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Quantum Dynamics of Trapped Bose–Einstein Condensates

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Abstract—In quantum optics, the most interesting processes occur due to nonlinear interactions between the electromagnetic field and various media. The parametric processes which produce nonclassical states of the electromagnetic field have analogs in the processes of photoassociation and dissociation of atomic and molecular Bose–Einstein condensates. Just as the optical processes need a full quantum theoretical treatment in some regimes, we show that photoassociation and dissociation require full quantum treatments to be confident of the theoretical predictions we can make. If the processes take place inside an optical cavity, we show that we may also need to consider the quantum nature of the intracavity electromagnetic field. As the process of intracavity photoassociation that we analyze has no exact mapping onto a Fokker–Planck equation, we show how quantum-field-theoretical techniques can be used to write stochastic difference equations in a generalized positive-P representation, which may be solved numerically.

1. INTRODUCTION

To date, a number of dynamical situations have been investigated for dilute gas Bose–Einstein condensates (BEC) which are described incorrectly in a mean-field approach using Gross-Pitaevski-type (GPE) equations [1]. These begin with the evaporative cooling by which a BEC is produced [2] and include molecular association of an atomic BEC using both laser light [3–5] and Feshbach resonances [6], as well as the photodissociation of a molecular condensate [7, 8].

In previous articles, we have shown that there is a simple dynamical process for which a quantum treatment of all the interacting fields is necessary, namely, the intracavity coherent photoassociation of an atomic condensate to form a molecular condensate [9, 10]. For this system, we have demonstrated that there are parameter regimes in which the quantum solutions, obtained using either positive-P representation equations truncated at second order or a full, generalized positive-P representation, give qualitatively different results to the semiclassical mean-field equations. This generalized positive-P representation is developed using methods described elsewhere [11–14]. In this work, we will investigate to what extent all fields need to be treated quantum mechanically. Our approach may also be useful to investigate the formation of Efimov states [15, 16] during the process of molecular association via Feshbach resonances. These states, being triatomic molecules, need a triple product of creation or annihilation operators for their full description and are hence not exactly treatable by the usual phase-space methods.

2. STOCHASTIC PROCESSES BEYOND THE FOKKER–PLANCK EQUATION

The phase-space methods of quantum optics have been a very useful tool for the investigation of nonlinear quantum systems [17]. Central to these methods is finding a master equation for the density matrix starting from the quantum Hamiltonian; this master equation is then mapped onto a Fokker–Planck equation (FPE) for the appropriate pseudoprobability distribution. As a rare exception, this FPE may be solved directly. Otherwise, using the well-known duality between FPEs and stochastic differential equations (SDEs), an SDE may be written. This can either be linearized to give analytical solutions or solved numerically using the well-developed techniques of stochastic integration.

The existence of an FPE depends on the system under consideration. For example, consider the two-mode interaction Hamiltonian

$$\mathcal{H} = i\hbar\kappa[\hat{X}^m\hat{Y}^{\dagger n}] + \text{h.c.}, \tag{1}$$

where $\hat{X}$ and $\hat{Y}$ are arbitrary bosonic annihilation operators. We find that for $m + n > 2$ there is no FPE for the Wigner distribution, as the differential equation for the Wigner function will have derivatives of higher than second order. For $m > 2$ or $n > 2$, there are no FPEs in the P or Q representations. The problem is that the FPE may not contain derivatives of higher than second order. Pawula's theorem [18] stipulates that a partial differential equation for the pseudoprobability distribution with derivatives of higher than second order has no mapping onto an SDE. A common method used to avoid this problem has been to truncate the equations at second order, especially in the Wigner representation. While often successful, there are known cases where

this approach gives erroneous results [19–22] and, perhaps worse, in cases where even the positive-P equations must be truncated, we have no systematic way of knowing how important the truncated terms may be.

The fact that Pawula's theorem only applies in the continuous time limit allows us to proceed. As we have previously demonstrated [13, 14, 23], stochastic difference equations (SΔE's) in discretized time may be devised for nonlinear Hamiltonians which would map onto generalized FPEs (that is, a partial differential equation for a pseudoprobability distribution with derivatives of higher than second order). These SΔEs are found directly from the Hamiltonian, without the need to derive master and Fokker–Planck equations [14]. The derivation, using a few simple rules, is also much simpler than the usual methods for systems which give a genuine FPE. As numerical simulation is often the only possible exact treatment for highly nonlinear systems, the development of SΔEs, even though they have no continuous time limit, is, for all practical purposes, sufficient.

3. THE SYSTEM

The system we consider is one with a trapped atomic condensate held in an electromagnetic cavity which is resonant at the frequency of the transition between the atomic and an excited molecular state of the condensate. Here, we make the approximation that all three fields can be represented as single modes, which is reasonable as long as we consider short interaction times where the kinetic energy may be ignored. We also ignore the vibrational and rotational levels of the molecular state, as the energy spacing between them is more than the laser linewidth. We also make the normal zero-temperature approximation of quantum optics, as condensates exist at temperatures of the order of nanokelvins.

The interaction Hamiltonian for this system in the rotating wave approximation is

$$\begin{aligned}\mathcal{H} &= \frac{i\hbar g}{2}[\hat{a}^{\dagger 2}\hat{b}\hat{e}^{\dagger} - \hat{a}^{2}\hat{b}^{\dagger}\hat{e}] \\ &+ \hbar\chi_a\hat{a}^{\dagger 2}\hat{a}^{2} + \hbar\chi_b\hat{b}^{\dagger 2}\hat{b}^{2} \\ &+ i\hbar(\epsilon\hat{e}^{\dagger} - \epsilon^{*}\hat{e}) \\ &+ \Gamma^{\dagger}\hat{e} + \Gamma\hat{e}^{\dagger},\end{aligned} \tag{2}$$

where g represents the effective coupling strength between the condensates and the electromagnetic field, $\hat{a}(\hat{b})$ is the annihilation operator for the atomic (molecular) condensate, and $\hat{e}$ is the annihilation operator for the intracavity electromagnetic field. The χ_j represent the self-interaction (collision) terms between the atoms or molecules, ϵ represents the classical pumping of the cavity, and Γ is a bath operator for the electromagnetic field.

4. GENERALIZED POSITIVE-P EQUATIONS

As the differential equation for the positive-P distribution of this system contains mixed third-order derivatives, it is not amenable to standard phase-space techniques [17]. Following our alternative approach, we can map the Hamiltonian onto the following set of coupled SΔEs in a generalized positive-P representation, (with $\alpha(t+\Delta t) = \alpha(t) + \Delta\alpha(t)$, and so on for the other variables):

$$\begin{aligned}\Delta\alpha &= \Big[-2i\chi_a\alpha^{\dagger}\alpha^{2} + ge^{\dagger}\alpha^{\dagger}\beta \\ &+ \frac{\sqrt{g}}{2}\Big(e^{\dagger} + \frac{\xi_1 + i\xi_2}{\sqrt{2}u}\Big)(\eta_1 + i\eta_3) \\ &+ \frac{\sqrt{g}}{2}\beta(\eta_1 - i\eta_3) + \sqrt{-2i\chi_a\alpha^{2}}\eta_5\Big]\Delta t, \\ \Delta\alpha^{\dagger} &= \Big[2i\chi_a\alpha^{\dagger 2}\alpha + ge\alpha\beta^{\dagger} \\ &+ \frac{\sqrt{g}}{2}\Big(e + \frac{\xi_3 - i\xi_4}{\sqrt{2}u}\Big)(\eta_2 - i\eta_4) \\ &+ \frac{\sqrt{g}}{2}\beta^{\dagger}(\eta_2 + i\eta_4) + \sqrt{2i\chi_a\alpha^{\dagger 2}}\eta_6\Big]\Delta t, \\ \Delta\beta &= \Big[-2i\chi_b\beta^{2}\beta^{\dagger} - \frac{g}{2}\alpha^{2}e + \sqrt{-2i\chi_b\beta^{2}}\eta_7\Big]\Delta t, \\ \Delta\beta^{\dagger} &= \Big[2i\chi_b\beta^{\dagger 2}\beta - \frac{g}{2}\alpha^{\dagger 2}e^{\dagger} + \sqrt{2i\chi_b\beta^{\dagger 2}}\eta_8\Big]\Delta t, \\ \Delta e &= \Big[\epsilon - \gamma e + \frac{g}{2}\alpha^{\dagger 2}\beta \\ &+ \sqrt{g}\alpha^{\dagger}(\eta_1 + i\eta_3) + \frac{u}{\sqrt{2}}(\xi_1 - i\xi_2)\Big]\Delta t, \\ \Delta e^{\dagger} &= \Big[\epsilon^{*} - \gamma e^{\dagger} + \frac{g}{2}\alpha^{2}\beta^{\dagger} \\ &+ \sqrt{g}\alpha(\eta_2 - i\eta_4) + \frac{u}{\sqrt{2}}(\xi_3 + i\xi_4)\Big]\Delta t,\end{aligned} \tag{3}$$

where u is a free parameter which may be chosen so as to improve the convergence of the numerics. These equations imply an equal discretization of the time axis, with Δt being the step of the time grid. In the above, all noise sources are real and have the properties

$$\begin{aligned}\overline{\eta_i(t)} &= 0, \quad \overline{\eta_j(t)\eta_k(t')} = \delta_{jk}\delta(t-t'), \\ \overline{\xi_i(t)} &= 0, \quad \overline{\xi_j(t)\xi_k(t')} = \delta_{jk}\delta(t-t').\end{aligned} \tag{4}$$

The δ function is to be understood in accordance with the time discretization: $\delta(t-t') = \delta_{tt'}/\Delta t$, where $\delta_{tt'}$

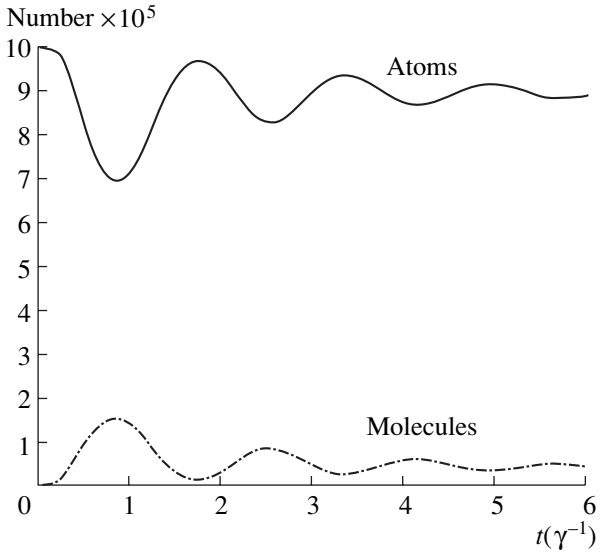

Fig. 1. Occupation numbers of the atomic and molecular condensates as a function of time according to 3×10^5 quantum trajectories. The parameters are $g = 10^{-5}$, $|\epsilon|^2 = 10^6$, $\chi_{a,b} = 10^{-9}$, and $|\alpha(0)|^2 = 10^6$. All quantities plotted in this and the following graphs are dimensionless.

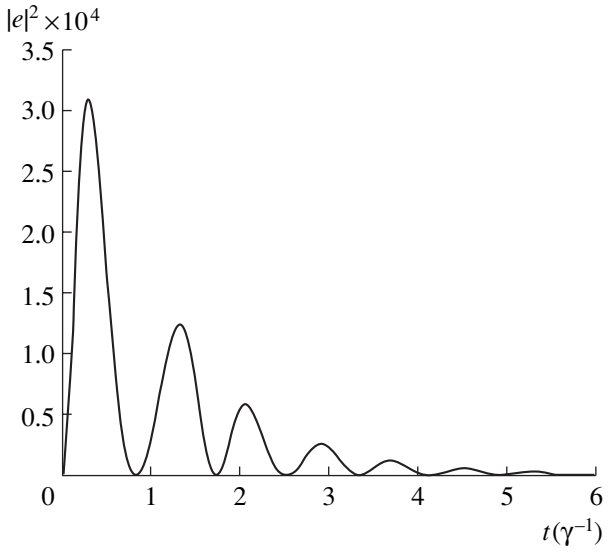

Fig. 2. The intracavity intensity (in units of photon number) of the electromagnetic field calculated quantum mechanically for the same parameters as in Fig. 1 showing the photon blockade effect.

is the Kronecker symbol. As in the usual positive-P distribution, there is a correspondence between the c-number variables [α, $\alpha^\dagger$, β, $\beta^\dagger$, e, $e^\dagger$] and the operators [$\hat{a}$, $\hat{a}^\dagger$, $\hat{b}$, $\hat{b}^\dagger$, $\hat{e}$, $\hat{e}^\dagger$], although a variable such as $\alpha^\dagger$ is not complex conjugate to α (except in the mean over a large number of stochastic trajectories) due to the independence of the noise sources.

5. RESULTS

We have solved Eq. (3) numerically for a range of parameters and found a behavior of the mean fields that is strikingly different from that found in the usual mean-field approximation, as well as from that in regimes where the mean-field approach is valid. In our simulations, we start with an atomic condensate inside an optical cavity which begins to be pumped at $t = 0$. Initially neither molecules nor an electromagnetic field are present, with the atomic field being treated as initially in a coherent state. We present the results here of numerical investigations of the regime where semiclassical and quantum predictions are different. In this regime, the quantum dynamics exhibit short-time oscillations and photon blockade.

In Fig. 1, we show the time development of the atomic and molecular fields as the cavity pumping is turned on for the parameters $g = 10^{-5}$, $|\epsilon|^2 = 10^6$, $\chi_{a,b} = 10^{-9}$, and $|\alpha(0)|^2 = 10^6$, which are all scaled in terms of the cavity loss rate. We have taken the means over 3×10^5 stochastic trajectories, which was more than sufficient to ensure excellent convergence. We can obtain some insight into the behavior exhibited here when we examine the dynamics of the intracavity electromagnetic field, as shown in Fig. 2. We find an initial buildup of intensity in the cavity, with this field also becoming oscillatory and eventually almost vanishing completely. The mean behavior of these three fields is identical to that found by truncating the positive-P distribution at second order [9].

For comparison, in Figs. 3 and 4, we show the solutions of Eq. (3) with all the noise terms removed. The disagreement between quantum and semiclassical solutions is even more striking than that previously found for pure travelling-wave SHG [24]. One way of explaining the quantum solutions is to consider that the interaction detunes the cavity. The linearized equation for the electromagnetic field contains a term $\frac{g}{2}\alpha^{\dagger 2}\beta$ which will have some imaginary component due to the self-interaction terms of the atomic and molecular fields. However, this term by itself cannot cause the blockade. What is needed is noise in the atomic and molecular fields. This noise can then act to cause a diffusion of the phase of the electromagnetic field, making it difficult for the cavity mode to sustain itself. In this respect, it is interesting to note that solution of the truncated Wigner equations for this system gives the same results as the positive-P solutions [25]. This indicates that the noise required need not be deeply quantum, as the truncated Wigner is equivalent to the semiclassical theory of stochastic electrodynamics [26].

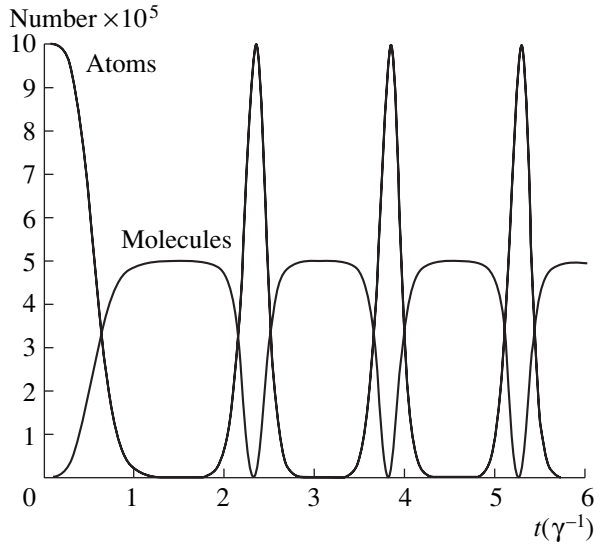

Fig. 3. Occupation numbers of the atomic and molecular condensates as a function of time calculated semiclassically for the same parameters as in Fig. 1.

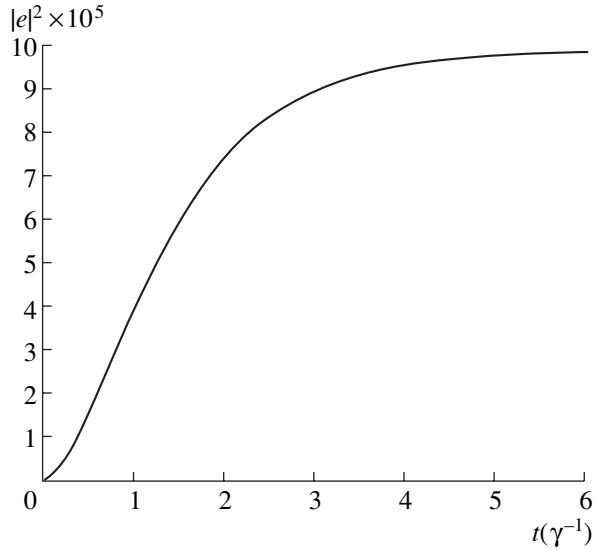

Fig. 4. The intracavity light field (in units of photon number) calculated semiclassically for the same parameters as in Fig. 1.

6. SPONTANEOUS MOLECULAR DISSOCIATION

One of the approximations made so far in this article is that we are considering times over which there will not be significant spontaneous dissociation of the excited molecules. Hence we have so far ignored this factor in the dynamics. As it is often stated that any damping can act to destroy quantum features, it is of interest to include this process. We will now add a phenomenological Born–Markovian damping term to the Hamiltonian for the molecular field:

$$\mathcal{H}_{\text{spon}} = \Gamma_b^{\dagger}\hat{b} + \Gamma_b\hat{b}^{\dagger}. \tag{5}$$

In the normal manner, this results in loss terms, $-\gamma_b\beta$ and $-\gamma_b\beta^{\dagger}$, being added to the equations for β and $\beta^{\dagger}$. What we find upon integration of the resulting equations [10] is that the behavior has changed, with the atom number undergoing an oscillatory decrease while the molecule number undergoes an oscillatory increase. The intracavity light field starts to revive as the atom number goes down. This is to be expected, as we have less interacting matter inside the cavity as the molecules are damped. However, to develop this picture any further would begin to exceed the limits of our single-mode-type approach. What is interesting is that the semiclassical predictions are still qualitatively wrong. The semiclassical light field again rises monotonically to its steady-state value, so that the differences should again be easily experimentally detectable.

7. SEMICLASSICAL TREATMENTS OF THE ELECTROMAGNETIC FIELD

For this system, it is simple and obvious how to treat all the fields either quantum mechanically or semiclassically. When we want to treat only the electromagnetic field semiclassically, there is some ambiguity. Removing the noise from the appropriate equations and representing the electromagnetic field by the c-number variable $\Omega(t)$, we find the following set of positive-P equations:

$$\begin{aligned}
\frac{d\alpha}{dt} &= -2i\chi_a\alpha^{+}\alpha^{2} + g\Omega^{*}\alpha^{+}\beta + \sqrt{g\Omega^{*}\beta - 2i\chi_a\alpha^{2}}\,\eta_1,\\
\frac{d\alpha^{+}}{dt} &= 2i\chi_a\alpha^{+2}\alpha + g\Omega\alpha\beta^{+} + \sqrt{g\Omega\beta^{+} + 2i\chi_a\alpha^{+2}}\,\eta_2,\\
\frac{d\beta}{dt} &= -2i\chi_b\beta^{+}\beta^{2} - \frac{g\Omega}{2}\alpha^{2} + \sqrt{-2i\chi_b\beta^{2}}\,\eta_3,\\
\frac{d\beta^{+}}{dt} &= 2i\chi_b\beta^{+2}\beta - \frac{g\Omega^{*}}{2}\alpha^{+2} + \sqrt{2i\chi_b\beta^{+2}}\,\eta_4,\\
\frac{d\Omega}{dt} &= \epsilon - \gamma\Omega + \frac{g}{2}\alpha^{+2}\beta,
\end{aligned} \tag{6}$$

where η_j are real Gaussian noise terms. There are now three choices. Although noise in the electromagnetic field has been explicitly removed, it is still implicit in the variables α^{+} and β. Solving the equations as written above is still not a semiclassical treatment of the electromagnetic field; it is more like a semiquantum treatment. Note that there is even more ambiguity here, as we could have retained the equation for $e^{\dagger} \longrightarrow \Omega^{*}$ instead of that for $e \longrightarrow \Omega$). One other option is to average the matter variables at each time step and use a fac-

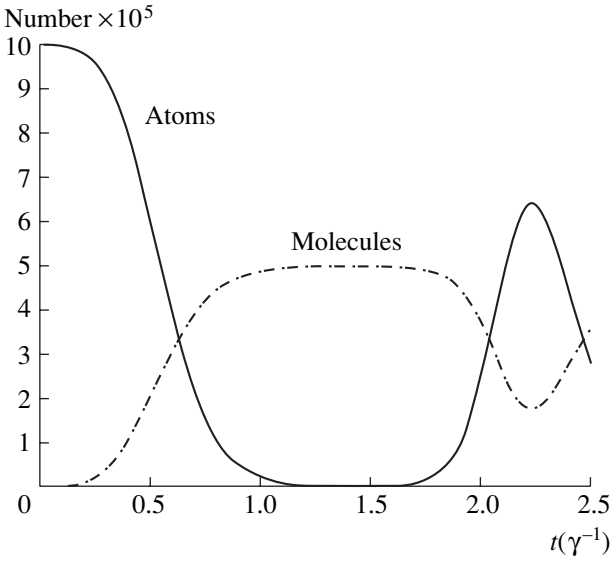

Fig. 5. The atomic and molecular occupation numbers for the same parameters as in Fig. 1, but with the electromagnetic field calculated without the contribution from the matter fields. This graphic is the result of 6.4×10^4 trajectories.

torization assumption, so that the last of the equations becomes

$$\frac{d\Omega}{dt} = \epsilon - \gamma\Omega + \frac{g}{2}\overline{\alpha^{+2}}\bar{\beta}. \quad (7)$$

Both these options give essentially the same results as the full equations. However, when we treat the electromagnetic field as if it were building up in an empty cavity, via the equation

$$\frac{d\Omega}{dt} = \epsilon - \gamma\Omega, \quad (8)$$

and leave the noise terms in the atomic and molecular equations, we find a different result altogether. The atomic and molecular field behave, as shown in Fig. 5, in a manner reminiscent of travelling-wave second-harmonic generation [24]. This is not at all surprising, as the equations are now mathematically equivalent to second-harmonic generation equations with an added $\chi^{(3)}$ component and a time-dependent coupling [27]. This demonstrates that it is the back action of the atomic and molecular fields on the electromagnetic field that is responsible for the dynamical features of this process and that at least a semiquantum treatment of the electromagnetic field is necessary, despite the large number of quanta present.

8. CONCLUSIONS

We have described and analyzed a situation in which the mean-field approach does not adequately describe the dynamics of a Bose–Einstein condensate. The differences are not of the order of the inverse of the system size but are qualitative. We have seen from numerical investigations that quantum solutions become closer to semiclassical solutions as the number of atoms or the coupling decreases. This is a sign of the nonlinearity of the quantum dynamics, where noise-driven correlations are built up between the three fields in a manner which has no semiclassical mean-field description, which was demonstrated using different semiclassical approaches to the modeling of the electromagnetic field.

We have also shown how the third-order terms in the equations of motion can be modeled. Although the third-order noises were found to have no noticeable effect within the limits of our model, the fact that they may be successfully modeled may be important for processes such as the formation of Efimov states in the process of molecular formation using Feshbach resonances and also for other processes which may be investigated in the future.

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