Analytical solution of a double-well Bose-Einstein Condensate

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We introduce a microscopic computation which shows that the Hamiltonian of a Bose-Einstein Condensate can be analytically solved in the two-mode approximation, in particular, in the case of an asymmetric double-well condensate in the dilute regime. Our model is exactly diagonalisable when the overlap of the quasilocalized modes in each well is small enough with respect to the trap asymmetry. For larger overlaps or highly symmetric traps, our diagonalisable Hamiltonian acquires extra terms that we treat within perturbation theory.

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The Hamiltonian of a two-mode Bose-Einstein condensate (BEC) has been extensively studied in the literature [1–5] due to its relative simplicity and application to double-well [4] or spin-1/2 [5] condensates.

In spite that the two-mode BEC corresponds to the most simple multi-mode situation, canonical models employed, such as the Bose-Hubbard Hamiltonian [1], cannot be solved analytically. Therefore, common techniques to study this system involve numerical methods, approximations (such as the use of Bethe ansatz) and semiclassical analysis (mean-field theory) where the modes are treated classically. However some of the authors of this paper have introduced a model which Hamiltonian can be diagonalized analytically [6, 7]. The model is a generalization of the Bose-Hubbard Hamiltonian which includes mode-exchange and coherent tunneling interactions previously ignored or neglected. Interestingly, physical effects produced by such interactions have been experimentally observed [8]. Since our model involves certain constraints among the different terms of the Hamiltonian, the question of to what extent it describes a realistic BEC remains open. This is the question that we address here.

In this paper we show that the exactly solvable model of the two-mode BEC introduced in [6, 7] can be derived from the microscopical description of a double-well BEC. Showing this simply involves a generalization of the modes commonly employed in the two-mode approximation. The microscopic calculation we carry out here yields directly the diagonalizable model plus extra-terms that can be treated perturbatively as long as the overlap between the quasi localised modes in each well is much smaller than the trap asymmetry. We find that this is indeed the case in a wide variety of experiments involving double-well BECs. The behaviour of the diagonalizable model under generic perturbations has already been studied in [9]. Exploiting these results we compute the relevant corrections of the eigenstates within perturbation theory. Thus, we provide a complete toolbox for the analytical description of a wide range of double-well BECs, which includes not only the ground state of the system but all the eigenvalues and eigenvectors.

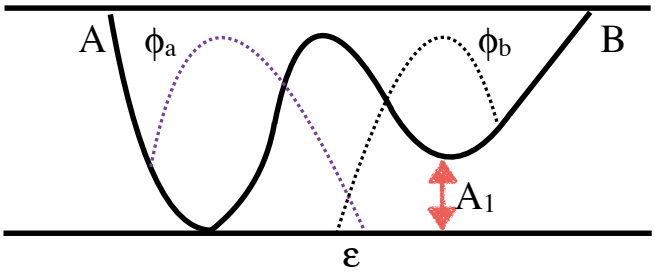

FIG. 1: An asymmetric double-well BEC consisting of wells A and B with energy offset A_1. ϕ_a, ϕ_B are almost-localised modes with a small overlap characterised by ϵ (see the text). In the Bose-Hubbard model, the two-mode approximation considers two equally balanced superpositions of ϕ_a and ϕ_b. Here, we consider a more general superposition (see Eq. (13) which allows to treat the Hamiltonian analytically, as long as $\epsilon << A_1$.

Let us discuss our results in more detail. We start with the microscopic description 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 collisions with s-wave scattering length a:

$$\begin{aligned}\hat{H} &= \hat{H}_1 + \hat{H}_2,\\ \hat{H}_1 &= \int d\mathbf{r}\big(-\frac{\hbar^2}{2m}\hat{\Psi}^\dagger\nabla^2\hat{\Psi} + \hat{\Psi}^\dagger V(\mathbf{r})\hat{\Psi}\big),\\ &= \int d\mathbf{r}\hat{\Psi}^\dagger H_t\hat{\Psi},\\ H_2 &= \frac{g}{2}\int d\mathbf{r}\hat{\Psi}^\dagger\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi},\end{aligned} \tag{1}$$

where $g = \frac{4\pi\hbar^2 a}{m}$ is the coupling strength and H_t is the Hamiltonian of the trap. The wavefunction $\hat{\Psi}$ can be expanded in terms of the eigenfunctions ϕ_i of the total Hamiltonian $\hat{H}$ and their corresponding annhilation operators $\hat{c}_i$ as

$$\hat{\Psi} = \sum_i \phi_i\hat{c}_i. \tag{2}$$

At absolute zero temperature and in the absence of particle collisions, all particles occupy the ground level of the single-particle Hamiltonian $\hat{H}_1$ producing a BEC. In this case, the ground-state wavefunction ϕ_S is symmetric. However, in the case that particles collide with interaction energy small compared to the single-particle energy, we can consider that particles occupy the two lowest eigenstates of the Hamiltonian, i.e the antisymmetric mode ϕ_A is also populated. In this case, a two-mode approximation is valid and the total wavefunction of the system is well described by

$$\hat{\Psi} = \phi_1 \hat{c}_1 + \phi_2 \hat{c}_2. \tag{3}$$

The real wavefunctions ϕ_1 and ϕ_2 are orthonormal modes $\int dr \phi_i \phi_j = \delta_{i,j}$ with $i, j = 1, 2$ which have a small transition amplitude such that

$$E_{12} = \int dr \phi_1 H_t \phi_2. \tag{4}$$

Typically, the modes in terms of the symmetric and antisymmetric solutions are written as,

$$\begin{aligned} \phi_1 &= \frac{1}{\sqrt{2}}(\phi_S + \phi_A), \\ \phi_2 &= \frac{1}{\sqrt{2}}(\phi_S - \phi_A). \end{aligned} \tag{5}$$

By substituting the two-mode approximation Eq. (10) in the Hamiltonian (1) we obtain,

$$\begin{aligned} H_1 &= E_1 c_1^\dagger c_1 + E_2 c_2^\dagger c_2 + E_{12}(c_1^\dagger c_2 + c_2^\dagger c_1) \\ H_2 &= U_{1111} c_1^{\dagger 2} c_1^2 + U_{2222} c_2^{\dagger 2} c_2^2 + +4U_{1212} c_1^\dagger c_2^\dagger c_1 c_2 \\ &+ 2U_{1112}(c_1^{\dagger 2} c_1 c_2 + h.c) + 2U_{2212}(c_2^{\dagger 2} c_1 c_2 + h.c) \\ &+ U_{1122}(c_1^{\dagger 2} c_2^2 + h.c) \end{aligned}$$

where

$$\begin{aligned} E_1 &= \int dr \phi_1 H_t \phi_1 \, , \, E_2 = \int dr \phi_2 H_t \phi_2, \\ U_{1111} &= \int dr \phi_1^2 \phi_1^2 \, , \, U_{2222} = \int dr \phi_2^2 \phi_2^2 \\ U_{1212} &= \int dr |\phi_1|^2 |\phi_2|^2 \, , \, U_{1112} = \int dr \phi_1^2 \phi_1 \phi_2 \\ U_{1222} &= \int dr \phi_2^2 \phi_1 \phi_2 \, , \, U_{1122} = \int dr \phi_1^2 \phi_2^2. \end{aligned} \tag{6}$$

The Hamiltonian Eq. (15)describes a constant number of particles $N = n_1 + n_2$ where

$$n_{1,2} = c_{1,2}^\dagger c_{1,2} \tag{7}$$

of them occupy mode $_{1,2}$ with corresponding energy $E_{1,2}$. The number of particles in each mode change with probability amplitude E_{12}. In addition to this, particles undergo same-mode collisions with scattering lengths U_{1111} and U_{2222}, elastic collisions between particles in different modes U_{1122} and mode-exchange collisions U_{1112}, U_{1222}, U_{1122}. While the latter terms are usually neglected, their effects have been observed in the laboratory [8] and they have been extensively discussed theoretically [7].

Let us now focus in double-well BECs and distinguish two cases of interest, namely symmetric and asymmetric potentials. We label the symmetric and antisymmetric solutions of the single particle Hamiltonian corresponding to the symmetric well as ϕ_A^s, ϕ_S^s and ϕ_A^a, ϕ_S^a the solutions in the asymmetric potential. Therefore, in the case of the symmetric potential the two-mode approximation corresponds to two almost-localized modes

$$\begin{aligned} \phi_1^s &= \frac{1}{\sqrt{2}}(\phi_S^a + \phi_A^a) \\ \phi_2^s &= \frac{1}{\sqrt{2}}(\phi_S^a - \phi_A^a). \end{aligned} \tag{8}$$

In the literature of double-well BECs [1], these modes are commonly labeled

$$\phi_1^s = \phi_a \, ; \, \phi_2^s = \phi_b \tag{9}$$

to emphasize that they are almost localized modes in well A and B respectively. We will use this notation here as well.

In the asymmetric potential case, we can write the modes ϕ_1^a and ϕ_2^a in terms of the symmetric quasilocalized modes,

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

It is easy to see that in terms of the symmetric and antisymmetric solutions of the symmetric potential we obtain

$$\begin{aligned} \phi_1^a &= \cos\Omega \phi_A^s + \sin\Omega \phi_S^s \\ \phi_2^a &= -\sin\Omega \phi_A^s + \cos\Omega \phi_S^s \end{aligned} \tag{10}$$

where $\Omega = \frac{1}{2}(\theta + \frac{\pi}{2})$. Note that we recover the symmetric case when $\theta = 0$.

We have introduced the set of quasilocalized modes because the integrals in the Hamiltonian are easily evaluated in the ϕ_a and ϕ_b basis. They are nearly normalized modes with $\int dr \phi_a \phi_a = 1 + \epsilon$, $\int dr \phi_b \phi_b = 1 - \epsilon$, where the amplitude of transition between them

$$\epsilon = \int dr \, \phi_a H_t \phi_b \tag{11}$$

is assumed to be very small. Therefore, all the fourth-order integrals containing both modes, such as :

$$I_1 = \int dr \phi_b^2 \phi_a^2 \, , \, I_2 = \int dr \phi_a^3 \phi_b, \, , \, I_3 = \int dr \phi_b^3 \phi_a \tag{12}$$

are of order $\mathcal{O}(\epsilon^2)$.

Relaxing the notation, the modes of the asymmetric potential are related with the quasilocalized modes by the transformation:

$$\begin{aligned}\phi_1 &= \cos(\theta/2)\phi_a - \sin(\theta/2)\phi_b \\ \phi_2 &= \cos(\theta/2)\phi_b + \sin(\theta/2)\phi_a. \end{aligned} \quad (13)$$

Note that for the case $\theta = 0$, the two-mode approximation becomes

$$\hat{\Psi} = \phi_a \hat{a} + \phi_b \hat{b}, \quad (14)$$

which yields a Hamiltonian which describe two non-interacting well-localised modes,

$$H = E_a a^\dagger a + E_b b^\dagger b + U_{aa} a^{\dagger 2} a^2 + U_{bb} b^{\dagger 2} b^2$$

with

$$\begin{aligned} E_a = \int dr \phi_a H_t \phi_a \, , \, U_{aa} = \int dr \phi_a^4, \\ E_b = \int dr \phi_b H_t \phi_b \, , \, U_{bb} = \int dr \phi_b^4. \end{aligned} \quad (15)$$

In this case the modes ϕ_a and ϕ_b become orthonormal. Another case of interest is that of $\theta = \pi/2$. In this case we obtain the two-mode approximation commonly used in the literature for a symmetric double well potential which leads to the well known Hubbard-Bose Hamiltonian after neglecting the terms corresponding to mode-exchange collisions U_{1212}, U_{1112}, U_{2212} and U_{1122}.

Here we consider a more general mode decomposition parametrized by the angle θ. However, this simple change has strong consequences. After evaluating the integrals in this new set of modes and adding the constant $-N$ we obtain the Hamiltonian,

$$H = \mathcal{H}_0 + \mathcal{H}^{'} + \mathcal{H}^{''} \quad (16)$$

where $\mathcal{H}_0$ is diagonalizable: [6, 7]

$$\begin{aligned} \mathcal{H}_0 &= A_1 \cos\theta (c_1^\dagger c_1 - c_2^\dagger c_2) + A_1 \sin\theta (c_1^\dagger c_2 + c_2^\dagger c_1) \\ &+ A_2 (1 + \cos^2\theta)(c_1^{\dagger 2} c_1^2 + c_2^{\dagger 2} c_2^2) + 4 A_2 \sin^2\theta c_1^\dagger c_2^\dagger c_1 c_2 \\ &+ 2 A_2 \cos\theta \sin\theta (c_1^{\dagger 2} c_1 c_2 - c_2^{\dagger 2} c_1 c_2 + h.c) \\ &+ A_2 \sin^2\theta (c_1^{\dagger 2} c_2^2 + h.c) \end{aligned} \quad (17)$$

and $\mathcal{H}^{'}$, $\mathcal{H}^{''}$ are of order $\mathcal{O}(\epsilon)$, $\mathcal{O}(\epsilon^2)$ respectively. Here

$$A_1 = \frac{1}{2}(E_a - E_b) \quad (18)$$

and

$$A_2 = \frac{1}{2} U \quad (19)$$

for $U = U_{aa} = U_{bb}$ assuming that the scattering length of particles in each mode is equal. Close attention must be taken in evaluating A_1 and A_2 since the wavefunctions must be renormalized before the integration is carried out. $\mathcal{H}_0$ describes a BEC in an asymmetric double-well potential. $c_1^\dagger c_1$ and $c_2^\dagger c_2$ correspond to the number of particles in each well. The wave functions ϕ_1 and ϕ_2 overlap giving rise to tunneling of particles through the potential barrier. Particles undergo on-site collisions $c_{1,2}^\dagger c_{1,2}^\dagger c_{1,2} c_{1,2}$ and in the overlapping region of the wavefuntions particles of different wells can collide $c_1^\dagger c_2^\dagger c_2 c_1$. Two other interesting effects are present in the Hamiltonian. One of them in coherent tunneling in which two particles collide and tunnel as a single particle $c_{1,2}^\dagger c_{1,2}^\dagger c_{2,1} c_{2,1}$. These effects has already been observed in laboratory. A less known effect is collision assisted tunneling in which a particle tunnels thanks to energy gained during a on-site collision $c_1^\dagger c_1^\dagger c_1 c_2$.

The eigenstates of the Hamiltonian $\mathcal{H}_0$ are

$$|\Phi_{n_1,n_2}\rangle = \exp(\frac{\theta}{2}(c_1^\dagger c_2 - c_1 c_2^\dagger))|n_1, n_2\rangle \quad (20)$$

with corresponding eigenenergy

$$E_{n_1,n_2} = A_1(n_1 - n_2) + A_2(n_1 - n_2)^2. \quad (21)$$

Note also that the two-mode approximation requires that on-site interactions are much stronger than the interactions between particles in different wells. This is possible if we restrict ourselves to small values of θ such that

$$\sin\theta \simeq \theta << 1 \, , \, \cos\theta \simeq 1. \quad (22)$$

Let us consider the term $\mathcal{H}^{'}$,

$$\mathcal{H}^{'} = -\epsilon(\frac{\theta}{2}(c_1^\dagger c_1 - c_2^\dagger c_2) + c_1^\dagger c_2 + c_2^\dagger c_1), \quad (23)$$

where we have already assumed the approximation in Eq. (22).

By comparing Eqs. (17) and (23), we see that we can treat $\mathcal{H}^{'}$ as a perturbation, as long as $\epsilon << A_1\theta$. This is indeed the case in a wide variety of experiments involving double-well condensates [10–12]. The tunnelling rate $E_{12} \simeq A_1\theta + \epsilon$ takes experimental values ranging from $5 \cdot 10^{-4}$ Hz $\times h$ [11] to 2 Hz $\times h$ [10], while the energy offset between the wells can be as high $A_1 = 530$ Hz $\times h$ [12]. Even if the wells are intended to be perfectly symmetric, the uncertainty in the trap depth leads us to assume a minimum trap asymmetry of $A_1 \simeq 20$ Hz $\times h$ [10].

Using the results in [9], we find the following non-vanishing matrix elements in perturbation theory:

$$\begin{aligned} \langle \Phi_{n_1\, n_2} | H^{'} | \Phi_{n_1\, n_2} \rangle &= -\frac{3}{2}\epsilon\, \theta\, (n_1 - n_2) \\ \langle \Phi_{n_1+1\, n_2-1} | H^{'} | \Phi_{n_1\, n_2} \rangle &= -\epsilon\sqrt{n_2\, (n_1 + 1)} \\ \langle \Phi_{n_1-1\, n_2+1} | H^{'} | \Phi_{n_1\, n_2} \rangle &= -\epsilon\sqrt{n_1\, (n_2 + 1)}. \end{aligned} \quad (24)$$

Now let us discuss the term $\mathcal{H}^{''}$, which includes all the fourth-order integrals containing both modes:

$$\begin{aligned} \mathcal{H}^{''} &= 4\, I_1 c_1^\dagger c_2^\dagger c_1 c_2 + 2\, I_2 (c_1^{\dagger 2} c_1 c_2 + h.c) \\ &+ 2\, I_3 (c_2^{\dagger 2} c_1 c_2 + h.c) + I_1 (c_1^{\dagger 2} c_2^2 + h.c) + \mathcal{O}(\theta) \end{aligned} \quad (25)$$

where the $\mathcal{O}(\epsilon^2)$ integrals I_1, I_2, I_3 are defined in Eq. 12. The leading contributions to the non-vanishing matrix elements of the perturbation are:

$$\begin{aligned}
\langle \Phi_{n_1\,n_2}|H^{'}|\Phi_{n_1\,n_2}\rangle &= 4\,n_1\,n_2\,I_1 \\
\langle \Phi_{n_1+1\,n_2-1}|H^{'}|\Phi_{n_1\,n_2}\rangle &= 2\,(I_2+\,I_3)\sqrt{n_2\,(n_1+1)} \\
\langle \Phi_{n_1-1\,n_2+1}|H^{'}|\Phi_{n_1\,n_2}\rangle &= 2\,(I_2+\,I_3)\sqrt{n_1\,(n_2+1)} \\
\langle \Phi_{n_1+2\,n_2-2}|H^{'}|\Phi_{n_1\,n_2}\rangle &= I_1\sqrt{(n_1+1)\,(n_1+2)\,n_2\,(n_2-1)} \\
\langle \Phi_{n_1-2\,n_2+2}|H^{'}|\Phi_{n_1\,n_2}\rangle &= I_1\sqrt{(n_2+1)\,(n_2+2)\,n_1\,(n_1-1)}
\end{aligned}$$

The behaviour of several physical quantities of interest in a model described by a Hamiltonian $\mathcal{H}_0$ under generic perturbations with the same mathematical structure as $\mathcal{H}^{'}$ and $\mathcal{H}^{''}$ was thoroughly discussed in [9].

In summary, we introduce a toolbox for the analytical description of a two-mode BEC. Our results are found by means of a generalisation of the modes commonly used in the two-mode approximation. The Bose-Hubbard model corresponds to a particular case of the modes we introduce here. An important advantage of our scheme is that it includes mode-exchange and coherent tunnelling interaction terms that have been observed experimentally and are typically neglected. Moreover, while the Bose-Hubbard hamiltonian is commonly solved numerically, our model can be fully treated with analytical methods. We not only find the ground state but the full spectrum and the eigenstates. We believe that this will be of great benefit for quantum information and metrology application with BEC setups. As a first example of interest, our discussion has been focused on the asymmetric double-well BEC. However, the theory we have here developed can be applied to a more general situation since the only assumptions we have made are that the condensate wavefunction can be approximated by two modes and that the transition amplitude between them is very small. For instance, a case of interest is a single-well Bose-Einstein condensate consisting of atoms in two hyperfine levels [5]. In such case, mode-exchange collisions have been predicted by microscopic calculations [13]. The exactly solvable model can be generalized to the multi-mode case (including optical lattices) and many-body interactions. It is therefore of great interest to explore as well the microscopic derivation of those cases.

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