PHYSICAL REVIEW
LETTERS

VOLUME 78 | 12 MAY 1997 | NUMBER 19

Large Amplitude Oscillations of a Bose Condensate

Augusto Smerzi[1,*] and Stefano Fantoni[1,2,†]
[1]*SISSA, via Beirut 2/4, I-34014, Trieste, Italy*
[2]*International Centre for Theoretical Physics, I-34014, Trieste, Italy*
(Received 25 November 1996)

We analyze the response of condensed trapped atoms to external driving magnetic fields. Solving the time-dependent Gross-Pitaewskii equation within a new, accurate algorithm, we found frequencies and relaxation times of collective oscillations in excellent agreement with the experimental results. Using simple scaling arguments we make quantitative predictions for future experiments. [S0031-9007(97)03147-5]

PACS numbers: 03.75.Fi, 02.70.Ns , 05.30.Jp, 32.80.Pj

The recent experimental observations of collective excitations of trapped atoms [1,2] are stimulating an increasing interest in the dynamical properties of a Bose condensate. The frequencies of these resonances have been studied solving the linearized Gross-Pitaewskii equation [3,4], but a theoretical analysis of the damping of the condensate oscillations is still lacking. Yet, to understand how relaxation and loss of coherence arise on the dynamics of finite, isolated quantum systems is a fundamental problem investigated in many area of physics [5]. For trapped bosons at temperature $T > T_c$ (with T_c the critical temperature), the damping of collective motions is mainly due to two-body collisions. The dynamics is governed by the classical Boltzmann equation modified to take into account the stimulated collisions induced by the Bose statistics [6]. At $T < T_c$ the thermal component of the density will damp the condensate oscillations mainly through one-body collisions (Landau damping) [7]. It has been suggested that at $T = 0$ the relaxation comes from the coupling of the collective vibration into high-frequency states due to the nonlinear mean-field interaction in the Gross-Pitaewskii equation (GPE) [8]. Let us remark that this coupling does not increase the entropy of the system. The transformation of the collective energy in temperature would require higher-order terms in the nonlinear interaction, and would lead to the loss of spatial coherence and to the appearence of a normal component of the density, an important, still poorly understood problem closely related with the appearence of the condensate at the critical temperature [9,10].

In the experimental setup of Refs. [1,2,11] trapped atoms are evaporatively cooled well below T_c to form a pure condensate, without signs of a thermal component. In Ref. [1] collective, coherent excitations are induced by a driving magnetic field with adjustable symmetries acting on the radial plane. The oscillations are studied turning off the trapping magnetic field and imaging the cloud after 7 ms of free expansion in space. Several distructive measurements are required to complete the spectroscopical analysis. Monopolar oscillations of a sample of $N = 4500 \pm 300$ atoms are observed at a frequency $\omega = (1.84 \pm 0.01)\omega_0$ (with ω_0 radial trap frequency) and lifetime $\tau_{\mathrm{rel}} = 110 \pm 25$ ms.

Collective oscillations can be studied theoretically solving the Gross-Pitaewskii equation [12]:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + [V_{\mathrm{ho}} + V_{\mathrm{sc}}]\psi \qquad (1)$$

with the self-consistent field:

$$V_{\mathrm{sc}} = \frac{4\pi\hbar^2 a}{m}\|\psi\|^2. \qquad (2)$$

The scattering length for ^{87}Rb is $a = 110a_0$, with a_0 the Bohr radius, and ψ is normalized to the total number of atoms. The trapping magnetic field can be parametrized

as a cylindrically symmetric harmonic potential $V_{\rm ho} = \frac{1}{2}m\omega_0^2(r^2 + \Lambda^2 z^2)$, with $\Lambda = \sqrt{8}$, $r^2 = x^2 + y^2$, and $\omega_0 = 2\pi \times 132$ Hz. The stationary ground state of GPE has been studied in Refs. [8,13,14,16] for positive and negative scattering lengths, but to find the general time-dependent solution is more challenging. The first (to our knowledge) numerical analysis of GPE using an external isotropic harmonic potential has been done in [8] within the Crank-Nicholson method. The major problem of this kind of lattice algorithms is the presence of small perturbations of the wave function caused by random numerical noise and the finite spatial step size of the grid. This noise, amplified by the nonlinear mean-field interaction in GPE, creates spurious excitations and unphysical damping, limitating the analysis of collective observables to short times [8].

In this Letter we describe a new, very accurate, algorithm to solve GPE that we apply to study the resonances observed experimentally.

Without loss of generality we can write the wave function as

$$\psi = R(\vec{r}, t) \exp\left[\frac{i}{\hbar} S(\vec{r}, t) \right] \tag{3}$$

with R and S real. Replacing Eq. (3) in Eq. (1) and equating the real and imaginary parts, the GPE becomes equivalent to two coupled equations:

$$\frac{\partial \rho}{\partial t} = \nabla\left(\rho \frac{\nabla S}{m} \right) = 0 , \tag{4}$$

$$\frac{\partial S}{\partial t} + \left(\frac{\nabla S}{2m} \right)^2 + V_{\rm ho} + V_{\rm sc} + U_q = 0 \tag{5}$$

with the "quantum potential" U_q given by

$$U_q = -\frac{\hbar^2}{4m}\left[\frac{\nabla^2 \rho}{\rho} - \frac{1}{2}\frac{(\nabla \rho)^2}{\rho^2} \right]. \tag{6}$$

Equation (4) represents the continuity equation for the macroscopic particle density $\rho = R^2$ while Eq. (5) can be interpreted as a classical Hamilton-Jacobi equation for the action S. The latter describes particles moving according to the classical and quantum force $\vec{F}_{cl} = -\nabla(V_{\rm ho} + V_{\rm sc})$ and $\vec{F}_q = -\nabla U_q$, respectively. In other words, Eqs. (4), (5) introduce a "quantum phase space" formed by real coordinates and canonical momenta *defined* as $\vec{p} = \frac{\nabla S}{m} = m\frac{d}{dt}\vec{r}$. Observables can be calculated from the quantum distribution function $f_q(\vec{r}, \vec{p}, t)$ as proper phase-space integrals in analogy with classical statistical mechanics. The monopole momentum and potential energy are $I(t) = \int r^2 f_q(\vec{r}, \vec{p}, t)\, d\vec{r} d\vec{p}$ and $V = \int (V_{\rm ho} + V_{\rm sc}) f_q(\vec{r}, \vec{p}, t)\, d\vec{r} d\vec{p}$, respectively. Attention should be paid to the calculation of the kinetic energy that is given by $T = \int (p^2/2m + U_q) f_q(\vec{r}, \vec{p}, t)\, d\vec{r} d\vec{p}$; in fact, the quantum potential U_q is originated from the Laplacian in the Schroedinger equation. Let us remark that f_q is positive definite and it represents a probability density in the quantum phase space; it should not be confused with the Wigner distribution function [19].

The quantum evolution of f_q is given by a generalized Liouville equation:

$$\frac{\partial}{\partial t} f_q + \frac{\vec{p}}{m} \nabla f_q - \nabla V_{\rm tot} \nabla_p f_q = 0 \tag{7}$$

with $V_{\rm tot} = V_{\rm ho} + V_{\rm sc} + U_q$. This equation can be numerically solved using the "quantum atomic dynamics" (QAD) algorithm as follows:

(1) The distribution function is parametrized as a sum of "weighted test particles" (WTP):

$$f_q(\vec{r}, \vec{p}, t) = K \sum_{i=1}^{N_{tp}} w(\vec{r} - \vec{r}_i(t)) w_p(\vec{p} - \vec{p}_i(t)) \tag{8a}$$

and we choose

$$\begin{aligned} w(\vec{r} - \vec{r}_i(t)) &= \exp[-\gamma(\vec{r} - \vec{r}_i(t))^2], \\ w_p(\vec{p} - \vec{p}_i(t)) &= \delta(\vec{p} - \vec{p}_i(t)) \\ K &= \frac{N}{N_{\rm tp}}\left(\frac{\gamma}{\pi} \right)^{3/2} \end{aligned} \tag{8b}$$

with γ fixed to reproduce the initial density profile (see below).

(2) The time evolution of WTP $\{\vec{r}_i, \vec{p}_i\}$ proceeds as in a classical particles dynamics where the mean-field and the quantum potential are calculated self-consistently at each time step. A second-order Runge-Kutta method gives [15]

$$\vec{p}_i(t + \tfrac{1}{2}\Delta t) = \vec{p}_i(t - \tfrac{1}{2}\Delta t) - \nabla V_{\rm tot}(\vec{r}, t)\Delta t , \tag{9a}$$

$$\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \vec{p}_i(t + \tfrac{1}{2}\Delta t)/m\Delta t . \tag{9b}$$

A total number of WTP $N_{\rm tp} = 8000$ and the time step $\Delta t = 0.002$ ms are needed to ensure the convergence of the results.

(3) The initial distribution of WTP in phase space requires special care. The stationary ground state solution of GPE is given by

$$\rho(\vec{r}, t = 0) = \int f_q(\vec{r}, \vec{p})\, d\vec{p} = \|\psi(\vec{r}, t = 0)\|^2, \tag{10a}$$

$$\vec{p}_i(t = 0) = \nabla S/m = 0 . \tag{10b}$$

Equation (10b) comes from the fact that in the ground state $S = \mu t$, with μ the chemical potential. The initial position of $\{\vec{r}_i\}$ can be chosen randomly by using the Metropolis algorithm [15] with the profile of ψ calculated, for example, as in [13]. However, this procedure introduces an undesired numerical noise. The classical nature of Eq. (7) suggests an exact, self-consistent solution to this problem. We add a small friction term $\vec{F}_{\rm fric} = -\epsilon \vec{p}/m$ to Eq. (9a), and we allow

the particles to propagate until they rearrange themselves to the state with $\{\vec{p}_i = 0\}$ and $\vec{F}_{\rm tot} = -\nabla V_{\rm tot} = 0$. This gives the exact initial conditions in the quantum phase space. Then the friction is switched off. The density profile so obtained is exactly the same as the one obtained with the standard method described in [13].

In the small amplitude limit (linear regime) and for isotropic external potentials, GPE describes undamped oscillations [9,17]. The simplest way to show this is to calculate the equation of motion for the monopole moment. From Eq. (1) we obtain

$$\frac{d^2I}{dt^2} + 5\omega_0^2 I - 6E + 2T = 0\,. \qquad (11)$$

The time evolution of I is related self-consistently to the kinetic energy T, but for a large number of particles and small oscillations T can be neglected. This roughly corresponds to satisfy the condition $\eta = \rho_0 g_0/\hbar\omega_0 \gg 1$ with ρ_0 the peak density of the condensate and $g_0 = \frac{4\pi\hbar^2 a}{m}$. Whitin this approximation, Eq. (11) describes undamped oscillations with frequency $\omega = \sqrt{5}\omega_0$. As a numerical test of our algorithm, in Fig. 1 we show the monopole moment versus time calculated for a system of 4500 atoms and with a small initial monopolar deformation, obtained by scaling the coordinates as $\vec{r}_i = (1 + \alpha)\vec{r}_i^{\rm gs}$, with $\alpha = 0.005$ and where $\vec{r}_i^{\rm gs}$ are the WTP positions in the ground state. The system exhibits undamped oscillations ($\tau_{\rm rel} > 10$ s that should be compared with $\tau_{\rm rel} = 0.110$ s of [1]) with a frequency of $\omega = 2.2\omega_0$. Further numerical tests, which will be presented elsewhere, were done to check that the total energy is conserved at each time-step. This condition is essential in order to avoid unphysical damping coming from numerical noise.

In the experiment [1], collective monopolar vibrations have been induced using a time-dependent magnetic field acting on the x-y plane during the first 0.05 s. In order to simulate exactly the experiments, we solve GPE by adding a time-dependent potential $V_d = \frac{1}{2}m\omega^2(t)r^2$ that oscillates with a frequency equal to that of the excitation under study and with an amplitude equal to 1.5% of the radial spring constant. In Fig. 2 we show the time evolution of the monopole moment calculated in the radial plane. The oscillations induced by the driving potential increase rapidly in amplitude during $t = 0.05$ s. Then the system oscillates freely in the anisotropic external trap. A fit with an exponential decaying cosine function gives a frequency of oscillations $\omega = 1.845\omega_0$ and a relaxation time $\tau_{\rm rel} = 135$ ms, in excellent agreement with the experimental values. The physical origin of the damping holds on the interplay between the anisotropy of the trap, which spreads the response of the system over two main frequencies (associated with atoms moving in the radial and in the axial plane), and the nonlinear self-consistent field that couples all the different modes of oscillation. Atoms moving faster or slower than the oscillating wave (that corresponds to a phonon in homogeneous systems) will lose or gain kinetic energy, leading to the relaxation of the system. In the linear regime, such a mechanism has been described by Landau in the study of plasma oscillations for homogeneous systems (Landau damping) [18]. An intriguing possibility, which deserves an accurate analysis, is that the damping of the collective motions is associated with the presence of

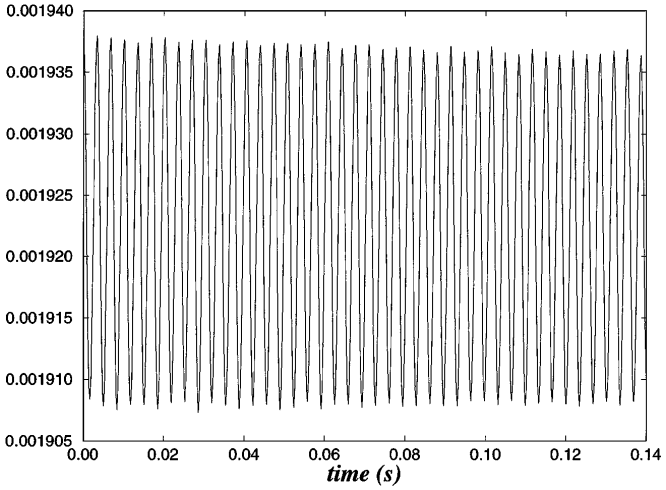

FIG. 1. Monopole moment (in arbitrary units) versus time for a system of $N = 4500$ atoms in an isotropic harmonic trap of frequency $\omega_0 = 2\pi \times 132$ Hz. The initial deformation is obtained by scaling the coordinate as $\vec{r} = (1 + \alpha)\vec{r}_i^{\rm gs}$ with $\alpha = 0.005$. For such a small initial deformation the system exibits undumped oscillations.

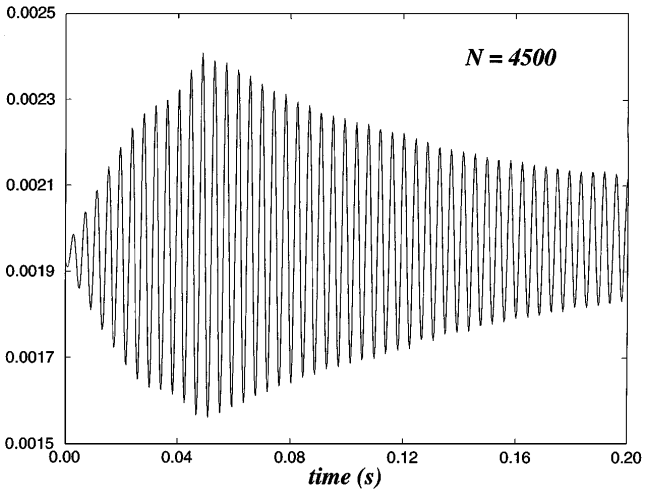

FIG. 2. Monopole moment (in arbitrary units) versus time for a system of $N = 4500$ atoms in an anisotropic external trap. A driving field acting for $t < 0.05$ ms increases the amplitude of oscillations. Then the system oscillates freely in the trap. The frequency is $\omega = 1.845\omega_0$ with a relaxation time $\tau_{\rm rel} = 135$ ms, in agreement with the experimental results $\omega = (1.84 \pm 0.01)\omega_0$ and $\tau_{\rm rel} = 110 \pm 25$ ms.

chaos in the trajectories of the test particles Eqs. (7)–(9). It is quite possible that this fact reflects some chaotic property of the trajectory of real atoms. The occurrence of a chaotic evolution of the condensate density and of the phase S has been recently investigated by Kagan *et al.* [21], solving the GPE equation in the Thomas-Fermi approximation. They have pointed out that such a stochastic behavior leads to real relaxation and irreversibility.

We note that in our simulation the monopole moment calculated along the radial plane is in exact opposition of phase with the one calculated along the transverse plane. However, the experimental results [1] indicate that the phase shift is not equal to π: this is connected with the free expansion of the cloud that preceeds the imaging [20].

A very important feature of the Gross-Pitaewskii equation is the possibility to gain simple scaling laws for the relaxation times and the frequencies of the collective oscillations. Rescaling Eq. (1) as $\vec{r} = \vec{r}_{\rm old}(\frac{2m\omega_0}{\hbar})^{\frac{1}{2}}$ and $t = t_{\rm old}\omega_0$, we obtain

$$i\frac{\partial\phi}{\partial t} = -\nabla^2\phi + \tfrac{1}{4}(r^2 + \Lambda^2 z^2)\phi + 8\pi a N\left(\frac{2m\omega_0}{\hbar}\right)^{\frac{1}{2}}\|\phi\|^2\phi \qquad (12)$$

with the normalization condition:

$$\int \|\phi\|^2 d\vec{r} = 1\,. \qquad (13)$$

A rapid look at Eq. (12) shows that the relaxation time can be written, for a given initial deformation, as $\tau_{\rm rel} = \omega_0^{-1}F(N\frac{a}{l_0})$, with the characteristic length for the harmonic oscillator $l_0 = (\hbar/m\omega_0)^{\frac{1}{2}}$. Regardless of the value of the number of atoms, trap frequencies, and, eventually, species of atoms with different masses and scattering length, we obtain that the relaxation times and the frequencies of two systems α, β are simply related as

$$\tau^{\alpha}_{\rm rel}/\tau^{\beta}_{\rm rel} = \omega^{\beta}/\omega^{\alpha} = \omega^{\beta}_0/\omega^{\alpha}_0 \qquad (14)$$

as far as we keep $N\frac{a}{l_0}$ costant *and* $\phi^{\alpha}(t=0) = \phi^{\beta}(t=0)$. A simple way to implement the last condition is to switch off the driving field at $t^{\alpha}_d = \frac{\omega^{\beta}_0}{\omega^{\alpha}_0}t^{\beta}_d$. It would be interesting to verify experimentally the scaling law Eq. (14), which could be also used to test under which conditions the Gross-Pitaewskii equation can be applied to study large amplitude collective motions. In fact, in GPE, the mean field approximation breaks down for too high energy vibrational modes [8]. Moreover, Eq. (14) could be used to calculate scattering length of different species of atoms.

There is a further comment that should be made here. The results presented so far clearly indicate that the oscillations induced experimentally cannot be studied in linear approximation. Theoretical calculations of the frequencies in [3,4] have been performed only in that limit, with an agreement with experimental data varying from 2% to 6% [4]. It is clear that the dependence of frequencies and relaxation times on the initial amplitude of the oscillation deserves an accurate analysis. Indeed, it is just the possibility of exploring the response of finite quantum systems in the nonlinear regime that makes the study of condensate trapped atoms of particular interest.

In conclusion, we have developed a new accurate algorithm to study collective coherent oscillations of trapped atoms. Frequencies and relaxation times of monopolar oscillations have been found in excellent agreement with the experimental data. The damping comes from the interplay between the anisotropy of the trap and the coupling of different modes of oscillations due to the nonlinear mean-field interaction for large amplitude oscillations. This damping could be associated with the presence of chaos in the trajectories of the test particles. Using simple scaling arguments for the relaxation times and the frequencies, we make quantitative predictions for future experiments.

Discussions with S. Stringari and E. Tosatti are acknowledged.

*Electronic address: smerzi@sissa.it
†Electronic address: fantoni@sissa.it

[1] D. S. Jin *et al.*, Phys. Rev. Lett. **77**, 420 (1996).
[2] M. O. Meves *et al.*, Phys. Rev. Lett. **77**, 988 (1996).
[3] S. Stringari, Phys. Rev. Lett. **77**, 2360 (1996).
[4] M. Edwards *et al.*, Phys. Rev. Lett. **77**, 1671 (1996).
[5] G. F. Bertsch and R. A. Broglia, *Oscllations in finite quantum systems* (Cambridge University Press, Cambridge, 1994).
[6] T. Lopez-Arias and A. Smerzi, "Kinetic Properties of a Boson Gas at Finite Temperature" (unpublished).
[7] S. H. Payne and A. Griffin, Phys. Rev. B, 7199 (1985).
[8] P. A. Ruprecht, M. J. Holland, and K. Burnett, Phys. Rev. A **51**, 4704 (1995).
[9] Yu. Kagan *et al.*, Phys. Rev. A **54**, 1753R (1996).
[10] For a review see *Bose-Einstein condensation*, edited by A. Griffin, D. W. Snoke, and S. Stringari (Cambridge University Press, Cambridge, England, 1995).
[11] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995); K. B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995); C. C. Bradley *et al.*, Phys. Rev. Lett. **75**, 1687 (1995).
[12] L. P. Pitaevskii, Sov. Phys. JETP **13**, 451 (1961); E. P. Gross, Nuovo Cimento **20**, 454 (1961); J. Math. Phys. **4**, 4704 (1963).
[13] F. Dalfovo and S. Stringari, Phys. Rev. A, 2477 (1996).
[14] G. Baym and C. J. Pethick, Phys. Rev. Lett. **76**, 6 (1996).
[15] S. E. Koonin and D. C. Meredith, *Computational Physics* (Addison-Wesley Publishing Company, 1990).

[16] A. Smerzi, "Bose-Einstein condensation of trapped atoms" (unpublished).
[17] L. P. Pitaewskii, Report No. cond. mat. 9605119 (unpublished).
[18] E. Lifshitz and L. P. Pitaevskii, *Kinetic Physics* (Pergamon, Oxford, 1980).
[19] A. Smerzi, Phys. Rev. A **52**, 4365 (1995); Phys. Rev. Lett. **76**, 559 (1996).
[20] S. Giovanazzi, A. Smerzi, and S. Fantoni (unpublished).
[21] Yu. Kagan, E. L. Surkov, and G. V. Shlyapnikov, Phys. Rev. A **55**, 18R (1997).