Quantum oscillations in a two-mode atom-molecule Bose-Einstein condensate – the discrete WKB approach

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Quantum effects in a system of coupled atomic and molecular Bose-Einstein condensates in the framework of a two-mode model are studied numerically and analytically, using the discrete WKB approach. In contrast to the mean-field approximation, the WKB analytical results are in a very good agreement with numerical results. The quantum fluctuations of the atomic and molecular populations are calculated, and found to be of the same order of magnitude as their mean values.

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I. INTRODUCTION

There is a growing interest in super-chemical properties of weakly interacting gases in the Bose-Einstein condensate (BEC) state. One of the major goals in this field is to produce a molecular Bose-Einstein condensate. To date, this has been achieved by creating it from an atomic BEC. Two routes are mainly used: ultra-cold molecules are formed by photo-association of atoms in a BEC or they are produced by applying a time-varying magnetic field near a Feshbach resonance.

One of the first theoretical attempts to describe the production of a molecular BEC via Raman photo-association of an atomic BEC has been put forward in Ref. [7]. There, the possibility of coherent formation of a molecular BEC is treated using a parametric field theory. In Ref. [8], a two-mode quantum Hamiltonian was proposed, that accounts for the statistics of both the atoms and the molecules. In this model, large amplitude nonlinear oscillations between atomic and molecular condensates are observed, that are damped away at long times. Using the same two-mode model, the dynamical evolution of an atomic-molecular BEC has been investigated in Ref. [9] and compared to the mean-field theory predictions. One of the conclusions drawn in this paper is that, large amplitude atomic-molecular oscillations, which were predicted in Ref. [8] on the basis of mean-field results, are damped by the rapid growth of fluctuations near the dynamically unstable molecular mode. Within the same framework, the bi-stability and quantum fluctuations in coherent photo-association of a BEC have been considered in Ref. [10]. The number statistics of the
two-mode model have also been compared to the number statistics of normal atomic Fermi gases and of Fermi systems with pair (BCS) correlations\textsuperscript{11}. Quite recently a coherent superposition of atoms and molecules condensate was observed in a Rb Bose-Einstein condensate by using a stimulated Raman adiabatic passage\textsuperscript{12}

In this paper, we show that, in the two-mode model proposed in Ref.\textsuperscript{8}, the expectation value of the population imbalance between atoms and molecules, as well as the level fluctuations, depend drastically on the initial value of the imbalance. We study this problem numerically and analytically. Our analytical results, based on the discrete WKB method developed in Ref.\textsuperscript{13}, are confirmed by the numerical solution of the exact quantum equations.

\section{II. THE MODEL}

We consider the simplest model of atomic-molecular condensate, consisting of an atomic mode $A$ and a molecular mode $B$. Let $b(b^\dagger)$ and $a(a^\dagger)$ be the annihilation (creation) operators for the molecular field $B$ and the atomic field $A$, respectively. The two modes are coupled coherently by an association-dissociation process of a Fermi-resonance\textsuperscript{14} type, and the effective Hamiltonian has the form

\begin{equation}
H = \frac{\Delta}{2} a^\dagger a + \frac{\chi}{\sqrt{V}} (b^\dagger a a + a^\dagger a^\dagger b) \tag{1}
\end{equation}

where the detuning parameter $\Delta = 2\mu_a - \mu_m$ characterizes the difference between the chemical potentials of the molecular ($\mu_m$) and the atomic ($\mu_a$) modes. In the case of coherent photo-association of a Bose-Einstein condensate, the Fermi-coupling parameter $\chi/\sqrt{V}$ (Rabi frequency) depends on the volume $V$ of the system\textsuperscript{15}.

Using Hamiltonian (1), the Heisenberg equations for the operators\textsuperscript{20}

\begin{equation}
\dot{n}(t) = a^\dagger(t) a(t), \quad \dot{x}(t) = b^\dagger(t) a(t)^2 + a^\dagger(t)^2 b(t) \quad \text{and} \quad \dot{y}(t) = i (b^\dagger(t) a(t)^2 - a^\dagger(t)^2 b(t)), \tag{2}
\end{equation}

are given by

\begin{equation}
\frac{d\hat{n}(t)}{dt} = \frac{\chi}{\sqrt{V}} \hat{y}(t), \quad \frac{d\hat{x}(t)}{dt} = -\Delta \hat{y}(t), \quad \frac{d\hat{y}(t)}{dt} = \Delta \hat{x}(t) - \frac{\chi}{\sqrt{V}} (3\hat{n}(t)^2 - 2N\hat{n}(t) - N). \tag{3}
\end{equation}

The total number of atoms in the system, $N = a^\dagger a + 2b^\dagger b$, is a conserved quantity.

In the mean-field approximation, $\langle \hat{n}^2 \rangle \approx \langle \hat{n} \rangle^2$, where $\langle \ldots \rangle$ stands for the average over the initial state of the system. Neglecting the term $\chi N/\sqrt{V}$ which is of order $N$ times less than the remaining terms in the right-hand side of Eq. (3), the equations of motion for $(x(t), y(t), n(t))$ have stationary point $(0, 0, 0)$, which corresponds to the entire population being in the molecular mode. However, for $\Delta^2 < 2\chi^2 \nu$, where $\nu = N/V$ is the concentration of atoms in the system, this state is dynamically unstable\textsuperscript{8}. It is one of the goals of this paper to go beyond the mean-field approximation and to clarify the behaviour of an atomic-molecular Bose-Einstein condensate in the limit of strong Fermi-coupling.

\section{III. DYNAMICAL EVOLUTION OF THE NUMBER OF ATOMS}

In what follows, we shall use the basis of states

\begin{equation}
|n_a, n_b\rangle = \frac{(a^\dagger)^n_a (b^\dagger)^n_b}{\sqrt{n_a! n_b!}} |0\rangle. \tag{4}
\end{equation}

Because the total number of atoms, $N$, is conserved, $|n_a, n_b\rangle = |n_a, (N - n_a)/2\rangle \equiv |n_a\rangle$. Notice that $n_a$ and $N$ have same parity. For the sake of simplicity, we assume $N$ even and put $N = 2P$, $n_a = 2p$ ($p \in \{0, 1, 2, \ldots, P\}$). We look
for a solution of the Schrödinger equation $H |\phi\rangle = E |\phi\rangle$ in the form $|\phi\rangle = \sum_{p=0}^{P} C_p |2p\rangle$. The coefficients $C_p$ satisfy the set of equations

$$EC_p = \Delta_p C_p + \frac{2}\sqrt{V} \left( f(p) C_{p-1} + f(p+1) C_{p+1} \right), \quad p \in \{0, 1, 2, \cdots, P\},$$  \tag{5}$$

with

$$f(p) = \sqrt{p(p-1)}(P + 1 - p).$$  \tag{6}$$

The number of possible energies and eigenstates, $\{E^{(\alpha)}, |\phi^{(\alpha)}\rangle\}$, is $P + 1$. In a system containing initially $n_0 = 2p_0$ atoms, the expectation value of the fraction of atoms, $z(t) = n(t)/N$, evolves according to

$$z(t) = \frac{1}{N} \left( n_0 e^{i\hat{H}t} n e^{-i\hat{H}t} |n_0\rangle \right) = \mathcal{Z} + \sum_{\alpha < \alpha'} I_{\alpha,\alpha'}(n_0) \cos \omega_{\alpha,\alpha'} t,$$  \tag{7}$$

where

$$\mathcal{Z} = \lim_{T \to \infty} \frac{1}{T} \int_0^T z(t) \, dt = \frac{2}{N} \sum_{\alpha} \left( \frac{C^{(\alpha)}_{p_0}}{C^{(\alpha)}_p} \right)^2 \sum_{p} p \left( \frac{C^{(\alpha)}_p}{C^{(\alpha)}_p} \right)^2$$  \tag{8}$$

represents the constant (dc-) part of $z(t)$ and

$$I_{\alpha,\alpha'}(n_0) = \frac{4}{N} C^{(\alpha')}_{p_0} C^{(\alpha)}_p \sum_{p} p C^{(\alpha')}_p C^{(\alpha)}_p$$  \tag{9}$$

are the respective intensities of the $P(P + 1)/2$ frequencies $\omega_{\alpha,\alpha'} = E^{(\alpha')} - E^{(\alpha)}$, $\alpha' > \alpha$, appearing in the system.

**IV. DISCRETE WKB SOLUTION**

To gain some insight into the dynamics of the system, we use the so-called discrete WKB-approach (see Ref. [13]) to solve the three-term recurrence equation [6] in the limit where $P \gg 1$. We introduce a new variable $x = p/P$ and consider the coefficients $C(p) = C(xP) \equiv c(x)$ as functions of the continuous variable $x$. Now, up to order 2 in $\epsilon \equiv 1/P$, Eq. [6] reads

$$\left( \lambda - \delta x \right) c(x) - \left( \epsilon (\partial_x F) \sinh (\epsilon \partial_x) + 2F \cosh (\epsilon \partial_x) \right) c(x) = 0$$  \tag{10}$$

where $\lambda = E/\sqrt{2\nu} P$, $\delta = \Delta/\sqrt{2\nu} P$ and $F(x) = P^{-3/2} f(xP + 1/2) \approx x \sqrt{1 - x}$. We now use the WKB method to treat equation [10]. We look for a solution in the form $c(x) = \exp \left\{ \frac{i}{\epsilon} S(x) \right\}$. Noting that $i \exp \left\{ i \partial_x S \right\} = i S' \exp \left\{ \frac{i}{\epsilon} S(x) \right\}$ and expanding the “action” $S(x)$ as a power series in $\epsilon$, $S = S_0 + \epsilon S_1$, we finally obtain

$$\epsilon^0 : \quad \cos S'_0 = \frac{\lambda - \delta x}{2F}, \quad \text{and} \quad \epsilon^1 : \quad S_1 = -\frac{1}{2} \ln (F \sin S'_0).$$  \tag{11}$$

The “classically allowed region” corresponding to this problem is determined by the inequality

$$x_{-}(\lambda) < x < x_{+}(\lambda),$$  \tag{12}$$

where the turning points $x_{\pm}(\lambda)$ are solutions to

$$\left( \lambda - \delta x \right)^2 = 4F^2(x).$$  \tag{13}$$
From (11), the semi-classical quantization rule for the spectrum can be shown to be given by

\[ S(\lambda) = \int_{x-(\lambda)}^{x+(\lambda)} dx \arccos \left( \frac{\lambda - \delta x}{2F(x)} \right) = (\alpha + \frac{1}{2}) \pi, \]

where \( \alpha \) is a non-negative integer [13]. This relation yields the number of states with energy lower than \( \lambda \), \( \alpha(\lambda) \), whose derivative is the density of state given by

\[ \rho(\lambda) = \left| \frac{d\alpha(\lambda)}{d\lambda} \right| = \frac{1}{\pi} \int_{x-(\lambda)}^{x+(\lambda)} \frac{dx}{v(x, \lambda)}. \]

The “velocity” \( v(x, \lambda) \) is given by \( v(x, \lambda) = \sqrt{4F^2(x) - (\lambda - \delta x)^2}. \) An approximate expression for the coefficients inside the allowed region is

\[ c(x, \lambda) = \frac{A}{\sqrt{v(x, \lambda)} \cos \left( \frac{1}{\epsilon} S_0(x, \lambda) + \theta \right)} \] where \( S_0(x, \lambda) = \int_{x-(\lambda)}^{x} dx' \arccos \left( \frac{\lambda - \delta x'}{2F(x')} \right) \).

The angle \( \theta \) depends on the position of the turning points [13] but its expression is not needed in what follows. We will consider that, outside the allowed region, \( c(x, \lambda) \) decays fast enough to be neglected. The normalization constant \( A \) is determined from the relation

\[ 1 = \sum_{p=0}^{P} |C_p(E)|^2 \approx P \int_{x-(\lambda)}^{x+(\lambda)} A^2 \cos^2 \left( \frac{1}{\epsilon} S_0(x, \lambda) + \theta \right) dx \approx P \pi A^2 \rho(\lambda). \]

To obtain the last equality, we have replaced the rapidly varying \( \cos^2(S_0/\epsilon) \) by its average value \( 1/2 \). This yields eventually

\[ c(x, \lambda) = \begin{cases} \sqrt{\frac{2}{\pi P\rho(\lambda)v(x, \lambda)}} \cos \left( \frac{1}{\epsilon} S_0(x, \lambda) + \theta \right), & x-(\lambda) \leq x \leq x+(\lambda) \\ 0, & \text{otherwise}. \end{cases} \]

V. ATOMIC AND MOLECULAR POPULATIONS

As already mentioned in the introduction, mean-field theory predicts the existence of large-amplitude coherent oscillations between atomic and molecular phases [6], while numerical simulations [9] suggest that these oscillations are strongly damped. It is therefore important to clarify the long-time behaviour of the atomic-molecular BEC. To do so, we propose to evaluate the \textit{dc-component} of the atomic population, \( \overline{z} \). It follows from Eqs. (8) and (18), that this quantity can be expressed as

\[ \overline{z} = \frac{1}{P} \sum_{\alpha} \left( \frac{C_{p_0}(\alpha)}{C_{p_0}} \right)^2 \sum_p p \left( \frac{C_p(\alpha)}{C_p} \right)^2 \approx P^2 \int_{\lambda-(x_0)}^{\lambda+(x_0)} d\lambda \rho(\lambda) c^2(x_0, \lambda) \int_{x-(\lambda)}^{x+(\lambda)} dx x c^2(x, \lambda) \approx \frac{1}{\pi^2} \lambda+(x_0) \left( \int_{x-(\lambda)}^{x+(\lambda)} \frac{x}{v(x, \lambda)} \right) \rho(\lambda) d\lambda, \]

where

\[ g(\lambda) = \int_{x-(\lambda)}^{x+(\lambda)} \frac{x}{v(x, \lambda)}. \]
In deriving Eqs. (19) and (20), we have taken into account the fast oscillating nature of $C_p(E)$ as a function of $p$ for $E$ fixed (see Fig.1), and therefore, $\cos^2\left(\frac{1}{r}S_0\right)$ has been systematically replaced by $1/2$. Integrations in Eqs. (19) and (20) can be carried out (see e.g. [17]) and as a result, we find the dc-component of the atom population to be

$$
\tau = \frac{1}{\pi} \int_{\lambda-(x_0)}^{\lambda+(x_0)} \left\{ x_t(\lambda) + (x_+ + x_0) \right\} \frac{E(m)}{K(m)} \frac{d\lambda}{v(x_0, \lambda)} \tag{21}
$$

where $x_t(\lambda)$ is the third root of Eq. (13) ($x_t \leq x_- \leq x_+$), $K(m)$ ($E(m)$) is the complete elliptic integral of the first (second) kind [16] with parameter $m = (x_+ - x_0)/(x_+ + x_0)$, and $\lambda_\pm = \delta x_0 \pm 2F(x_0)$. For weak detuning, $|\delta| < \sqrt{1-x_0}$, expression (21) is well approximated by

$$
\tau \approx \frac{2}{\pi} (1-\delta^2) \left\{ \arcsin \left( \frac{\sqrt{\lambda_+/(\lambda_+ - \lambda_-)}}{\ln (8(1-\delta^2)/\lambda_+)} \right) + \arcsin \left( \frac{\sqrt{\lambda_-/(\lambda_- - \lambda_+)}}{\ln (8(1-\delta^2)/|\lambda_-|)} \right) \right\}. \tag{22}
$$

Fig. 2 shows the dc-component of the expectation value of the molecular mode population $z_{mol} \equiv (1-\tau)/2$, in the resonant case $\delta = 0$, as a function of the initial value of the atomic mode population $z_0 \equiv z(0)$. The agreement between the numerical solution to Eq. (4) and the analytical result (21) obtained within the discrete WKB approach is quite remarkable. We also present here the dc-component of $\langle \hat{n}(t) \rangle$ obtained from the set of equations (13) in the mean-field approximation. In the resonant case $\delta = 0$ the atomic mode population is governed by the mean-field equation

$$
\frac{d^2z}{d\tau^2} + 3z^2 - 2z = 0 \tag{23}
$$

where $\tau = \chi \sqrt{\nu} t$ is a rescaled time. Under the initial conditions

$$
z(0) = z_0, \quad \frac{dz}{d\tau}|_{\tau=0} = 0
$$

the solution to Eq. (23) has the form

$$
z = z_0 - z_0 (1 - q_+) \text{sn}^2 \left( z_0 \sqrt{z_0(1-q_-)} \tau \bigg| \mu \right) \tag{24}
$$

where sn($u$|$\mu$) is the elliptic sine function with modulus $\mu = (1-q_+)/(1-q_-)$ and where

$$
q_\pm = \frac{1}{2z_0} \left( 1 - z_0 \pm \sqrt{1 + 2z_0 - 3z_0^2} \right).
$$

It is straightforward to obtain from Eq. (24) that the dc-component of the atomic population in the mean-field approximation has the form

$$
z_{m,f} = z_0 \left( q_- + (1 - q_-) \frac{E(\mu)}{K(\mu)} \right) \tag{25}
$$

Fig. 2 shows that the numerical and analytical WKB-solutions follow closely the mean-field solution (dashed line) near the ends of the interval $z_0 \in (0, 1)$ (for small and large initial atomic populations). However, in the main part of the interval, there is a significant discrepancy between numerical solution and mean-field solution. Note that the approximate formula for the dc-component given in (22) is also in a rather good agreement with these results: the relative error does not exceed 0.08. Fig. 3 displays the dc-component of the molecular population versus $\delta$ and $z_0$. As observed from this graph, for a wide range of initial atomic populations, $z_0$, a significant part of the population is on average in the molecular mode.
VI. POPULATION FLUCTUATIONS

To clarify the relevance of the molecular population behaviour shown in Figs. 2 and 3 to other physical properties of the system, we need to estimate the fluctuations of these quantities. To this end we consider the dc-component of the mean square fluctuation of the number of atoms

\[
(\Delta n)^2 \equiv \langle \hat{n}(t)^2 \rangle - \langle \hat{n}(t) \rangle^2 = \lim_{T \to \infty} \frac{1}{T} \int_0^T \langle \hat{n}(t)^2 \rangle \, dt.
\]  

(26)

From Eqs. (3) we find that the equation for the operator of the number of atoms \( \hat{n}(t) \) is

\[
\frac{d^2 \hat{n}(t)}{dt^2} + 3 \chi^2 V \hat{n}(t)^2 + \left( \Delta^2 - 2 \chi^2 N \right) \hat{n}(t) - \chi^2 VN - 2\Delta H = 0 
\]

(27)

where \( H \) is the Hamiltonian of the system (1). Now, averaging this last equation with respect to any quantum state and taking its dc-part, yields the following result exact for any quantum state and any total number of particles \( N \)

\[
\langle \hat{n}(t)^2 \rangle / N^2 = \frac{2}{3} \left( 1 - \delta^2 \right) \zeta + \frac{1}{3N} + \frac{2}{3} \frac{\Delta}{\chi^2} \frac{H}{N} 
\]

(28)

From Eqs. (1) and (28), we find that, for an initial state given by Eq. (4) with \( n_a = n_0 \) \((n_b = (N - n_0)/2)\), the mean square fluctuation of the number of molecules in the atomic-molecular BEC is

\[
(\Delta n_b)^2 / N^2 = \frac{1}{6} \left( 1 - \delta^2 \right) \zeta + \frac{1}{6} \delta^2 z_0 - \frac{\zeta^2}{4} + \frac{1}{12N} 
\]

(29)

with the dc-component of the atom population \( \zeta \) given by Eq. (21). The relative fluctuation of the number of molecules is given by the expression \( v = \sqrt{(\Delta n_b)^2 / \langle n_b \rangle} \). From Fig. 4 it can be seen that the fluctuations of the number of molecules are of the same order of magnitude as their mean values. It is worth recalling that the mean square fluctuations of the number of particles in an ideal gas is of the order of \( 1/N \) and are exceedingly small in macroscopic assemblies. On the other hand, the mean square fluctuations of the populations of individual energy states in an ideal Bose-Einstein gas are known to be greater than 1 (see e.g. [18]). The two-mode atom-molecule BEC is then an intermediate system with mean square fluctuations both less than 1 (see Fig. 4) and greater than \( 1/N \). Given the large fluctuations experienced by the populations around their average values, there is, strictly speaking, no convergence (in time) towards any state.

VII. CONCLUSION

In summary, we have considered the two-mode model of atom-molecule Bose-Einstein condensate, and studied quantum effects on atom-molecule population oscillations. We used numerical simulations and analytical approaches. We found numerically eigenvalues and eigenvectors of the full N-body problem. Analytical calculations were performed by using the discrete WKB approach. We found excellent agreement between the results of direct numerical simulations and analytical results. In contrast, the results of the widely used mean-field approach deviate significantly from the numerics for a wide range of atom concentrations. We studied also quantum fluctuations in coherent atom-molecule transformations. We found that that the fluctuations of the number of atoms (molecules) are of the same order of magnitude as their mean values. Thus, the two-mode BEC is seen to be in an intermediate regime: molecules and atoms can still be treated as separate phases, but their populations are highly fluctuating.
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FIG. 1: Coefficients $C_p(E)$ (arbitrary units) obtained from Eq. (5) for $\delta = 0$ and $N = 500$ ($P = 250$) and placed at the corresponding energy $E \simeq 1580.8$ (thin dashed line). The allowed region is enclosed by thick upper and lower lines. Coefficients $C_p(E)$ are clearly oscillating in this region and rapidly decaying outside.

FIG. 2: Normalized dc-component of the molecular population $z_{mol} = (1 - \tau)/2$ versus the normalized initial number of atoms, $z(0)$ for a zero detuning parameter, $\delta = 0$. Exact numerical results are obtained from Eqs. (5) and (8) for $N = 500$ cannot be distinguished from the analytical expression (21) shown as the solid line. The dashed curve represents the same quantity obtained in the framework of the mean field approach.
FIG. 3: De-component of the molecular population, $z_{\text{mol}} = (1 - z)/2$, versus the detuning parameter $\delta$ and the initial value of the atomic population $z_0$.

FIG. 4: De-component of the relative fluctuation of the number of molecules, $v = \sqrt{(\Delta n_b)^2/(n_b)}$, for different values of the detuning parameter $\delta$: $\delta = 0$ (solid line), $\delta = 0.5$ (dashed line) and $\delta = 0.75$ (dot-dashed line).