Low Energy Excitations of a Bose-Einstein Condensate: A Time-Dependent Variational Analysis

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We solve the time-dependent Gross-Pitaevskii equation by a variational ansatz to calculate the excitation spectrum of a Bose-Einstein condensate in a trap. The trial wave function is a Gaussian which allows an essentially analytical treatment of the problem. Our results reproduce numerical calculations over the whole range from small to large particle numbers, and agree exactly with the Stringari results in the strong interaction limit. Excellent agreement is obtained with the recent JILA experiment and predictions for the negative scattering length case are also made. [S0031-9007(96)01917-5]

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Very recently, the prediction [1] that a system of weakly interacting bosons would undergo a phase transition to a state having a macroscopic population of the ground level at very low temperatures (Bose-Einstein condensation, BEC) has been experimentally tested [2–4]. The requirements for BEC (low temperatures and high densities) have been successfully achieved by combining laser cooling [5] with evaporative cooling [6] techniques in samples of rubidium [2], lithium [3], and sodium [4,7] atoms. These experiments open up both experimental and theoretical challenges to understand and study the properties of this new state of matter. In particular, the collective excitations of a Bose condensed dilute gas in a trap have been measured for the first time in a recent experiment at JILA [8].

From the theoretical point of view a Bose-Einstein condensate at zero temperature is described by the nonlinear Schrödinger equation (NLSE) (in this context, also known as the Gross-Pitaevskii equation) [9]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(r)\psi + U_0 |\psi|^2 \psi , \qquad (1)$$

where m is the atomic mass, $V(\vec{r})$ is the trapping potential, and $U_0 = 4\pi\hbar^2 a/m$, where a is the scattering length. This nonlinear equation, which is well known in other areas of physics [10], describes the evolution of the macroscopic wave function of the condensate ψ. In the context of BEC solutions of this equation have essentially been studied with numerical methods [11]. This includes calculations of the ground state, expansion of the condensate, and collective (Bogoliubov) excitations in the trap which can be excited adding a (weak) time-dependent driving term to Eq. (1). Analytical work has been based mainly on the Thomas-Fermi (TF) approximation where the kinetic energy term is neglected in comparison to the interatomic and trap interactions. Very recently, the Bogoliubov excitation spectrum in a harmonic trapping potential has been derived by Stringari in the TF approximation, valid in the limit when the interatomic interaction energy is much larger than the excitation energies of the bare trap, i.e., in the large particle limit [12]. Theoretical predictions for the excitation spectrum based on numerical solution and the Stringari formulas are in remarkable agreement with the recent JILA experiment [8], and confirm the quantitative validity of the NLSE (1) to describe the evolution of the condensate wave function.

The purpose of this Letter is to develop a variational technique [14], based on Ritz's optimization procedure, to analyze the *time-dependent* NLSE (1) [15]. In particular, we will derive the low energy collective excitations of a Bose gas both for positive and negative scattering lengths based on Gaussian trial wave functions. The essential features of our treatment in comparison with the previous theoretical work are as follows: We derive analytical expressions for the frequencies of the dominant collective modes in a 3D anisotropic trap, valid for the arbitrary ratio of the atom-atom interactions to trap excitation energies, and positive and negative scattering lengths. In the large particle number case our expressions contain as a limit the spectrum derived by Stringari [12]. We typically reproduce results from numerical calculations on the few percent level [16], and our results are in good agreement with the recent JILA experiment [8]. In the case of the negative scattering length, our predictions could be tested in current or planned experiments.

The basic idea behind the variational method is to take a trial function with a fixed shape, but with some free (time-dependent) parameters. Using a variational principle, we find a set of Newton-like second order ordinary differential equations for these parameters which characterize the solution. This technique has been widely used in nonlinear problems [17,18], and it is specially suited for three-dimensional problems, whereby numerical simulations are very expensive or impossible. Furthermore, it allows one to derive analytical approximations that provide a deep physical insight into the problem. Although not exact, this technique is a good qualitative guide to study the propagation of wave functions having a simple shape, allowing some analytical results.

We consider a sample of bosons at zero temperature, confined in a harmonic potential

$$V(\vec{r}) = \frac{1}{2} m\nu^2(\lambda_x^2 x^2 + \lambda_y^2 y^2 + \lambda_z^2 z^2). \qquad (2)$$

Here the r's account for anisotropies of the trap. For example, for a cylindrically symmetric trap we have $\lambda_x = \lambda_y = 1$, and $\lambda_z = \nu_z/\nu$ the quotient between the trap (angular) frequency along the z direction ν_z and the radial one $\nu_r \equiv \nu$. Thus, the behavior of the condensate wave function is determined by Eq. (1), with $V(\vec{r})$ given in (2). The normalization condition for ψ is $\int d^3\vec{r}|\psi|^2 = N$, where N is the mean number of atoms.

The problem of solving Eq. (1) can be restated as a variational problem corresponding to the minimization of the action related to the Lagrangian density

$$\mathcal{L} = \frac{i}{2}\hbar\left(\psi\frac{\partial\psi^*}{\partial t} - \psi^*\frac{\partial\psi}{\partial t}\right) - \frac{\hbar^2}{2m}|\nabla\psi|^2 + V(r)|\psi|^2 + \frac{2\pi a\hbar^2}{m}|\psi|^4, \qquad (3)$$

where the asterisk denotes a complex conjugate. In order to obtain the evolution of the condensate wave function we will minimize $\mathcal{L}$ within a set of trial functions. Obviously, the selection of the proper form of the trial functions is crucial. In our case, a natural choice is a Gaussian, since in the linear limit (no interactions) it is precisely the ground state of the linear Schrödinger equation, i.e., we take

$$\psi(x,y,z,t) = A(t)\prod_{\eta=x,y,z} e^{-\frac{[\eta-\eta_0(t)]^2}{2w_\eta^2} + i\eta\alpha_\eta(t) + i\eta^2\beta_\eta(t)}. \qquad (4)$$

At a given time t, this function defines a Gaussian distribution centered at the position (x_0, y_0, z_0). The other variational parameters are A (amplitude), w_η (width), α_η (slope), and β_η [(curvature)$^{-1/2}$], where $\eta = x,y,z$. All these parameters are real numbers. As it has been shown in [19], the imaginary terms appearing in the exponent of (4) are essential if one wants to obtain reliable results. Our goal is to find the equations giving the evolution of all these variational parameters. To this aim, we insert (4) into (3) and calculate an effective Lagrangian L by integrating the Lagrangian density over the space coordinates

$$L = \langle\mathcal{L}\rangle = \int_{-\infty}^{\infty}\mathcal{L}\, d^3\vec{r}. \qquad (5)$$

Once we have this function, using Lagrange equations for each variational parameter, after a tedious although straightforward algebra one can derive the corresponding evolution equations. The first equation concerns the particle number conservation, $\pi^{3/2}|A(t)|^2 w_x(t)w_y(t)w_z(t) = N$. It is also possible to find the equations of the motion of the center of the condensate

$$\ddot{\eta}_0 + \lambda_\eta^2\nu^2\eta_0 = 0 \qquad (\eta = x,y,z). \qquad (6)$$

This equation shows explicitly that the center of the condensate will oscillate harmonically with the bare frequencies $\lambda_\eta\nu$. It is interesting, and intuitively clear that, in the case of a harmonic potential, this motion does not depend on the number of particles N, and therefore it is not affected by the nonlinear effects. This fact implies that the "center of mass" of the condensate responds like a classical particle to the external potential (note that this is not necessarily true for other potentials).

The widths of the condensate satisfy the following equations:

$$\ddot{w}_x + \lambda_x^2\nu^2 w_x = \frac{\hbar^2}{m^2 w_x^3} + \sqrt{\frac{2}{\pi}}\frac{a\hbar^2 N}{m^2 w_x^2 w_y w_z}, \qquad (7)$$

and two similar equations for w_y and w_z obtained by a cyclic permutation of the indices x,y,z in Eq. (7). The rest of the variational parameters can be obtained from the widths and the center coordinates through the equations

$$\beta_\eta = -\frac{m\dot{w}_\eta}{2\hbar^2 w_\eta}, \qquad \alpha_\eta = -\frac{m\dot{\eta}_0}{\hbar^2} - 2\beta_\eta\eta_0. \qquad (8)$$

Once we know the behavior of both the center of the condensate and the widths, we can calculate the evolution of the rest of the parameters, and then completely characterize the evolution of the Gaussian-like atomic cloud. Given that the solutions to Eq. (6) are readily derived, the whole problem reduces to solving the system of ordinary differential equations (7).

We find it convenient to define new dimensionless variables and constants according to $\tau = \nu t$, $w_\eta = a_0 v_\eta$ ($\eta = x,y,z$), and $P = \sqrt{2/\pi}\,Na/a_0$, where $a_0 = [\hbar/(m\nu)]^{1/2}$ is the size of the ground state for a harmonic potential of frequency ν (except for a factor of $\sqrt{2}$). Note that P basically gives the strength of the atom-atom interactions related to the bare harmonic potential. With these definitions, Eq. (7) becomes

$$\frac{d^2}{d\tau^2}v_x + \lambda_x^2 v_x = \frac{1}{v_x^3} + \frac{P}{v_x^2 v_y v_z}, \qquad (9a)$$

$$\frac{d^2}{d\tau^2}v_y + \lambda_y^2 v_y = \frac{1}{v_y^3} + \frac{P}{v_y^2 v_x v_z}, \qquad (9b)$$

$$\frac{d^2}{d\tau^2}v_z + \lambda_z^2 v_z = \frac{1}{v_z^3} + \frac{P}{v_z^2 v_y v_x}. \qquad (9c)$$

Equations (9a)–(9c) give us a simple picture of the evolution of the width of the condensate when we associate with them the classical motion of a ficticious particle with coordinates (v_x, v_y, v_z) in an effective three-dimensional potential

$$V_{\mathrm{eff}}(v_x, v_y, v_z) = \frac{1}{2}(\lambda_x^2 v_x^2 + \lambda_y^2 v_y^2 + \lambda_z^2 v_z^2) + \frac{1}{2v_x^2} + \frac{1}{2v_y^2} + \frac{1}{2v_y^2} - \frac{P}{v_x v_y v_z}. \quad (10)$$

The interpretation of Eqs. (9a)–(9c) is straightforward. (i) The left-hand side of these equations corresponds to three harmonic oscillators; (ii) the first term on the right-hand side, which is proportional to v_η^{-3} $(\eta = x, y, z)$, tends to spread the wave packet, and corresponds to the dispersion provided by the kinetic energy; (iii) finally, the last term comes from the nonlinear interaction between the particles. Depending on the sign of the scattering length a (i.e., the sign of P) this term can be either repulsive (positive scattering length) or attractive (negative scattering length). We wish to emphasize that Eqs. (9a)–(9c) for the scaled widths v_η $(\eta = x, y, z)$ contain all the information about the dynamics of the condensate, provided its shape does not depart too much from a Gaussian one, and therefore can be regarded as the starting point to study the dynamics of the condensate under different conditions [20].

We next focus our attention on the frequencies of the low energy excitations of the condensate. They correspond to the small oscillations around the equilibrium points. Under the present analysis, they can be calculated by first finding the equilibrium points of Eq. (6), (8), and (9a)–(9c) and then expanding the solutions around these points. In view of the fact that the α's and β's can be expressed in terms of the center coordinates, the widths, and their derivatives [cf., Eqs. (8)], these frequencies will be completely determined by Eq. (6) and (9a)–(9c). It is apparent that the frequencies coming from Eq. (6) are the bare frequencies $\lambda_x \nu, \lambda_y \nu, \lambda_z \nu$, and the respective modes correspond to the harmonic motion of the center of the condensate in the bare potential $V(\vec{r})$. Thus, in the following we will concentrate on the frequencies coming from Eqs. (9a)–(9c). Furthermore, we will restrict ourselves to the case of an anisotropic trap with cylindrical symmetry, which is the most interesting one from the experimental point of view [8]. In this case we have $\lambda_x = \lambda_y = 1$, $\nu \equiv \nu_r$.

The equilibrium points of Eqs. (9a)–(9c) correspond to the stable (or unstable) stationary states of the condensate. They satisfy the equations

$$v_0 = \frac{1}{v_0^3} + \frac{P}{v_0^3 v_{0z}}, \qquad \lambda_z^2 v_{0z} = \frac{1}{v_{0z}^3} + \frac{P}{v_{0z}^2 v_0^2}, \quad (11)$$

where $v_0 = v_{0x} = v_{0y}$. For the positive scattering length $(P > 0)$ there is only one stable equilibrium point. On the other hand, for the negative scattering length $(P < 0)$ the situation is different: depending on the values of the parameters involved in the problem it is possible to find either no equilibrium points or two equilibrium points, one stable and the other unstable. In the first case (no equilibrium points) a collapse of the condensate would occur, whereas in the second one (two equilibrium points) a stable condensate can exist. The condition under which collapse occurs derived from these equations [20] is similar to the one given in Ref. [13].

Expanding Eqs. (9a)–(9c) around the equilibrium points defined by (11), we find the following expressions for the low excitation frequencies:

$$\nu_a = 2\nu\sqrt{1 - 2P_{4,1}}, \quad (12a)$$

$$\nu_{b,c} = 2\nu\left[\frac{1}{2}(1 + \lambda_z^2 - P_{2,3}) \pm \frac{1}{2}\sqrt{(1 - \lambda_z^2 + P_{2,3})^2 - 8P_{3,2}}\right]^{1/2}, \quad (12b)$$

where we have defined $P_{i,j} = P/(4v_0^i v_{0z}^j)$. The corresponding modes are graphically represented in Fig. 1. Because of the cylindrical symmetry of the trap, the angular momentum along the z axis is conserved, and we can thus label the modes by azimuthal angular quantum numbers m [11,12]: we find $|m| = 2$ for mode a, and $m = 0$ for modes b and c [21].

In Fig. 2 we have plotted the three excitation frequencies as functions of P for parameters corresponding to the parameters in the JILA [8] [Fig. 2(a)], MIT [7] [Fig. 2(b)], and Rice experiments [3] [Fig. 2(c)], for which $\lambda_z = \sqrt{8}$, $18/132$, $117/163$, respectively. Let us analyze first the case of *positive scattering length* [Figs. 2(a) and 2(b)]. Figure 2(a) shows the results for the Rb experiment at JILA. We have included the experimental data reported in [8], taking $a = 6$ nm and $N = 4400$. The agreement between theory and experiment is remarkably good, despite the fact that for these parameters the wave function of the condensate is closer to the Thomas-Fermi solution with parabolic dependence [11,12] than to a Gaussian. The reason for that is that if one performs the Thomas-Fermi approximation in the NLSE (after an appropriate unitary transformation), the Gaussian approximation to describe the frequency spectrum is exact [11]. On the other hand they agree with the numerical calculations [16] to the percent level. The frequency close to $5\nu_r$ has not been measured in the experiment. The results of Fig. 2(b) correspond to the latest Na experiment at MIT (the experimental value of $P \simeq 1500$ lies out of the plot; the corresponding frequencies almost coincide with the asymptotes). The dashed lines give the asymptotic behavior $P \gg 1$, for which the energy of interaction

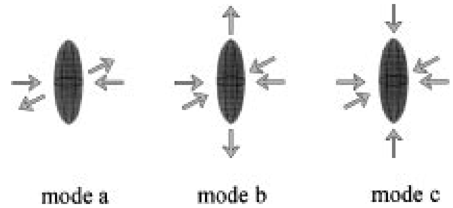

FIG. 1. Oscillation modes of the condensate.

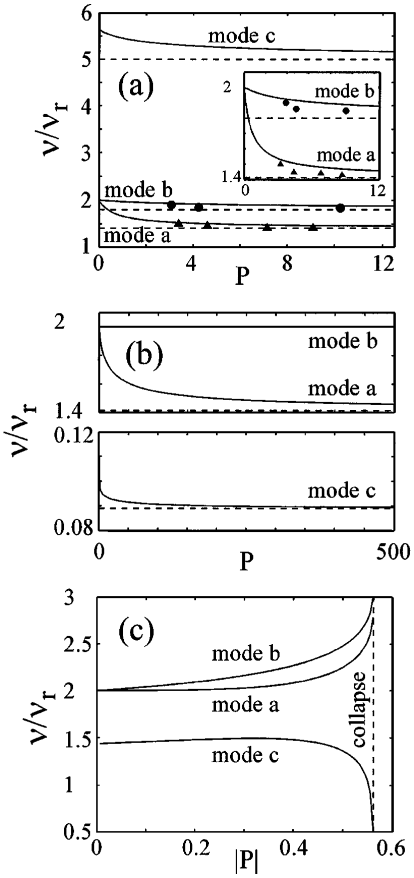

FIG. 2. Oscillation frequencies as functions of the parameter P for positive (a),(b) and negative (c) scattering length. (a) $\lambda_z = \sqrt{8}$, and the symbols represent experimental results mentioned in the text, taking $a = 6$ nm and $N = 4400$; (b) $\lambda_z = 18/132$; (c) $\lambda_z = 117/163$. The dashed lines correspond to the limit $P \rightarrow \infty$. The labels on the curves refer to different oscillation modes (see text).

predominates over the kinetic energy. In this case we have

$$\nu_a = \sqrt{2}\,\nu\,, \tag{13a}$$

$$\nu_{b,c} = \frac{\nu}{\sqrt{2}}[4 + 3\lambda_z^2 \pm \sqrt{16 + 9\lambda_z^4 - 16\lambda_z^2}\,]^{1/2}, \tag{13b}$$

which reproduces in this limit the formulas derived by Stringari [12]. This agreement is remarkable since the spectrum of Ref. [12] is based on the Thomas-Fermi approximation (valid for $P \gg 1$) which for the ground state predicts a parabolic dependence for the condensate wave function instead of the Gaussian assumed in our trial wave function. In the opposite limit, $P \rightarrow 0$ one recovers the bare trap results $\nu_a = \nu_b = 2\nu$ and $\nu_c = 2\lambda_z\nu$. In Fig. 2(c) we have plotted the results for *negative scattering length*. For small P we recover again the bare trap results. For larger values of P the interactions become more and more important, up to the point in which a stable condensate is not possible since it would collapse. Note that the width of the condensate remains finite at the edge of the collapse region.

In summary, we have shown that the variational formalism can explain in a very simple and elegant way some features observed in present experiments dealing with Bose-Einstein condensation. In particular, it predicts quite accurately the low energy excitation spectrum of the condensate for both positive and negative scattering lengths. We believe that this method can be used to treat analytically many problems related to the evolution of a Bose-Einstein condensate. A more detailed analysis will be presented elsewhere.

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