Bose-Einstein Condensates beyond Mean Field Theory: Quantum Backreaction as Decoherence

A. Vardi and J. R. Anglin

ITAMP, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138
(Received 12 July 2000)

We propose an experiment to measure the slow $\log(N)$ convergence to mean field theory (MFT) around a dynamical instability. Using a density matrix formalism instead of the standard macroscopic wave function approach, we derive equations of motion which go beyond MFT and provide accurate predictions for the quantum break time. The leading quantum corrections appear as decoherence of the reduced single-particle quantum state.

A Bose-Einstein condensate (BEC) is described in mean field theory (MFT) by a c-number macroscopic wave function, obeying the Gross-Pitaevskii nonlinear Schrödinger equation. MFT is closely analogous to the semiclassical approximation of single-particle quantum mechanics, with the inverse square root of the number N of particles in the condensate playing the role of $\hbar$ as a perturbative parameter. Since in current experimental condensates N is indeed large, it is generally difficult to see qualitatively significant quantum corrections to MFT. In the vicinity of a dynamical instability in MFT, however, quantum corrections appear on time scales that grow only logarithmically with N [1]. We propose an experiment to detect such quantum corrections, and present a simple theory to predict them. We show that, as the Gross-Pitaevskii classical limit of a condensate resembles single-particle quantum mechanics, so the leading quantum corrections appear in the single-particle picture as decoherence.

We consider a condensate in which particles can only effectively populate two second-quantized modes. This model can be realized with a condensate in a double well trap [2–7], or with an effectively two-component spinor condensate [8,9] whose internal state remains uniform in space [10]. Two internal states may be coupled by a near-resonant radiation field [11,12], and if collisions do not change spin states, there is also a simple nonlinear interaction among them. In either case the total number operator commutes with the Hamiltonian, and may be replaced with the c number N. Dropping c-number terms, we may thus write the two-mode Hamiltonian

$$H = -\frac{\omega}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{\eta}{2}[(\hat{a}_1^\dagger)\hat{a}_1 - (\hat{a}_2^\dagger)\hat{a}_2]^2,$$

(1)

where ω is the coupling strength between the two condensate modes, η is the two-body interaction strength, and $\hat{a}_1$, $\hat{a}_1^\dagger$, $\hat{a}_2$, and $\hat{a}_2^\dagger$ are particle annihilation and creation operators for the two modes. We will take η and ω to be positive, since the relative phase between the two modes may be redefined arbitrarily, and since without dissipation the overall sign of H is insignificant.

Instead of considering the evolution of $\hat{a}_j$ and its expectation value in a symmetry-breaking ansatz, we will exam-ine the evolution of the directly observable quantities $\hat{a}_i^\dagger \hat{a}_j$, whose expectation values define the reduced single-particle density matrix (SPDM) $R_{ij} \equiv \langle \hat{a}_i^\dagger \hat{a}_j \rangle / N$. It is convenient to introduce the Bloch representation, by defining the angular momentum operators,

$$\hat{L}_x \equiv \frac{\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1}{2}, \qquad \hat{L}_y \equiv \frac{\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1}{2i},$$
$$\hat{L}_z = \frac{\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2}{2}.$$

(2)

The Hamiltonian Eq. (1) then assumes the form,

$$H = -\omega \hat{L}_x + \frac{\eta}{2}\hat{L}_z^2,$$

(3)

and the Heisenberg equations of motion for the three angular momentum operators of Eq. (2) read

$$\frac{d}{dt}\hat{L}_x = -i[\hat{L}_x, H] = -\frac{\eta}{2}(\hat{L}_y\hat{L}_z + \hat{L}_z\hat{L}_y),$$
$$\frac{d}{dt}\hat{L}_y = -i[\hat{L}_y, H] = +\omega\hat{L}_z + \frac{\eta}{2}(\hat{L}_x\hat{L}_z + \hat{L}_z\hat{L}_x),$$
$$\frac{d}{dt}\hat{L}_z = -i[\hat{L}_z, H] = -\omega\hat{L}_y.$$

(4)

The mean field equations for the SPDM in the two-mode model may be obtained, without invoking U(1) symmetry breaking, by approximating second order expectation values $\langle \hat{L}_i \hat{L}_j \rangle$ as products of the first order expectation values $\langle \hat{L}_i \rangle$ and $\langle \hat{L}_j \rangle$:

$$\langle \hat{L}_i \hat{L}_j \rangle \approx \langle \hat{L}_i \rangle \langle \hat{L}_j \rangle.$$

(5)

Defining the single-particle Bloch vector $\vec{s} = (S_x, S_y, S_z) = (\frac{2\langle \hat{L}_x \rangle}{N}, \frac{2\langle \hat{L}_y \rangle}{N}, \frac{2\langle \hat{L}_z \rangle}{N})$, $\kappa = \eta N/2$ and using Eq. (5), we obtain the nonlinear Bloch equations

$$\dot{S}_x = -\kappa S_z S_y,$$
$$\dot{S}_y = \omega S_z + \kappa S_z S_x,$$
$$\dot{S}_z = -\omega S_y.$$

(6)

Mean field trajectories $\vec{s}(t)$ at four different κ/ω ratios are plotted in Fig. 1. The norm $|\vec{s}|$ is conserved in MFT, and so for a pure SPDM, Eqs. (6) are equivalent to the two-mode Gross-Pitaevskii (Bose-Josephson) equation [3–5]. The
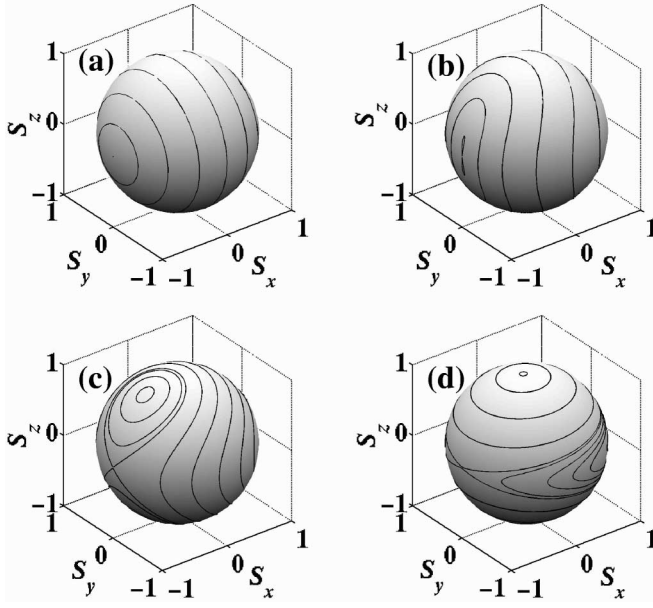
FIG. 1.　Mean field trajectories at (a) $\kappa = 0$, (b) $\kappa = 1.02\omega$, (c) $\kappa = 2\omega$, and (d) $\kappa = 20\omega$.

nonlinear Bloch equations (6) depict a competition between linear Rabi oscillations in the $S_y S_z$ plane and nonlinear oscillations in the $S_x S_y$ plane. For a noninteracting condensate (Fig. 1a) the trajectories on the Bloch sphere are circles about the S_x axis, corresponding to harmonic Rabi oscillations. As κ increases the oscillations become more anharmonic until, above the critical value $\kappa = \omega$ (Fig. 1b), the stationary point $\vec{s} = (-1, 0, 0)$ becomes dynamically unstable, and macroscopic self-trapping can occur (oscillations with a nonvanishing time averaged population imbalance $\langle S_z \rangle_t \neq 0$) [5]. In the vicinity of the dynamically unstable point, MFT will break down on a time scale only logarithmic in N, and so an improved theory is desirable.

If we assume that the condensate remains mildly fragmented, so that the two eigenvalues of R_{ij} are f and $1 - f$ for small f, we can take $\hat{L}_i = L_i + \widehat{\delta L_i}$, where the c number L_i is $\mathcal{O}(N)$ and, throughout the Hilbert subspace through which the system will evolve, all matrix elements of $\widehat{\delta L_i}$ are no greater than $\mathcal{O}(N\sqrt{f})$. The second order moments

$$\Delta_{ij} = 4N^{-2}(\langle \hat{L}_i \hat{L}_j + \hat{L}_j \hat{L}_i \rangle - 2\langle \hat{L}_i \rangle \langle \hat{L}_j \rangle), \quad (7)$$

will then be of order f. We can retain these, and so improve on MFT, if we truncate the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy of expectation value equations of motion at one level deeper: we eliminate the approximation (5), and instead impose

$$\langle \hat{L}_i \hat{L}_j \hat{L}_k \rangle \approx \langle \hat{L}_i \hat{L}_j \rangle \langle \hat{L}_k \rangle + \langle \hat{L}_i \rangle \langle \hat{L}_j \hat{L}_k \rangle + \langle \hat{L}_i \hat{L}_k \rangle \langle \hat{L}_j \rangle$$
$$- 2\langle \hat{L}_i \rangle \langle \hat{L}_j \rangle \langle \hat{L}_k \rangle. \quad (8)$$

This approximation is accurate to within a factor of $1 + \mathcal{O}(f^{3/2})$, better than (5) by one factor of $f^{1/2}$. Succes-

sively deeper truncations of the hierarchy yield systematically better approximations as long as f is small.

Applying (7) and (8) to (4), we obtain the following set of equations, in which the mean field Bloch vector drives the fluctuations Δ_{ij}, and is in turn subject to backreaction from them:

$$\dot{S}_x = -\kappa S_z S_y - \frac{\kappa}{2} \Delta_{yz},$$
$$\dot{S}_y = \omega S_z + \kappa S_z S_x + \frac{\kappa}{2} \Delta_{xz},$$
$$\dot{S}_z = -\omega S_y,$$
$$\dot{\Delta}_{xz} = -\omega \Delta_{xy} - \kappa S_z \Delta_{yz} - \kappa S_y \Delta_{zz},$$
$$\dot{\Delta}_{yz} = \omega(\Delta_{zz} - \Delta_{yy}) + \kappa S_z \Delta_{xz} + \kappa S_x \Delta_{zz}, \quad (9)$$
$$\dot{\Delta}_{xy} = (\omega + \kappa S_x)\Delta_{xz} - \kappa S_y \Delta_{yz} + \kappa S_z(\Delta_{xx} - \Delta_{yy}),$$
$$\dot{\Delta}_{xx} = -2\kappa S_y \Delta_{xz} - 2\kappa S_z \Delta_{xy},$$
$$\dot{\Delta}_{yy} = 2(\omega + \kappa S_x)\Delta_{yz} + 2\kappa S_z \Delta_{xy},$$
$$\dot{\Delta}_{zz} = -2\omega \Delta_{yz}.$$

In what follows, we will refer to (9) as evolution under "Bogoliubov backreaction" (BBR).

We note that Eqs. (9) are identical to the equations of motion one would obtain, for the same quantities, using the Hartree-Fock-Bogoliubov Gaussian ansatz. And if the second order moments Δ_{ij} may initially be factorized as $\Delta_{ij} = \delta_i \delta_j$ ($i, j = x, y, z$), then the factorization persists and the time evolution of δ_x, δ_y, and δ_z is equivalent to that of perturbations of the mean field equations (6):

$$\dot{\delta}_x = -\kappa(S_z \delta_y + S_y \delta_z),$$
$$\dot{\delta}_y = \omega \delta_z + \kappa(S_z \delta_x + S_x \delta_z), \quad (10)$$
$$\dot{\delta}_z = -\omega \delta_y.$$

Thus our equations for Δ_{ij} are in a sense equivalent to the usual Bogoliubov equations. The quantitative advantage of our approach therefore lies entirely in the wider range of initial conditions that it admits, which may more accurately represent the exact initial conditions. For instance, a Gaussian approximation will have $\Delta_{xx} = \mathcal{O}(1)$ in the ground state, where in fact $\Delta_{xx} = \mathcal{O}(N^{-1})$. This leads to an error of order $N^{-1/2}$ in the Josephson frequency computed by linearizing (9) around the ground state, even though the Gaussian backreaction result should naively be accurate at this order. Our SPDM approach does not have this flaw.

For finite motion of the Bloch vector, our formalism offers an efficient method to depict the backreaction of the Bogoliubov equations on the mean field equations via the coupling terms $-\kappa \Delta_{yz}/2$ and $\kappa \Delta_{xz}/2$ in (9). Because in general $\Delta_{yz}(t) \neq \Delta_{xz}(t)$, this backreaction has the effect of breaking the unitarity of the mean field dynamics. Consequently, the BBR trajectories are no longer confined to the surface of the Bloch sphere, but penetrate to the interior (representing mixed-state R_{ij}, with two nonzero

eigenvalues). Thus although decoherence is generally considered as suppressing quantum effects, decoherence of the single-particle quantum state of a condensate is itself the leading quantum correction (due to interparticle entanglement) to the effectively classical MFT.

In order to confirm this decoherence, and demonstrate how the BBR equations (9) improve on the mean field equations (6), we compare the trajectories obtained by these two formalisms to exact quantum trajectories, obtained by fixing the total number of particles $N = 50$, thereby obtaining an $N + 1$ dimensional representation of the operators in Eq. (4) and solving it numerically, using a Runge-Kutta algorithm. The results for the experimentally realizable initial state where all particles are in one of the modes (corresponding to the initial conditions $S_x = S_y = 0$, $S_z = -1$, $\Delta_{xx} = \Delta_{yy} = 2/N$, $\Delta_{xy} = \Delta_{xz} = \Delta_{yz} = \Delta_{zz} = 0$) and $\kappa = 2\omega$ are shown in Fig. 2. The MFT trajectory approaches the dynamical unstable point $\vec{\mathbf{s}} = (-1, 0, 0)$. Consequently, the quantum trajectory sharply breaks away from the MFT trajectory as it approaches this point, entering the Bloch sphere interior. While still periodic on a much shorter time scale than the exact evolution, the BBR evolution (dashed curve) provides an excellent prediction of the time of the breaking away from MFT (the "quantum break time").

The quantum break time near a dynamical instability is expected to grow logarithmically with N. In Fig. 3 we plot the von Neumann entropy

$$S = -\frac{1}{2} \ln\left[\frac{(1 + |\vec{\mathbf{s}}|)^{(1+|\vec{\mathbf{s}}|)}(1 - |\vec{\mathbf{s}}|)^{(1-|\vec{\mathbf{s}}|)}}{4} \right] \quad (11)$$

of the exact reduced single-particle density operator, as a function of the rescaled time ωt with $N = 10, 20, 40, 80, 160$, and 320 particles, for the same initial conditions as in Fig. 2. Since the MFT entropy is always zero, S serves as a measure of convergence. The quantum break time is clearly evident, and indeed increases as $\log(N)$. The

single-particle entropy is measurable, in the internal state realization of our model, by applying a fast Rabi pulse and measuring the amplitude of the ensuing Rabi oscillations, which is proportional to the Bloch vector length $|\vec{\mathbf{s}}|$. (Successive measurements with Rabi rotations about different axes, i.e., by two resonant pulses differing by a phase of $\pi/2$, will control for the dependence on the angle of $\vec{\mathbf{s}}$.) In a double well realization, one could determine the single-particle entropy by lowering the potential barrier, at a moment when the populations on each side were predicted to be equal, to let the two parts of the condensate interfere. The fringe visibility would then be proportional to $|\vec{\mathbf{s}}|$.

Decoherence of quantum systems coupled to reservoirs shows similar behavior to Fig. 3. The entropy of a dynamically unstable quantum system coupled to a reservoir [13], or of a stable system coupled to a dynamically unstable reservoir, is predicted to grow linearly with time, at a rate independent of the system-reservoir coupling, after an onset time proportional to the logarithm of the coupling. This shows that one can really consider the Bogoliubov fluctuations as a reservoir [14], coupled to the mean field with a strength proportional to $1/N$. But one can also consider decoherence due to a genuine reservoir (unobserved degrees of freedom, as opposed to unobserved higher moments). For example, thermal particles scattering off the condensate mean field will cause phase diffusion [15] at a rate Γ which may be estimated in quantum kinetic theory as proportional to the thermal cloud temperature. For internal states not entangled with the condensate spatial state, Γ may be as low as 10^{-5} Hz under the coldest experimental conditions, whereas for a double well the rate may reach 10^{-1} Hz. Further sources of decoherence may be described phenomenologically with a larger Γ.

Evolving the full N-particle density matrix under the appropriate quantum kinetic master equation [4], we again solve for $\vec{\mathbf{s}}$ either numerically or in BBR approximation.
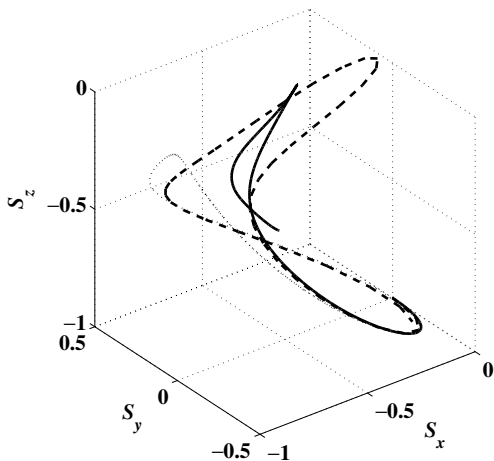

FIG. 2. Mean field ($\cdots$), Bogoliubov backreaction ($---$), and exact 50 particles (—) trajectories starting with all particles in one mode, at $\kappa = 2\omega$.
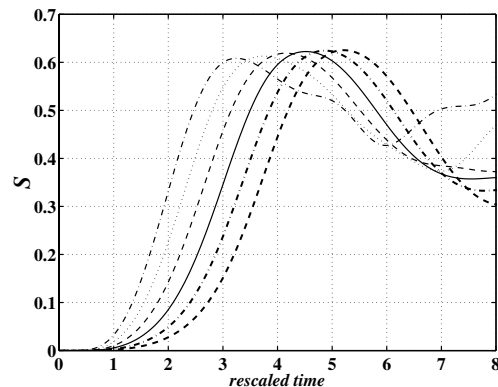

FIG. 3. Growth of the von Neumann entropy S of the quantum reduced single-particle density operator, at $\kappa = 2\omega$, for $N = 10$ ($-\cdot-$), 20 ($\cdots$), 40 ($---$), 80 (—), 160 ($-\cdot-\cdot-$), and 320 ($----$) particles. Initial conditions are the same as in Fig. 2.
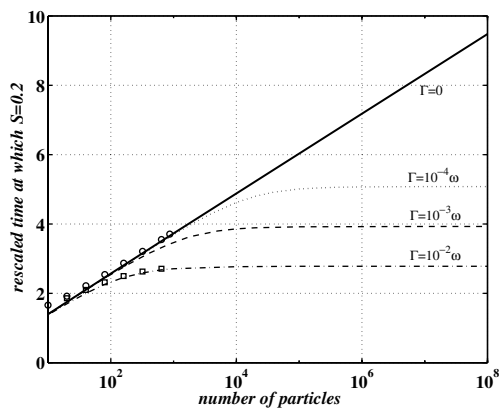
FIG. 4. Time at which S reaches 0.2 as a function of the particle number N, according to the BBR equations (9), modified to include thermal phase diffusion. Four different values of Γ are shown: $\Gamma = 0$ (—), $\Gamma = 10^{-4}\omega$ ($\cdots$), $\Gamma = 10^{-3}\omega$ (— — —), and $\Gamma = 10^{-2}\omega$ (— · —). Exact quantum results are presented for $\Gamma = 0$ (circles) and $\Gamma = 10^{-2}\omega$ (squares). Initial conditions κ and ω are the same as in Figs. 2 and 3.

In Fig. 4 we show the time at which the single-particle entropy reaches a given value, as a function of the number of particles, for various Γ, according to the modified BBR equations. The exact quantum results (limited by computational power to $N \sim 10^3$) are presented for the two limiting values of Γ, showing excellent agreement with the BBR predictions. In addition to showing the usefulness of the BBR theory in describing regimes beyond the reach of exact numerical solutions, the results of Fig. 4 show how quantum corrections can be experimentally distinguished from ordinary thermal effects: they provide a quantum saturation of the dephasing rate at low temperature. Such saturation is a common phenomenon in decoherence, which further supports our view of quantum backreaction as decoherence.

To conclude, we have shown that significant quantum corrections to the Gross-Pitaevskii MFT, in the vicinity of its dynamical instabilities, can be measured in a two-mode BEC under currently achievable experimental conditions. We have derived a simple theory that accurately predicts the leading quantum corrections and the quantum break time. Our picture of quantum backreaction in BECs as decoherence suggests new lines of investigation for both experiment and theory: measurements of single-particle entropy in condensates, descriptions of condensates with mixed single-particle states (instead of the usual macroscopic wave functions), and general questions of de-

coherence under nonlinear evolution. Exploring these possibilities, beyond the two-mode model considered here, provides many goals for further research.

[1] Y. Castin and R. Dum, Phys. Rev. Lett. **79**, 3553 (1997).

[2] J. Javanainen, Phys. Rev. Lett. **57**, 3164 (1986); J. Javanainen and S. Yoo, Phys. Rev. Lett. **76**, 161 (1996).

[3] M. Jack, M. Collett, and D. Walls, Phys. Rev. A **54**, R4625 (1996); G. J. Milburn, J. Corney, E. M. Wright, and D. F. Walls, Phys. Rev. A **55**, 4318 (1997); A. S. Parkins and D. F. Walls, Phys. Rep. **303**, 1 (1998).

[4] J. Ruostekoski and D. F. Walls, Phys. Rev. A **58**, R50 (1998).

[5] A. Smerzi, S. Fantoni, S. Giovanazzi, and S. R. Shenoy, Phys. Rev. Lett. **79**, 4950 (1997); S. Raghavan, A. Smerzi, S. Fantoni, and S. R. Shenoy, Phys. Rev. A **59**, 620 (1999); I. Marino, S. Raghavan, S. Fantoni, S. R. Shenoy, and A. Smerzi, Phys. Rev. A **60**, 487 (1999).

[6] I. Zapata, F. Sols, and A. Leggett, Phys. Rev. A **57**, R28 (1998).

[7] P. Villain and M. Lewenstein, Phys. Rev. A **59**, 2250 (1999).

[8] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, M. J. Holland, J. E. Williams, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. **83**, 3358 (1999).

[9] C. J. Myatt, E. A. Burt, R. W. Ghrist, E. A. Cornell, and C. E. Wieman, Phys. Rev. Lett. **78**, 586 (1997).

[10] Uniformity becomes stable when the effective healing length for phase separation ($[n|\sqrt{a_{11}a_{22}} - a_{12}|]^{-1/2}$ for n the total density) is larger than the size of the sample. This can be achieved with alkali metal condensates of $\sim 10^4$ atoms in traps of frequency ~ 100 Hz. See A. Vardi and J. R. Anglin (to be published).

[11] M. R. Matthews, D. S. Hall, D. S. Jin, J. R. Ensher, C. E. Wieman, E. A. Cornell, F. Dalfovo, C. Minniti, and S. Stringari, Phys. Rev. Lett. **81**, 243 (1998); J. Williams, R. Walser, J. Cooper, E. Cornell, and M. Holland, Phys. Rev. A **59**, R31 (1999).

[12] Patrik Öhberg and Stig Stenholm, Phys. Rev. A **59**, 3890 (1999).

[13] W. H. Zurek and J. P. Paz, Phys. Rev. Lett. **72**, 2508 (1994).

[14] S. Habib, Y. Kluger, E. Mottola, and J.-P. Paz, Phys. Rev. Lett. **76**, 4660 (1996).

[15] J. R. Anglin, Phys. Rev. Lett. **79**, 6 (1997).