\rangle,
\]

(28)

\[
E_n^2 = \left(p + \frac{1}{2}\right)\hbar \omega_2, \quad |\psi_n^2\rangle = \frac{1}{\sqrt{p!}}(a_2^+)^p |\psi_0^2\rangle.
\]

(29)

So the stationary states of the full Hamiltonian (18) are

\[
|\psi_{n,p}\rangle = |\psi_n^1\rangle|\psi_p^2\rangle = \frac{1}{\sqrt{n!p!}}(a_1^+)^n(a_2^+)^p |\varphi_{0,0}\rangle.
\]

(30)

and the corresponding energies are

\[
E_{n,p} = E_n^1 + E_p^2 = \left(n + \frac{1}{2}\right)\hbar \omega_1 + \left(p + \frac{1}{2}\right)\hbar \omega_2.
\]

(31)

We note that since the Hamiltonian (13) preserved the original parity symmetry of the original Hamiltonian (12), its eigenstates could also be classified according to their parity under \(a \to -a\) and \(b \to -b\). Since \(a_1\) and \(a_2\) are linear combinations of \(a, b\), the eigenstates can also be classified by their parity under \(a_{1,2} \to -a_{1,2}\). Using (30), it is then clear that the even eigenstates are those with \(n+p\) even and the odd eigenstates are those with \(n+p\) odd. So we can define the parity of a state as \((-1)^{n+p}\).
We stress that this spectrum is not unbounded because an infinite number of unphysical high energy states have been added. Thus, a constraint has to be included in order to satisfy the conditions \( |b^a| \ll 2J^a \), \( |b^b| \ll 2J^b \). Solving these constraints will give limits to the value of \( n \) and \( p \) and we will recover a finite-dimensional Hilbert space. Let us note that, through the repeated action of the operators \( a_1^\dagger \) and \( a_1^\dagger \), we can obtain stationary states of the system with a given number of quanta in each mode. The action of \( a_1^\dagger \), \( a_1 \), \( a_2^\dagger \), \( a_2 \) on the stationary states \( |\psi_{n,p}\rangle \) is as follows:

\[
\begin{align*}
    a_1^\dagger |\psi_{n,p}\rangle &= \sqrt{n+1} |\psi_{n+1,p}\rangle, \\
    a_1 |\psi_{n,p}\rangle &= \sqrt{n} |\psi_{n-1,p}\rangle \\
    a_2^\dagger |\psi_{n,p}\rangle &= \sqrt{p+1} |\psi_{n,p+1}\rangle, \\
    a_2 |\psi_{n,p}\rangle &= \sqrt{p} |\psi_{n,p-1}\rangle.
\end{align*}
\]

(32)

(33)

Generically, \( \omega_1 \) and \( \omega_2 \) are incommensurate with each other and there are no degenerate levels since two different pairs of integers \( \{n, p\} \) and \( \{n', p'\} \) do not exist such that \( n\omega_1 + p\omega_2 = n'\omega_1 + p'\omega_2 \). Such degeneracy may exist in the non-generic case where the ratio \( \omega_2/\omega_1 \) is a rational number. In the presence of degeneracy, the nonlinear terms that we have neglected can lift the degeneracy, unless the states have different parity.

4. Quantum dynamics

We are interested in the time evolution of the mean values of the observables \( J_x^a, J_x^b \), that is, the population imbalance between the left and right well of the potential of each bosonic species. In order to carry out such a program and to impose the correct initial conditions, it is much more convenient to start from the Heisenberg equations of motion for the observables \( Q_1, Q_2, P_1, P_2 \):

\[
\frac{d}{dt} \langle Q_i \rangle = \frac{1}{\hbar} \langle [Q_i, H_{2BJ}] \rangle = \langle P_i \rangle,
\]

(34)

\[
\frac{d}{dt} \langle P_i \rangle = -\frac{1}{\hbar} \langle [P_i, H_{2BJ}] \rangle = -\omega_i^2 \langle Q_i \rangle,
\]

(35)

which give rise to the following time evolution:

\[
\langle Q_i \rangle(t) = \langle Q_i \rangle(0) \cos \omega_i t + \frac{\langle P_i \rangle(0)}{\omega_i} \sin \omega_i t,
\]

(36)

\[
\langle P_i \rangle(t) = \langle P_i \rangle(0) \cos \omega_i t - \omega_i \langle Q_i \rangle(0) \sin \omega_i t.
\]

(37)

All we need now is to express \( J_x^a, J_x^b \) in terms of \( Q_1, Q_2, P_1, P_2 \) by means of equations (14), (15), (20), (21); in this way, the initial conditions \( \langle J_x^a \rangle(0), \langle J_x^b \rangle(0), \langle J_x^a \rangle(0), \langle J_x^b \rangle(0) \) are well known.

Starting from equations (20)–(21) we find

\[
Q_1 = \frac{a^\dagger}{\sqrt{K_b \sqrt{J^b}}} J_x^b - \frac{b^\dagger}{\sqrt{K_a \sqrt{J^a}}} J_x^a,
\]

(38)

\[
Q_2 = \frac{a^\dagger}{\sqrt{K_b \sqrt{J^b}}} J_x^b - \frac{b^\dagger}{\sqrt{K_a \sqrt{J^a}}} J_x^a,
\]

(39)

whose inverse transformation gives \( J_x^a \) and \( J_x^b \) in terms of \( Q_1, Q_2 \) and permits us to readily obtain the time evolution of their averages:

\[
\langle J_x^a \rangle(t) = \frac{a^\dagger \langle Q_2 \rangle(t) - a^\dagger \langle Q_1 \rangle(t)}{\sqrt{K_a \sqrt{J^a}}} - \frac{a^\dagger \langle Q_2 \rangle(t) - a^\dagger \langle Q_1 \rangle(t)}{\sqrt{K_b \sqrt{J^b}}}.
\]

(40)

\[
\langle J_x^b \rangle(t) = \frac{b^\dagger \sqrt{K_a \sqrt{J^a}} \langle Q_2 \rangle(t) - b^\dagger \langle Q_1 \rangle(t)}{\sqrt{K_b \sqrt{J^b}}}.
\]

(41)

The coefficients \( a^\dagger, b^\dagger, a^\dagger, b^\dagger \) are defined in the appendix. The initial conditions relevant to our study are the ones with a small imbalance between the two wells for each species and the coherent initial states. For the first case, we choose \( \langle J_x^a \rangle(0) = \pm 1, \langle J_x^b \rangle(0) = \pm 1, \langle J_x^a \rangle(0) = 0, \langle J_x^b \rangle(0) = 0 \), while the particle number is equal to \( j_a = j_b = 1000 \). Concerning the chosen values of the interaction strengths \( \Lambda_a, \Lambda_b \) and \( \Lambda_{ab} \), in the following we refer to the mixture of \(^{85}\)Rb and \(^{87}\)Rb atoms realized by the JILA group [16].

Figures 1 and 2 show the dynamics of \( J_x^a, J_x^b \) in the case in which there is a small imbalance between the two wells, specifically, we consider the case in which there is one unit difference in the left and in the right well, in the absence of imbalance between the two species (the corresponding parameters are reported in the figure captions). Here we note a coherent tunnelling between the two wells.

Figures 3 and 4 show instead the behaviour of \( J_x^a, J_x^b \) in the case of imbalance between the two species, with an imbalance between the two wells of one and two units and for
two different values of $\Lambda_{ab}$ (0.8 and 1). As one can note, at increasing $\Lambda_{ab}$ one approaches a phase separation instability in which the two species tend to separate in the different wells. This behaviour can be understood in terms of the behaviour of the eigenfrequencies $\omega_{1,2}$ versus $\Lambda_{ab}$. In figures 5 and 6 one of the two frequencies becomes imaginary for a critical value of $\Lambda_{ab}$, thus signalling an instability. Let us note that the instability point is a function of $\Lambda_a$, $\Lambda_b$ and usually takes place for a critical positive value of the interspecies interaction, as discussed in section 2, equations (22) and (25). In the case in which this interaction is attractive the system is always in a coherent tunnelling regime.

A few comments on the dynamics of the system are in order here. Compared to our previous analysis [25], the present analysis does not allow for the study of long-time scale phenomena since their detection is abruptly increased with $N$; thus, only short-time scale effects are reliable. Furthermore

we point out that the dynamics should become aperiodic in the general case.

When the initial state is a coherent spin state for each species, $|\psi(0)\rangle = |\psi(0)\rangle_a |\psi(0)\rangle_b$, where $|\psi(0)\rangle_i = C_i \sum_{m_i=-N_i/2}^{N_i/2} \frac{N_i!}{m_i! (N_i/2-m_i)!} \frac{e^{-im_i2\pi}}{2} e^{-i\phi_i} |m_i\rangle_i$, $C_i = \sin^{N_i/2}(\frac{\pi}{2}) \cos^{N_i/2}(\frac{\pi}{2}) e^{-i\frac{2\pi}{4}}$, $i = a, b$, the initial conditions are

$$\langle J^x_i(0) \rangle = -\frac{N_i}{2} \cos \theta_a, \langle J^y_i(0) \rangle = -\frac{N_i}{2} \cos \theta_b, \langle J^z_i(0) \rangle = \frac{N_i}{2} \sin \theta_a \sin \phi_a, \langle J^y_i(0) \rangle = \frac{N_i}{2} \sin \theta_b \sin \phi_b.$$

In this case the same type of behaviour, as for the small imbalance, is observed. In figure 7 we take the values $\theta_a = \theta_b = \pi/2$ and $\phi_a = \phi_b = \pi/4$.

The quantum dynamics investigated above could be experimentally reproduced. If we refer for instance to the mixture of $^{85}\text{Rb}$ and $^{87}\text{Rb}$ atoms realized by the JILA group [16], a wide tuning of s-wave interactions is possible via Feshbach resonances. In particular it is possible to fix the scattering length of $^{87}\text{Rb}$ and to tune the scattering length as well as the interspecies one. That allows one to explore the parameter space in a wide range and to realize the symmetric regime $\Lambda_a = \Lambda_b = \Lambda$ as well as the asymmetric one. Furthermore, one can tune the inter-well coupling, i.e. the parameters $K_a, K_b$, in such a way as to get the semiclassical limit. Another possible realization of the phenomena described above could be obtained with the mixture of $^{41}\text{K}$ and $^{85}\text{Rb}$ atoms produced by the LENS group [15], which offers a wide possibility of driving from the weak to the strong interacting regime because of the presence of several magnetic Feshbach resonances [33].
5. Semiclassical dynamics

In this section, we briefly introduce the semiclassical limit of our model within the linear approximation in order to make a comparison with the quantum results obtained above. A detailed semiclassical analysis has been already carried out in the recent literature (see [18–22]). Here we only recall the classical equations of motion to give a physical interpretation of $q_{a,b}$ and $p_{a,b}$ in equation (14). From the Hamiltonian (9), we can derive the following equations of motion for the components of the vectors $\vec{J}^{a,b}$:

$$\frac{dJ^a_z}{dt} = -\Lambda_a J^a_y J^a_z - \Lambda_{ab} J^a_y J^b_z,$$

$$\frac{dJ^b_z}{dt} = -\Lambda_b J^b_y J^b_z - \Lambda_{ab} J^a_y J^b_z,$$

$$\frac{dJ^a_y}{dt} = \Lambda_a J^a_z J^a_y + \Lambda_{ab} J^b_z J^a_y + K_a J^a_y,$$

$$\frac{dJ^b_y}{dt} = \Lambda_a J^b_z J^a_y + \Lambda_{ab} J^a_z J^b_y + K_b J^b_y,$$

$$\frac{dJ^a_x}{dt} = -K_a J^a_y,$$

$$\frac{dJ^b_x}{dt} = -K_b J^b_y.$$  

These equations imply that $(\vec{J}^{a})^{2} = (J^{a}_x)^{2} + (J^{a}_y)^{2} + (J^{a}_z)^{2}$ and $(\vec{J}^{b})^{2} = (J^{b}_x)^{2} + (J^{b}_y)^{2} + (J^{b}_z)^{2}$ are constants, so we can introduce

$$J^{a}_x = ||J^{a}|| \sin \theta_a \cos \varphi_a,$$

$$J^{a}_y = ||J^{a}|| \sin \theta_a \sin \varphi_a,$$

$$J^{a}_z = ||J^{a}|| \cos \theta_a,$$

and

$$J^{b}_x = ||J^{b}|| \sin \theta_b \cos \varphi_b,$$

$$J^{b}_y = ||J^{b}|| \sin \theta_b \sin \varphi_b,$$

$$J^{b}_z = ||J^{b}|| \cos \theta_b.$$  

Using (48) and (49) in (42)–(47), we obtain the equations [20]

$$\frac{d\theta_a}{dt} = K_a \sin \varphi_a,$$

$$\frac{d\theta_b}{dt} = K_b \sin \varphi_b,$$

$$\frac{d\varphi_a}{dt} = (\Lambda_a J^a \cos \theta_a + \Lambda_{ab} J^b \cos \theta_b) + K_a \cot \theta_a \cos \varphi_a,$$

$$\frac{d\varphi_b}{dt} = (\Lambda_b J^b \cos \theta_b + \Lambda_{ab} J^a \cos \theta_a) + K_b \cot \theta_b \cos \varphi_b.$$  

These equations coincide with equations (5)–(8) in [20], equations (5) in [22] and equations (3) in [21]. The energy conservation introduces one extra constraint, so that the phase space is actually three dimensional. This may permit in certain conditions the observation of classical chaos. If we linearize equations (50)–(53) around the point $\theta_a = \theta_b = \pi/2, \varphi_a = \varphi_b = 0$, we find the equations of motion

$$\frac{d\delta\theta_a}{dt} = K_a \delta\varphi_a,$$

$$\frac{d\delta\theta_b}{dt} = K_b \delta\varphi_b,$$

$$\frac{d\delta\varphi_a}{dt} = -(\Lambda_a J^a \delta\theta_a + \Lambda_{ab} J^b \delta\theta_b) - K_a \delta\varphi_a,$$

$$\frac{d\delta\varphi_b}{dt} = -(\Lambda_b J^b \delta\theta_b + \Lambda_{ab} J^a \delta\theta_a) - K_b \delta\varphi_b,$$

where $\theta_a = \pi/2 + \delta\theta_a$ and $\theta_b = \pi/2 + \delta\theta_b$. These equations are derived from the Hamiltonian

$$H_{\text{eff}} = K_a J^a \varphi_b^2 + K_b J^b \varphi_a^2 + \frac{1}{2}((\Lambda_a J^a)^2 + K_a J^a)(\delta\theta_a)^2 + (\Lambda_b J^b)^2 + K_b J^b)(\delta\theta_b)^2 + 2\Lambda_{ab} J^a J^b \delta\theta_a \delta\theta_b,$$

with the Poisson brackets $\{\varphi_a, J^a \delta\theta_a\} = 1$ and $\{\varphi_b, J^b \delta\theta_b\} = 1$. By rescaling the variable $\varphi$ and $\delta\theta$ ($i = a, b$) as $\varphi_i \rightarrow \frac{1}{\sqrt{\Lambda_i}} \varphi_i$ and $\delta\theta_i \rightarrow \sqrt{\frac{\Lambda_i}{2}} \delta\theta_i$, we obtain the corresponding classical Hamiltonian of (16) with Poisson brackets $\{\varphi_i, J^i \delta\theta_i\} = 1$. This Hamiltonian can be diagonalized in a standard way by introducing a linear combination of the variables $\tilde{\varphi}_i$ and $\tilde{\delta}\theta_i$ that preserves the Poisson brackets. The diagonalized Hamiltonian will be that of two independent classical harmonic oscillators of variables $\varphi_1, \varphi_2$ and $\delta\theta_1, \delta\theta_2$. Applying then the Bohr–Sommerfeld quantization, we reobtain spectrum (31), giving the desired connection between the semiclassical and the quantum approach. This also leads to a physical interpretation of the conjugate variables $q_{a,b}$ and $p_{a,b}$ in equation (14) as the azimuthal angles of the pseudospins $\vec{J}^{a,b}$. The full classical solution of equations (50)–(53) can be found in [18–22].

6. Conclusions and perspectives

In this paper we investigated the quantum dynamics of a Bose–Josephson junction made of a binary mixture of BECs loaded in a double-well potential within the two-mode approximation. Focussing on the regime where the number of atoms is very large, a mapping onto an SU(2) spin problem together with a Holstein–Primakoff transformation has been performed to calculate the time evolution of the imbalance between the two wells. This approach allows one to exactly solve the system under the assumption of weak interatomic interactions. The results show an instability towards a phase separation above a critical positive value of the interspecies interaction while the system evolves towards a coherent tunnelling regime for negative interspecies interactions. The detection of a phase separation could be experimentally achieved in current experiments with a mixture of $85\text{Rb}$ and $87\text{Rb}$ atoms [16].

We point out that all of the above results are obtained within the linear approximation. It would be interesting to extend our model beyond the linear regime; in such a case, the classical dynamics may exhibit a chaotic behaviour in some parameter range because the phase space is three dimensional.
At the quantum level, these features will show up in the spectrum as well as the eigenstates of the Hamiltonian. Indeed the Hamiltonian is not time reversal invariant because of the terms linear in $J_x/J_z$, and we expect that the distribution of spacings between energy levels should follow the GUE (Gaussian unitary ensemble) statistics [34]. Regarding the dynamics, we conjecture that the short time scale behaviour of the quantum system will look chaotic, but the long time behaviour will not. Such an analysis will be carried out in detail in a forthcoming publication.

7. Appendix. Coefficients

The coefficients $a'$, $b'$, $a''$, $b''$ are defined as follows:

$$a' = \frac{2\omega_{ab}}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_b - \omega_a\right)^2 + \left(\omega_a - \omega_b\right)^2 \right]}}$$  \hspace{1cm} (A.1)

$$b' = \frac{\omega_{ab}^2}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_b - \omega_a\right)^2 + \left(\omega_a - \omega_b\right)^2 \right]}}$$  \hspace{1cm} (A.2)

$$a'' = \frac{2\omega_{ab}}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_b - \omega_a\right)^2 - \left(\omega_a - \omega_b\right)^2 \right]}}$$  \hspace{1cm} (A.3)

$$b'' = \frac{\omega_{ab}^2}{\sqrt{4\omega_{ab}^2 + \left[\left(\omega_b - \omega_a\right)^2 - \left(\omega_a - \omega_b\right)^2 \right]}}$$  \hspace{1cm} (A.4)

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