Fermionic stabilization and density-wave ground state of a polar condensate

O. Dutta, R. Kanamoto and P. Meystre
Department of Physics and College of Optical Sciences,
The University of Arizona, Tucson, AZ 85721, USA

(Dated: February 1, 2008)

We examine the stability of a trapped dipolar condensate mixed with a single-component fermion gas at $T = 0$. Whereas pure dipolar condensates with small $s$-wave interaction are unstable even for small dipole-dipole interaction strength, we find that the admixture of fermions can significantly stabilize them, depending on the strength of the boson-fermion interaction. Within the stable regime we find a region where a ground state is characterized by a density wave along the soft trap direction.

PACS numbers: 05.30.Fk 03.75.Hh

The recent demonstration of a condensate of chromium atoms \[1\] opens up the study of quantum-degenerate gases that interact via long range, anisotropic magnetic dipole interactions. In a parallel development, it can be expected that quantum degenerate samples of heteronuclear polar molecules will soon be available through the use of Feshbach resonances \[2, 3\], photoassociation \[4, 5\], or a combination of the two approaches, other possible routes including buffer-gas cooling \[6\], collisional beam cooling \[7\], reactive scattering \[8\] and stark deceleration \[9\] alone or in combination. When in their vibrational ground state these molecules interact primarily via the electric dipole interaction, and may therefore also form dipole-dominated condensate.

As a result of the dipole-dipole interaction, a number of novel phenomena have been predicted to occur in low-density quantum-degenerate atomic and molecular systems, both in conventional traps and in optical lattices. The existence of a variety of quantum phases including a “supersolid” phase for dipolar bosons in optical lattices have been predicted in Ref. \[10\]. A supersolid phase was also predicted for hardcore bosons in two-dimensional triangular lattices \[11, 12\], in Kagome lattices \[13\], and in an extended multi-band Bose-Hubbard Hamiltonian \[14\], although recent quantum Monte Carlo simulations \[15\] did not find any supersolid phase for bosons in a Kagome lattice. The authors of Ref. \[16\] studied Bose-Fermi mixtures in two-dimensional square lattices, and found a bosonic supersolid transition induced by a modulation of the fermionic density resulting from a nesting effect. However, the situation is much different in the absence of a lattice structure: the only stable state of dipolar condensates in a pancake-shaped trap has a Gaussian-like density profile \[17, 18, 19\], and states with a periodic density modulation are always unstable \[20\], although Ref. \[21\] has shown that modulating periodically the strength of a laser-induced dipole-dipole interaction can result in stable density-modulated condensates.

In this note we consider a mixture of dipolar bosons and non-interacting single-component fermions confined to a cigar-shaped trap. Such a mixture might be realized using isotopes of chromium, or during the production of heteronuclear molecules via either a Feshbach resonance or the photoassociation of two different fermionic species of atoms. Using linear response theory to determine the fermion-induced interaction between bosons we find that it significantly stabilizes the dipolar bosonic condensate. We then identify a region in parameter space where the stable ground state displays a density-modulated structure along the long axis of the trap.

We assume for simplicity that both the dipolar bosons and the fermions are trapped in the transverse direction by a tight harmonic potential of frequency $\omega_\perp$ and in the longitudinal direction by a much softer harmonic potential of frequency $\omega_\parallel$. The dipoles are taken to be polarized by an electric or magnetic field in a direction $y$ perpendicular to the long axis of the trap. The dipole-dipole interaction between two bosonic particles separated by a distance $r$ is given by $V_{\text{dd}}(r) = g_{\text{dd}} (1 - 3y^2/r^2) / r^3$, where $g_{\text{dd}}$ is the dipole-dipole interaction strength. In the mean-field approximation, the energy functional for the order parameter $\phi(r)$ of the dipolar condensate is

$$E = \int \phi^*(r) H_0 \phi(r) d^3r + \frac{N g}{2} \int |\phi(r)|^4 d^3r$$

$$+ \frac{N}{2} \int |\phi(r)|^2 V_{\text{dd}}(r - r') |\phi(r')|^2 d^3r' d^3r' + E_{\text{ind}},$$

where $H_0 = -\hbar^2 \nabla^2 / (2m) + m \omega_\perp^2 (x^2 + y^2 + \lambda z^2) / 2$ is the sum of the kinetic energy and the trapping potential, $m$ is the mass and $N$ the total number of bosonic particles, and $\lambda = \omega_\parallel / \omega_\perp$. The second term in $E$ is the boson-boson $s$-wave interaction of strength $g$, and the third term describes the nonlocal dipole-dipole interaction between bosons. Note that that term also contains a short-range contact contribution \[22, 23, 24\]. The last term $E_{\text{ind}}$ accounts for the fermion-induced interaction $V_{\text{ind}}(\mathbf{k})$ between bosons. It is given by

$$E_{\text{ind}} = \frac{1}{2} g_{\text{ff}} N \int V_{\text{ind}}(\mathbf{k}) n(\mathbf{k}) n(-\mathbf{k}) d^3k,$$

where $n(\mathbf{k})$ is the momentum-space bosonic density.

In deriving Eq. \[2\] we have assumed a contact boson-fermion interaction of strength $g_{\text{ff}}$, with a corresponding interaction energy of the form $g_{\text{ff}} \int n_f(\mathbf{k}) n(-\mathbf{k}) d^3k$, $n_f(\mathbf{k})$ being the fermion density. The linear response of the fermions to a bosonic density fluctuation $n(\mathbf{k})$ can
be expressed as $n_f(k) = V_{\text{ind}}(k)n(k)$, and Eq. (2) is obtained by substituting that expression back into to the boson-fermion interaction energy. The explicit form of the induced potential is $V_{\text{ind}}(k) = \frac{g_{\text{ind}}}{2 \lambda} \chi_f(k)$, where $\chi_f$ is the density response function related to the dynamical structure factor $S(k, \omega)$, the probability of exciting particle-hole pairs with momentum $k$ out of the Fermi sea, by $\chi_f(k) = -2\int_0^\infty d\omega |S(k, \omega')/\omega'|$. For a non-interacting single-component Fermi system we have

$$S(k, \omega) = \sum_{p<k_f} \delta(\omega - \omega_{pk}).$$ (3)

Here $p = |p|$, $k_f$ is the Fermi momentum, and the excitation energy is $\omega_{pk} = pk \cos \theta/m_f + k^2/(2m_f)$, $\theta$ being the relative angle between $p$ and $k$, and $m_f$ the mass of the fermions. This expression assumes that the fermions are locally free, so that there is a Fermi sphere in momentum space.

Using the form of $S(k, \omega)$ from Ref. [25] we find

$$\chi_f(k) = -\frac{\nu k_f}{2k} \left[ \frac{k}{k_f} + \left(1 - \frac{k^2}{4k_f^2}\right) \ln \left| \frac{2k_f + k}{2k_f - k} \right| \right]$$ (4)

where $\nu$ is the three-dimensional density of states at the Fermi surface. Here $[.]$ is used to denote absolute value. Substituting Eq. (4) into the expression $V_{\text{ind}}(k) = g_{\text{ind}}\chi_f(k)$ and carrying out a series expansion to lowest order in the non-local terms we have

$$V_{\text{ind}}(k) \approx \begin{cases} \frac{g_{\text{ind}}}{12} \left(2k_f/\nu\right)^2, & k < 2k_f, \\ \frac{g_{\text{ind}}}{12} \left(2k_f/\nu\right)^2, & k > 2k_f. \end{cases}$$ (5)

The negative contribution to this potential describes an effective attractive interaction between bosons in the long wavelength limit, while its positive part corresponds to a nonlocal repulsive interaction.

With the form (5) of the bosonic energy functional and the potential $V_{\text{ind}}$ at hand, we now proceed to determine the stability of the dipolar condensate, using a variational wave function in the parameter space of the fermion-induced interaction and dipolar strength. For this purpose, the condensate order parameter $\phi(r)$ is assumed to factorize as $\phi(r) = \phi_\perp(x, y)\phi_\parallel(z)$ with the normalization $\int d^3r|\phi(r)|^2 = 1$. The transverse wave function is $\phi_\perp(x, y) = \exp[-(x^2 + y^2)/(2d^2)]/\sqrt{\pi d^2}$, $d$ being a variational parameter, while the longitudinal component is $\phi_\parallel(z) = \exp[-z^2/(2d_z^2)]/\sqrt{\pi^{1/2}d_z}$, $d_z$ being likewise a variational parameter.

Substituting this Gaussian ansatz and its Fourier transform into Eqs. (1) and (2), the energy of the condensate becomes

$$\frac{2m}{\hbar^2} \frac{d^2 D}{d^2} E_g = \left(1 + \frac{\lambda^2}{2\eta^2}\right) \frac{d^2 D^2}{d^2} + \left(1 + \frac{\lambda^2}{2\eta^2}\right) \frac{d^2 D^2}{d^2}$$ (6)

FIG. 1: Stability diagram of a dipolar condensate in ($g_{\text{ind}}, g_{\text{bd}}$) space for $g_s = 0.2$ and $\lambda = 0.05$. In region I the stable ground state has a Gaussian-like density distribution and in region II it is characterized by a density modulation, i.e., $\phi_{\text{ind}} > 0$.

$$+ g_{\text{bd}} \frac{d^2}{d^2} \left[ (gs - 1)\eta + \eta^2 \left\{ F(\eta) + g_{\text{ind}} \frac{d^2}{d^2} + \frac{g_{\text{ind}}k^2}{\eta^2} \right\} \right],$$

where $\eta = d/d_z$, $\tilde{k}_f = k_f d_z$, $d_z = \sqrt{\hbar/m \omega_z}$ is the transverse oscillator length, and

$$F(x) = \frac{\tan^{-1}(\sqrt{x^2 - 1})}{(x^2 - 1)^{3/2}} - \frac{1}{x^2(x^2 - 1)}.$$ (7)

The first term in Eq. (6) denotes the short range part of $V_{\text{bd}}$, and the second term results from the difference between the boson-boson $s$-wave interaction and the attractive part of the interaction in $V_{\text{ind}}(k)$. To calculate the fermion-induced interaction energy $E_{\text{ind}}$ we have assumed that $2\tilde{k}_f > 1$. In Eq. (6) we have introduced the effective three-dimensional dipole-dipole interaction $g_{\text{bd}} = N g_{\text{bd}} m/(\sqrt{2}\pi \hbar^2 d_z)$, the effective contact potential $g_s = 1/3 + (g - g_{\text{bd}}^2\nu)/(2\pi g_{\text{bd}})$, and the induced interaction $g_{\text{ind}} = g_{\text{bd}}^2\nu/(12\pi g_{\text{bd}}^2 k^2)$.

The energy functional (6) is minimized with respect to $d/d_z$ and $\eta = d/d_z$ for various combinations of the parameters $g_{\text{bd}}, g_{\text{ind}}$. The results of these simulations are summarized in Fig. (II). All numerical results presented in the following are for $\lambda = 0.05$, $g_s = 0.2$, and $\tilde{k}_f = 2$ (a value typical of the situation for a fermionic gas of $10^3$ atoms in a a transverse trap length of $d_z \sim 1\mu m$ and $\lambda = 0.05$). We found that the condensate typically collapses for $\eta \gtrsim 1$ or $d \to 0$, while the stable regime is characterized by $\eta \lesssim 0.1$ and $d \sim d_z$. Region I is characterized by stable ground states with a Gaussian-like density profile, while in Region II the ground state exhibits density modulations that are further discussed later on.

In the absence of fermion-induced effective boson-fermion interaction $g_{\text{ind}} = 0$, the dipolar condensate is found to be unstable to collapse even for very small dipolar strength $g_{\text{bd}}$. For $g_{\text{ind}} \neq 0$, in contrast, the condensate becomes stable for a range of values of $g_{\text{bd}}$ that increases with increasing $g_{\text{ind}}$. This can be understood from the form of the non-local part of the induced interac-
eral values of the fermion-induced interaction $g_{\text{ind}}$. Here we assumed that $d \sim d_L$. The zero potential level is shown as a horizontal dashed line.

**FIG. 2:** Effective one-dimensional potential, Eq. (8), for several values of $g_{\text{ind}}$. We proceeded by first demonstrating the existence of a roton minimum in the Bogoliubov excitation spectrum of a homogeneous condensate along the trap axis, and show that by increasing the effective dipolar strength $g_{3d}$ this minimum can touch the zero-energy axis. The roton-like spectrum follows from the attractive nature of dipolar interaction for high momenta [17, 18, 26, 27] and touching the zero energy indicates an instability toward a nonuniform ground state [25].

Integrating Eqs. (1) and (2) in the transverse direction yields the effective longitudinal potential

$$V_{\text{eff}}(\tilde{k}_z) = g_s - \frac{\tilde{k}_z^2}{2} \exp\left(\frac{\tilde{k}_z^2}{2}\right) E_1\left(\frac{\tilde{k}_z^2}{2}\right) + g_{\text{ind}} \frac{d^2}{d^2} \tilde{k}_z^2,$$  

where $\tilde{k}_z = k_z d$ is a scaled wave vector, $k_z$ being the longitudinal momentum, and $E_1(x) = \int_0^x dx \exp(e^{-x} / x)$ is the exponential integral. In obtaining Eq. (8) we have assumed that $\tilde{k}_z < k_f$ which justifies keeping only the contribution to the induced potential [5] with $k < 2k_f$. Figure 2 shows that as $g_{\text{ind}}$ is increased the one-dimensional potential becomes less attractive for higher momenta, and also that the non-local part of $V_{\text{eff}}(\tilde{k}_z)$ becomes repulsive again for sufficiently strong $g_{\text{ind}}$.

Assuming a homogeneous condensate of length $L$ along the long axis of the trap then yields the Bogoliubov spectrum

$$\Omega^2(\tilde{k}_z) = \frac{\tilde{k}_z^2}{2} \left[ \frac{\tilde{k}_z^2}{2} + \frac{2g_{3d}}{L} V_{\text{eff}}(\tilde{k}_z) \right],$$

with the appearance of a roton minimum for large enough effective dipolar strength, see Fig. 3. By increasing $g_{3d}$ further, the roton minima can touch the zero-energy axis. This suggests that at this point the structure of the condensate ground state can undergo a transition, with the appearance of a density modulation along the long axis of the trap.

To verify this possibility we introduce a new longitudinal variational wave function that includes a density-wave component of amplitude $a_{d\text{w}}$

$$\phi_{||,d\text{w}}(z) = \phi_{||}(z) + a_{d\text{w}} \cos\left(\frac{k_0 z}{d}\right),$$  

with the normalization constraint $a^2 + a_{d\text{w}}^2 / 2 = 1$. The excess energy of this density-modulated state, as compared to a broad Gaussian order parameter, can be expressed as

$$\epsilon(k_0, a_{d\text{w}}) = \frac{2md^2}{\hbar^2} \left( E_{d\text{w}} - E_g \right)$$

$$= \frac{a^2_{d\text{w}}}{2} \left( k_0^2 + \sqrt{2g_{3d}} \frac{d^2}{d^2} \left[ 2a^2 V_{\text{eff}}(\tilde{k}_0) + a_{d\text{w}}^2 V_{\text{eff}}(2\tilde{k}_0) \right] \right).$$

Limiting ourselves to the stable region of Fig. 1, we first choose the values of $d$ and $d_z$ that minimize the energy [8], and then minimize $\epsilon(k_0, a_{d\text{w}})$ with respect to the variational parameters $k_0$ and $a_{d\text{w}}$. Density-wave ground state is characterized by $\min \{ \epsilon \} < 0$ and $a_{d\text{w}} \neq 0$. The region of density-wave ground state determined in this fashion corresponds to region II of Fig. 1. For $g_{\text{ind}} \geq 0.023$, a transition from a Gaussian-like state to a density-wave state is observed when the dipole-dipole interaction $g_{3d}$ is increased. This transition is smooth in the sense that $a_{d\text{w}}$ increases gradually from zero as
we increase the dipolar strength $g_{3d}$ beyond the critical value. Figure 4 illustrates the gradual emergence of density waves for a fixed induced strength $g_{\text{ind}} = 0.058$. We find that by gradually increasing $g_{3d}$ to a modest value the density profile acquires periodic zeros along the longitudinal direction.

One possible candidate to observe the predicted density wave region is a mixture of bosonic $^{52}$Cr and fermionic $^{51}$Cr atoms. Bosonic Chromium has a magnetic dipole moment of $6\mu_B$ and a s-wave scattering length $\sim 100a_0$. The trap considered in this paper has a transverse frequency $\omega_\perp \sim 200\text{Hz}$ and aspect ratio $\lambda = \frac{500}{a_0}$. For this geometry the density wave state in region II of Fig. 1 can be reached for a boson-fermion scattering length of $\sim 500a_0$, for bosonic and fermionic atoms numbers of $10^4$ and $10^3$, respectively.

In summary, we have analyzed the stability of ultracold dipolar bosons mixed with non-interacting fermions. A central result of our analysis is that the fermions help stabilize the dipolar condensate, as a consequence of the fact that the non-local induced interaction is repulsive in the limit of moderate wavelengths. In the stable region we found a transition in the shape of the condensate ground-state from a Gaussian-like profile to a modulated density profile along the axis of the trap. Our analysis is mean-field, implying that the system is assumed to be condensed with phonon-like low energy excitations along the longitudinal direction. The density modulation emerges as a result of the additional breaking of the translational symmetry of the condensate and can be called a superfluid density wave.

Future work will discuss the effect of the strength of the contact interaction and of the Fermi momentum on the stability of the condensate and the density wave, with possible extensions to pancake geometries and to rotating systems. A number of exotic states are likely to be found in that regime. An extension to finite temperatures will allow us to investigate possible classical phase transitions between superfluid and various kinds of density-wave states.

This work is supported in part by the US Office of Naval Research, by the National Science Foundation, and by the US Army Research Office.

[1] A. Griesmaier et. al., Phys. Rev. Lett. 94, 160401 (2005).
[2] C. A. Stan et. al., Phys. Rev. Lett. 93, 143001 (2004).
[3] S. Inouye et. al., Phys. Rev. Lett. 92, 033004 (2004).
[4] J. M. Sage, S. Sainis, T. Bergeman, and D. DeMille, Phys. Rev. Lett. 94, 203001 (2005).
[5] J. D. Weinstein et. al., Nature 395, 148 (1998).
[6] M. S. Elioff, J. J. Valentini, D. W. Chandler, Science 302, 1940 (2003).
[7] N.-N. Liu and H. Loesch, Phys. Rev. Lett. 98, 103002 (2007).
[8] J. Bochinski et. al., Phys. Rev. Lett. 91, 243001 (2003).
[9] K. Góral, L. Santos and M. Lewenstein, Phys. Rev. Lett. 88, 170406 (2002).
[10] M. Boninsegni and N. Prokof’ev, Phys. Rev. Lett. 95, 237204 (2005).
[11] S. Wessel and M. Troyer, Phys. Rev. Lett. 95, 127205 (2005); D. Heidarian and K. Damle Phys. Rev. Lett. 95, 127206 (2005); and R. G. Melko et. al., Phys. Rev. Lett. 95, 127207 (2005).
[12] G. Murthy, D. Arovas, and A. Auerbach, Phys. Rev. B 55, 3104 (1997).
[13] V. W. Scarola and S. Das Sarma, Phys. Rev. Lett. 95, 033003 (2005).
[14] K. Damle and T. Senthil, Phys. Rev. Lett. 97, 067202 (2006); S. V. Isakov et. al., Phys. Rev. Lett. 97, 147202 (2006).
[15] H. P. Büchler and G. Blatter, Phys. Rev. Lett. 91, 130404 (2003).
[16] S. Ronen, D. C. E. Bortolotti, and J. L. Bohn, Phys. Rev. Lett. 98, 030406 (2007).
[17] L. Santos, G. V. Shlyapnikov and M. Lewenstein, Phys. Rev. Lett. 90, 250403 (2003).
[18] L. Santos, G. V. Shlyapnikov, P. Zoller, and M. Lewenstein, Phys. Rev. Lett. 85, 1791 (2000).
[19] S. Komineas, N.R. Cooper, Phys. Rev. A. 75, 023623 (2007).
[20] S. Giovanazzi, D. O’Dell, and G. Kurizki, Phys. Rev. Lett. 88, 130402 (2002).
[21] S. Ronen, D. C. E. Bortolotti, D. Blume and J. L. Bohn, Phys. Rev. A 74, 033611 (2006).
[22] S. Yi and L. You, Phys. Rev. A 61, 041604(R) (2000); Phys. Rev. A 63, 053607 (2001).
[23] A. Derevianko, Phys. Rev. A 67, 033607 (2003).
[24] P. Nozières and D. Pines, The Theory of Quantum Liquids (Perseus Books, 1999). Pg.108-110 contains the mathematical form of $S(k, \omega)$.
[25] S. Giovanazzi and D. H. J. O’Dell, Eur. Phys. J. D 31, 439 (2004).
[26] U. R. Fischer, Phys. Rev. A 73, 031602(R) (2006).
[27] Y. Pomeau and S. Rica, Phys. Rev. Lett. 72, 2426 (1994); C. Josserand, Y. Pomeau and S. Rica, Phys. Rev. Lett. 74, 160401 (2000).
98, 195301 (2007).

[29] J. Werner et al., Phys. Rev. Lett. 94, 183201 (2005).

[30] A. Griesmaier et al., Phys. Rev. Lett. 97, 250402 (2006).

[31] Jinwu Ye, cond-mat/0512480.