Quantum Bose–Josephson junction with binary mixtures of BECs

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Abstract
We study the quantum behaviour of a binary mixture of Bose–Einstein condensates in a double-well potential starting from a two-mode Bose–Hubbard Hamiltonian. We focus on the small tunnelling amplitude regime and apply perturbation theory up to second order. Analytical expressions for the energy eigenvalues and eigenstates are obtained. Then, the quantum evolution of the number difference of bosons between the two potential wells is fully investigated for two different initial conditions: completely localized states and coherent spin states. In the first case both the short- and the long-time dynamics is studied and a rich behaviour is found, ranging from small amplitude oscillations and collapses and revivals to coherent tunnelling. In the second case, the short-timescale evolution of number difference is determined and a more irregular dynamics is evidenced. Finally, the formation of Schrödinger cat states is considered and shown to affect the momentum distribution.

1. Introduction
The experimental discovery of Bose–Einstein condensation [1] in dilute systems of trapped alkalimetal atoms, such as rubidium (Rb), lithium (Li), sodium (Na) and ytterbium (Yb), has spurred a renewed interest into the investigation of macroscopic quantum phenomena and interference effects, allowing for a deeper understanding of the conceptual foundations of quantum mechanics [2]. This fascinating research area has been growing, thanks to the high degree of experimental manipulation and control [3]. Interference between condensates released in a potential with a barrier was first observed in 1997 [4] and that paved the way for further investigations on the problem of Bose condensates in a double-well potential. Then Josephson oscillations were observed in one-dimensional optical potential arrays [5]. A single bosonic Josephson junction was produced for the first time in 2005 with Rb atoms and its dynamics was experimentally investigated both within the tunnelling and self-trapping regime [6–8]. More recently, mixtures of $^{85}$Rb and $^{87}$Rb atoms have been produced and experimentally investigated [9] as well, whose intraspecies scattering lengths could be tunable via magnetic and optical Feshbach resonances. Furthermore the realization of heteronuclear mixtures of $^{87}$Rb and $^{41}$K atoms with tunable interspecies interactions [10] paved the way to the exploration of double-species Mott insulators and, in general, of the quantum phase diagram of the two-species Bose–Hubbard model [11]. The interplay between the interspecies and intraspecies scattering has deep consequences for the properties of the condensates, such as the density profile [12] and the collective excitations [13]. However, the wide tunability of such interactions makes a BEC mixture a very interesting subject of investigation, both from the experimental and theoretical side, as a means of studying new macroscopic quantum tunnelling phenomena as well as the interplay between quantum coherence and nonlinearity. Indeed, novel and richer behaviours are expected in such a multicomponent BEC.

On the theoretical side, a bosonic Josephson junction with a single species of BEC has been widely investigated by means of a two-mode approximation [14–16], within the classical as well as the quantum regime. In the classical regime, characterized by large particle numbers and weak repulsive interactions, the Gross–Pitaevskii equation provides a reliable description. Within the two-mode approximation it reduces to two generalized Josephson equations which describe the time evolution of the relative phase and the population imbalance between the wells [15] and differ from...
their superconducting counterpart [17] by the presence of a nonlinear term which couples the variables. Because of such a term, a bosonic Josephson junction exhibits a variety of novel phenomena which range from $\pi$-oscillations to macroscopic quantum self-trapping (MQST) [15]. While the $\pi$-oscillations, as well the usual Josephson ones, deal with a symmetric oscillation of the condensate about the two wells, the MQST phenomenon is characterized by a broken symmetry phase with a population imbalance between the wells. In the quantum regime, characterized by smaller values of the particle number and strong interactions, an increase in phase fluctuations is observed together with the suppression of number fluctuations. Furthermore the time evolution is characterized by phase collapse and revival [18]. The quantum behaviour of bosonic Josephson junctions has been deeply investigated by means of the usual quantum phase model [19–21] as well as by starting from a two-mode Bose–Hubbard Hamiltonian [22–24]. In this context the phase coherence of the junction has been characterized by studying the momentum distribution [20, 25]. The generation and detection of Schrödinger cat states have been investigated as well; indeed the presence of such kind of states reflects in the strong reduction of the momentum–distribution contrast [24, 26].

More recently such a theoretical analysis has been successfully extended to a binary mixture of BECs in a double-well potential [27–30]. The semiclassical regime in which the fluctuations around the mean values is 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. In particular, two different MQST states with broken symmetry have been found [29], 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 variation of some parameters or initial conditions, the phase-separated MQST states evolve towards a symmetry-restoring phase where the number difference of bosons between the two wells is suppressed, and their influence on the contrast in the momentum distribution is studied. Finally, in section 6, some conclusions and outlooks of this work are presented.

2. The model

A binary mixture of Bose–Einstein condensates [28, 29] loaded in a double-well potential is described by the general many-body Hamiltonian

\[
H = H_a + H_b + H_{ab},
\]

where

\[
H_a = \int d\mathbf{r} \left( -\frac{\hbar^2}{2m_a} \nabla^2 \psi_a + \psi_a^* V_a(\mathbf{r}) \psi_a \right) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \psi_a^* (\mathbf{r}) \psi_a^* (\mathbf{r}') U_{aa}(\mathbf{r} - \mathbf{r}') \psi_a (\mathbf{r}) \psi_a (\mathbf{r}')
\]

\[
H_b = \int d\mathbf{r} \left( -\frac{\hbar^2}{2m_b} \nabla^2 \psi_b + \psi_b^* V_b(\mathbf{r}) \psi_b \right) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \psi_b^* (\mathbf{r}) \psi_b^* (\mathbf{r}') U_{bb}(\mathbf{r} - \mathbf{r}') \psi_b (\mathbf{r}) \psi_b (\mathbf{r}')
\]

\[
H_{ab} = \int d\mathbf{r} d\mathbf{r}' \psi_a^* (\mathbf{r}) \psi_b^* (\mathbf{r}') U_{ab}(\mathbf{r} - \mathbf{r}') \psi_a (\mathbf{r}) \psi_b (\mathbf{r}')
\]

are the Hamiltonians for bosons of species $a$ and $b$ respectively and

\[
H_{ab}
\]
The interaction term between bosons of different species. For dilute mixtures one can replace the interaction potentials \( U_{ab}, U_{bb} \) with the effective contact interactions:

\[
\begin{align*}
U_{aa}(\mathbf{r} - \mathbf{r}') = & \ g_{aa} \delta(\mathbf{r} - \mathbf{r}'), \\
U_{ab}(\mathbf{r} - \mathbf{r}') = & \ g_{ab} \delta(\mathbf{r} - \mathbf{r}'), \\
U_{bb}(\mathbf{r} - \mathbf{r}') = & \ g_{bb} \delta(\mathbf{r} - \mathbf{r}'),
\end{align*}
\]

where \( g_{aa} = \frac{4\pi\hbar^2}{m_a} \) and \( g_{bb} = \frac{4\pi\hbar^2}{m_b} \) are the intraspecies coupling constants of the species \( a \) and \( b \) respectively, and \( m_a, m_b \) being the atomic masses and \( a_{ab}, g_{ab} \) the s-wave scattering lengths; furthermore, \( g_{ab} = \frac{4\pi\hbar^2}{m_{am}} \) is the interspecies coupling constant, where \( m_{ab} = \frac{m_a m_b}{m_{am}} \) is the reduced mass and \( a_{ab} \) is the associated s-wave scattering length. In this way the Hamiltonian (1)–(4) can be rewritten as

\[
H_i = \int d^3r \left( -\frac{\hbar^2}{2m_i} \nabla^2 \psi_i + V_i(\mathbf{r}) \psi_i \right) + \frac{g_{ii}}{2} \int d^3r \nabla_i \psi_i \nabla_i \psi_i, \quad i = a, b
\]

\[
H_{ab} = g_{ab} \int d^3r \psi_a^\dagger \psi_b \psi_a \psi_b.
\]

Here \( V_i(\mathbf{r}) \) is the double-well trapping potential and, in the following, we assume \( V_a(\mathbf{r}) = V_b(\mathbf{r}) = V(\mathbf{r}) \); \( \psi^\dagger_i(\mathbf{r}), \psi_i(\mathbf{r}) \), \( i = a, b \), are the bosonic creation and annihilation operators for the two species, which satisfy the commutation rules

\[
[\psi_i(\mathbf{r}), \psi_j(\mathbf{r}')] = \delta_{ij} \delta(\mathbf{r} - \mathbf{r}'), \quad [\psi_i(\mathbf{r}), \psi_j^\dagger(\mathbf{r}')] = 0,
\]

\[
[\psi_i(\mathbf{r}), \psi_j^\dagger(\mathbf{r}') \] = \delta_{ij} \delta(\mathbf{r} - \mathbf{r}'), \quad i, j = a, b
\]

and the normalization conditions

\[
\int d^3r |\psi_i(\mathbf{r})|^2 = N_i, \quad i = a, b,
\]

where \( N_i, i = a, b \), being the number of atoms of species \( a \) and \( b \) respectively. The total number of atoms of the mixture is \( N = N_a + N_b \). In the following we refer to values of the coupling constants \( g_{aa}, g_{bb}, g_{ab} \) such that the condition of stability of the binary mixture, \( g_{aa} g_{bb} \geq g_{ab}^2 \), is met and the phase separation regime is avoided.

Now 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 and that allows us to reduce the dimension of the Hilbert space of the initial many-body problem. Indeed for low energy excitations and low temperatures it is possible to consider only these two states and neglect the contribution from the higher ones, the so-called two-mode approximation [14–16]. In this way, by taking into account for each of the two species \( a \) and \( b \) the mean-field ground states \( \phi_{ga}^a, \phi_{ga}^b \) and the mean-field excited states \( \phi_{ge}^a, \phi_{ge}^b \), the wavefunctions \( \psi_i, i = a, b \), can be rewritten as

\[
\psi_a = a_g \phi_{ga}^a + a_e \phi_{ge}^a,
\]

\[
\psi_b = b_g \phi_{ga}^b + b_e \phi_{ge}^b,
\]

where \( \int d^3r |\phi_{g/e}^i|^2 = 1, i = a, b, a_{e}^a, b_{e}^b, a_{e}^b, b_{e}^a \) (\( a_g, b_g \) and \( a_e, b_e \)) are the creation (annihilation) operators for a particle of the species \( a, b \) in the ground and the excited state respectively. They satisfy the usual bosonic commutation relations \([a_i, a_{j}^\dagger] = [b_i, b_{j}^\dagger] = \delta_{ij} \). Furthermore, \( \phi_{g/e}^i(\mathbf{r}) = (\phi_i^a)^\dagger \phi_i^a = 0 \), which simplifies the calculations. Let us change the basis and switch to the atom number states in such a way that the expectation value of the population of the left and right well can be defined. The new annihilation operators are \( a_L = \frac{1}{\sqrt{2}}(a_g + a_e), a_R = \frac{1}{\sqrt{2}}(a_g - a_e) \) and \( b_L = \frac{1}{\sqrt{2}}(b_g + b_e), b_R = \frac{1}{\sqrt{2}}(b_g - b_e) \) for the species \( a \) and \( b \) respectively, so that the wavefunctions (11) become

\[
\psi_a = \frac{1}{\sqrt{2}} a_L (\phi_g^a + \phi_e^a) + \frac{1}{\sqrt{2}} b_R (\phi_g^a - \phi_e^a),
\]

\[
\psi_b = \frac{1}{\sqrt{2}} b_L (\phi_g^b + \phi_e^b) + \frac{1}{\sqrt{2}} b_R (\phi_g^b - \phi_e^b).
\]

By substituting equations (12) into the Hamiltonian (6)–(7), after some algebra we obtain its second quantized version within the two-mode approximation:

\[
H = \frac{E^a}{8} (a_L^\dagger a_R - a_L^\dagger a_L)^2 - \frac{E^b}{2N_b} (a_L^\dagger a_L + a_L^\dagger a_R)
\]

\[
+ \frac{\delta E^a (a_L^\dagger a_L + a_L^\dagger a_R)^2}{4N_b} + \frac{E^b}{8} (b_R^\dagger b_R + b_L^\dagger b_L)^2
\]

\[
- \frac{E^b}{2N_b} (b_R^\dagger b_R + b_L^\dagger b_L) + \frac{\delta E^b (b_L^\dagger b_L + b_R^\dagger b_R)^2}{4N_b}
\]

\[
\times (\kappa_{g,e}^a + \kappa_{e,g}^a + \kappa_{g,e}^b + \kappa_{e,g}^b) + \frac{1}{2} N_a (E_g^a + E_e^a)
\]

\[
+ \frac{1}{4} N_a (N_a - 2) (\kappa_{g,e}^a + \kappa_{g,e}^a + \kappa_{g,e}^b + \kappa_{g,e}^b) + \frac{1}{4} N_b (N_b - 2) (\kappa_{g,e}^b + \kappa_{g,e}^b) + \frac{1}{4} N_a N_b (\kappa_{g,e}^a + \kappa_{g,e}^a + \kappa_{g,e}^b + \kappa_{g,e}^b),
\]

where \( N_i = N_{L} + N_{R}, i = a, b \), is the number of atoms of species \( a \) and \( b \) respectively, expressed as a sum of numbers of atoms in the left and right well. The parameters are defined as follows:

\[
E_{g}^i = \int d^3r \left( -\frac{\hbar^2}{2m_i} \phi_i^a \nabla^2 \phi_i^a + \phi_i^a \nabla^2 \phi_i^a \right), \quad i = a, b
\]

\[
E_{e}^i = \int d^3r \left( -\frac{\hbar^2}{2m_i} \phi_i^a \nabla^2 \phi_i^e + \phi_i^a \nabla^2 \phi_i^e \right), \quad i = a, b
\]

\[
\kappa_{i,j}^a = \frac{g_{aa}}{2} \int d^3r |\phi_i^a|^2 |\phi_j^a|^2, \quad i, j = g, e
\]

\[
\kappa_{i,j}^b = \frac{g_{bb}}{2} \int d^3r |\phi_i^b|^2 |\phi_j^b|^2, \quad i, j = g, e
\]
In equation (13), the terms proportional to \( E_{ij} \), \( i = a, b \), describe tunnelling of particles of species \( a \) and \( b \) from one to the other well while the terms proportional to \( E_{11} \), \( i = a, b \), deal with the local interaction within the two wells and the terms proportional to \( \delta E \) correspond to additional two-particle processes. Finally the terms proportional to \( \Delta_{ab} \) and \( \kappa_{ab} \) couple the two species and then various constant terms follow, which will drop for simplicity.

In this paper, we focus on the small tunnelling amplitude regime where number fluctuations are suppressed and a Mott-insulator behaviour is established, so it is convenient to introduce the angular momentum representation for the species \( a \) and \( b \) as follows:

\[
J^a_i = \frac{1}{2} (a_i^a a_i^L + a_i^L a_i^a), \quad J^b_i = \frac{1}{2} (a_i^b a_i^L - a_i^L a_i^b), \quad J^a_z = \frac{1}{2} (a_i^a a_i^L - a_i^L a_i^a), \quad J^b_z = \frac{1}{2} (a_i^b a_i^L + a_i^L a_i^b), \quad J^b_i = \frac{1}{2} (b_i^b b_i^L + b_i^L b_i^b), \quad J^b_z = \frac{1}{2} (b_i^b b_i^L - b_i^L b_i^b),
\]

where the operators \( J^a_i \), \( J^b_i \), \( i = x, y, z \), obey to the usual angular momentum algebra and the following relations hold:

\[
(J^a_i)^2 = \frac{N_a}{2} \left( \frac{N_a}{2} + 1 \right), \quad (J^b_i)^2 = \frac{N_b}{2} \left( \frac{N_b}{2} + 1 \right).
\]

In particular, the components \( J^a_1 = \frac{1}{2} (N_a - N_{1L}) \), \( i = a, b \), give the difference of the number of bosons of the species \( a \), \( N_{1L} \), and \( N_{1R} \), occupying the two minima of the double-well potential, i.e. the population imbalances, which are experimentally observable quantities. Thus, Hamiltonian (13) can be cast in the following form:

\[
H = \frac{E_a^a}{2} \left( J^a_i \right)^2 - \frac{2 E_{1i}}{N_a} J^a_i + 4 \Delta^A \left( J^a_i \right)^2 + \frac{4 E_b^b}{2} \left( J^b_i \right)^2 - \frac{2 E_{1j}}{N_b} J^b_i + 4 \Delta^B \left( J^b_i \right)^2 + \Delta_{ab} J^a_i J^b_i - J^a_i J^b_i
\]

\[
\times \left( \kappa_{e,e}^{ab} + \kappa_{e,g}^{ab} - \kappa_{e,e}^{ab} - \kappa_{e,g}^{ab} \right),
\]

where the constant terms have been dropped. Let us now simplify the notation by introducing the following parameters:

\[
\Lambda_a = E_a^a, \quad \Lambda_a = 4 \Delta^A, \quad K_a = \frac{2 E_{1i}}{N_a},
\]

\[
\Lambda_b = E_b^b, \quad \Lambda_b = 4 \Delta^B, \quad K_b = \frac{2 E_{1j}}{N_b},
\]

\[
D_{ab} = \kappa_{e,e}^{ab} + \kappa_{e,g}^{ab} - \kappa_{e,e}^{ab} - \kappa_{e,g}^{ab},
\]

and rewrite the Hamiltonian (25) as

\[
H = \frac{1}{2} \Lambda_a \left( J^a_i \right)^2 - \Lambda_a J^a_i + C_a \left( J^a_i \right)^2 + \frac{1}{2} \Lambda_b \left( J^b_i \right)^2 - \Lambda_b J^b_i + C_b \left( J^b_i \right)^2 + \Delta_{ab} J^a_i J^b_i - D_{ab} J^a_i J^b_i.
\]

Within the experimental parameters range it is possible to show that \( C_i \ll \Lambda_i, K_i, i = a, b \), and \( D_{ab} \ll \Lambda_{ab} \) [7, 29]; 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 a simple two-mode approximation maps to two Ising-type spin models in a transverse magnetic field. It is possible, also in this case of binary mixtures of BECs, to take into account the overlap between wavefunctions localized in different wells and then retain the terms just neglected, as done in [16] for the single-species Bose–Josephson junction. In this way an improved two-mode model can be defined, which gives rise to a quantitative agreement with the results of a numerical integration of the coupled Gross–Pitaevskii equations describing the system [33]. We would point out that throughout the paper we adopt a simple two-mode approximation because we are interested in the qualitative features of the quantum dynamics of a binary mixture of BECs in a double well.

In the following we will focus on the symmetric case \( \Lambda_a = \Lambda_b = \Lambda \) and \( K_a = K_b = K \) because it allows us to perform analytical calculations while capturing many relevant phenomena characterizing the physics of the system. An investigation of the full parameter space will require numerical calculations and will be the subject of a future publication together with a detailed comparison between analytical and numerical results and a quantitative evaluation of the validity of the two-mode approximation [34]. So the model Hamiltonian (25) becomes

\[
H = H_0 + H_I,
\]

\[
H_0 = \frac{1}{2} \Lambda \left( J^a_i \right)^2 + \frac{1}{2} \Lambda \left( J^b_i \right)^2 + \Delta_{ab} J^a_i J^b_i,
\]

\[
H_I = -K \left( J^a_i + J^b_i \right),
\]

where, in the small tunnelling amplitude regime, \( H_I \) is considered as a perturbation. The total Hamiltonian commutes with \( (J^a_i)^2 \) and \( (J^b_i)^2 \), which leads to the conservation of total angular momentum with quantum numbers \( j_a = N_a/2 \) and \( j_b = N_b/2 \) respectively. So the whole Hilbert space has finite dimension, equal to \( (2j_a + 1) \otimes (2j_b + 1) = (N_a + 1) \otimes (N_b + 1) \); thus it depends on the number of bosons of the species \( a \) and \( b \) respectively. The whole basis \( \{|m_a, m_b|\} \) is given by the eigenvectors of \( J^a_1 \) \( (J^b_1|m_a = m_b| m_a) \) and \( J^a_1 \) \( (J^b_1|m_b = m_b| m_b) \) with \( m_a = -N_a/2, \ldots, N_a/2 \) and \( m_b = -N_b/2, \ldots, N_b/2 \).

As a first step we need to diagonalize the unperturbed Hamiltonian (29), which can be done by performing the following \( \theta = \frac{\pi}{4} \) rotation on the operators \( J^a_1, J^b_1 \):

\[
\tilde{J}^a_1 = a_1 J^a_1 - a_2 J^b_1, \quad a_1 = a_2 = \frac{1}{\sqrt{2}},
\]

\[
\tilde{J}^b_1 = a_1 J^a_1 + a_2 J^b_1.
\]
while an analogous rotation needs to be carried out on \( \hat{J}^x \), \( \hat{J}^y \) entering the perturbation \((30)\). As a result we get
\[
\hat{H} = \frac{1}{2}(\Lambda - \Lambda_{ab})(\hat{O})^2 + \frac{1}{2}(\Lambda + \Lambda_{ab})(\hat{J}^z)^2 - 2K\hat{J}^z.
\] (32)
which, by defining \( \Lambda_1 = \Lambda - \Lambda_{ab} \), \( \Lambda_2 = \Lambda + \Lambda_{ab} \) and
\[
\hat{O}^1 = \frac{\Lambda_1}{\sqrt{2}}, \quad \hat{O}^2 = \frac{\Lambda_2}{\sqrt{2}}, \quad \hat{J}^2 = \hat{J}^z, \quad \hat{J}^x = \frac{\hat{J}^x}{\sqrt{2}}
\] can be cast in the final form
\[
\hat{H} = \Lambda_1 (\hat{O}^1)^2 + \Lambda_2 (\hat{O}^2)^2 - 2K\hat{J}^z. \tag{33}
\]
In the following section we will find analytical expressions for the eigenvalues and the eigenvectors up to second order by performing perturbation theory in the tunnelling amplitude.

### 3. Stationary states

In the present section we apply second-order perturbation theory to the Hamiltonian of equation \((33)\) in the small tunnelling amplitude limit, which allows us to derive analytical expressions for the stationary states of the system.

In order to pursue this task let us rewrite equation \((33)\) in a dimensionless form by assuming \(\frac{\Delta}{\hbar} \) as the unit of energy:
\[
\hat{H} = 2(\hat{O}^1)^2 + 2\lambda (\hat{J}^z)^2 - 2k\hat{J}^z. \tag{34}
\]
where \(\lambda = \frac{\Delta}{\hbar} \) and \(k = \frac{2\hbar}{\Lambda} \). Then take
\[
\hat{H}_0 = 0 = 2(\hat{O}^1)^2 + 2\lambda (\hat{J}^z)^2 \tag{35}
\]
as unperturbed Hamiltonian and
\[
\hat{H}_I = -2k\hat{J}^z, \tag{36}
\]
as a small perturbation term. Here \(\hat{J}^i \), \(i = x, y, z\), obey the usual angular momentum algebra and the following relation holds:
\[
(\hat{J}^z)^2 = \frac{N_z}{2} \left( \frac{N_z}{2} + 1 \right), \tag{37}
\]
where
\[
N_z = \frac{N_a + N_b}{2}. \tag{38}
\]
In principle, the rotated basis \(\{|m_1, m_2\}\} = \{|m_1 = \frac{1}{2}(m_a - m_b)\}, \{|m_2 = \frac{1}{2}(m_a + m_b)\}\} of the unperturbed Hamiltonian \((35)\) is given by the eigenvectors of \(\hat{O}^1 = \frac{\Lambda_1}{\sqrt{2}}\). \(\hat{O}^1|m_1\rangle = m_1|m_1\rangle\) and \(\hat{O}^2\)
\[
(\hat{J}^z)|m_2\rangle = m_2|m_2\rangle\)
with \(m_1 = \frac{1}{2}(-m_a - m_b), \ldots, \frac{1}{2}(m_a + m_b)\) and \(m_2 = \frac{1}{2}(-m_a + m_b), \ldots, \frac{1}{2}(m_a + m_b)\), whose corresponding eigenvalues are \(E_{m_1,m_2} = (m_1)^2 + 2\lambda(m_2)^2\).

The presence of the operator \(\hat{O}^1\), which does not commute with the perturbation term \(\hat{H}_I\), makes the problem of finding eigenvalues and eigenvectors of the full Hamiltonian \((34)\) within perturbation theory much more involved. In order to simplify the treatment and carry out analytical calculations while retaining the relevant phenomenology, we concentrate on the particular case of a binary mixture where the two species are equally populated, i.e. \(N_a = N_b\), and have the same population imbalance between the two wells, i.e. \(m_a = m_b\).

This situation allows us to describe the quantum dynamics of the system in correspondence of the MQST regime, for which we need a completely localized initial state. That fixes \(m_1 = 0\) while \(m_2 = m_a = -\frac{N_a}{2}, \ldots, \frac{N_a}{2}\) could be an even or odd integer depending on \(N_a\) even or odd, and leads to the zero-order eigenvalues \(E_{0,m_2}^{(0)} = 2\lambda(m_2)^2 = \frac{\lambda}{2}(m_a + m_b)^2\). Each eigenvalue is two-fold degenerate, with the only exception of the ground state for \(N_a\) even, \(E_{0,0}^{(0)} = 0\), which is nondegenerate. The two-dimensional subspace of degeneracy is spanned by the states \(|0, \pm m_2\rangle\) (where \(\hat{J}^2|0, \pm m_2\rangle = \pm m_2|0, \pm m_2\rangle\)) and the corresponding zero-order eigenvectors are
\[
|\hat{P}_{0,m_2}^{(0)}\rangle = |0, m_2^\pm\rangle = \frac{1}{\sqrt{2}}(|0, m_2\rangle \pm |0, -m_2\rangle). \tag{39}
\]
By switching on the perturbation term \((36)\) it is possible to show that the degeneration is lifted starting from the levels with smaller \(m_2\): in general the double degeneracy of the zero-order eigenvalues \(E_{0,m_2}^{(0)}\) will be lifted at the \(2m_2\)-th order of perturbation theory \([22]\). By applying perturbation theory \([35]\) up to order \(k^2\), we obtain the following corrected eigenvalues:
\[
E_{0,m_2}^{(2)} = 2\lambda(m_2)^2 + \frac{k^2}{\lambda} \left( \frac{j_2(j_2 + 1) + (m_2)^2}{3} - 1 \right), \quad m_2 \neq 1, \frac{1}{2}, \tag{40}
\]
\[
E_{0,1/2}^{(2)} = 2\lambda + \frac{k^2}{\lambda} \left( \frac{j_2(j_2 + 1) + 1/4}{3} + \frac{j_2(j_2 + 1)}{2} \right). \tag{41}
\]
\[
E_{0,1/2}^{(2)} = 2\lambda + \frac{k^2}{\lambda} \left( \frac{j_2(j_2 + 1) + 1/4}{3} - \frac{k^2}{4\lambda} \left( j_2(j_2 + 1) - 3/4 \right) \right). \tag{42}
\]
where \(j_2 = \frac{N_a}{2}\). Furthermore, for \(N_a\) even, the nondegenerate ground state \(|0, 0\rangle\) belongs to the symmetry class of \(|0, m_2\rangle\). The corresponding eigenvectors, up to order \(k^2\), are given in the appendix.

As a final remark we would make some qualitative considerations on the precision of the second-order perturbative results we just obtained. In the previous section we pointed out that the tunnelling amplitude \(K\) (and, then, the renormalized tunnelling amplitude \(k\)) must be chosen sufficiently small in order to realize a weak link. Furthermore, we are considering a regime very close to the Mott-insulator one; so, the onsite energies being much larger than the tunnelling amplitudes, a perturbation theory in \(k\) gives reliable results. In general, the perturbative corrections to the eigenvalues in equations \((40)-(42)\) behave as powers of \(k j_2 \sim k N_2\) for large \(N_2\). As a consequence, the bigger the value of \(N_2\), the smaller the value of \(k\) at which the perturbative expansion is reliable, as shown in detail in \([22]\) for the single-species Bose–Hubbard dimer. For the ground state, and in general for the lower-energy states, the divergence of the perturbative results abruptly increases with \(N_2\). So, for BEC mixtures such as the one of the JILA setup with \(N_2 \sim 6.5 \times 10^4\) \([9]\) the perturbative results for the lower-energy eigenvalues should be valid for very small values of \(k\). Conversely, for the higher-energy
levels (i.e. \( m_2 = \frac{N_2}{2} \)) the second-order corrections to equation (40) go as \( k^2 \frac{N_2}{N_2-1} \) instead of \((k N_2)^2\) of the low-lying states and then decrease as \( N_2 \) increases. As a consequence, the higher-order corrections are much more strongly decreasing functions of \( N_2 \) and the perturbative results are accurate to larger values of \( k \).

In the following sections we use the analytical expressions of energy eigenvectors derived in the appendix, see equations (62)–(69), in order to study the quantum evolution of \( \langle \hat{J}_z^2(\tau) \rangle = \frac{1}{2} (J_a^2(\tau) + J_b^2(\tau)) \), that is, the number difference of bosons of species \( a \) and \( b \) between the two wells of the potential.

4. Dynamics: completely localized initial states

In this section we investigate the quantum evolution of the number difference of bosons of species \( a \) and \( b \) between the two wells assuming a completely localized state as the initial condition. That could be interesting in order to elucidate the quantum behaviour of the system in correspondence of the classical MQST regime and to put in evidence new phenomena including quantum coherence in a multicomponent system. In such a case we will study both the short- and the long-time dynamics: as a result a rich behaviour emerges, ranging from small amplitude oscillations and collapses and revivals to coherent tunnelling. Although such a physics is well known for the single-component Bose–Josephson junction, in our case, the dynamics shows that the two species can coexist in the same potential well despite the repulsive interaction between them.

As a first step let us recall the general formula which gives the time evolution of the mean value of \( \langle \hat{J}_z^2(\tau) \rangle = \frac{1}{2} (J_a^2(\tau) + J_b^2(\tau)) \) [35]:
\[
\langle \hat{J}_z^2(\tau) \rangle = \sum_{n=m_1^2}^{m_2^2} \sum_{n'=m_1^2}^{m_2^2} \phi_n^* \phi_{n'} \langle \hat{J}_{0,n}^2 \rangle \langle \hat{J}_{0,n'}^2 \rangle e^{i (\hat{E}_{0,n} - \hat{E}_{0,n'}) \tau},
\]

where \( \tau = \frac{\hbar}{\Delta} t \) is the dimensionless time, the sums are over all the eigenvectors \( \langle \hat{J}_{0,n}^2 \rangle \), with \( m_2 = 0 \) or \( \frac{1}{2} \), \( \frac{N_2}{2} \), and \( \phi_n \) are the projections of the initial state \( |\psi(0)\rangle \) on the basis \( \langle \hat{J}_{0,m}^2 \rangle \):
\[
|\psi(0)\rangle = \sum_{n=m_2^2}^{m_1^2} \phi_n \langle \hat{J}_{0,n} \rangle.
\]

So it is clear how the knowledge of eigenvalues and eigenvectors is enough in order to study the quantum evolution of \( \hat{J}_z^2 \), the Bohr frequencies involved, \( \hat{E}_{0,n} - \hat{E}_{0,n'} \), and the corresponding weights \( \phi_n^* \phi_{n'} \langle \hat{J}_{0,n}^2 \rangle \langle \hat{J}_{0,n'}^2 \rangle \).

Let us now study the dynamics of the system when all the bosons of species \( a \) and \( b \) are initially contained in one of the two wells of the potential, say the right one, and then the imbalances of the two species coincide, so that \( N_{a,R} = N_a \), \( N_{b,R} = 0 \), \( N_{a,L} = N_0 \), \( N_{b,L} = 0 \); furthermore, the two species are equally populated, i.e. \( N_a = N_b \). That implies \( m_1 = 0 \) and \( m_2 = \frac{N_2}{2} = \frac{N_2}{2} \) in our centre of mass rotated basis. The corresponding initial condition is
\[
|\psi(0)\rangle = \left| 0, \frac{N_2}{2} \right\rangle.
\]

In order to investigate the short-timescale evolution we need to keep terms up to second order in the tunnelling amplitude \( k \) when we compute the weights in equation (43). We find that
\[
\langle \hat{J}_z^2(\tau) \rangle = \frac{N_2}{2} + \frac{k^2 N_2}{2 \lambda^2 (N_2 - 1)^2} \left[ \cos(\omega_{\mu}(\tau)) - 1 \right],
\]

where the frequency involved is
\[
\omega_{\mu} = \frac{\Delta E_0(\frac{\mu}{2} - 1)^2}{\Delta E_0(\frac{\mu}{2} + 1)^2} = \frac{k^2 N_2}{\lambda (N_2 - 1)} - \frac{k^2 N_2}{\lambda (N_2 - 1)^2} - \frac{N_2}{\lambda} \left( \frac{N_2}{2} - \frac{N_2}{4} \right).
\]

At short timescales small amplitude oscillations with frequency \( \omega_{\mu} \) around the initial condition \( (N_{2R} = N_2, N_{2L} = 0) \) are observed and that coincides with a strongly self-trapped regime.

In order to investigate the dynamics at longer timescales we have to take into account also the small splittings \( \Delta E_0(\frac{\mu}{2} - 1)^2 \) and \( \Delta E_0(\frac{\mu}{2} + 1)^2 \) of the two higher pairs of quasidegenerate eigenvalues which provide two further frequencies (see [23] for the derivation):
\[
\omega_0 = \Delta E_0(\frac{\mu}{2} + 1)^2 = \frac{k^2 N_2}{\lambda^2 (N_2 - 1)^2} \left( N_2 - 1 \right)!
\]
\[
\omega_1 = \Delta E_0(\frac{\mu}{2} - 1)^2 = \frac{k^2 N_2}{\lambda^2 (N_2 - 1)^2} \left( N_2 - 2 \right)!
\]

The whole result is
\[
\langle \hat{J}_z^2(\tau) \rangle = \frac{N_2}{2} \left[ \cos(\omega_0 \tau) + \frac{k^2 N_2}{4 \lambda^2 (N_2 - 1)^2} \right] \times \left[ \frac{N_2}{2} \left( \cos(\omega_1 \tau) - \cos(\omega_0 \tau) \right) \right] + 2 \cos(\omega_0 \tau) \cos(\omega_1 \tau) - \cos(\omega_0 \tau) - \cos(\omega_1 \tau).
\]

and, by putting \( \omega_0 = \omega_1 = 0 \), the short timescale dynamics, equation (46), is recovered. Summarizing, at longer timescales the two-species bosons are still localized in the initial potential well but the quantum dynamics exhibits collapses and complete revivals. Indeed the coefficient \( \cos(\omega_0 \tau) \), which multiplies the higher-frequency term \( \cos(\omega_1 \tau) \), gives rise to the beat, which is responsible for the observed collapses and revivals at timescales fixed by \( \omega_1 \), as shown in figure 1. Finally, at very large timescales determined by the frequency \( \omega_0 \) all the bosons tunnel coherently back and forth between the two traps; only the first term \( \cos(\omega_0 \tau) \) is responsible of such a coherent tunnelling, since all harmonic functions containing frequencies \( \omega_0 \) and \( \omega_1 \) are small in amplitude and proportional to \( k^2 \); thus, they are unable to transfer bosons from one trap to the other.

The tunnelling dynamics within macroscopic quantum self-trapping regime described above is analogous to that of the \( \pi \)-mode fixed point obtained by the Gross–Pitaevskii approach [29] where the two species localize in the same well despite the repulsive interaction between them. Let us finally note that, despite the explicit dependence on \( \lambda \) of the frequencies (47)–(48), the different physics related to the three timescales described above is simply due to the
energy splitting introduced by the renormalized tunnelling for small $\Lambda_{ab}$. Thus in the case of a mixture of BECs with equal population the dynamics remains similar to that of a single-component BEC, apart from the coexistence of the two species in the same well. This is shown in figure 1 where the tunnelling dynamics for the single-species BEC is also reported.

As for the experimental detection of the long-timescale phenomena (collapses/revivals and coherent tunnelling), since the time for their appearance is abruptly increased with $N_2$, this implies a rapid decrease of the characteristic frequencies rendering more difficult the observation of the intermediate and long-time behaviour in current BEC experiments. Indeed, by a comparison of equations (47)–(48), we clearly see that the frequency $\omega_{\mu}$ is of order $k_0^0$ while $\omega_0$ and $\omega_1$ are of order $kN_2$ and $kN_2^{-2}$ respectively. That reflects on the dimensionless timescales for such phenomena, which range from order 1 for short-time dynamics to $10^7$ and $10^{11}$ for the intermediate and long-time dynamics, respectively. Indeed pure condensates consisting of $1150 \pm 150$ atoms of $^{87}$Rb loaded in a double well have been recently realized [6, 7] thus rendering the detection of the short-time behaviour possible. Mixtures with a number of atoms ranging from $9 \times 10^3$ and $5 \times 10^3$ ($^{87}$Rb and $^{41}$K [10]) to $4 \times 10^4$ and $9 \times 10^4$ ($^{85}$Rb and $^{87}$Rb [9]) have also been recently realized, but in this case very small characteristic frequencies are implied. However, these phenomena may be relevant for molecular systems where the number of vibrational excited quanta is small, allowing also for the experimental observation of intermediate and long-time dynamics.

In the next section we will further investigate the dynamics of the system by assuming as the initial state a simple coherent state and then study the formation of a particular superposition of such coherent states, the so-called Schrödinger cat states.

5. Dynamics: coherent spin initial states and Schrödinger cat states

In this section we choose as the initial condition a simple coherent spin state [36] and study the short-timescale evolution of number difference; in this way a more complex dynamics will appear. Finally, we study the generation of Schrödinger cat states; in particular, we focus on the contrast in the

Figure 1. Time evolution of the relative boson number difference between the two traps for different timescales. The value of $k = 0.5$ and the boson number is $N_2 = 10$, while $\lambda = 1$ on the left panels and $\lambda = 1.3$ on the right panels. The case $\lambda = 1$ corresponds to the single species BEC, i.e. $\Lambda_{ab} = 0$. 
momentum distribution and show how it vanishes for a two-component cat state.

Let us start by considering as initial condition the following coherent spin state [36]:

\[
|\psi(0)\rangle = C \sum_{m_3=-N_2/2}^{N_2/2} \sqrt{\frac{N_2!}{(\frac{N_2}{2} + m_3)! (\frac{N_2}{2} - m_3)!}} \times \tan^{m_3} \left(\frac{\theta}{2}\right) e^{-im_3\phi} |0, m_3\rangle,
\]

(50)

where the coefficient \(C\) is

\[
C = \sin^{N_2/2} \left(\frac{\theta}{2}\right) \cos^{N_2/2} \left(\frac{\theta}{2}\right) e^{-i\pi N_2/2 \phi},
\]

(51)

and \(\theta\) and \(\phi\) are two angles characterizing the superposition. The time evolution of the mean value of \(\hat{J}_z\) up to first order in the tunnelling amplitude \(k\) is given by

\[
\langle (\hat{J}_z)^{(1)}(\tau) \rangle = \langle (\hat{J}_z)^{(0)}(\tau) \rangle + \frac{k}{\lambda} \left(\sin(\theta)\right)^{N_2} \times \left[ C_1 \cos(\omega_0 \tau) - 1 \right] + C_2 \sin(\omega_0 \tau) + \sum_{n=0}^{N_2/2-1} \frac{N_2!}{(\frac{N_2}{2} + n)! (\frac{N_2}{2} - n)!} \left(\frac{N_2}{2} - 2n\right) \tau^2 \cos(\theta) \sin(\theta) \right),
\]

(52)

where

\[
A_n = \tan^{2n+1} \left(\frac{\theta}{2}\right) \left[ \cos(F_n \tau + \phi) - \cos(\phi) \right]
\]

(53)

with frequencies \(F_n = \frac{\pi}{N_2} \cos(\theta) + \frac{1}{N_2} \sin(\theta) \). Furthermore, the coefficients \(C_1\) and \(C_2\) are given by

\[
C_1 = \frac{N_2!}{(\frac{N_2}{2} + 1)! (\frac{N_2}{2} - 1)!} \cos(\phi) \left(\frac{N_2}{6} - \frac{1}{3}\right) \times \left[ \tan^3 \left(\frac{\theta}{2}\right) - \frac{1}{\tan^3 \left(\frac{\theta}{2}\right)} \right] - \left(\frac{N_2}{2} + 1\right),
\]

(54)

\[
C_2 = \frac{N_2!}{(\frac{N_2}{2} + 1)! (\frac{N_2}{2} - 1)!} \left[ \tan \left(\frac{\theta}{2}\right) + \frac{1}{\tan \left(\frac{\theta}{2}\right)} \right] \times \left[ \tan^3 \left(\frac{\theta}{2}\right) - \frac{1}{\tan^3 \left(\frac{\theta}{2}\right)} \right],
\]

(55)

for \(N_2\) even, and

\[
C_1 = \frac{N_2!}{(\frac{N_2}{2} + 1)! (\frac{N_2}{2} - 1)!} \cos(\phi) \times \left[ \tan^2 \left(\frac{\theta}{2}\right) - \frac{1}{\tan^2 \left(\frac{\theta}{2}\right)} \right],
\]

(56)

\[
C_2 = \frac{N_2!}{(\frac{N_2}{2} + 1)! (\frac{N_2}{2} - 1)!} \left[ \tan \left(\frac{\theta}{2}\right) + \frac{1}{\tan \left(\frac{\theta}{2}\right)} \right] \times \left[ \tan \left(\frac{\theta}{2}\right) + \frac{1}{\tan \left(\frac{\theta}{2}\right)} \right],
\]

(57)

for \(N_2\) odd. Finally, for \(N_2\) even, the zero-order mean value \(\langle (\hat{J}_z)^{(0)}(\tau) \rangle \) is given by

\[
\langle (\hat{J}_z)^{(0)}(\tau) \rangle = -\frac{N_2}{2} \cos(\theta) \left(\sin(\theta)\right)^{N_2} \times \left[ \tan^2 \left(\frac{\theta}{2}\right) - \frac{1}{\tan^2 \left(\frac{\theta}{2}\right)} \right] \times \left[ \cos(\omega_0 \tau) - 1 \right] + 2 \sin(2\phi) \sin(\omega_0 \tau),
\]

(58)

where the dominant frequency \(\omega_0\) is equal to \(\omega_0 = \frac{\pi}{N_2} \cos(\theta) + \frac{1}{N_2} \sin(\theta) \). The corresponding expression for \(N_2\) odd is

\[
\langle (\hat{J}_z)^{(0)}(\tau) \rangle = -\frac{N_2}{2} \cos(\theta) \left(\sin(\theta)\right)^{N_2} \times \left[ \tan^2 \left(\frac{\theta}{2}\right) - \frac{1}{\tan^2 \left(\frac{\theta}{2}\right)} \right] \times \left[ \cos(\omega_0 \tau) - 1 \right] + 2 \sin(\phi) \sin(\omega_0 \tau),
\]

(59)

where \(\omega_0 = \frac{\pi}{N_2} \cos(\theta) + \frac{1}{N_2} \sin(\theta) \times 2k \sqrt{\frac{N_2}{2} (\frac{N_2}{2} - 1) + \frac{1}{4}} \). As one can see, the dominant frequency is gradually suppressed with the number of bosons \(N_2 = \frac{1}{2} (N_0 + N_0) \) [22]. This is clearly seen in figure 2 where the boson number difference between the two traps is plotted for different \(N_2\) values as a function of the dimensionless time \(\tau\). One also notices a decrease of the oscillation amplitude at increasing \(N_2\).

The effect of \(\lambda\) is instead shown in figure 3 where the short-time dynamics of the boson number difference is analysed for two values of the interspecies interaction. When \(\lambda\) increases the amplitude of the oscillations decreases. The detection of the mixture dynamics is thus more favourable for values of \(\lambda\) smaller than unity.

5.1. Cat states

Let us consider the coherent spin state (50); the expectation value of the Hamiltonian (34) on such state is given by

\[
\langle \psi(0) | \hat{H} | \psi(0) \rangle = 2 \lambda n^2 / 2 - 2k \sqrt{(N_2/2)^2 - n^2} \cos \phi.
\]

(60)
where \( n = -(N_2/2) \cos \theta \) and has the maximum value for \( \phi = 0, \theta = \pi/2 \). This result also corresponds to the mean-field result for the energy. Now, starting from the coherent spin state \( \text{Schrödinger cat states} \) we are interested in looking for Schrödinger cat states. Such states are quantum superposition of macroscopic states and their realization has already been suggested for a single species Bose–Josephson junction in \([24]\).

Also in the case of a Bose–Josephson junction with binary mixtures one might realize cat states from the time evolution of an initially coherent state following a sudden rise of the barrier between the two wells. Thus, we consider at time \( t = 0^+ \) a zero inter-well coupling \( k \), i.e. the time evolution is governed by the Hamiltonian \( H_0 \) in equation \( (35) \). For each basis vector \( |0, m_2\rangle \) of the coherent state \( |\psi(T)\rangle \), the time evolution is given by \( |0, m_2\rangle(t) = e^{i2\pi m_2^2/T} |0, m_2\rangle \). The value of \( \theta \) is the so-called revival time such that \( |\psi(T)\rangle = |\psi(0)\rangle \). Considering now the times \( T/2p \) and \( p \) being the integer, the time evolution of the coherent state is governed by the factor \( \exp\left( -i\pi m_2^2 / p \right) \) which satisfies the property \( \exp( -i\pi (m^2 + p^2) / p ) = ( -1 )^p \exp( -i\pi m_2^2 / p ) \), depending on the parity of \( p \). For the choice of even \( p \), a discrete Fourier transform leads to the cat state

\[
|\psi(T/2p)\rangle = \sum_{k=0}^{p-1} u_k e^{i2\pi kN_2/p} e^{-i2\pi k/p |\psi\rangle},
\]

i.e. a superposition of \( p \) coherent states, where \( u_k = 1/p \sum_{m=0}^{p-1} e^{-i2\pi m^2 / p} e^{i2\pi km / p} \). In particular, the cat state affects the momentum distribution. This dependence could be important to probe experimentally their existence. In particular, when considering the two-component cat state, i.e. for the choice \( p = 2 \), one obtains that the contrast in the momentum distribution, i.e. the expectation value of \( \bar{J}_z^2 \) on the unperturbed state, vanishes \([24]\).

Furthermore, the amplitude of the intervals of time in which the contrast is zero increases with increasing \( N_2 \) as clearly shown in figure \( 4 \).

It should be noted that despite the close similarity in the behaviour of the contrast between the single-component BJ and the double one, the mixture could be a better candidate for the creation and detection of cat states. In fact their creation time is \( \pi \hbar / \lambda \) and, since for repulsive interaction between the two species and \( \Lambda > \Lambda_{ab} \) we get \( \lambda = -[(1 + \Lambda/\Lambda_{ab})/(1 - \Lambda/\Lambda_{ab})] > 1 \), such a time can be made short enough to render their detection more favourable. But in order to establish if the mixture will be a useful candidate for the creation and detection of cat states, it would be necessary to study the influence of the various decoherence mechanisms. In general, the main decoherence mechanism which limits the lifetime and the size of BECs is the three-body recombination. Three-body losses strongly influence the formation and evolution of complex superpositions of states of different phases, i.e. the mechanism of quantum collapse and revival of the phase \([37]\) which is adopted as a protocol to realize cat states \([32]\). In order to establish the robustness of Schrödinger cat states against three-body losses it is then mandatory to compare the decoherence time and the revival time keeping in mind that if the decoherence timescale is much faster than the revival time, revivals will not occur and intermediate superpositions of states are destroyed.

In general, for atomic three-body decay the recombination loss at each site is characterized by the decay rate \( \gamma = K_x \int dx |w(x)|^2 \), where \( w(x) \) is the localized wavefunction at the site \( x \) and \( K_3 \) is the three-body rate constant \([37]\). It can be shown \([38]\) that, for a binary mixture of BECs, such a decay rate takes the form \( \gamma_{BM} = \frac{K_x}{\pi} \int dx |w(x)|^2 \), where the oscillator length \( a_{ho} \) is a parameter which is fixed by the geometry of the trapping potential and \( a_{ho}, a_{ab} \) are the scattering lengths. Such a decay rate should be compared with the creation rate \( \Lambda_{RR}^2 \). However, it should be noted that since the decay rate depends on external parameters as the harmonic trapping frequency and since the scattering length could be controlled by Feshbach resonances, it should be possible to realize a regime where the creation rate is much larger than \( \gamma_{BM} \) and detection of cat states is possible. Let us finally note that by fixing the ratio of \( Rb^{85}Rb^{87} \) interaction\( \gamma_{BM} \) to \( Rb^{85}Rb^{85} \) interaction as 2.13, a parameter accessible in the JILA setup\([9]\), the detection time is twice smaller than the case of a single-component BEC.

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.

Figure 3. Time evolution of the relative boson number difference between the two traps for \( N_1 = 10 \). The value of \( \kappa = 0.1 \) while \( \lambda = 1.3 \) (dashed line) and \( \lambda = 0.3 \) (straight line), while \( \theta = \pi/2 \) and \( \phi = \pi/4 \).

Figure 4. Contrast in the time evolution of \( \langle J_z^2 \rangle \) for \( \theta = \pi/2 \) and \( \phi = \pi/4 \) and even number of bosons. The red line is for \( N_2 = 10 \), the blue one for \( N_2 = 14 \) and the black one for \( N_2 = 20 \). The interval in which the contrast is zero increases with increasing \( N_2 \).
We focused on the small tunnelling amplitude limit and adopted the angular momentum representation for the Bose–Hubbard dimer Hamiltonian. Perturbation theory up to second order in the tunnelling amplitude enabled us perform analytical calculations in the symmetric case where \( \Lambda_a = \Lambda_b = \Lambda \) and \( K_a = K_b = K \). In this way we obtained the energy eigenvalues and eigenstates, whose knowledge is mandatory in order to investigate the quantum evolution of the number difference of bosons between the two potential wells. In order to study the quantum dynamics more easily and analytically, we restricted 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. We concentrated on the two initial conditions: completely tunable via Feshbach resonances. In particular it is possible to realize the symmetric regime \( \text{sym} \). This allowed us to obtain analytical approximation and of the precision of the perturbative results and will be the subject of a future publication together with different couplings between the two bosonic species and/or different populations needs to resort to numerical calculations and will be the subject of a future publication together with a quantitative evaluation of the validity of the two-mode approximation and of the precision of the perturbative results obtained in this work [34]. Another interesting issue which deserves further investigation is a careful analysis of the quantum manifestations of the self-trapping transition and in general of the MQST phenomenon in this more general context.

The complex dynamics of the generalized Bose–Josephson junctions investigated in the present paper could be experimentally testable within the current technology. For instance, the JILA group recently [9] succeeded in producing a mixture of \(^{85}\)Rb and \(^{87}\)Rb atoms, whose interactions are widely tunable via Feshbach resonances. In particular it is possible to fix the scattering length of \(^{87}\)Rb as well as the interspecies one and to tune the scattering length of \(^{85}\)Rb. That allows one to explore the parameter space in a wide range and also to realize the symmetric regime \( \Lambda_a = \Lambda_b = \Lambda \). Because of the high degree of experimental control, such a setup could be employed to reproduce the phenomenology described in this work.

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Appendix. Order \( k^2 \) eigenvectors

The eigenvectors of the full Hamiltonian (34), up to order \( k^2 \), are

\[
\begin{align*}
\left| \phi_{0,0}^{(2)} \right> &= \left(1 - \frac{k^2}{32\lambda^2} \right) \left| 0, 0 \right> + \frac{k}{4\lambda} \sqrt{j_2(j_2+1)-\frac{3}{4}} \left| j_2(j_2+1)-\frac{3}{4} \right> \left| 0, \frac{1}{2} \right> + \frac{k^2}{16\lambda^2} \left[ j_2(j_2+1)-\frac{3}{4} \right] \left| j_2(j_2+1)-\frac{3}{4} \right> \left| 0, \frac{3}{2} \right> + \frac{k^2}{64\lambda^2} \left[ j_2(j_2+1)-\frac{3}{4} \right] \left| j_2(j_2+1)-\frac{3}{4} \right> \left| 0, \frac{3}{2} \right>, \\
\left| \phi_{0,1}^{(2)} \right> &= \left(1 - \frac{k^2}{72\lambda^2} \right) \left| 0, 1 \right> + \frac{k}{6\lambda} \sqrt{j_2(j_2+1)-\frac{3}{4}} \left| j_2(j_2+1)-\frac{3}{4} \right> \left| 0, \frac{1}{2} \right> + \frac{k^2}{96\lambda^2} \left[ j_2(j_2+1)-\frac{3}{4} \right] \left| j_2(j_2+1)-\frac{3}{4} \right> \left| 0, \frac{3}{2} \right>.
\end{align*}
\]
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