Order parameter at the boundary of a trapped Bose gas

F. Dalfovo,[1] L. Pitaevskii,[2,3] and S. Stringari[1]

[1]*Dipartimento di Fisica, Università di Trento, I-38050 Povo, Italy*
and Istituto Nazionale di Fisica della Materia, I-38050 Povo, Italy
[2]*Department of Physics, Technion, Haifa 32000, Israel*
[3]*Kapitza Institute for Physical Problems, ulica Kosygina 2, 117334 Moscow, Russia*

Through a suitable expansion of the Gross-Pitaevskii equation near the classical turning point, we obtain an explicit solution for the order parameter at the boundary of a trapped Bose gas interacting with repulsive forces. The kinetic energy of the system, in terms of the classical radius R and of the harmonic oscillator length a_{HO}, follows the law $E_{kin}/N \propto R^{-2}[\ln(R/a_{HO}) + \text{const}]$, approaching, for large R, the results obtained by solving numerically the Gross-Pitaevskii equation. The occurrence of a Josephson-type current in the presence of a double trap potential is finally discussed. [S1050-2947(96)09411-5]

The recent experimental realization of Bose-Einstein condensation in atomic gases confined in magnetic traps [1–3] is stimulating new interest in the study of inhomogeneous Bose condensed systems where the order parameter exhibits an important spatial dependence on a macroscopic scale [4].

The purpose of the present work is to investigate the behavior of the wave function of the condensate near the classical turning point, that is, at the boundary of the trapped gas. This region is particularly important for the determination of the kinetic energy associated with the atoms of the condensate [5,6]. It is also crucial for the description of Josephson-type effects taking place in the presence of a barrier in the confining potential.

The order parameter $\psi(\mathbf{r})$ associated with the ground state of a dilute Bose gas obeys the Gross-Pitaevskii equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m}|\psi(\mathbf{r})|^2 \right]\psi(\mathbf{r}) = \mu\psi(\mathbf{r}), \quad (1)$$

where V_{ext} is the external confining potential, μ is the chemical potential and a is the s-wave scattering length. The condensate wave function $\psi(\mathbf{r})$ is normalized to the number N of atoms and is related to the atomic density through $\rho(\mathbf{r}) = |\psi(\mathbf{r})|^2$. The solution of Eq. (1) has been recently found by direct numerical integration [6–9]. In the following we will consider systems interacting with repulsive forces ($a>0$). When the scattering length (or the number of atoms in the trap) is sufficiently large, the solution of Eq. (1), in the region where $\mu > V_{ext}(\mathbf{r})$, takes the simplified Thomas-Fermi form

$$\psi(\mathbf{r}) = \left[\frac{m}{4\pi\hbar^2 a}[\mu - V_{ext}(\mathbf{r})] \right]^{1/2}. \quad (2)$$

Equation (2) is obtained by neglecting the kinetic energy term $\nabla^2\psi(\mathbf{r})$ in the Schrödinger-like equation (1) and provides an accurate description of the exact solution in the interior of the atomic cloud where the gradients of the wave function are small, as shown in Fig. 1. Several physical quantities, such as the potential energy and the chemical potential, can be safely calculated starting from Eq. (2) [5,6].

For other quantities the Thomas-Fermi approximation is instead inadequate. This is the case, for instance, of the kinetic energy associated with the condensate

$$E_{kin} = \int d\mathbf{r} \frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2, \quad (3)$$

for which the Thomas-Fermi approximation yields a logarithmic divergency arising at the boundary [5]. In this region, where $V_{ext}(\mathbf{r}) \sim \mu$, the kinetic energy term in Eq. (1) can no longer be ignored and the Thomas-Fermi approximation (2) fails. In the following we will explore the correct behavior of the order parameter in the boundary region at $T=0$, starting from the Gross-Pitaevskii equation (1). With respect to similar procedures used in the study of the single-particle Schrödinger equation in the presence of an external field [11], the present method includes explicitly the interatomic forces which are responsible for crucial nonlinear effects in the equations of motion.

Let us consider for simplicity a spherical trap [10]. The Gross-Pitaevskii equation (1) takes the form

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\psi - \frac{\hbar^2}{mr}\frac{d}{dr}\psi + [V_{ext}(r) - \mu]\psi + \frac{4\pi\hbar^2 a}{m}\psi^3 = 0. \quad (4)$$

Let R be the boundary of the system, determined by the equation $\mu = V_{ext}(R)$. Near this point, where $|r-R| \ll R$, one can carry out the expansion

$$V_{ext}(r) - \mu = (r-R)F + o(r-R), \quad (5)$$

where F is the modulus of the attractive external force $\mathbf{F} = -\nabla V_{ext}$ evaluated at $r=R$. Moreover, for values of R much larger than the thickness of the boundary [see Eq. (8) below] the second term in Eq. (4) is negligible. Indeed one can easily check that the effect of the first derivative is much smaller than the one of the second derivative in determining the shape of the profile close to R, when R is sufficiently large. So, one can approximate the Gross-Pitaevskii equation (4), in this limit, with the new equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\psi+(r-R)F\psi+\frac{4\pi\hbar^2 a}{m}\psi^3=0 . \quad (6)$$

Let us introduce the dimensionless variable

$$\xi=\frac{(r-R)}{d}, \quad (7)$$

where

$$d=\left(\frac{2m}{\hbar^2}F\right)^{-1/3} \quad (8)$$

is a typical thickness of the boundary giving, as we will see later, the distance from the classical radius R where the Thomas-Fermi approximation starts failing. Then we introduce the adimensional function ϕ defined by

$$\psi(\mathbf{r})=\frac{1}{d(8\pi a)^{1/2}}\phi(\xi). \quad (9)$$

In terms of ϕ the Gross-Pitaevskii equation (6) takes the universal form

$$\phi''-(\xi+\phi^2)\phi=0. \quad (10)$$

Notice that the nonlinear term ϕ^3 arises from the internal potential energy in Eq. (1). When $\xi\rightarrow+\infty$ this term can be neglected and Eq. (10) takes the simpler form $\phi''-\xi\phi=0$ which is the equation defining the Airy function. The asymptotic behavior then has the form

$$\phi(\xi\rightarrow\infty)\simeq\frac{A}{2\xi^{1/4}}\exp\left(-\frac{2}{3}\xi^{3/2}\right), \quad (11)$$

where the constant A must be determined by numerical integration of Eq. (10). In the opposite limit $\xi\rightarrow-\infty$ one can neglect the second derivative ϕ'' and the asymptotic behavior is given by

$$\phi(\xi\rightarrow-\infty)\simeq\sqrt{-\xi}. \quad (12)$$

The full behavior of the function ϕ is shown in Fig. 2. The value of the constant A is found to be 0.397.

The solution of Eq. (10) provides, via Eqs. (7)–(9), the proper structure of the wave function of the condensate near the classical turning point R. It is worth noting that Eq. (10) does not depend on the form of the external potential nor on the size of the interatomic force. These physical parameters enter the transformations (7) and (9) which fix, together with the solution of Eq. (10), the actual behavior of the wave function ψ.

Equations (2) and (9) determine the behavior of the wave function in two distinct regions of space: the former in the interior of the cloud, the latter in the boundary region. For sufficiently large N these two regions are sufficiently extended to match each other. An example is shown in Fig. 1 for $N=10^5$.

A third interesting region is the one at large distances beyond the boundary R where the system is very dilute and one can ignore the interaction term in Eq. (1). In this region the wave function can be written in the following way [11]:
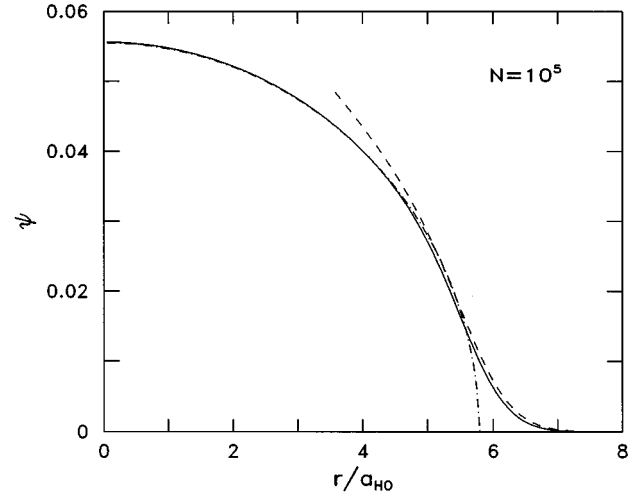

FIG. 1. Condensate wave function for 10^5 atoms of ^{87}Rb (scattering length $a=5.29\times10^{-7}$ cm) in a spherical harmonic trap of length $a_{HO}=1.22\times10^{-4}$ cm. Solid line: numerical solution of the Gross-Pitaevskii equation (1). Dot-dashed line: Thomas-Fermi approximation (2) (indistinguishable from the solid line in the inner part). Dashed line: surface profile obtained from the universal equation (10).

$$\psi(r)=\frac{1}{r}\left(\frac{\hbar R^2}{16\pi d^3 a}\right)^{1/2}\frac{A}{\{2m[V_{ext}(r)-\mu]\}^{1/4}}$$

$$\times\exp\left(-\sqrt{\frac{2m}{\hbar^2}}\int_R^r[V_{ext}(r')-\mu]^{1/2}dr'\right). \quad (13)$$

The effects of the interatomic interactions enter here only through the value of the chemical potential. It is worth noticing that the case $V_{ext}\equiv0$ would correspond to the asymptotic behavior of the order parameter for saturating systems in the absence of confining forces as happens, for example, outside the free surface of superfluid helium [12]. The coefficient of proportionality in Eq. (13) has been fixed in order to obtain the proper matching with the solution of Eqs. (9) and (10) taking place in the region of r where $R\gg r-R\gg d$ [see Eq. (11)].

Let us apply the formalism discussed above to the simplest case of an isotropic harmonic trap:

$$V_{ext}(r)=\frac{1}{2}m\omega_{HO}^2 r^2. \quad (14)$$

For $r<R$, the Thomas-Fermi wave function (2) takes the form

$$\psi_{TF}(r)=\left[\frac{R^2-r^2}{8\pi a_{HO}^4 a}\right]^{1/2}, \quad (15)$$

where we have used the expression $\mu=(1/2)m\omega_{HO}^2 R^2$ for the chemical potential and introduced the harmonic oscillator length $a_{HO}=(\hbar/m\omega_{HO})^{1/2}$. The radius R is fixed by imposing the normalization of the wave function (15) to the total number of particles:
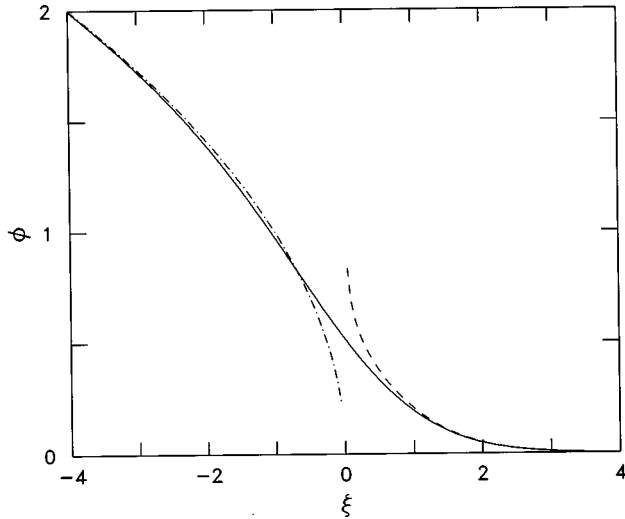
FIG. 2. Solution of the universal equation (10). The two asymptotic limits (12) (dot-dashed line) and (11) (dashed line) are also shown.

$$N=\frac{R^5}{15aa_{\mathrm{HO}}^4} \tag{16}$$

and increases very slowly with N.

Near the boundary the wave function is instead given by Eq. (9) where the thickness d, from Eq. (8), is

$$d=\left(\frac{a_{\mathrm{HO}}^4}{2R}\right)^{1/3}. \tag{17}$$

A similar result for the boundary thickness has been recently found by Baym and Pethick (see note 14 in Ref. [5]). Note that the ratio d/R tends to zero as N increases. Taking large and negative values of ξ as in Eq. (12) means moving from the boundary to the interior of the cloud until $(R-r)\gg d$. In this region the asymptotic behavior (12) holds and one obtains

$$\psi(r)\rightarrow\left[\frac{R(R-r)}{4\pi aa_{\mathrm{HO}}^4}\right]^{1/2}. \tag{18}$$

This exactly coincides with ψ_{TF} given in Eq. (15) provided $(R-r)\ll R$. In conclusion the wave function in the boundary region properly matches the Thomas-Fermi wave function (15) for values of r satisfying the conditions

$$d\ll(R-r)\ll R. \tag{19}$$

For distances from the boundary less than d the Thomas-Fermi approximation (15) fails; vice versa, for distances comparable to the radius R, Eq. (9) becomes inadequate. The matching of the two approximations at the surface is clearly visible in Fig. 1 for 10^5 atoms of ^{87}Rb. It is worth noticing that, near the boundary where ψ vanishes smoothly, the shape of the order parameter obtained with the universal equation (10) (dashed line) follows closely the exact solution of the Gross-Pitaevskii equation (solid line). For larger val-

ues of N the two curves becomes practically indistinguishable, thereby confirming the validity of the approximations used to derive Eq. (10).

Let us apply the above results to the calculation of the kinetic energy of the system. The integral (3) can be naturally divided into two parts:

$$E_{\mathrm{kin}}=\frac{4\pi\hbar^2}{2m}\left(\int_0^{R-\epsilon}|\psi'(r)|^2r^2dr+\int_{R-\epsilon}^{+\infty}|\psi'(r)|^2r^2dr\right), \tag{20}$$

where the distance $\epsilon>0$ from the boundary R is chosen in such a way that the conditions (19), with $(R-r)=\epsilon$, are satisfied. This permits us to evaluate the first term using the Thomas-Fermi approximation (15) and the second one using the solution (9) of the universal equation (10). Clearly the sum of the two terms should not depend on the explicit value of ϵ.

The first integral of Eq. (20) is easily evaluated and becomes

$$\int_0^{R-\epsilon}|\psi'(r)|^2r^2dr=\frac{R^3}{16\pi a_{\mathrm{HO}}^4a}\left[\ln\frac{2R}{\epsilon}-\frac{8}{3}\right], \tag{21}$$

where we have neglected corrections vanishing as ϵ/R.

The relevant range of integration for the second integral is the boundary region where the universal equation (10) holds. In fact the contribution coming from the region far beyond the surface, where the correct behavior of the wave function is given by Eq. (13), gives rise to higher order corrections. To the leading order one then finds

$$\int_{R-\epsilon}^{+\infty}|\psi'(r)|^2r^2dr=\frac{R^3}{4\pi a_{\mathrm{HO}}^4a}\int_{-\epsilon/d}^{+\infty}(\phi')^2d\xi, \tag{22}$$

where $\phi'=d\phi/d\xi$. If the ratio $\epsilon/d=(R-r)/d$ is sufficiently large [see condition (19)] the integral on the right-hand side is easily calculated and takes the value

$$\int_{-\epsilon/d}^{+\infty}(\phi')^2d\xi=\frac{1}{4}\ln\frac{2\epsilon}{d}+C \tag{23}$$

with

$$C=-\int_{-\infty}^{+\infty}\log(\sqrt{1+\xi^2}+\xi)\frac{d}{d\xi}[(\phi')^2\sqrt{1+\xi^2}]d\xi=0.176. \tag{24}$$

In Eq. (24) we have ignored corrections vanishing as d/ϵ. Collecting the above results and using the explicit expression (17) for the boundary thickness d in terms of the oscillator length a_{HO}, one finally finds the following result for the kinetic energy per particle:

$$\frac{E_{\mathrm{kin}}}{N}=\frac{5}{2}\frac{\hbar^2}{mR^2}\left[\ln\left(\frac{R}{a_{\mathrm{HO}}}\right)+C'\right]=\frac{5}{2}\frac{\hbar^2}{mR^2}\ln\left(\frac{R}{1.3a_{\mathrm{HO}}}\right), \tag{25}$$

where $C'=(7/4)\ln 2-2+3C$. Note that we have used the Thomas-Fermi expression (16) for N. Corrections to N coming from the modified structure of the surface affect the ki-
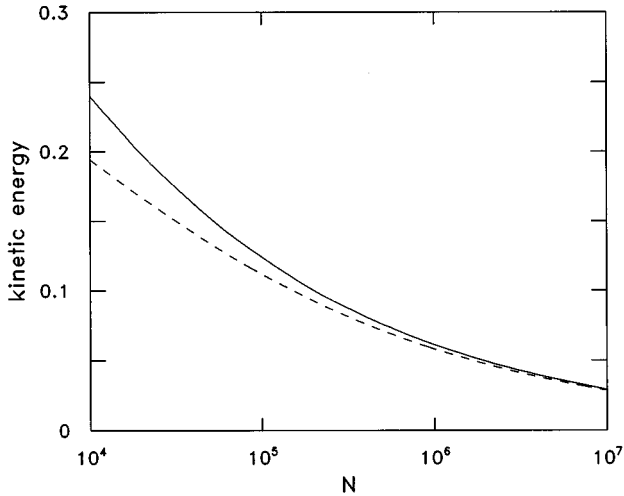
FIG. 3. Kinetic energy per particle, in units of $\hbar\omega_{\text{HO}}$, for ^{87}Rb in a spherical harmonic trap as a function of the number of condensed atoms. Solid line: from the solution of the Gross-Pitaevskii equation (1). Dashed line: approximation (25).

netic energy only to higher orders. Equation (25) provides the correct asymptotic behavior of the kinetic energy in the limit of large N where $R \gg a_{\text{HO}}$. This is confirmed by the comparison with the exact value of the kinetic energy obtained by solving numerically the Gross-Pitaevskii equation (1), as shown in Fig. 3.

We conclude this paper by discussing an interesting application of the formalism to a Josephson-type effect. The physical idea is to consider a confining potential with two wells separated by a barrier. When the chemical potential in the two traps is different, an oscillating flux of atoms is generated. Let us consider the simplest one-dimensional problem (extension to 3D will be the object of a future work) and let the external field V_{ext} consist of two symmetric traps, trap 1 and trap 2, as shown schematically in Fig. 4. A difference between the chemical potentials μ_1 and μ_2 of the atoms in the two traps can be achieved, for example, by filling them with a different number of atoms. In order to obtain a first analytic result for the flux of atoms generated by the difference in the chemical potentials we will assume that the bar-
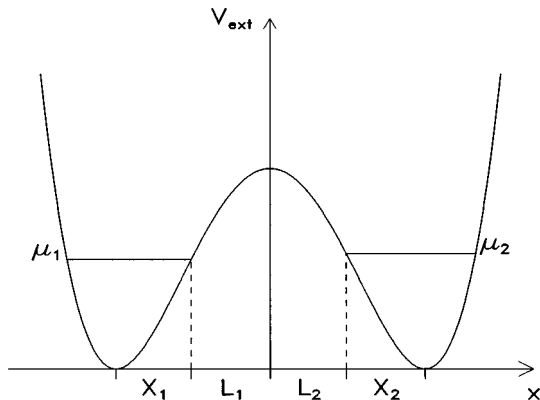
rier between the two wells is high enough. In this case the overlap between the wave functions relative to the two traps occurs only in the classically forbidden region where interaction effects can be ignored and one can safely use approximation (13) for the wave function. Furthermore we will ignore the variation of μ_1 and μ_2 generated by the corresponding flux of particles. In 1D the factor $1/r$ in the wave function (13) is absent and it is convenient to take the origin of axes at the symmetry point of the external potential (see Fig. 4).

The Gross-Pitaevskii equation has two natural solutions in this case. The first one with chemical potential μ_1 is localized in the trap 1. Its behavior in the classically forbidden region $x > -L_1$ is given by

$$\psi_1(x) = \left(\frac{\hbar X_1^2}{16\pi d_1^3 a}\right)^{1/2} \frac{A}{\{2m[V_{\text{ext}}(x) - \mu_1]\}^{1/4}}$$
$$\times \exp\left(-\sqrt{\frac{2m}{\hbar^2}} \int_{-L_1}^{x} [V_{\text{ext}}(x') - \mu_1]^{1/2} dx'\right), \quad (26)$$

where X_1 is the distance between the center of trap 1 and the classical turning point, d_1 is its boundary thickness [see Eq. (8)], and L_1 is the distance between the classical turning point and the symmetry point of the external potential (see Fig. 4).

The second solution with chemical potential μ_2 is instead localized in the trap 2 and its behavior in the region $x < L_2$ is given by

$$\psi_2(x) = \left(\frac{\hbar X_2^2}{16\pi d_2^3 a}\right)^{1/2} \frac{A}{\{2m[V_{\text{ext}}(x) - \mu_2]\}^{1/4}}$$
$$\times \exp\left(-\sqrt{\frac{2m}{\hbar^2}} \int_{x}^{L_2} [V_{\text{ext}}(x') - \mu_2]^{1/2} dx'\right). \quad (27)$$

It is immediate to verify that the linear combination

$$\psi(x,t) = \psi_1(x)\exp\left(-i\frac{\mu_1 t}{\hbar}\right) + \psi_2(x)\exp\left(-i\frac{\mu_2 t}{\hbar}\right) \quad (28)$$

is solution of the time dependent Schrödinger equation. In fact the wave functions ψ_1 and ψ_2 significantly overlap only in the classically forbidden region where nonlinear effects due to the interatomic potential are negligible. The current density

$$I = \frac{i\hbar}{2m}\left(\psi(x,t)\frac{\partial}{\partial x}\psi^*(x,t) - \psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)\right) \quad (29)$$

associated with the wave function (28) can be easily calculated and takes the typical Josephson form

$$I = I_0\sin\frac{(\mu_1 - \mu_2)t}{\hbar} \quad (30)$$

FIG. 4. Geometry of the double trap for the Josephson effect (see text).

with $I_0 = (\hbar/m)(\psi_1\psi_2' - \psi_2\psi_1')$. Using the explicit results (26) and (27) for the wave functions ψ_1 and ψ_2 and taking $\mu_1 \sim \mu_2 = \mu$ and $L_1 \sim L_2 = L$ in the evaluation of I_0, we find that the current I_0 is uniform in the interval $(-L, +L)$. Its explicit value is given by the useful result

$$I_0 = \frac{\hbar A^2 X^2}{16\pi m d^3 a} \exp\left(-\sqrt{\frac{2m}{\hbar^2}}\int_{-L}^{+L}[V_{\text{ext}}(x') - \mu]^{1/2}dx'\right).$$

$$(31)$$

As a consequence of the Josephson current the number of atoms in the two traps will oscillate in time according to the law [13]

$$\frac{d}{dt}N_1 = -\frac{d}{dt}N_2 = -I_0\sin\frac{(\mu_1 - \mu_2)t}{\hbar}, \qquad (32)$$

thereby providing the anticipated result for the flux of particles through the barrier separating the two traps.

We have considered here the Josephson effect only in the simplest one-dimensional case. We note that quasi-one-dimensional devices are already under experimental investigation [14], using strongly anisotropic magnetic traps to obtain a cigar-shaped order parameter and optical methods to create a potential barrier. Extension of our formalism to 3D will be the object of future work.

In conclusion we have obtained an explicit solution of the Gross-Pitaevskii equation near the classical turning point where the Thomas-Fermi approximation turns out to be completely inadequate. Using this solution we have been able to derive an analytic expression for the kinetic energy of the system holding for large values of N. We have finally discussed possible Josephson-type oscillations of atoms through the barrier separating two traps.

[1] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, Science **269**, 198 (1995).

[2] C.C. Bradley, C.A. Sackett, J.J. Tollett, and R.G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).

[3] K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).

[4] *Bose Einstein Condensation*, edited by A. Griffin, D.W. Snoke, and S. Stringari (Cambridge Univ. Press, Cambridge, 1995). This volume collects various review discussions on Bose-Einstein condensation in different physical systems.

[5] G. Baym and C. Pethick, Phys. Rev. Lett. **76**, 6 (1996).

[6] F. Dalfovo and S. Stringari, Phys. Rev. A **53**, 2477 (1996).

[7] P.A. Ruprecht, M.J. Holland, K. Burnett, and M. Edwards, Phys. Rev. A **51**, 4704 (1995).

[8] M. Holland and J. Cooper, Phys. Rev. A **53**, R1954 (1996).

[9] M. Edwards, R.J. Dodd, C.W. Clark, P.A. Ruprecht, and K. Burnett, Phys. Rev. A **53**, R1950 (1996).

[10] The formalism is straightforwardly extended to anisotropic traps. In this case the distance $r - R$ entering Eqs. (5)–(7) should be replaced by the quantity $(\mathbf{R} - \mathbf{r})\cdot\mathbf{F}/F$.

[11] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics* (Pergamon Press, Oxford, 1965).

[12] A. Griffin and S. Stringari, Phys. Rev. Lett. **76**, 259 (1996).

[13] The resulting oscillations of N_1 and N_2 imply a time dependence in the difference between the chemical potentials in the two traps. Such an effect should be small in order to justify the use of Eqs. (28)–(32). This implies the inequality $I_0\partial\mu/\partial N \ll (\mu_1 - \mu_2)^2$, where we have used $\partial\mu_1/\partial N_1 \sim \partial\mu_2/\partial N_2 = \partial\mu/\partial N$.

[14] W. Ketterle (private communication).