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Effects of three-body collisions in a two-mode Bose-Einstein condensate

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We study the effects of three-body collisions in the physical properties of a two-mode Bose-Einstein condensate. The model introduced here includes two-body and three-body elastic and mode-exchange collisions and can be solved analytically. We will use this fact to show that three-body interactions can produce drastic changes in the probability distribution of the ground state and the dynamics of the relative population. In particular, we find that three-body interactions under certain circumstances may inhibit the collapse of the relative population. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4936314>]

I. INTRODUCTION

Most of our understanding of condensed matter is based on models that consider two-body collisions. However there are many situations where three-body or higher order collisions are relevant in the physical properties of such systems.¹⁻³ For example, it is known that three-body collisions are important in systems that show exotic quantum phases, such as topological phases² or spin liquids.³ Moreover, it is suspected that many-body collisions are important in the coldest phases of Bose-Einstein condensates (BECs), where the dilute regime breaks down.⁴ Microscopic calculations show that polar molecules driven by microwave fields undergo three-body interactions.⁵ The interaction potentials of molecules trapped in an optical lattice give rise to Hubbard models with strong nearest-neighbour two-body and three-body interactions.

In this paper, we find the exact analytic solution of a generalized two-mode Bose-Hubbard model that includes two-body and three-body elastic and mode-exchange collisions. Then we show that three-body collisions can change dramatically the properties of the ground state of a two-mode Bose-Einstein condensate. The effects are also observable in the evolution of the relative population inhibiting, in some cases, quantum collapse. It is well known that three-body collisions are responsible for particle loss in Bose-Einstein condensates, through a process called three-body recombination.⁶ During three-body collisions, the particles recombine to form a molecule that is not trapped by the potential. However it is now possible to inhibit molecular three-body recombination in atomic Bose-Einstein condensates via the application of resonant 2π laser pulses.⁷ In such situations, our model becomes of special interest, since it takes into account three-body collisions where particles do not recombine and remain trapped in the potential.

The model we introduce can describe the physics of a double-well Bose-Einstein condensate or a spin-1/2 Bose-Einstein condensate consisting of particles with two internal degrees of freedom trapped in a single well. In the context of the double-well Bose-Einstein condensate, the mode-exchange collisions included here are known as generalized nearest neighbour interactions⁸ and give rise to coherent tunneling effects.^{9,10} Recent analysis shows that stronger two-body interactions are

correlated with two-body coherent tunneling dynamics in which two particles simultaneously tunnel through the barrier.¹⁰ This effect, also known as second order tunneling, has been observed in the laboratory.⁹ Mode-exchange collisions are called inelastic collisions in the context of spin-1/2 condensates and occur when cold collisions take place in the presence of light fields. Such is the case of spin-1/2 condensates where a laser field is used to induce Josephson-type interactions, which produce transitions among the spin degrees of freedom.¹¹

II. MODEL

We consider a general model of a two-mode Bose-Einstein condensate that includes two-body and three-body collisions given by the Hamiltonian $\mathcal{H}_3 = H_1 + H_2 + H_3$, where (taking $\hbar = 1$)

$$\begin{aligned}
 H_1 &= \lambda_{a|a} a^\dagger a + \lambda_{b|b} b^\dagger b + \lambda_{a|b} (a^\dagger b + b^\dagger a), \\
 H_2 &= \mathcal{U}_{aa|aa} a^\dagger a^\dagger a a + \mathcal{U}_{bb|bb} b^\dagger b^\dagger b b + \mathcal{U}_{ab|ab} a^\dagger b^\dagger a b \\
 &\quad + U_{aa|ab} (a^\dagger a^\dagger a b + h.c.) + U_{bb|ab} (b^\dagger b^\dagger a b + h.c.) \\
 &\quad + U_{aa|bb} (a^\dagger a^\dagger b b + h.c.), \\
 H_3 &= \mathcal{U}_{aaa|aaa} a^\dagger a^\dagger a^\dagger a a a + \mathcal{U}_{bbb|bbb} b^\dagger b^\dagger b^\dagger b b b \\
 &\quad + \mathcal{U}_{aab|aab} a^\dagger a^\dagger b^\dagger a a b + \mathcal{U}_{abb|abb} a^\dagger b^\dagger b^\dagger a b b \\
 &\quad + U_{aaa|aab} (a^\dagger a^\dagger a^\dagger a a b + h.c.) \\
 &\quad + U_{bbb|abb} (b^\dagger b^\dagger b^\dagger a b b + h.c.) \\
 &\quad + U_{aaa|abb} (a^\dagger a^\dagger a^\dagger a b b + h.c.) \\
 &\quad + U_{bbb|aab} (b^\dagger b^\dagger b^\dagger a a b + h.c.) \\
 &\quad + U_{aab|abb} (a^\dagger a^\dagger b^\dagger a b b + h.c.) \\
 &\quad + U_{aaa|bbb} (a^\dagger a^\dagger a^\dagger b b b + h.c.). \tag{1}
 \end{aligned}$$

The operators a^\dagger, a and b^\dagger, b are associated with two modes, labeled A and B, with respective frequencies $\lambda_{a|a}$ and $\lambda_{b|b}$. These modes correspond either to atoms with two different hyperfine levels¹² or two spatially separated condensates^{13,14} (see Fig. 1). The Josephson-type interaction, in which one particle is annihilated in one mode and created in the other, has coupling constant $\lambda_{a|b}$. This process is induced by applying a magnetic field gradient¹³ or a laser.¹² The terms in H_2 , which have four bosonic operators, describe two-particle collisions. The two-body elastic scattering strengths are given by $\mathcal{U}_{aa|aa}$ and $\mathcal{U}_{bb|bb}$ for same mode collisions and $U_{ab|ab}$ when the particles colliding belong to different modes. Mode-exchange collisions have interaction strengths $U_{aa|ab}, U_{bb|ab}$ when two particles collide and one of them is transformed into the other mode and interaction strength $U_{aa|bb}$ when the collision transforms two particles in one mode into the other mode. This process is also known as second order tunneling in the context of a double-well BEC.^{9,10}

The Hamiltonian $\mathcal{H}_2 = H_1 + H_2$ has been studied in detail in Ref. 15. This two-body interaction Hamiltonian coincides with the two-mode Bose-Hubbard model if mode-exchange collisions are neglected, i.e., $U_{aa|ab} = U_{bb|ab} = U_{aa|bb} = 0$. However, microscopic calculations show that such

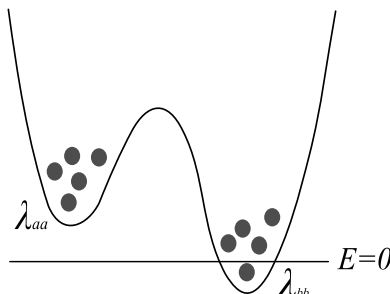


FIG. 1. A Bose-Einstein condensate in an asymmetric double-well potential, characterised by the single well energies $\lambda_{a|a}$ and $\lambda_{b|b}$.

interactions, known as inelastic collisions in the context of spin-1/2 Bose-Einstein condensates, should be considered since they occur when particles collide in the presence of a laser field.¹¹ Surprisingly, including such collisions allows for an exact analytical solution.^{15–18} Here we include a three-body collision term given by H_3 , where three-body interactions consist of products of six operators (three creation and three annihilation). This term includes all possible three-body collisions where $\mathcal{U}_{aaa|aaa}$, $\mathcal{U}_{bbb|bbb}$, $\mathcal{U}_{aab|aab}$, and $\mathcal{U}_{abb|abb}$ correspond to elastic scattering lengths and $\mathcal{U}_{aaa|aab}$, $\mathcal{U}_{aaa|abb}$, and $\mathcal{U}_{aaa|bbb}$ correspond to mode-exchange collisions where one, two, and three particles change mode, respectively.

We have found that the Hamiltonian \mathcal{H}_3 has six families of exact analytical solutions. In this paper, we present the solution which we consider of greatest physical interest. The other solutions will be presented elsewhere.

We start by considering the double-well potential shown in Fig. 1. Particles undergo two- and three-body collisions and we assume that first, second, and third order tunneling events can occur. In second (third) order tunneling, two (three) tunneling events can occur coherently. Therefore single particles can coherently tunnel two (three) times and two (three) particles can tunnel simultaneously during a collision.

We consider that a particle in well A (or B) has probability amplitude $A_1 \cos \theta$ (or $-A_1 \cos \theta$) of staying in well A (or B) and probability amplitude $A_1 \sin \theta$ of tunneling to well B (or A). A_1 is the first order tunneling strength and θ is the tunneling phase. Note that the minus sign appears because we chose for simplicity well B to have negative energy corresponding to $\lambda_{b|b} = -\lambda_{a|a}$. We consider A_2 and A_3 to be second and third order tunneling strengths. Therefore, $A_2 \sin^2 \theta$ and $A_3 \sin^2 \theta \cos \theta$, for example, are the second and third order probability amplitudes, respectively, for a single particle in well A to tunnel back and forth.

The coefficients in the single particle Hamiltonian H_1 are found by considering all possible single particle events including second and third order tunneling. For example,

$$\begin{aligned} \lambda_{a|a} &= A_1 \cos \theta + A_2(\cos^2 \theta + \sin^2 \theta) \\ &+ A_3 \cos \theta(\cos^2 \theta + \sin^2 \theta) = A_2 + (A_3 + A_1) \cos \theta \end{aligned} \quad (2)$$

is the probability amplitude for a single particle in well A to end in well A. The general two-body and three-body scattering lengths $U_{ij|lm}$ and $U_{ijk|lmn}$ are given by the product of the corresponding second and third order tunneling strengths times the appropriate tunneling phase amplitudes ($\sin \theta$ if the particle tunnels during the collision and $\pm \cos \theta$ if the particle stays). For example, consider a three-body collision during which two particles change state. The total probability amplitude will be

$$U_{aaa|abb} = 3A_3 \cos \theta \sin^2 \theta. \quad (3)$$

The factor 3 comes from the fact that there are three possible events that give rise to the same final outcome, according to the different time orderings of the events.

In the case of two-body collisions, we consider that during a collision, two and three tunneling events can occur. So collisions in which two particles in well A end up both in well B are given by

$$\begin{aligned} U_{aa|bb} &= A_2 \sin^2 \theta \\ &+ 3A_3(\cos \theta \sin^2 \theta - \sin^2 \theta \cos \theta) = A_2 \sin^2 \theta, \end{aligned} \quad (4)$$

where again the factor 3 comes from the time ordering. Such considerations give rise to the parameters

$$\begin{aligned} \lambda_{a|a} &= A_2 + (A_3 + A_1) \cos \theta, \\ \lambda_{b|b} &= A_2 - (A_3 + A_1) \cos \theta, \\ \lambda_{a|b} &= (A_1 + A_3) \sin \theta, \\ \mathcal{U}_{aa|aa} &= (A_2 \cos \theta + 3A_3) \cos \theta, \\ \mathcal{U}_{bb|bb} &= (A_2 \cos \theta - 3A_3) \cos \theta, \\ \mathcal{U}_{ab|ab} &= 2A_2(\sin^2 \theta - \cos^2 \theta), \\ U_{aa|ab} &= (3A_3 + 2A_2 \cos \theta) \sin \theta, \\ U_{bb|ab} &= (3A_3 - 2A_2 \cos \theta) \sin \theta, \end{aligned}$$

$$\begin{aligned}
\mathcal{U}_{aa|bb} &= A_2 \sin^2 \theta, \\
\mathcal{U}_{bbb|bbb} &= -\mathcal{U}_{aaa|aaa} = -A_3 \cos^3 \theta, \\
\mathcal{U}_{abb|abb} &= -\mathcal{U}_{aab|aab} = -A_3(2 \cos \theta \sin^2 \theta - \cos^3 \theta), \\
U_{aaa|aab} &= U_{bbb|abb} = 3A_3 \cos^2 \theta \sin \theta, \\
U_{aaa|abb} &= 3A_3 \cos \theta \sin^2 \theta, \\
U_{bbb|aab} &= -3A_3 \cos \theta \sin^2 \theta, \\
U_{aab|abb} &= 3A_3(\sin^3 \theta - \cos^2 \theta \sin \theta), \\
\mathcal{U}_{aaa|bbb} &= A_3 \sin^3 \theta.
\end{aligned} \tag{5}$$

At this point, it is important to illustrate the connection of this model with a physical model of a BEC. Consider the many-body energy functional for bosonic particles of mass m trapped in a potential $V(\mathbf{r})$ undergoing two-body and three-body collisions,

$$\begin{aligned}
H &= H_0 + H_{I2} + H_{I3}, \\
H_0 &= \int d\mathbf{r} \left(-\frac{\hbar^2}{2m} \hat{\Psi}^\dagger \nabla^2 \hat{\Psi} + \hat{\Psi}^\dagger V(\mathbf{r}) \hat{\Psi} \right) \\
&= \int d\mathbf{r} \hat{\Psi}^\dagger H_t \hat{\Psi}, \\
H_{I2} &= \frac{g_2}{2} \int d\mathbf{r} \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi}, \\
H_{I3} &= \frac{g_3}{2} \int d\mathbf{r} \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi} \hat{\Psi},
\end{aligned} \tag{6}$$

where g_2, g_3 are two-body and three-body coupling strengths, respectively, and H_t is the Hamiltonian of the trap. The wavefunction $\hat{\Psi}$ can be expanded in terms of a certain set of functions ϕ_i and their corresponding annihilation operators \hat{c}_i as

$$\hat{\Psi} = \sum_i \phi_i \hat{c}_i. \tag{7}$$

We employ the standard two-mode approximation

$$\hat{\Psi} = \phi_1 \hat{c}_1 + \phi_2 \hat{c}_2 \tag{8}$$

and then the rotation

$$\begin{aligned}
\phi_1 &= \cos(\theta/2) \phi_a - \sin(\theta/2) \phi_b, \\
\phi_2 &= \cos(\theta/2) \phi_b + \sin(\theta/2) \phi_a,
\end{aligned} \tag{9}$$

where ϕ_a, ϕ_b are nearly normalized modes¹⁹ with $\int dr \phi_a \phi_a = 1 + \epsilon$, $\int dr \phi_b \phi_b = 1 - \epsilon$, where the amplitude of transition between them

$$\epsilon = \int dr \phi_a H_t \phi_b \tag{10}$$

is assumed to be very small. We obtain the Hamiltonian \mathcal{H}_3 described above with

$$\begin{aligned}
A_1 &= \frac{1}{2}(E_1 - E_2), \quad A_2 = \frac{1}{2}U_2, \quad U_2 = U_{11} = U_{22}, \quad A_3 = \frac{1}{2}U_3, \quad U_3 = U_{111} = U_{222}, \\
E_1 &= \int dr \phi_1 H_t \phi_1, \quad U_{11} = \int dr \phi_1^4, \quad U_{111} = \int dr \phi_1^6, \\
E_2 &= \int dr \phi_2 H_t \phi_2, \quad U_{22} = \int dr \phi_2^6, \quad U_{222} = \int dr \phi_2^6
\end{aligned} \tag{11}$$

plus several terms of order ϵ , ϵ^2 , and ϵ^3 which can be treated perturbatively^{17,18} as long as $\epsilon \ll A_1 \theta$. We will discuss the experimental validity of this approximation in Sec. IV.

III. RESULTS

Surprisingly, the Hamiltonian $\mathcal{H}_3 = H_1 + H_2 + H_3$ has an exact analytic solution for this set of parameters. The analytic expression of its eigenstates is

$$|E_m\rangle = e^{-\frac{\theta}{2}(a^\dagger b - ab^\dagger)} |J, m\rangle, \quad (12)$$

where $|J, m\rangle$ are the Fock states for $2J = N$. N is the total number of particles, given by the operator

$$\hat{N} = n_a + n_b = a^\dagger a + b^\dagger b, \quad (13)$$

and m is the eigenvalue of the relative population operator,

$$\hat{m} = (a^\dagger a - b^\dagger b)/2. \quad (14)$$

Since the number of particles in the system N is constant, m is restricted to values $m = -J, \dots, J$. The unitary operator $e^{-\frac{\theta}{2}(a^\dagger b - ab^\dagger)}$ is known as the two-mode displacement operator with real displacement parameter θ .

Interestingly, the eigenstate for $m = -J$ corresponds to a coherent state, which gives an appropriate description of several physical aspects of the two-mode Bose-Einstein condensate.²⁰ It is easy to verify that $e^{-\frac{\theta}{2}(a^\dagger b - ab^\dagger)} |J, m\rangle$ are the eigenstates of Hamiltonian (1). One must simply apply the two-mode displacement operator to the Hamiltonian,

$$H_0 = A_1(a^\dagger a - b^\dagger b) + A_2(a^\dagger a - b^\dagger b)^2 + A_3(a^\dagger a - b^\dagger b)^3, \quad (15)$$

which is diagonal in the Fock basis. The result of this transformation is the Hamiltonian \mathcal{H}_3 with the coefficients shown in (5), except for an energy shift. For this reason, both Hamiltonians have the same energy spectrum and their eigenvectors are related by the displacement operator. The ground state of the system is $|E_g\rangle = e^{-\frac{\theta}{2}(a^\dagger b - ab^\dagger)} |J, m_0\rangle$, where m_0 is the integer that minimizes the energy $E_m = A_1 m + A_2 m^2 + A_3 m^3$. This number can be determined with the expressions,

$$m_0^\pm = \frac{A_2}{3A_3} \left(-1 \pm \sqrt{1 - \frac{3A_1 A_3}{A_2^2}} \right), \quad A_3 \neq 0, \\ m_0 = -\frac{A_1}{2A_2}, \quad A_3 = 0. \quad (16)$$

If $3A_1 A_3 / A_2^2 > 1$, m_0 is a complex number and the energy has no local minimum. Therefore, the minimum energy will correspond to the extreme point $m_{ex} = -NA_3/|A_3|$. On the other hand, if $3A_1 A_3 / A_2^2 < 1$ then the minimum, which is given by Eq. (16), is m_0^+ for $A_3 > 0$ and m_0^- when $A_3 < 0$. However, if the size of the system is big enough, then the cubic part of the energy prevails for $|m| \gg 0$. Under these circumstances, the energy of the extreme point $E_{m_{ex}}$ is smaller than the local minimum $E_{m_0^\pm}$.

A quantity of interest is the probability distribution of the relative population for the ground state, which is given by

$$P = |\langle N, m | \psi_0 \rangle|^2 = |d_{m, m_0}^N|^2, \quad (17)$$

where

$$d_{m, m_0}^N = \sum_k (-1)^{k-m_0+m} \frac{\sqrt{(N+m_0)!(N-m_0)!(N+m)!(N-m)!}}{(N+m_0-k)!k!(N-k-m)!(k-m_0+m)!} \\ \times \left(\cos \frac{\theta}{2}\right)^{2N-2k+m_0-m} \left(\sin \frac{\theta}{2}\right)^{2k-m_0+m} \quad (18)$$

are the Wigner rotation matrix elements.²¹ Note that the sum must be done for the values of k such that none of the arguments of the factorials in the denominator are negative. Different ground states parametrized by m_0 are obtained by changing the rate $A_1 A_3 / A_2^2$. We plot in Fig. 2 an example for $N = 100$ particles with $A_3 = 0$ (i.e., assuming that there are no third order tunneling and three-body collisions) and $m_0 = A_1 / 2A_2 = -50$. Such a state has a multi-peak distribution. However, if $A_3 = 0.0035$, we get a single peak distribution corresponding to $m_0 = -100$, i.e., a coherent state. Each figure has an inset

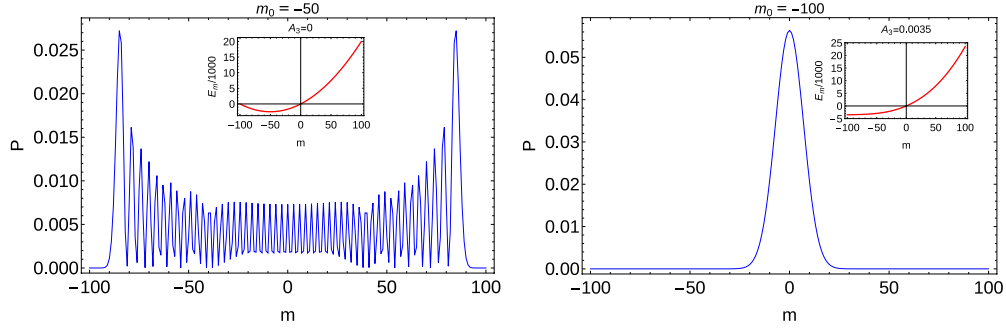


FIG. 2. Probability distribution P of the relative population for the ground state with $N = 100$, $A_1/A_2 = 100$ and (left) $A_3 = 0$, (right) $A_3 = 0.0035$. The ground state distribution changes from a multi-peak to a single peak distribution if three-body collisions are included. The insets show the change in the spectrum.

with a plot of the corresponding spectrum, where we can see that three body processes generate a shift of the minimum. This shows how three-body collisions and third order tunneling drastically change the structure of the ground state of the system. Moreover, the energy gap between the ground and first excited states is larger in Fig. 2(b). This is a typical feature of the self-trapping regime²² which suggests that three-body terms tend to favor localization. We will confirm this insight below.

We now analyze the effects of three-body collisions on the evolution of the average relative population $\langle m \rangle = \langle a^\dagger a - b^\dagger b \rangle$, for an initial condition $|\psi(t=0)\rangle$. The evolution of the relative population is given by

$$\langle m \rangle = \cos \theta \sum_{-N}^N m |C_m|^2 - \sin \theta \sum_{-N+1}^N C_m C_{m-1} \sqrt{N(N+1) - m(m-1)} L_m, \quad (19)$$

$$L_m = \cos[(E_{m-1} - E_m)t], \quad (20)$$

where the coefficients C_m are defined by

$$|\psi(t=0)\rangle = \sum_{m=-N}^N C_m e^{\frac{-\theta}{2}(a^\dagger b - ab^\dagger)} |N, m\rangle. \quad (21)$$

In Fig. 3, we plot Equation (19) for $N = 100$, $A_1 = 100$, $A_2 = 1$ and the initial condition $|\psi(t=0)\rangle = |N, N\rangle$, i.e., all the particles start in a single well. We can see that the relative population shows collapses and revivals for two body collisions. We can also observe that a small rate of three-body collisions ($A_3 = 1/100$) has a noticeable effect on the behaviour of the time evolution of the system, and in fact, it tends to break down the perfect collapse-revival cycles of the relative population. These cycles are characteristic of a delocalized dynamics, while the small-amplitude oscillations of the population imbalance in Fig. 3(b) point to a self-trapped dynamics. This confirms that the three-body terms tend to favor localization in this model.

IV. DISCUSSION AND CONCLUSIONS

At this point, let us discuss the experimental relevance of our results. In the case of a double-well potential, the modes a and b are quasilocated modes in wells A and B and A_1 corresponds to the asymmetry between the two wells. Thus, ϵ and A_1 can be experimentally tuned by changing the distance and the energy offset between the wells, respectively. Indeed, as discussed in Ref. 17, the condition $\epsilon \ll A_1 \theta$ holds in a wide variety of experiments with double-well BECs.^{23–25} More specifically, the linear tunnelling rate $U_{1|2} = \int dr \phi_1 H_i \phi_2 \simeq A_1 \theta + \epsilon$ takes experimental values ranging from $5 \cdot 10^{-4}$ Hz h²⁴ to 2 Hz h,²³ while the energy offset between the wells can be as high as $A_1 = 530$ Hz h.²⁵ Even if the wells are intended to be perfectly symmetric, the

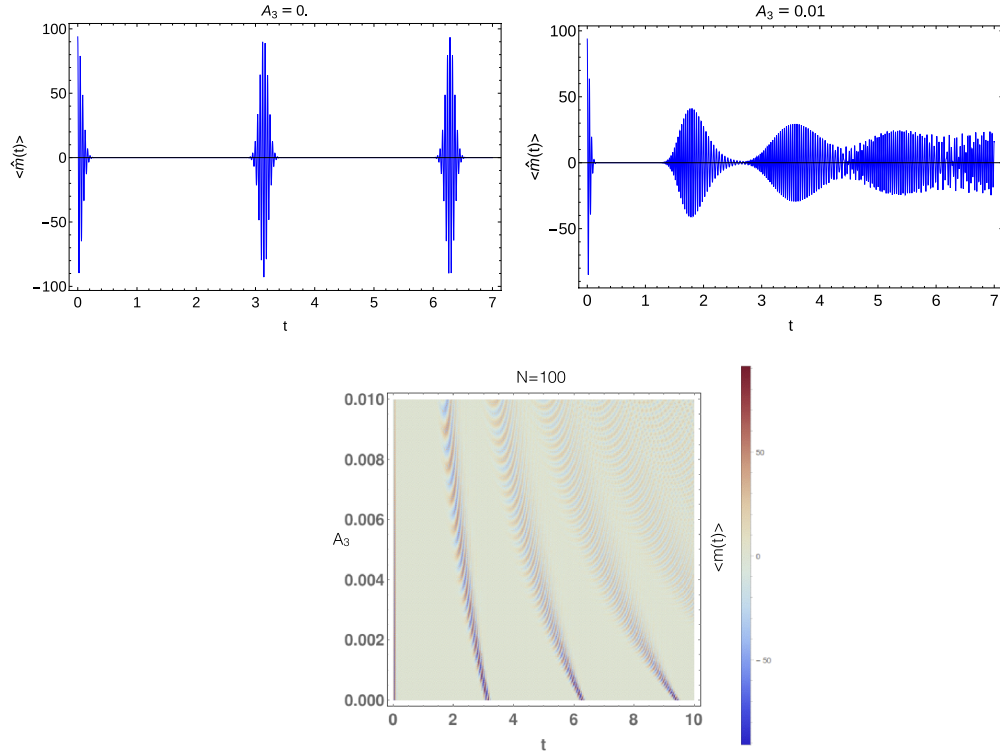


FIG. 3. Evolution of the relative population $\langle m \rangle$ for $N = 100$ particles with $A_1 = 100$, $A_2 = 1$, and A_3 specified in each figure. The initial state corresponds to $|\psi(t=0)\rangle = |N, N\rangle$. We observe that the presence of three-body collisions changes the dynamics of the system and in fact tends to break down perfect quantum collapse-revival cycles. We show that this phenomenon occurs in a continuous fashion with respect to the parameter A_3 .

uncertainty in the trap depth leads us to assume a minimum trap asymmetry of $A_1 \approx 20 \text{ Hz h}$.²³ Regarding the other parameters, A_2 and A_3 represent the two-body and three-contributions to the potential energy. It has been estimated the latter represent a few percent of the former. For instance, in He,¹ A_3 is around 2% of the total potential energy. All these values are in line with the plots in Sec. III. Note also that the three-body terms represent the leading-order corrections to the standard two-body interaction. It is reasonable to assume that four-body and higher order terms will be small with respect to the three-body ones and overall negligible. We can conclude that our model is suitable to describe a wide variety of experiments involving double-well BECs. It would be interesting to explore as well the microscopic derivation of a spin-1/2 BEC in order to determine the connection with our model.

In summary, we introduced a model of two-mode Bose-Einstein condensate which includes not only two-body but also three-body interactions. We find an analytic solution and provide the full spectrum of eigenvalues and the corresponding eigenvectors. This allows us to analyse the role of three-body interactions in physical quantities of interest, such as the probability distribution of the relative population or the time evolution of its expectation value. We find that three-body collisions have non-trivial effects, such as significant changes in the probability distribution of the ground state or the inhibition of collapses in the evolution of the relative population of the modes. Our work provides insights into the effects of higher order collisions in the physics of a two component Bose-Einstein condensate. Following the formalism employed in this paper, higher-order collisions can also be included in the model.¹⁶

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