Expansion of a dipolar condensate

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(Received 30 October 2002; revised manuscript received 14 January 2003; published 17 April 2003)

We discuss the expansion of an initially trapped dipolar condensate. When the nominal isotropic s-wave interaction strength becomes tunable through a Feshbach resonance, anisotropic dipolar effects are shown to be detectable under current experimental conditions [E. A. Donley *et al.*, Nature London **412**, 295 (2001)].

DOI: 10.1103/PhysRevA.67.045601 PACS number(s): 03.75.−b, 05.30.−d, 32.80.Pj

Atomic Bose-Einstein condensates (BEC's) are realized at extremely low temperatures [1–3], when short-range atom-atom interaction can be described by a single parameter: the s-wave scattering length a_{sc}. This is a valid approximation as all higher-order partial, wave collisions die away in a short-range potential when the collision energy approaches zero. In more realistic models, however, even ground-state atoms may be polarized such as in an external magnetic trap, when the direction of its spin (of the valence electron for alkali) becomes aligned. BEC with dipole-dipole interaction has attracted considerable attention in recent years [4–9], and trapped fermionic dipoles have also been studied [10].

Despite the fact that dipolar interactions are now widely known to exist in a trapped BEC, it has not been directly detected yet. This is because the dipole interaction is much weaker than the contact interaction under most circumstances. Recently, we have studied the small amplitude shape oscillation of a dipolar condensate [7]. When the s-wave scattering length a_{sc} is tuned near to zero as realizable in the ^{85}Rb experiment [11,12], we showed that the anisotropic dipolar effect becomes detectable under current experimental conditions.

The free expansion of an interacting condensate after its sudden release from the trap is now a standard diagnostic tool in BEC physics [13,14]. It has also been extended to the case of an interacting Fermi gas [15]. In this paper, we investigate the free expansion of a dipolar condensate. Our results show that this may also lead to the experimental detection of dipolar interactions. This paper is organized as follows; first, we briefly review the formulation for a dipolar BEC; we then discuss our study of its expansion with both variational and numerical methods. We will subsequently concentrate on a detailed study for situations corresponding to the ^{85}Rb experiment [11]. Then we conclude with some different results on the shape and stability of a dipolar condensate.

For simplicity, we study a trapped dipolar BEC assuming all atomic dipole moments are equal and aligned along the z axis. The atom-atom interaction simplifies to

$$V(\vec{R}) = g_0 \delta(\vec{R}) + g_2 \frac{1-3\cos^2\theta_R}{R^3}, \tag{1}$$

where $\vec{R} = \vec{r} - \vec{r}\,'$, θ_R is the polar angle of $\vec{R}$, $g_0 = 4\pi\hbar^2 a_{sc}/M$ representing the contact interaction, and in atomic units $g_2 = \alpha^2(0)\mathcal{E}^2$ [$\alpha(0)$ is the atomic polarizability] or μ^2 (μ is the magnetic dipole moment). The corresponding Gross-Pitaevskii equation (in adimensional form) is then

$$i\dot{\psi}(\vec{r}) = \left[-\frac{\nabla^2}{2} + V_{ext}(\vec{r}) + \sqrt{(2\pi)^3} P_0 |\psi(\vec{r})|^2 + \frac{3}{2}\sqrt{2\pi} P_2 \int d\vec{r}\,' \frac{1-3\cos^2\theta}{R^3} |\psi(\vec{r}\,')|^2 \right] \psi(\vec{r}), \tag{2}$$

where $\psi(\vec{r})$ is the condensate wave function (normalized to unity) and a cylindrical symmetric harmonic trap in dimensionless unit $V_{ext}(\vec{r}) = (x^2 + y^2 + \lambda^2 z^2)/2$, with an aspect ratio λ. The length unit is $a_\perp = \sqrt{\hbar/M\omega_\perp}$ and energies are measured in units of $\hbar\omega_\perp$ ($\omega_\perp$ is the radial frequency of the trap). $P_0 = \sqrt{2\pi} N a_{sc}/a_\perp$ measures the contact interaction strength while $P_2 = \sqrt{2\pi} N g_2/(3\hbar\omega_\perp a_\perp^3)$ denotes the strength of the dipole-dipole interaction. The ground-state wave function of a dipolar condensate can be found by replacing the left-hand side of Eq. (2) with $-\mu\psi$, where μ is the chemical potential.

To proceed with the study of the condensate free expansion; we can solve the Eq. (2) numerically. We initialize the wave function to the self-consistently solved ground state in the presence of the trap V_{ext}, then find the time evolved wave function from the Eq. (2) by employing a self-adaptive Runge-Kutta method without the V_{ext}. In practice, this becomes an expensive calculation as we have to use a rather large spatial grid to accommodate the ever-expanding wave function and to obtain sufficient accuracy. We find that it is necessary to check the accuracy of solutions repeatedly on different sized grids.

Alternatively, the variational approach as developed earlier [4] can be used. In this case, we assume that the wave function always takes the form of a Gaussian, and transform the Eq. (2) into the following equations for variational parameters q_r and q_z:

$$\ddot{q}_r + q_r = \frac{1}{q_r^3} - \frac{1}{q_r^3 q_z}[P_2 f(\kappa) - P_0], \tag{3}$$

$$\ddot{q}_z + \lambda^2 q_z = \frac{1}{q_z^3} - \frac{1}{q_r^2 q_z^2}[P_2 g(\kappa) - P_0], \tag{4}$$

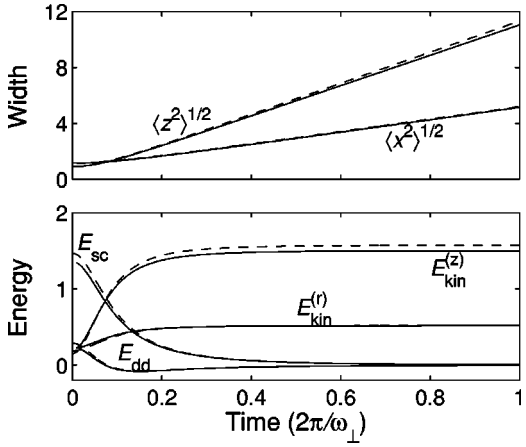

FIG. 1. Comparisons of free expansion results from the numerical (solid line) and the variational (dashed line) approaches as discussed in the text, for $\lambda=2$, $P_0=10$, and $P_2=10$. The upper panel is for the condensate widths (in units of $a_\perp$) and the lower panel is for the various energy components (in units of $\hbar\omega_\perp$).

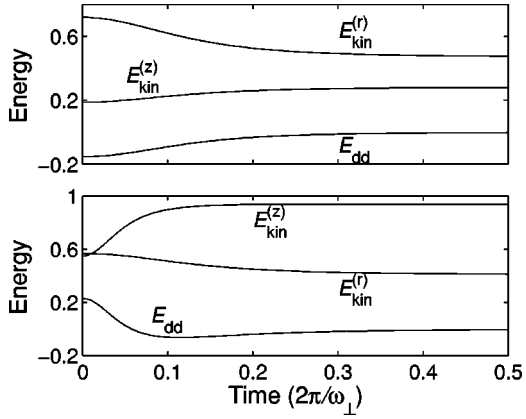

FIG. 2. The time dependence of various energy components (in units of $\hbar\omega_\perp$) during free expansion for $\lambda=1$ (upper panel) and 3 (lower panel). Other parameters are $P_0=0$ and $P_2=1$.

which in fact represent the widths of the condensate in the radial and axial directions, respectively, as $q_r=\sqrt{\langle x^2\rangle/2}=\sqrt{\langle y^2\rangle/2}$ and $q_z=\sqrt{\langle z^2\rangle/2}$. $\kappa=q_r/q_z$ is the condensate aspect ratio, generally different from the trap aspect ratio λ, and $f(\kappa)=[-4\kappa^4-7\kappa^2+2+9\kappa^4H(\kappa)]/2(\kappa^2-1)^2$, $g(\kappa)=[-2\kappa^4+10\kappa^2+1-9\kappa^2H(\kappa)]/(\kappa^2-1)^2$ with $H(\kappa)=\tanh^{-1}\sqrt{1-\kappa^2}/\sqrt{1-\kappa^2}$. The equilibrium widths of the (trapped) condensate can be obtained by setting $\ddot{q}_r=\ddot{q}_z\equiv 0$, which are then used as initial conditions to study the free expansion dynamics by simply dropping the terms q_r and $\lambda^2 q_z$ on the right-hand side of Eqs. (3) and (4). The kinetic and interaction energy per atom of the expanding condensate can then be expressed in terms of condensate widths according to

$$E_{\rm kin}=E_{\rm kin}^{(r)}+E_{\rm kin}^{(z)}=\frac{1}{2}\left(\frac{1}{q_r^2}+\dot{q}_r^2\right)+\frac{1}{4}\left(\frac{1}{q_z^2}+\dot{q}_z^2\right),$$

$$E_{\rm int}=E_{\rm sc}+E_{\rm dd}=\frac{P_0}{2q_r^2q_z}+P_2\frac{2\kappa^2+1-3\kappa^2H(\kappa)}{2q_r^2q_z(\kappa^2-1)}. \qquad (5)$$

The validity of the variational solution has been checked thoroughly for the frequencies of condensate small amplitude shape oscillations [6,7]. Goral and Santos have briefly considered the expansion of a dipolar condensate [8] using the same time-dependent variational method. We have checked over a wide range of parameters to justify its use in the free expansion problem. This allowed us tremendous freedom in exploring the expansion dynamics without resorting to the time consuming numerical solutions. Figure 1 shows the time dependence of condensate widths and energy components, assuming $\lambda=2$ and $P_0=P_2=10$. We see that the variational approach indeed gives a very good approximation to the numerical calculations. This result is also confirmed for λ from 0.1 to 3.

The time dependence of various energy components is also interesting. As shown in Fig. 2, $E_{\rm dd}$ always approaches zero asymptotically during the expansion irrespective of its initial signs. In the early stages, however, its behavior depends on trap geometry due to the anisotropic nature of the interaction. For small λ, the initial dipole-dipole interaction energy is negative; during the expansion, it always gains energy from the kinetic energy and approaches zero monotonically. For large λ, when the initial dipole-dipole interaction energy is positive, the condensate first releases its interaction energy until $E_{\rm dd}$ becomes negative, then gains energy and finally, approaches zero.

The effects of dipolar interaction on the kinetic energies are rather simple. We find that, independent of λ, the dipolar interaction always decreases $E_{\rm kin}^{(r)}$ while increases $E_{\rm kin}^{(z)}$ with time, i.e., the dipole-dipole interaction causes the transfer of radial kinetic energy into the axial direction. This phenomenon is observed even when $P_0\neq 0$. This result contradicts intuition, because along the z axis, the dipole-dipole interaction is attractive, one would expect that the $E_{\rm kin}^{(z)}$ would decrease with time because the atoms are being slowed down due to the dipolar attraction. To resolve this puzzle, we note that the kinetic energy along radial or axial directions, each has two parts: one from the gradient of the wave function $(1/2q_r^2)$ which decreases with time, and the other from the expanding gas $(\dot{q}^2/2)$ which increases with time. This observed phenomena shows that in the radial direction, the increase of the kinetic energy due to $\dot{q}_r^2/2$ cannot compensate for the decrease due to $1/2q_r^2$. Similarly, we can understand the net increase of kinetic energy along the axial direction.

For the remainder of this paper, we will focus our studies on ^{85}Rb condensate as in the JILA experiment [11,12], where the tuning of the scattering length has been demonstrated in a remarkable fashion utilizing the Feshbach resonance. In this case, the magnetic-dipole moment of the trapped state $|F=2,M_F=2\rangle$ is $\mu=2\mu_B/3$ (μ_B is the Bohr magneton). We adopt the radial frequency $\omega_\perp=2\pi\times 17.35$ (Hz) as from the

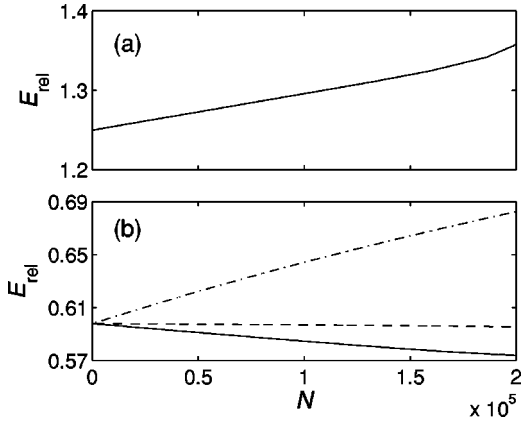

FIG. 3. The atom number dependence of $E_{\rm rel}$ (in units of $\hbar\omega_\perp$) for a ^{85}Rb condensate with $\lambda=3$ (a) and $\lambda=6.8/17.35$ (b). The s-wave scattering lengths are $a_{\rm sc}=0$ (solid line), $0.1a_0$ (dashed line), and $0.5a_0$ (dash-dotted line) with a_0 the Bohr radius.

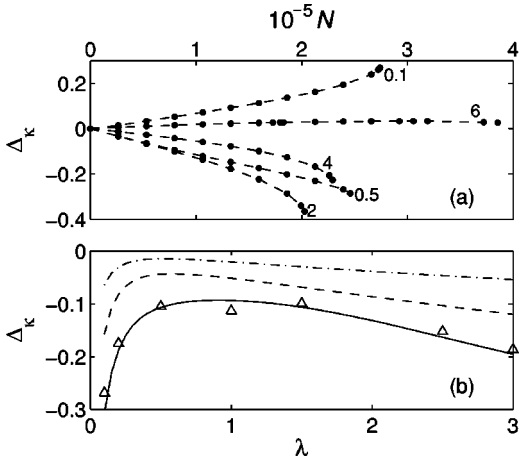

FIG. 4. The relative change of condensate aspect ratio due to dipole-dipole interaction. (a) For the ground state in the trap (before expansion) with $\lambda=0.1$, 0.5, 2, 4, and 6. (b) The relative change of asymptotic condensate aspect ratio (after expansion) for $N=2\times10^5$ (solid line), 10^5 (dashed line), and 4×10^4 (dash-dotted line). Triangle markers show the results for $N=2\times10^5$ from numerically calculated expansions.

experiment [11,12] and assume that the asymmetric parameter λ can be adjusted. The resulting dipolar interaction strength is $P_2=5.0\times10^{-6}N$.

The release energy $E_{\rm rel}=E_{\rm kin}+E_{\rm int}$ is the total energy per atom after switching off the trapping potential. It's values can be strongly affected by the atom-atom interaction. For noninteracting atoms, the release energy per atom $E^0_{\rm rel}=(1+\lambda/2)/2$ is independent of the atom number. For interacting atoms, it depends on the total number of atoms, since both P_0 and P_2 are proportional to N. If the interaction is repulsive, the release energy per atom always increases with N. For attractive interaction, the release energy always decreases (increases) with N if N is above (below) some critical value. Depending on the geometry of the trapping potential, the overall dipole-dipole interaction can be either repulsive or attractive, and the release energy also shows different behaviors for different trapping potentials. In Fig. 3(a), we present the atom number dependence of the release energy for $\lambda=3$. Since the dipole-dipole interaction is predominately repulsive in this case, the release energy increases with N. Figure 3(b) is plotted for $\lambda=6.8/17.35$ case, when $P_0=0$ (solid line), the release energy decreases with N. This behavior holds even for a very small positive scattering length as shown in Fig. 3(b).

The dipolar interaction also changes the condensate aspect ratio. We introduce the relative change of (the ground state) condensate aspect ratio, defined as

$$\Delta_\kappa=\frac{\kappa(P_2\neq0)-\kappa(P_2=0)}{\kappa(P_2=0)}, \tag{6}$$

to quantify this effect. In Fig. 4(a), we plot the numerical results of $\Delta_\kappa(P_0=0,P_2)$ for the trapped ground-state condensate with various values of λ. We see that the relative changes can become as high as 30% for a wide range of trap aspect ratio λ. An experimental measurement of these differences will represent a direct detection of dipolar effects, although the following technical difficulty remains; The condensates produced in current ^{85}Rb experiments [11] contain rather small number of atoms that an *in situ* direct optical imaging is very challenging. The free expansion as discussed in this paper, leads to larger condensate sizes as shown in Fig. 1, thus allowing for easier imaging of condensate aspect ratios. We find that the condensate aspect ratio changes during the expansion and eventually approaches a constant value, which we call the asymptotical aspect ratio. Not surprisingly, this asymptotical aspect ratio depends on the dipole-dipole interaction. In Fig. 4(b), we present the λ dependence of the relative change of the asymptotical condensate ratios for various values of N. We see that for carefully chosen parameters, $\Delta_\kappa(P_0=0,P_2)$ can become large enough to be observed experimentally. In reality, the tuning of $a_{\rm sc}$ to zero $(P_0=0)$, using Feshbach resonance, is limited by the precision of experimental calibrations. To address this point,

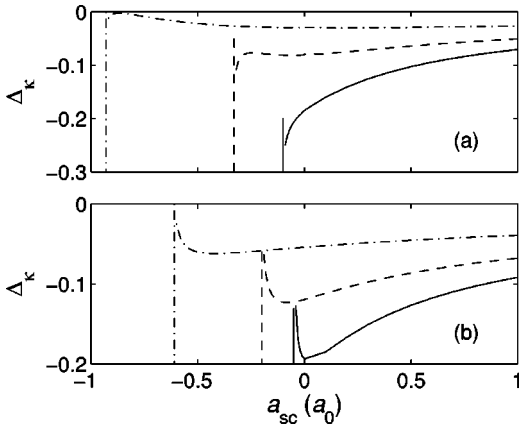

FIG. 5. The dependence of the relative change of condensate asymptotic aspect ratio on the scattering length (from variational calculations) for $\lambda=0.2$ (a) and 3 (b). Atom numbers are $N=2\times10^5$ (solid line), 10^5 (dashed line), and 4×10^4 (dash-dotted line). The vertical lines indicate the critical scattering lengths, where a condensate collapses.

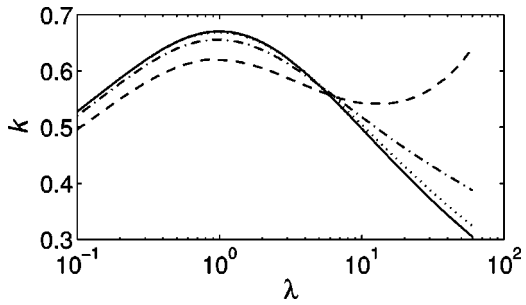

FIG. 6. The effect of dipole-dipole interaction on the stability coefficient k (from variational calculations) for a condensate of ^{85}Rb atoms with $a_{sc}=-0.5a_0$ (dashed line), $-1.0a_0$ (dash-dotted line), and $-3.0a_0$ (dotted line). The solid line corresponds to the absence of dipolar interaction.

we have also investigated the relative change of asymptotic condensate aspect ratio against the scattering length as displayed in Fig. 5. We see clearly that for $N=2\times10^5$, Δ_κ is still reasonably large even for $a_{sc}=1(a_0)$.

Finally, as already studied extensively before, the partially attractive nature of the dipole-dipole interaction can destabilize the condensate ground state in traps with small values of λ (<5.2) [4,6]. The stability coefficient $k=N_{cr}|a_{sc}|/a_{ho}$ [with $a_{ho}=\sqrt{\hbar/m\bar{\omega}}$ and $\bar{\omega}=(\omega_x\omega_y\omega_z)^{1/3}$] is frequently used to measure the stability of a condensate [16]. In Fig. 6, we plot the λ dependence of k for various scattering lengths as obtained from variational study. We see that for a small negative scattering length, when λ is small, the dipole-dipole interaction decreases the k value. On the other hand, when λ is large, the two-dimensional droplet like confinement enhances the repulsive aspect of the dipolar interaction, which in turn balances out the attractive s-wave interaction, resulting in an increase of the k value. In between, the s-shaped dashed curve (for $a_{sc}=-0.5a_0$) seems to be a universal signature (for all values of $a_{sc}<0$). This plot could thus potentially also be used for directly detecting the dipolar interaction.

In conclusion, we have studied the free expansion of a dipolar condensate. We have shown that the weak dipole-dipole interaction may become detectable through several observations, of which the measurement of the condensate aspect ratio after an expansion period seems the most promising. We also discussed briefly, the effects of the dipolar interaction on condensate stability when a_{sc} is tuned close to zero, a situation close to the recent experimental measurement of k in ^{85}Rb condensates [17].

Note added. Our result is consistant with, and directly applicable to situations as discussed in Ref. [18], which showed up after the initial submission of this paper.

We thank Dr. Raman for helpful discussions. This work was supported by the NSF Grant No. PHYS-0140073.

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