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Strong-field driving of a dilute atomic Bose-Einstein condensate

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A hydrodynamical version of the time-dependent Gross-Pitaevskii equation has been formulated and applied to the description of a Bose-Einstein condensate (BEC) of ^{87}Rb atoms in the JILA time-averaged orbiting potential (TOP) trap. The response of the BEC to time-dependent modulations of the trap potential is computed and the characteristic frequencies of a BEC oscillation agree well with those observed in recent experiments. For the axially symmetric $m=0$ mode of the TOP trap, we find a weak dependence of the oscillatory frequency on the strength of the driving amplitude under conditions comparable to those of current experiments. The free ringing of the BEC that is induced by a transient change in the potential is found to be periodic, in agreement with the predictions of Thomas-Fermi theory. We analyze the harmonic content of the spectral response and consider possibilities for high-harmonic generation in the context of nonlinear atom optics.
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I. INTRODUCTION

First observed in 1995, Bose-Einstein condensation of trapped neutral alkali-metal atom gases [1–3] has become a vehicle for the detailed experimental and theoretical investigation of macroscopic quantum systems. During the past year, the mechanical response of a Bose-Einstein condensate (BEC) to disturbances of its confining potential has been measured [4,5]. In the weak-driving regime, the resonant response of the BEC agrees well with the predictions of linear-response theory applied to the time-dependent mean-field Gross-Pitaevskii (GP) equation [5–7]. However, there is no apparent experimental difficulty in entering the strong-driving regime, where nonlinear response of the BEC will be encountered; this is already displayed in the observation of the amplitude dependence of resonant collective excitation frequencies [8] and we expect that many more examples will be seen. Therefore, we have developed a method for a general numerical solution of the time-dependent GP equation for trapped BECs and apply it here to cases of transient disturbance of the trapping potential comparable to those of current experiments. We find good agreement with experimental results for the amplitude dependence of the frequency of the $m=0$ mode observed in the JILA experiments by Jin *et al.* [4] and identify some simple mechanisms for controlling the nonlinear driven response.

II. SMALL-AMPLITUDE RESPONSE OF A DRIVEN BEC

An approach to describing the response of a confined BEC to small time-dependent disturbances has been described by Ruprecht *et al.* [9] within the framework of the Bogoliubov approximation [10]. In this approach, one identifies the normal modes of free oscillation of the confined BEC by solving an eigenvalue problem. The response of the BEC to a general weak disturbance is then treated like that of any mechanical system without damping: normal modes are excited independently, with amplitudes that depend upon the matching of their spatial and spectral characteristics with those of the disturbance. In particular, a normal mode of frequency ν_i will respond to monochromatic driving at frequency ν with an amplitude proportional to $1/(\nu_i^2-\nu^2)$, just as in the case of a simple harmonic oscillator. This suggests an obvious method of experimental spectroscopy of BEC normal modes, which is to observe BEC density fluctuations induced by modulations of the trapping potential near resonance.

This analysis has been applied to the case of the JILA time-averaged orbiting potential (TOP) trap [6] and gives predictions of the frequencies and spatial profiles of normal-mode excitations that agree well with experiments using BECs of several thousand ^{87}Rb atoms. That particular experiment focused on two low-lying normal modes, characterized by azimuthal angular momentum quantum numbers that reflect the cylindrical symmetry of the trap: a shape oscillation with $m=0$, which will be discussed in the present paper, and a quadrupole oscillation with $m=2$.

The theoretical description of normal modes simplifies considerably when the number N_0 of condensate atoms becomes large. One may then treat the GP equation within the Thomas-Fermi approximation and the normal mode frequencies become independent of N_0 [11]. This approximation gives results that agree well with experiments [5,7] on ^{23}Na with $N_0>10^5$.

III. STRONG-FIELD DRIVING OF BEC

For strong external disturbances of a BEC, we can no longer expect the response to be small and must go beyond a linearized theory. The most straightforward approach is to solve the full time-dependent GP equation, which is reasonable if the driving does not disturb the underlying quantum coherence of the BEC. This has been done by Ruprecht *et al.* [9] for the case of a spherical trap, by direct numerical integration of the time-dependent GP equation, treated as an initial-value problem with the BEC in its ground state at $t=0$. Ruprecht *et al.* observed nonlinear behavior analogous to that encountered in nonlinear optics: harmonic generation, i.e., the oscillation of the condensate at integer multiples of a normal mode frequency, and sum- and difference-frequency generation. These analogs are expected to become of considerable interest as the field of ''atom optics'' develops [12] and our present approach is motivated by the desire to explore the full potential of the BEC as a nonlinear atom-optical device.

In the Thomas-Fermi limit, the GP equation for a condensate in a harmonic potential with time-varying spring constants can be solved quite easily by an approach described by Kagan *et al.* [13] and generalized by Castin and Dum [7]. The approach of Kagan *et al.* treats the isotropic harmonic potential $V(\mathbf{r})=f(t)r^2$, where $f(t)$ is an arbitrary function of time. This approach reduces the solution of the time-dependent GP partial differential equation to the solution of one nonlinear ordinary differential equation for a scaling parameter $b(t)$: the condensate density $\rho_c(\vec{r},t)$ is then given by $\rho_c(\vec{r},t)=b(t)^{-3}\rho_c(\vec{r}/b(t),t=0)$, where $\rho_c(\vec{r},t=0)$ is a solution of the appropriate time-independent GP equation in the Thomas-Fermi approximation. Thus the variation of the trap potential is equivalent to a time-dependent dilatation of the length scale, so the BEC always maintains the same shape. Furthermore, this approach shows that for a transient disturbance, i.e., one for which $f(t)=$ const for $t>t_0$, the motion of the condensate is strictly periodic for $t>t_0$, with the period being determined by the value of $b(t_0)$. This is much different from the behavior of a general linear system, where a transient disturbance gives rise to ringing at a combination of normal mode frequencies, which need not be commensurate. Thus the generic response of a transiently driven BEC in this approximation is *harmonic generation*, where the fundamental frequency is established by the time history of excitation: it is not an intrinsic property of the time-independent system.

However, the integration of the time-dependent GP equation under general conditions applicable to current experiments still requires the solution of a time-dependent nonlinear partial differential equation in two or three spatial dimensions. We now describe the method we have developed for this task.

IV. QUANTUM HYDRODYNAMIC FORMULATION OF THE TIME-DEPENDENT GP EQUATION

The simplest description of a zero-temperature, dilute BEC of trapped atoms is based on mean-field theory with the atom-atom interaction approximated by a delta-function pseudopotential [10]. This gives the time-dependent GP equation for the condensate wave function $\Psi(\vec{r},t)$:

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+V_{trap}(\vec{r},t)+\frac{4\pi\hbar^2 a}{m}|\Psi(\vec{r},t)|^2\right)\Psi(\vec{r},t), \tag{1}$$

where $V_{trap}(\vec{r},t)$ is the confining potential, m the atomic mass, and a the s-wave scattering length. In this paper we present results for potentials V_{trap} that describe isotropic and cylindrically symmetric harmonic oscillators, which reduce the problem to treatment of one and two spatial dimensions, respectively. The basic time variation of V_{trap} that we have considered is a brief sinusoidal modification of the spring constants, similar to those studied experimentally.

Our approach involves solving the hydrodynamical version of the GP equation

$$\frac{\partial\rho_c}{\partial t}+\vec{\nabla}\cdot(\rho_c\vec{v}_c)=0,$$

$$\frac{\partial\vec{v}_c}{\partial t}+\vec{\nabla}\left(\frac{4\pi\hbar^2 a}{m^2}\rho_c+\frac{V_{trap}}{m}+\frac{\vec{v}_c^{\,2}}{2}-\frac{\hbar^2}{2m^2}\frac{\nabla^2\sqrt{\rho_c}}{\sqrt{\rho_c}}\right)=0, \tag{2}$$

where the condensate density $\rho_c(\vec{r},t)$ and velocity $\vec{v}_c(\vec{r},t)$ fields are those of the standard hydrodynamic representation of the Schrödinger equation developed by Madelung [14]. Equations (2) are of hyperbolic type and we treat them by a modified version of the time-dependent density-functional approach that we have applied previously to the treatments of a Fermi liquid [15]. The principal modification, which also has constituted the biggest numerical challenge, is the treatment of the so-called quantum pressure, which is the term proportional to $(\nabla^2\sqrt{\rho_c})/\sqrt{\rho_c}$. This term is not present in the treatments of the system that utilize the Thomas-Fermi approximation and it will be important in regions of strong density variation.

We solve Eqs. (2) as an initial-value problem, with the initial value of the velocity field $\vec{v}_c(\vec{r},t=0)=0$ everywhere and the intial condensate density $\rho_c(\vec{r},t=0)$ given by the solution of the time-independent GP equation. To find $\rho_c(\vec{r},t=0)$ for the isotropic trap, we used a standard shooting method [16] for direct numerical solution of the ordinary differential equation; for the cylindrically symmetric trap we use a basis-set solution that was obtained elswhere [17]. To propagate the initial density we employed the Lax [16] algorithm and the boundary conditions that have been discussed previously in Ref. [15]. Our algorithms were tested successfully on comparable solvable systems: the free expansion of the Gaussian wave packet, the motion of a Gaussian wave packet in the harmonic potential, and the maintenance of the stationarity the ground state of both the spherically and axially symmetric condensates.

V. RESULTS FOR CYLINDRICALLY SYMMETRIC AND ISOTROPIC TRAPS

We first discuss a simulation of the JILA TOP trap experiment reported in Ref. [4]. We treat a condensate of

$N_0 = 3500$ ^{87}Rb atoms confined in a cylindrically symmetric trap with an axial frequency $\nu_z = 373$ Hz and radial frequency $\nu_\rho = 132$ Hz. [The ratio $\nu_z/\nu_\rho = \sqrt{8}$ is a characteristic of the TOP trap, where ρ and z designate the radial and axial coordinates of the conventional cylindrical coordinate system. It is convenient to refer the length scale to the characteristic distance $d = (2\pi)^{-1}\sqrt{h/m\nu_z}$, which describes the width (in the z direction) of the condensate wave function in the noninteracting limit, and to measure time in units of the corresponding axial period $T = 1/\nu_z$.] The condensate is externally disturbed by modulation of the radial frequency of the form

$$\nu_\rho(t) \to \nu_\rho[1 + A(t)\sin(2\pi\nu_d t)], \tag{3}$$

where $A(t) = A_0$ for $0 < t < t_0$ and $A(t) = 0$ otherwise. We report results here for $\nu_d = 170$ Hz and for values of A_0 ranging from 0.02 to 0.6, with t_0 of the order of 10 ms. Although the identification of constants of motion of the nonlinear Schrödinger equation is not straightforward in general, it is easy to demonstrate that a cylindrically symmetric disturbance preserves the axial symmetry present in the initial state. Thus the trap modulation described by Eq. (3), applied to an initial state of definite m, will produce a time-dependent wave function with the same value of m always (this is because the time derivative of the wave function at $t = 0$ must then also have the same m, so by approximate evolution of Ψ with finite time steps, m is preserved). Thus, for symmetric modulations it is appropriate to treat m as a good quantum number even in the strong-driving limit, so $m = 0$ characterizes the excitation described here (on the other hand, the $m = 2$ mode, which is observed [4] in torsional excitation in the linear-response limit, will evolve into a time-dependent state of more complex angular character as the strength of the drive increases). Thus it is appropriate to express Eqs. (2) in the usual cylindrical coordinates (ρ, z) and to solve them as an initial-value problem in time t for flow of fluid in the two-dimensional space (ρ, z).

Our numerical procedure is summarized as follows. We apply a finite-difference discretization scheme to approximate the spatial derivatives in Eqs. (2), using the standard central difference formula accurate to $O(\delta)$ on a uniform grid of spacing $\delta \approx 0.05d$. A typical grid size was 400×400 points, with edge boundary conditions defined as in Ref. [15]: the normal derivatives of ρ_c and $\vec{v}_c$ are required to vanish on the boundary, though in practice very little atomic density reaches it. The Laplacian operator that defines the quantum pressure was evaluated using a five-point central difference formula. Propagation of the flow in time was treated by the Lax method [16], which provides a conditionally stable propagator accurate to $O(\tau)$ in the time step τ; values of $\tau \approx 0.001T$ were adequate to get results converged to the accuracy reported here.

Figure 1 shows the radial and axial shape oscillations of the BEC for the case $A_0 = 0.02, t_0 = 0.01$ s, after the pulse has been turned off. The radial and axial widths displayed are the mean values $\langle\rho\rangle$ and $\langle z^2\rangle$, respectively, in units of the

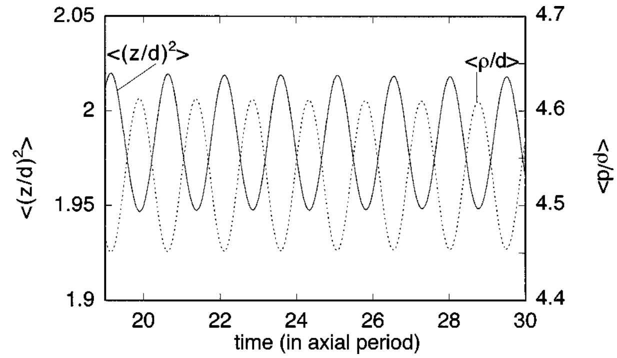

FIG. 1. Response of an ^{87}Rb BEC with $N_0 = 3500$ in the JILA TOP trap ($\nu_z = 373$ Hz) to weak (2%), $m = 0$, driving with a 10-ms modulation of ν_ρ, as described in the text. Axial and radial oscillations are given in units of the characteristic radial length $d = (2\pi)^{-1}\sqrt{h/m\nu_z}$ vs time in units of the axial period. Radial oscillations of the condensate's shape (at the frequency in agreement with [8]) are accompanied by a sympathetic response of the axial width, approximately 180° out of phase.

characteristic length $d = (2\pi)^{-1}\sqrt{h/m\nu_z}$, where $\langle\rho\rangle = \int \rho\rho_c(\vec{r})d^3r$ and $\langle z^2\rangle = \int z^2\rho_c(\vec{r})d^3r$. The observed frequency of radial breathing is $0.68\nu_z$, which is within 3% of the value predicted by linear-response theory in this case. The periodic behavior of the response is the same as in the Thomas-Fermi limit, but Fig. 1 of Ref. [6] shows that that limit has not quite been attained in this case. Note that sympathetic axial breathing occurs approximately 180° out of phase with the radial breathing, as seen in the JILA experiment by Jin *et al.* [4]. This is the behavior expected of a low-compressibility fluid confined in a potential: when squeezed radially, it will expand along the axial direction.

Figure 2 quantifies the frequency response function for $A_0 = 0.02$ and shows its behavior as A_0 increases. Note that the dependence of the fundamental frequency upon driving amplitude is weak: we estimate the uncertainty of our calculations to be 1.5% and the shift of the fundamental peak between $A_0 = 0.02$ and $A_0 = 0.6$ is within this range, consistent with the very weak observed variation of this frequency

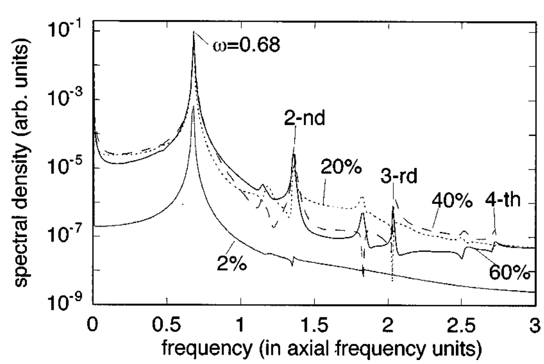

FIG. 2. Fourier transform (in arbitrary units) of the oscillations of $\langle\rho\rangle$ vs frequency in units of axial frequency ν_z for the excitation scheme of Fig. 1, for $A_0 = 0.02$, 0.2, 0.4, and 0.6 (respectively 2–60 %). No shift of the fundamental frequency occurs within the 1.5% accuracy of our calculations.

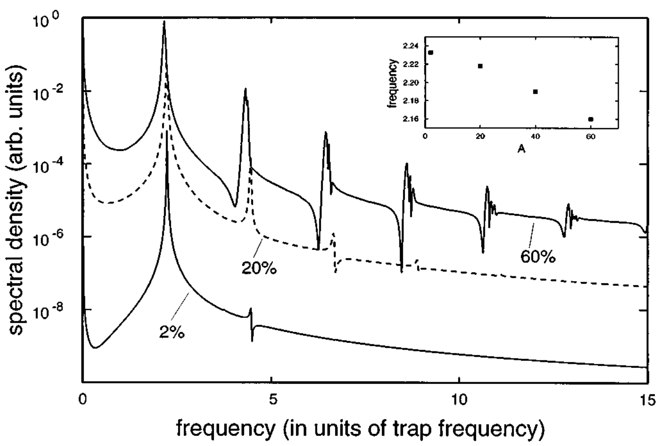

FIG. 3. Spectral response function (not normalized) of oscillations of $\langle r(t)\rangle$ for an ^{87}Rb BEC with $N_0=80\,034$, contained in a spherical trap with a radial frequency $\nu_r=300$ Hz, modulated with $\nu_d=170$ Hz, $t_0=10$ ms, and $A_0=0.02,0.2,0.6$. The ordinate is measured in units of ν_r. The inset shows the shift of the fundamental frequency as a function of driving amplitude, as determined from the displacement of the highest peak.

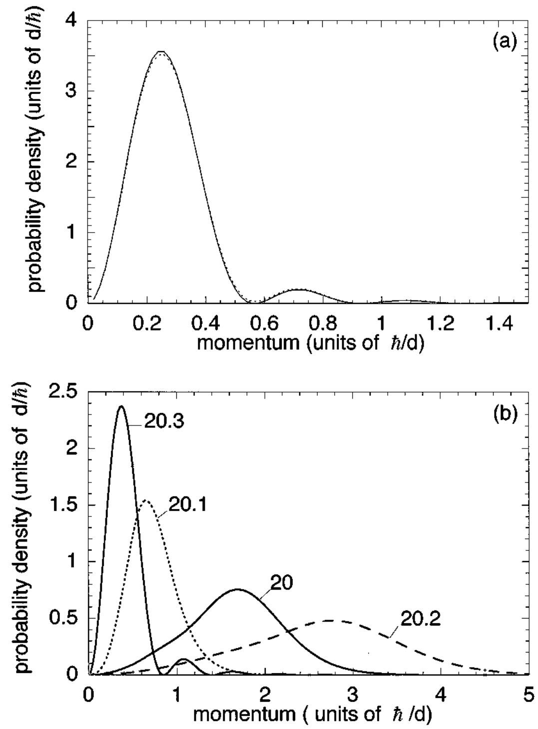

FIG. 4. (a) Typical probability density in momentum space for a weak (2%) driving (dashed line) compared with the initial momentum distribution (solid line). Units are defined by the characteristic oscillator length scale $d=(2\pi)^{-1}\sqrt{h/m\nu_r}$. (b) Probability density (multiplied by p^2) for a strong (60%) disturbance at times corresponding to 20.0, 20.1, 20.2, and 20.3 units of the trap period. Units are defined as in (a).

[8]. The most important deviations from a monochromatic response are the presence of harmonics, though for larger modulations some additional weak spectral features are visible.

A major goal of current BEC research is the development of a bright source of coherent matter waves, or "atom laser" [18], whose operation is described by atom optics in the "strong-field" regime, i.e., in which many bosons occupy the same mode of the matter field. For an electromagnetic field *in vacuo*, the speed of wave propagation is independent of the field amplitude (ignoring the negligible relativistic effect of light-light scattering by particle pair production), so the spatial structure of a normal mode of the field is independent of the number of photons that occupy it. In contrast, the corresponding spatial modes of a matter-wave field $\Psi(\vec{r},t)$ are described by the GP equation (1), and their structure depends upon the boson occupation number N_0 due to the presence of the nonlinear term $(4\pi\hbar^2 a/m)|\Psi(\vec{r},t)|^2$ in the effective potential. Thus the atom laser is governed by intrinsically nonlinear atom optics, similar to that of an optical laser with a photorefractive cavity medium. It is thus desirable to develop some insight into the qualitative features of nonlinear atom optical response.

We hypothesize that the weak nonlinearity observed in radial squeezing of the TOP trap is related to the anisotropy of the driving force. This force is applied radially and so the condensate will be able to flow in the axial direction whose potential is undisturbed. If the trap potential is squeezed in all directions at once, on the other hand, there should be a more uniform compression of the condensate, which will lead to a higher peak density and thus more pronounced influence of the nonlinear term in the GP equation. Indeed, we find a discernibly greater nonlinear response in the case of an isotropic harmonic trap, with an isotropic modulation of the radial frequency. Figure 3 shows the results for an ^{87}Rb BEC with $N_0=80034$, contained in a spherical trap with a radial frequency $\nu_r=300$ Hz. The radial frequency is modulated as in Eq. (3), with $\nu_d=170$ Hz and $t_0=10$ ms. In this case, we observe a decrease of the induced oscillation frequency with increasing A_0. For small A_0, the observed frequency is very close to $\sqrt{5}\nu_r$, which is the value obtained in the Thomas-Fermi limit [11,13]. Equation (14) of Ref. [13] implies that this frequency should approach $2\nu_r$ for large A_0 in the Thomas-Fermi limit, which is consistent with the direction observed here. Again, the dominant nonlinear response in these spectra appears to be harmonic generation. We have compared our results for $\langle r(t)\rangle$ with those obtained by solving the ordinary differential equation of Ref. [13] and find no difference that is significant within the accuracy of our method. Thus this case seems to be well described by the Thomas-Fermi approximation.

The appearance of these harmonics in spatial distributions leads us to inquire how they are manifested in momentum space and so might be used to modify the de Broglie spectrum of a BEC in situations where the trap is suddenly turned off. In Fig. 4 we plot a series of snapshots of the probability density in momentum space both for weak and strong spherically symmetric modulation of the condensate as depicted in Fig. 3. The snapshots are taken after a 10-ms disturbance and several milliseconds of free oscillations in the trapping potential. The probability density is calculated from the formula

$$|\widetilde{\Psi}(k,t)|^2 \sim \left[\int_0^\infty r^2 j_0(kr) R(r,t) \cos S(r,t)\, dr\right]^2 + \left[\int_0^\infty r^2 j_0(kr) R(r,t) \sin S(r,t)\, dr\right]^2,$$

where $j_0(r)$ is a spherical Bessel function of zeroth order and the amplitude $R(r,t)$ and the phase $S(r,t)$ of the wave function in a position space can be recovered from the density and velocity fields $\rho_c(\vec{r},t)$ and $\vec{v}_c(\vec{r},t)$.

For the weak (2%) modulation, the density in momentum space is practically time independent. It exibits only a small wiggle [Fig. 4(a)] connected with the localization of the wave packet in position space. For 60% modulation, however, the momentum distribution changes rapidly [Fig. 4(b)]. Both the central frequency and width of the peak of the momentum distribution vary by about a factor of 3 over the course of one oscillation. If the trap were to be turned off suddenly at $t=t_1$, we should expect to see the BEC evolve as a free dilute Bose gas with an initial momentum distribution given by that at $t=t_1$. Thus, in this system we can hope to use the trap modulation as a tool for significant modification of the evolution of a released BEC if the trap can be turned off over a small fraction of its period.

VI. CONCLUSION

We have developed a hydrodynamic formulation of the time-dependent Gross-Pitaevski equation and applied it to forced oscillations of a dilute Bose-Einstein condensate in harmonic traps. Its results are consistent in the small-amplitude limit with linear-response theory and replicate the very-weak-amplitude dependence of the frequency of the $m=0$ mode as observed in the JILA TOP trap. We argue that the nonlinear response can be enhanced by using uniformly compressive versus anisotropic driving and show that this is consistent with differences in the nonlinear response of cylindrical and spherical traps.

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