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Numerical solution of the nonlinear Schrödinger equation for small samples of trapped neutral atoms

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We present a numerical technique to solve the time-independent nonlinear Schrödinger equation with an external potential. We apply it to the case of a dilute Bose-condensed assembly of trapped neutral atoms where the potential varies on the same scale as the condensate. This situation should soon be accessible to experimental observation.

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I. INTRODUCTION

It may soon be possible to produce samples of Bose-condensed, neutral atoms in magnetic traps [1,2]. In some cases dilute gases will be composed (especially in experiments that just get to condensation) of a modest number of atoms and may be very inhomogeneous due to the variation of the trap potential on the scale of the sample [2]. This is particularly true in the laser plus evaporative cooling route. This means that they can exhibit features that are difficult to observe in homogeneous gases. In particular, we shall show that nonlinear excitations of the condensate are stabilized by the presence of the potential. As long as we are outside the region of critical fluctuations [1], we can determine the shape of the condensate in the trap using the relevant nonlinear Schrödinger equation, i.e., the Gross-Pitaevskii equation [3]. Approximate semiclassical solutions of this equation have been presented elsewhere for magnetostatic traps [4].

In this paper, we present an account of the solutions obtained by a direct numerical solution of the Gross-Pitaevskii equation for atoms in a spherical harmonic trap. We then compare these solutions with those obtained using the well-known and much-used approximation, which assumes the kinetic energy term in the Schrödinger equation can be neglected. We shall present solutions for the case where all the atoms are in the condensate, i.e., for the case $T=0$. It is not difficult, however, to extend the numerical method to include the effect of any uncondensed atoms on the mean field acting upon the atoms [5]. This ground-state solution can also be used as an input to techniques that predict the spectrum of elementary excitations in the trap [6]. It is also needed in theories of the optical properties of condensed atoms [7]. We have given a fairly full account of the way we proceed to maximize the usefulness to others who wish to find such solutions.

II. THE NONLINEAR SCHRÖDINGER EQUATION

Mean field theory for a dilute assembly of bosons at $T=0$ results in an effective nonlinear Schrödinger equation for the condensate's "wave function." This equation, the Gross-Pitaevskii, nonlinear Schrödinger equation (NLSE) for condensed neutral atoms in an harmonic trap, has the following form [8]:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+\tfrac{1}{2}m\omega_{\text{trap}}^2r^2\Psi(\mathbf{r},t)+NU_0|\Psi(\mathbf{r},t)|^2\Psi(\mathbf{r},t)\ . \qquad (2.1)$$

Here $\Psi(\mathbf{r},t)$ is the Bose-Einstein condensate (BEC) wave function, m is the mass of a single atom, ω_{trap} is the angular frequency of the trap, N is the number of atoms in the condensate, and U_0 characterizes the atom-atom interaction and is given by

$$U_0=\frac{4\pi\hbar^2a}{m}\ , \qquad (2.2)$$

where a is the scattering length. Using this approximation for the interaction is valid at sufficiently low energies and when one can exclude all but s-wave interactions between atoms [10]. We shall assume, for the purposes of this discussion, that a is positive. We shall return to this issue later in the paper when we consider the results for specific examples.

To find a stationary solution we write $\Psi(\mathbf{r},t)=e^{-i\mu t/\hbar}\psi(\mathbf{r})$, (where μ is the chemical potential of the condensate); inserting this equation into Eq. (2.1), we find the following equation for $\psi(\mathbf{r})$:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+\tfrac{1}{2}m\omega_{\text{trap}}^2r^2\psi(\mathbf{r})+NU_0|\psi(\mathbf{r})|^2\psi(\mathbf{r})=\mu\psi(\mathbf{r})\ . \qquad (2.3)$$

The BEC ground-state wave function is spherically symmetric, thus, we can write it in the form

$$\psi(r)=A\frac{\phi(r)}{r}\ . \qquad (2.4)$$

Inserting Eq. (2.4) into (2.3) gives

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dr^2}+\tfrac{1}{2}m\omega_{\text{trap}}^2r^2\phi(r)+NU_0A^2\left[\frac{\phi^2(r)}{r^2}\right]\phi(r)=\mu\phi(r)\ . \qquad (2.5)$$

To obtain an equation suitable for numerical work, we transform to dimensionless length units by letting $r=(\hbar/2m\omega_{\text{trap}})^{1/2}x$, which yields

$$\frac{d^2\phi}{dx^2}+\left[\beta-\tfrac{1}{4}x^2-NA^2\gamma\left[\frac{\phi^2(x)}{x^2}\right]\right]\phi(x)=0\ , \tag{2.6}$$

where

$$\gamma=\frac{2mU_0}{\hbar^2}=8\pi a \tag{2.7}$$

and

$$\beta=\frac{\mu}{\hbar\omega_{\text{trap}}}\ . \tag{2.8}$$

The norm of $\Psi(\mathbf{r})$ must be equal to one (since N appears explicitly in the NLSE), thus

$$4\pi\left[\frac{\hbar}{2m\omega_{\text{trap}}}\right]A^2\int_0^\infty|\phi(x)|^2dx=1\ . \tag{2.9}$$

Furthermore, $\psi(\mathbf{r})$ must vanish as $|\mathbf{r}|\to\infty$ and it also must be regular at the origin. Translating these two conditions into equations suitable for numerical work can be done more easily after the asymptotic behavior of $\phi(x)$ has been determined. This behavior is considered in the next section.

III. THE ASYMPTOTIC BEHAVIOR OF THE WAVE FUNCTION

A. Behavior as $x\to\infty$

Since the full wave function must vanish as $|\mathbf{r}|\to\infty$, the nonlinear term inside the square brackets in Eq. (2.6) must eventually become negligible compared to the other two terms. Thus, this equation has the following approximate form for large x:

$$\frac{d^2\phi}{dx^2}+[\beta-\tfrac{1}{4}x^2]\phi(x)\approx 0\ . \tag{3.1}$$

The solution of this equation is a parabolic cylinder function [9] and there are two solutions only one of which vanishes as $x\to\infty$. The asymptotic form of the correctly behaving parabolic cylinder function is well known and has the form

$$\phi(x)\sim Ce^{-x^2/4+(\beta-1/2)\ln(x)}\ ,\quad (x\to\infty)\ , \tag{3.2}$$

where C is a constant that depends on the wave-function norm.

B. Behavior as $x\to 0$

Now consider Eq. (2.6) as $x\to 0$. The nonlinear term inside the square brackets approaches a constant in this limit because of the regularity of the wave function at $x=0$. Thus, we can write

$$\phi(x)\approx\phi'(0)x\ ,\quad (x\to 0)\ , \tag{3.3}$$

where, hereafter, the prime denotes differentiation with respect to x. Note that $\phi(x)$ must vanish at $x=0$. Equation (2.6) can, therefore, be approximated in this limit by

$$\frac{d^2\phi}{dx^2}+\{\beta-NA^2\gamma[\phi'(0)]^2\}\phi(x)\approx 0\ . \tag{3.4}$$

Differentiating the solution of the above equation that vanishes at the origin and setting $x=0$ yields an algebraic equation for $\phi'(0)$, which can be solved to obtain

$$\phi'(0)\approx\left[\frac{\beta}{NA^2\gamma+1}\right]^{1/2}\ . \tag{3.5}$$

This equation is useful in numerical work because it serves as a starter for the Runge-Kutta integration.

C. Boundary conditions on ϕ

We are now in a position to write down the boundary conditions satisfied by $\phi(x)$. For $x\to 0$,

$$\phi(0)=0 \tag{3.6}$$

and

$$\phi'(0)\approx\left[\frac{\beta}{NA^2\gamma+1}\right]^{1/2}\ , \tag{3.7}$$

and for $x\to\infty$

$$\phi(x)\sim e^{-x^2/4+(\beta-1/2)\ln(x)}\equiv\phi_{\text{asym}}(x) \tag{3.8}$$

and, since asymptotic expansions may be differentiated,

$$\phi'(x)\sim[-x/2+(\beta-1/2)(1/x)]\times e^{-x^2/4+(\beta-1/2)\ln(x)}\equiv\phi'_{\text{asym}}(x)\ . \tag{3.9}$$

Note that the constant C is absent in Eq. (3.8). This constant depends on the overall normalization of the wave function and is set to one in practice as the normalization is determined independently. Imposing this condition ensures that the wave-function norm will not be unity. We shall show how we find a solution with unit norm later in the paper.

The four equations above, together with the normalization condition [Eq. (2.9)], form the basis for the numerical technique for finding the ground-state solution of the NLSE. We turn now to a description of this technique.

IV. NUMERICAL INTEGRATION TECHNIQUE

The numerical method divides into two parts. The first part consists of finding a solution of Eq. (2.6) that satisfies the boundary conditions summarized in Eqs. (3.6)–(3.9). The norm of such a solution will not be equal to one. The second part involves finding a related solution whose norm is one, but which corresponds to a condensate *containing a different number of atoms.* We shall discuss each of these steps in turn.

The parameters on which the solution of Eq. (2.6) depend are N, γ, β, and A. When all of these parameters have been assigned numerical values, both the values of $\phi(0)$ and $\phi'(0)$ are determined from Eqs. (3.6) and (3.7). The Runge-Kutta method [11] is used to propagate the solution of Eq. (2.6) out to large values of x for given values of the parameters. The resulting solution does not, however, satisfy the boundary conditions at *large* x. Thus, many different sets of the above parameters must be tried in order to find the set of values for which boundary conditions at both large and small x are satisfied. In this work, the values of N, γ, and β were held constant and A was varied.

So, for a given value of A, Eq. (2.6) was integrated out to $x_{\rm max}$. Let us call the resulting numerically determined solution $\phi_{\rm num}(A,N;x)$. After the integration, the asymptotic form of the wave function $\phi_{\rm asym}(x)$ was renormalized to be equal to $\phi_{\rm num}(x_{\rm max})$ at $x=x_{\rm max}$ and the Wronskian of this function with $\phi_{\rm num}(A;x)$ was computed at $x=x_{\rm max}$. The value of A was incremented and the above process was repeated yielding another value of the Wronskian.

The process ended when the sign of the Wronskian changed. Letting the value of A, for which the Wronskian vanishes be A_0, the wave function $\phi_{\rm num}(A_0,N;x)$ satisfies all of the boundary conditions described above except that its norm is not equal to one. It is possible to use these results to find a solution that satisfies all of the boundary conditions; we turn to this procedure next.

The wave function $\phi_{\rm num}(A_0,N_0;x)$ is a solution of

$$\frac{d^2\phi_{\rm num}}{dx^2}+\left[\beta-\frac{1}{4}x^2-N_0A_0^2\gamma\left[\frac{\phi^2_{\rm num}(A_0,N_0;x)}{x^2}\right]\right]\times\phi_{\rm num}(A_0,N_0;x)=0\ . \tag{4.1}$$

Now consider a new wave function $\phi_1(A_1,N_1;x)$ that is a solution of the equation

$$\frac{d^2\phi_1}{dx^2}+\left[\beta-\frac{1}{4}x^2-N_1A_1^2\gamma\left[\frac{\phi^2_1(A_1,N_1;x)}{x^2}\right]\right]\times\phi_1(A_1,N_1;x)=0\ . \tag{4.2}$$

The two solutions, $\phi_{\rm num}(A_0,N_0;x)$ and $\phi_1(A_1,N_1;x)$, will be different unless

$$N_0A_0^2=N_1A_1^2 \tag{4.3}$$

because, in this case, the defining differential equations and boundary conditions for the two solutions are identical and we have

$$\phi_1(A_1,N_1;x)=\phi_{\rm num}(A_0,N_0;x)\ . \tag{4.4}$$

The *full* wave functions corresponding to $\phi_1(A_1,N_1;x)$ and $\phi_{\rm num}(A_0,N_0;x)$ will be different: However,

$$\psi_0(A_0,N_0,r)=\left[\frac{A_0}{r}\right]\phi_{\rm num}(A_0,N_0;r) \tag{4.5}$$

and

$$\psi_1(A_1,N_1,r)=\left[\frac{A_1}{r}\right]\phi_1(A_1,N_1;r)=\left[\frac{A_1}{r}\right]\phi_{\rm num}(A_0,N_0;r)\ . \tag{4.6}$$

The new wave function $\psi_1(A_1,N_1,x)$ is written in terms of the numerically determined wave function and has a different norm. Thus, by simultaneously changing both A and N, we can find new solutions of the NLSE with different normalizations for condensates having different numbers of particles. The only undetermined quantity in Eq. (4.6) is A_1. Its value is simply determined by the normalization condition, Eq. (2.9);

$$4\pi\left[\frac{\hbar}{2m\omega_{\rm trap}}\right]A_1^2\int_0^\infty|\phi_{\rm num}(A_0,N_0;x)|^2dx=1\ . \tag{4.7}$$

Since both A_0 and $\phi_{\rm num}(A_0,N_0;x)$ are known, we can solve the above equation for A_1

$$A_1=\left[4\pi\left[\frac{\hbar}{2m\omega_{\rm trap}}\right]\int_0^\infty|\phi_{\rm num}(A_0,N_0;x)|^2dx\right]^{-1/2}\ . \tag{4.8}$$

Once A_1 has been determined, the number of atoms in the condensate to which the new wave function applies, is determined by Eq. (4.3);

$$N_1=\left[\frac{A_0}{A_1}\right]^2N_0\ . \tag{4.9}$$

And the final solution is given by

$$\psi(A_1,N_1;r)=\frac{A_1}{r}\phi_{\rm num}(A_0,N_0;r)\ , \tag{4.10}$$

where $\phi_{\rm num}(A_0,N_0;r)$ and A_0 are obtained numerically from the Runge-Kutta integration, A_1 is subsequently determined from Eq. (4.8), and N_1 is obtained from Eq. (4.9).

V. RESULTS

In this section we shall present results for some specific examples and make comparison with a commonly used approximation. In Fig. 1 we give the solution for the case of $N\sim10^5$ particles in a trap of frequency 10 Hz. This is a reasonable case that one might expect to realize in the case of the alkali-metal atoms, say Cs [1]. We have assumed that we are dealing with a case where the scattering length is positive. In some cases, this will require the selection of particular ground states or the application of an external field [12]. If the scattering length were negative, there would not, in general, be a stable solution of the NLSE, i.e., no stable condensate [13]. We have, therefore, taken the typical value $a\approx3$ nm for the scattering length in this investigation. We have also plotted the approximate solution obtained by assuming one can neglect the kinetic energy term in the NLSE. If one can make this approximation, Eq. (2.3) takes the form

$$\tfrac{1}{2}m\omega^2_{\rm trap}r^2\psi(\mathbf{r})+NU_0|\psi(\mathbf{r})|^2\psi(\mathbf{r})=\mu\psi(\mathbf{r})\ . \tag{5.1}$$

This has the solution

$$|\psi(r)|^2=\frac{\mu-(1/2)m\omega^2_{\rm trap}r^2}{NU_0} \tag{5.2}$$

for $r<r_c$, where

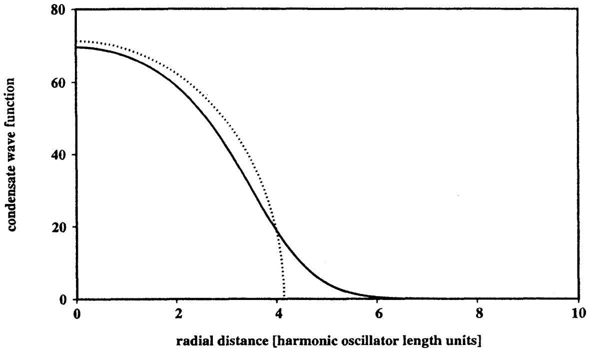

FIG. 1. This figure contains plots of the exact (solid line) and approximate (dotted line) condensate wave functions for a condensate having 10 648 atoms. The form of the approximate wave function is given by Eq. (5.2) where the number of condensate atoms was taken to be the same as for the exact solution but the chemical potential was determined by normalization as in Eq. (5.4). The value of the chemical potential for the exact case is $4.3\hbar\omega_{\text{trap}}$. Note that the horizontal axis is scaled in harmonic oscillator length units whose value is given by $x_{\text{harmonic}}=(\hbar/2m\omega_{\text{trap}})^{1/2}$. The vertical axis is scaled by this number as well so that $A\phi(x)/x$ is plotted instead of $A\phi(x)/r$.

$$r_c=\left[\frac{2\mu}{m\omega_{\text{trap}}^2}\right]^{1/2}, \tag{5.3}$$

and is zero for $r>r_c$. This value of μ in the above equation is fixed by normalization and has the value

$$\mu=\left[\frac{15NU_0}{8\pi}\right]^{2/5}(\tfrac{1}{2}m\omega_{\text{trap}}^2)^{3/5}. \tag{5.4}$$

This solution will obviously fail in the region close to $r\approx r_c$. This failure is clearly exhibited in Fig. 1. For very large numbers of atoms in a trap, one may be able to ignore the role of this term. For small condensates, however, a significant amount of the condensate formed will be in this region. In that case, the precise solutions found using the method we have described will be needed. This will certainly be the case when one considers light scattering from these small condensates and the artificially sharp edge of the approximate solution would cause significant errors in the predictions.

The ground-state condensate wave function also appears as a potential term in the coupled equations that describe the condensate's response to an external light field [6]. An artificially sharp edge appearing in this potential will cause the solution of these equations to oscillate rapidly near $r=r_c$ thus introducing high-frequency noise into the Fourier transform of the solution. As it is this transform that is of interest in the light scattering problem, this limits the usefulness of the predicted condensate response function based on the approximate ground state.

In Fig. 2, we have plotted the variation of the ground-state energy—the chemical potential—as a function of the total number of atoms in the condensate. One can see how this deviates from the "free," i.e., noninteracting, value as the number of atoms in the condensate is increased.

So far we have limited our discussion to ground states. In the presence of the external potential it may be possible to observe nonlinear excitations of the condensate. One such solution is shown in Fig. 3. This corresponds to $N=1993$ with a chemical potential the same as the condensate of Fig. 1. Such nonlinear "excitations" of the condensate may play a role as the gas proceeds via metastable states in the cooling process. In a homogeneous gas, such amplitude variations would be quickly damped away [14]. One has, of course, to ask about the stability of such excitations and this is a matter that we intend to address in detail in our future work. There will also be excitations of the condensate that are not spherically symmetric, i.e., vortex solutions. Some of these could be found by separation in cylindrical coordinates (this would work if the vortex occurs at the center of the trap.) More general solutions are also possible that cannot be found using the techniques described here. Finding these may warrant direct solution in three-dimensions of the NLSE for trapped Bose-condensed atoms.

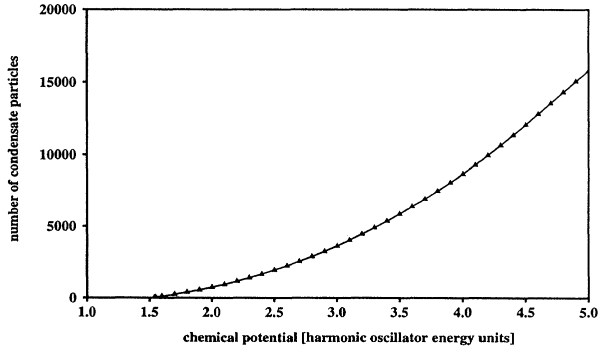

FIG. 2. A plot of the number of condensate atoms as a function of the chemical potential. The horizontal axis is scaled in units of the harmonic oscillator energy spacing, $\hbar\omega_{\text{trap}}$.

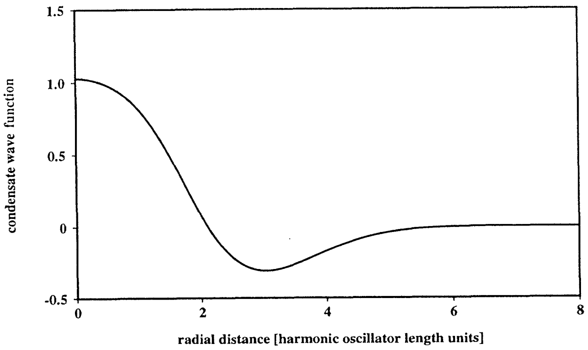

FIG. 3. A plot of a second solution of the NLSE for a condensate having the same chemical potential as in Fig. 1 but containing only 1993 atoms.

VI. CONCLUSIONS

We have presented a technique for solving the NLSE for a sample of Bose-condensed trapped atoms. We have shown when and how the solution deviates from the simplest, often-used approximation. The detailed nature of the nonlinear excitations (vortices, etc.) of these confined condensates should soon be accessible to direct experimental observation. This will provide motivation to extend the investigations described here to more general and complex geometries. The simpler solutions we have produced do, however, already exhibit the interesting features we have described.

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