Expansion of a dipolar condensate

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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 412, 295 (2001)].

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Atomic Bose-Einstein condensates (BEC) are realized at extremely low temperatures, 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, and trapped fermionic dipoles have also been studied.

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 studied the small amplitude shape oscillation of a dipolar condensate, and 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. It has also been extended to the case of an interacting Fermi gas. 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; then we 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. Then we conclude with some new 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 is then simplified to be

\[
V(\vec{R}) = g_0\delta(\vec{R}) + g_z 1 - \frac{3 \cos^2 \theta_R}{R^3}
\]

where \( \vec{R} = \vec{r} - \vec{r}' \), \( \theta_R \) is the polar angle of \( \vec{R} \), \( g_0 = 4\pi\hbar^2a_{sc}/M \) representing the contact interaction, and in atomic units \( g_z = \frac{\alpha(0)q^2\ell^2}{\sqrt{2\mu}} \) (\( \alpha(0) \) atomic polarizability) or \( \mu^2 \) (\( \mu \) magnetic dipole moment). The corresponding Gross-Pitaevskii equation (in adimensional form) is then

\[
i\frac{\partial\psi}{\partial t} = \left[ -\frac{\nabla^2}{2} + V_{\text{ext}}(\vec{r}) + \sqrt{(2\pi)^3} P_0 |\psi(\vec{r})|^2 \right. \\
\left. + \frac{3}{2}\sqrt{2\pi} P_2 \int d\vec{r}' \frac{1 - 3 \cos^2 \theta}{R^3} |\psi(\vec{r}')|^2 \right] \psi(\vec{r}), \tag{2}
\]

where \( \psi(\vec{r}) \) is the condensate wave function (normalized to 1) and a cylindrical symmetric harmonic trap in dimensionless unit \( V_{\text{ext}}(\vec{r}) = (x^2 + y^2 + \lambda^2 z^2)/2 \), with an aspect ratio \( \lambda \). 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). \( P_0 = \sqrt{2\pi Na_{sc}/a_\perp} \) 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 lhs of Eq. (2) with \(-\mu\psi\), where \( \mu \) 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 \( V_{\text{ext}} \), then find the time evolved wavefunction from the Eq. (2) by employing a self-adaptive Runge-Kutta method without the \( V_{\text{ext}} \). In practice, this becomes an expansive 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 can be used. In this case, we assume that the wave function always takes the form of a Gaussian, and transform the Equation (2) into the following equations for variational parameters

\[
\ddot{q}_r + q_r = \frac{1}{q_r^2} - \frac{1}{q_r^4} [P_2 f(\kappa) - P_0], \tag{3}
\]

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

where in fact represent the radial and axial condensate widths of the expanding condensate as \( q_r = \sqrt{x^2}/2 \) and \( q_z = \sqrt{z^2}/2 \). \( \kappa = q_r/q_z \) is the condensate...
aspect ratio, generally different from the trap aspect ratio $\lambda$, and $f(\kappa) = [-4\kappa^4 - 7\kappa^2 + 2 + 9\kappa^4 H(\kappa)]/(2(\kappa^2 - 1))^2$, $g(\kappa) = [-2\kappa^4 + 10\kappa^2 + 1 - 9\kappa^2 H(\kappa)]/(\kappa^2 - 1)^2$ with $H(\kappa) = \tan^{-1}\sqrt{1 - \kappa^2}/\sqrt{1 - \kappa^2}$. The kinetic and interaction energy per atom can then be expressed in terms of condensate widths according to

$$
E_{\text{kin}} = E_{\text{kin}}^{(r)} + E_{\text{kin}}^{(z)} = \frac{1}{2} \left( \frac{1}{q_r^2} + \frac{1}{q_z^2} \right) + \frac{1}{4} \left( \frac{1}{q_r^2} + \frac{1}{q_z^2} \right),
$$

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

The validity of the variational solution has been checked thoroughly for the frequencies of condensate small amplitude shape oscillations \[3\]. \[4\]. We have checked over a wide range of parameters before concluding that it is also justified for use in the free expansion problem. This enabled 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 $\lambda$ from 0.1 to 3.

The time dependent behavior of the energy components is rather interesting. As shown in Fig. 2, irrespective of the initial signs of the overall dipole interaction energy, it always approaches zero asymptotically during the expansion. In the early stages, however, its behavior depends on trap geometry due to the anisotropic nature of the interaction. For small $\lambda$, 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 $\lambda$ when the initial dipole-dipole interaction energy is positive, the condensate first releases its interaction energy until $E_{\text{dd}}$ 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 $\lambda$, the dipolar interaction always decreases $E_{\text{kin}}^{(r)}$ while increases $E_{\text{kin}}^{(z)}$ 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 $E_{\text{kin}}^{(z)}$ 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 $(q_r^2/2)$ which increases with time. This observed phenomena shows that in the radial direction the increase of the kinetic energy due to $q_r^2/2$ 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.
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 \( \mu = 2 \mu_B / 3 \) (\( \mu_B \) is the Bohr magneton). We adopt the radial frequency \( \omega_\perp = 2\pi \times 17.35 \) (Hz) as from the experiment [11, 12] and assume that the asymmetric parameter \( \lambda \) can be adjusted. The resulting dipolar interaction strength is \( P_2 = 5.0 \times 10^{-6} N \).

The release energy \( E_{\text{rel}} = E_{\text{kin}} + E_{\text{int}} \) is the total energy of the condensate after switching off the trapping potential. It’s values can be strongly affected by the atom-atom interaction. For non-interacting atoms, the release energy per atom \( E_{\text{rel}}^0 = (1 + \lambda / 2) / 2 \), 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 the upper panel of Fig. 3, 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 \( N \). In the lower panel for \( \lambda = 6.8/17.35 \), when \( P_0 = 0 \) (solid line), the release energy decreases with \( N \). We find that this behavior holds even for a very small positive scattering length as shown in Fig. 3. As one might have expected, only for very small values of the s-wave scattering length, are the effects of dipole-dipole interaction important.

The dipolar interaction can also change the condensate aspect ratio. To quantify this effect, we use the relative difference of the (ground state) condensate aspect ratio

\[
\Delta \kappa = \frac{|\kappa(P_2 \neq 0) - \kappa(P_2 = 0)|}{\kappa(P_2 = 0)}.
\]

In Fig. 4 (a), we plot the numerical results of \( \Delta \kappa(P_0 = 0, P_2) \) for various values of \( \lambda \). We see that the relative differences can become as high as 30% for a wide range of trap aspect ratio \( \lambda \). 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 \(^{85}\text{Rb} \) experiments [11] contain rather small number of atoms that a 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. 3, 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 also depends on the dipole-dipole interaction. In Fig. 4 (b), we present the \( \lambda \) dependence of the relative change of the asymptotical condensate ratios for various values of \( N \). We see that for
FIG. 5: The effects of dipole-dipole interaction on the stability coefficient $k$ for a $^{85}\text{Rb}$ condensate with scattering length $a_{sc} = -0.5a_0$ (dashed line), $-1.0a_0$ (dash-dotted line), and $-3.0a_0$ (dotted line). The solid line indicates the stability coefficient when dipole-dipole interaction is not included.

carefully chosen parameters $\Delta \kappa (P_0 = 0, P_2)$ can become large enough to be observed experimentally.

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 $\lambda$ ($< 5.2$). The stability coefficient $k = N_{cr} |a_{sc}|/a_{ho}$ (with $a_{ho} = \sqrt{\hbar/m \omega}$ and $\omega = (\omega_x \omega_y \omega_z)^{1/3}$) is frequently used to measure the stability of a condensate. In Fig. 3, we plot the $\lambda$ dependence of $k$ for various scattering lengths as obtained from variational study. We see that for a small negative scattering length, the dipole-dipole interaction changes the $k$ value dramatically, another signature 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 destabilizing the condensate when the nominal s-wave scattering is tuned close to zero, a situation close to the recent experimental measurement of $k$ in $^{85}\text{Rb}$ condensates.

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