## Coupled atomic-molecular condensates in a double-well potential: decaying molecular oscillations

H.  $\mathrm{Jing}^{1,2,3,\mathrm{a}},\,\mathrm{S.}~\mathrm{Gu}^{1,3},\,\mathrm{and}$  M.  $\mathrm{Zhan}^{1,3}$ 

<sup>1</sup> State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics,

Wuhan Institute of Physics and Mathematics, Chinese Academe of Science, Wuhan 430071, P.R. China

 $^{2}\,$  Department of Chemistry, Hong Kong University of Science and Technology, Kowloon, Hong Kong

<sup>3</sup> Center for Cold Atoms, Chinese Academe of Science, P.R. China

Received 30 October 2005 / Received in final form 10 February 2006 Published online 5 May 2006 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2006

**Abstract.** We present a four-mode model that describes coherent photo-association (PA) in a doublewell Bose-Einstein condensate, focusing on the *average* molecular populations in certain parameters. Our numerical results predict an interesting strong-damping effect of molecular oscillations by controlling the particle tunnellings and PA light strength, which may provide a promising way for creating a stable molecular condensate via coherent PA in a magnetic double-well potential.

**PACS.** 03.75.Nt Other Bose-Einstein condensation phenomena – 03.75.Mn Multicomponent condensates; spinor condensates – 05.30.Jp Boson systems

The remarkable realizations of Bose-Einstein condensates (BEC) in cold dilute atomic gases have provided a rich playground to manipulate and demonstrate various properties of quantum degenerate gases [1]. Recently rapid advances have been witnessed for creating a quantum degenerate molecular gaze via a magnetic Feshbach resonance [2,3] or an optical photo-association (PA) [4,5] in an atomic BEC, and the appealing physical properties of the formed atom-molecule mixtures were investigated very extensively under the quasi-homogeneous trapping conditions [2–5]. The coherent PA process not only produces a new species of BEC but also leads to many interesting quantum statistical effects due to its nonlinear coupling nature in the dynamics [6]. On the other hand, the pure atomic condensates in a double-well potential also attracted considerable interest since many intriguing quantum phenomena really can appear in this system [7], hence a natural question arises about the possible new properties of a hybrid atom-molecule condensate in a double-well potential, by adding an additional associating light. This problem is also related to that of molecular formations via PA in an optical lattice [8].

In fact, our previous work in three-mode case already showed that [9], the coherent PA process in the case of an atomic output coupler really leads to some novel quantum statistical phenomena, e.g., the squeezing-free effect for molecules formed by photo-association of atoms in the propagating mode [9]. In this paper, we present an effective mean field approach (MFA) to study the average molecular populations in two wells by numerically solving the general depleted case beyond short-time limits. We find that, just for valid MFA parameters range, the new freedoms of atomic tunnelling and then the formed molecules can *strongly* influence the molecular occupations, meanwhile the associating light strength also can play a notable different role. In particular, the novel effect of strong decaying molecular oscillations (without or with molecular tunnelling in the deep- or shallow-well case) can be revealed by adjusting these two parameters. A simple physical picture for this effect is given by comparing with the well-known two-color free-bound-bound PA case [10], which clearly shows a promising way to create a stable molecular condensate via coherent "double-well PA" technique.

Turning to the situation of Figure 1, we assume for simplicity that large number of Bose-condensed atoms are loaded into, say, the right side of a double-well magnetic potential, and the coherent PA only happens in the left site. The dynamics of double-well atomic condensates can be described by a simple model [7] which includes the Kerr-type atomic interactions occupying the same or different wells. However, the atomic collisions effects on the dynamics of double-well condensates are wellknown [7,11] and its strength can be tuned by the technique of magnetic-field-induced Feshbach resonance [12], hence, to see clearly the results of nonlinear PA interactions in presence of particles tunnelling, we naturally ignore it for present purpose (the strengths for the molecules or atom-molecule collisions are yet not known [5]). In the

<sup>&</sup>lt;sup>a</sup> e-mail: jinghui@wipm.ac.cn



Fig. 1. A sketch of the coherent photo-association (PA) process in a magnetic double-well potential. Initially, the atomic component A is entirely trapped in the right site, the coherent PA only happens in the left site.

second quantized notation, boson annihilation operators for trapped atoms and molecules in two wells are denoted by  $a_1, a_2, b_1$  and  $b_2$ , respectively. The free part of the total Hamiltonian are written as  $H_0 = -\Delta a_1^{\dagger} a_1 - \delta b_1^{\dagger} b_1$ , where  $\Delta$  and  $\delta$  are the magnetic and optical detunings respectively, and generally, one should also consider the possible effects of these detunings [5], but here we focus attention on the most interested effects in this system due to the interactions of different modes (i.e., the resonance case). Defining the optical Rabi coupling frequency as  $\gamma$ , the four-mode Hamiltonian can be written as  $H = H_0 + H_{int}$ , where the interaction part is ( $\hbar = 1$ )

$$H_{int} = -G_a(a_1^{\dagger}a_2 + a_2^{\dagger}a_1) - G_b(b_1^{\dagger}b_2 + b_2^{\dagger}b_1) -\gamma(a_1^{\dagger^2}b_1 + b_1^{\dagger}a_1^2),$$
(1)

and  $G_a$  ( $G_b$ ) is the atomic (molecular) tunnelling term, and  $\gamma$  represents an effective Rabi frequency characterizing the coherent PA process applied for an *arbitrary* time interval. For simplicity, we have ignored the incoherent process of the excited-state molecular damping or the effect of molecular dissociating into those non-condensate atomic modes [13]. It is important to realize that the tunnelling rate of the molecules is exponentially suppressed compared to the tunnelling rate of the atoms since the molecule is twice as heavy as the atom and the tunnelling amplitude is proportional to  $e^{-\sqrt{2mV_0/\hbar^2}d}$ , where m is the mass,  $V_0$  the barrier height, and d the barrier thickness. This means that the values of  $G_a$  and  $G_b$  are correlated instead of two independent parameters. Obviously a conserved quantity exists for the present system:  $\sum_{i=1}^{2} (a_i^{\dagger} a_i + 2b_i^{\dagger} b_i) \equiv N$ , where N is the total atom number for a condensate of all atoms or twice the total molecule number of a condensate of all molecules.

Note that the main feature of our present scheme is that the coherent PA process starts not directly in the initial trapped atomic condensate, but in the "developing" atomic mode which is initially in a vacuum state. The Heisenberg equations of motion for the atomic and molecular modes read

$$\dot{a}_1 = iG_a a_2 + 2i\gamma a_1^{\dagger} b_1, \quad \dot{a}_2 = iG_a a_1; \dot{b}_1 = iG_b b_2 + i\gamma a_1^2, \qquad \dot{b}_2 = iG_b b_1.$$
(2)

The mean field approximation replaces the operators  $a_i$ and  $b_i$  by *c*-numbers, i.e.  $a_i \rightarrow \alpha_i$ ,  $b_i \rightarrow \beta_i$  (i = 1, 2), then we have the following simple *c*-number differential equations

$$\dot{\alpha}_1 = iG_a\alpha_2 + 2i\gamma\alpha_1^*\beta_1, \quad \dot{\alpha}_2 = iG_a\alpha_1; \dot{\beta}_1 = iG_b\beta_2 + i\gamma\alpha_1^2, \qquad \dot{\beta}_2 = iG_b\beta_1,$$
(3)

where  $\alpha_i$  and  $\beta_i$  (i = 1, 2) are two complex numbers. Such replacement is the so-called semiclassical approach analogous to the Gross-Pitaevskii approximation used to describe an alkali condensate [3,4]. It is completely accessible to also incorporate the molecular damping terms  $\xi \beta_i$ phenomenologically into the molecular-mode equations for our numerical study ( $\xi$  is proportional to the molecular damping rate), but we would not consider it here for two physical reasons: firstly we mainly focus on the role of coherent PA process in the double-well situation and, comparing with the well-known single-well PA case, these additional damping terms fail to bring any qualitatively new results for the evolutions of average molecular occupations in our model; secondly, some techniques can be used to minimize the effects of these quasi-bound molecular damping terms, such as the Feshbach-resonanceassisted stimulated adiabatic passage (STIRAP) method, proposed by Ling et al. through the MFA [14].

We remark that the MFA in our model should have a limited range of validity. In particular, it certainly should break down and be replaced by a fully quantized theory when the effects of quantum *fluctuations* become important. For example, by directly starting from equation (2), we have analyzed the quantum dynamics and statistics in the short-time and undepleted limits (without molecular tunnelling) [9]. Of course, the precise criteria for the validity of MFA in our model will be known only when the generalization to the more interested long-time depleted case is available. Nevertheless, one would expect that its range of validity should include a certain variety of phenomena of interest, especially when the concerned problem is the average molecule numbers under certain parameters [6]. In fact, the coherent two-color PA process in an atomic BEC was already experimentally realized most recently which can be well described by a mean-field three-mode model [4]. Interestingly, we will see that some nontrivial results really can be revealed by the MF approach also in the present model.

To see concrete examples, we have analyzed the different dynamical behaviors for the molecule numbers in two wells under the conditions of deep- and shallow-well cases, respectively, and compared these behaviors with that of single-well case, which indicates a quite different but interesting way to create a stable molecular condensate by using this double-well potential.



Fig. 2. (Color online) The molecular numbers in a deep doublewell case (a), (b) without or (c), (d) with molecular tunnelling. The decaying molecular oscillations can be seen in (c), (d) for larger PA strength. The two couplings (in units KHz) and temporal length can be limited within validity range of MF approach [6].

(i) Deep double-well case. The results about the dynamical evolutions of molecular numbers can be shown as Figure 2 by numerically solving equation (3). The initial atoms is typically 5000 [5]. Clearly, if one only consider the atomic tunnelling, the PA leads to an increasing of molecule number in left site, as it should be. However, comparing with the single-well case (see the later), the molecular formation which happens in an initial vacuum instead of a trapped condensate will not need a strong PA light. More interestingly, when we take the molecular tunnelling into account, similar phenomena like that of two-color PA with "molecular tunnelling" term [10] can be observed, i.e., almost all the formed molecules accumulate in *right* site, meanwhile the strong PA light leads to decaying molecular oscillations with time. A similar physical picture can also be given for this [14]: the *interference* of two transitions (i.e., the transition of left-well atoms to the molecules and then the transition of left-well molecules to right-well molecules) under certain parameters leads to its effectively zero occupation and then the accumulations of photoassociated molecules in a different site. Note that, for ensuring the validity range of MFA, the two couplings and the temporal length are carefully reduced [6, 14].

(ii) Shallow double-well case. The evolutions of the molecular numbers are shown in Figure 3, which clearly shows the different roles of atomic and molecular tunnellings in coherent molecular formations. For much strong ratomic tunnelling and strong PA light, we find strong decaying molecular oscillations which, together with other useful techniques [5,10,14], may provide a promising way to obtain more stable molecular condensate via a double-well potential. Note that, this results are based on our mean-field zero-dimensional model under the approximation of density homogeneity within two

wells, although it can be possible to estimate the inhomogeneity effect in the Thomas-Fermi limit [14].

(iii) Single-well case. For a clear comparison, we also plot the short- and long-time behaviors of molecule numbers evolutions for single well case as in Figures 4a and 4b, respectively. The only control parameter now is the PA light strength. Obviously, although stronger PA light induces rapid molecules increasing, it also leads to rapid molecular oscillations for long evolution time, which should be avoided in any actual experiment. Thereby the considerable decaying of molecular oscillations in our scheme, especially for long evolution time, obtained by controlling particle tunnellings and PA light strength, may shed some new light on current experimental efforts towards a stable molecular condensate.

We should emphasis again that, in our mean-field zerodimensional model, the only used approximation is the atomic density homogeneity within two wells. Although we have ignored the atomic collisions and the molecular damping as explained above, these terms would be simple to include in the model especially in the high coupling limits where their effects on the spatial structure can be much reduced. Also it would be interesting to adopt the MFA beyond zero-dimensional model [5,15].

Summing up, we have numerically examined an interesting scheme for creating a molecular condensate via coherent PA of the Josephson tunnelling atoms in a doublewell potential, focusing on the *average* molecular numbers in two wells. Since one of the main problems of creating molecules by PA is that the same lasers also tend to destroy the molecules and and thus it is of interest to be able to move the molecules away from the lasers as quickly as possible. Our scheme here may provide a promising way for creating a stable molecular condensate via PA process



Fig. 3. (Color online) The molecular numbers in a shallow doublewell case with (a), (b) weak or (c), (d) strong molecular tunnelling. Stronger couplings are not probed (for reducing valid evolutions [6]). The tunnelling strength of molecules is dependent on that of atoms. The decaying oscillations also can be seen in, e.g., (d).

Fig. 4. (Color online) The populations of atoms  $N_a (= |\alpha|)^2$  and molecules  $N_b (= |\beta|^2)$  in a single well, for (a), (b) the short-time or (c), (d) the long-time case (for the comparison with the double-well PA case).

in a double-well potential. Based on a non-linear meanfield theory of a four mode model, we found that for certain parameter regimes the molecules accumulate in the well without the PA laser. We analyzed the different roles of atomic and molecular tunnellings and that of PA light strength in the molecular formations, through which an interesting strong-decaying effect was observed for the rightsite molecular oscillations in the case of strong atomic tunnelling and strong PA light strength (with PA process only happening in the left site). This is quite different from the simple single-well case. In fact our scheme can be viewed as further generalization of two-color PA (only with "molecular tunnelling" [10,14]).

Of course, even more important phenomena due to quantum fluctuations of matter-wave fields, like the quantum statistics of the resulting fields, can be investigated only by methods beyond any mean-field approach. A powerful numerical technique based on the *c*-number stochastic equations in the positive-P representation of quantum optics [16] may be used to study these intriguing subjects as in the extensive studies of two-color PA process [5, 15], which may comprise the future works.

Note added: After the submission of this paper, we note a very recent work of Olsen and Drummond in which a similar model was presented and then solved by the methods of *c*-number stochastic equations within, however, a quite different framework of (coupled intracavity) optical downconverters [17].

We are grateful to the referees for their kind suggestions which have lead to considerable improvement of this paper. We also thank Shuai Kang, Jing Cheng and Yi-Jing Yan for their helpful discussions. This work was supported by Wuhan Youth Chenguang Project and the NSFC (10304020, 10574141).

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