Manifestations of the Roton Mode in Dipolar Bose-Einstein Condensates

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We investigate the structure of trapped Bose-Einstein condensates (BECs) with long-range anisotropic dipolar interactions. We find that a small perturbation in the trapping potential can lead to dramatic changes in the condensate's density profile for sufficiently large dipolar interaction strengths and trap aspect ratios. By employing perturbation theory, we relate these oscillations to a previously identified "rotonlike" mode in dipolar BECs. The same physics is responsible for radial density oscillations in vortex states of dipolar BECs that have been predicted previously.

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The study of ultracold atomic and molecular gases is notable for its connection to denser condensed matter systems. Ultracold gases can show a strong resemblance to condensed matter systems such as vortex lattices, superfluids, and Mott insulators. Part of the attraction to these analogies is the ability to control an ultracold atomic or molecular gas, allowing researchers to explore regions of parameter space that are difficult to access in a naturally occurring system.

A recent example of this connection between ultracold gases and "conventional" condensed matter systems arises in dilute Bose-Einstein condensates (BECs) consisting of dipolar particles. An early theoretical study investigated a gas of dipoles that are free to move in a plane, but are confined in the direction orthogonal to the plane and that are polarized in this same direction. This system is predicted to exhibit an anomalous dispersion relation that possesses a minimum at a characteristic momentum, reminiscent of the roton dispersion well known in superfluid He [1]. Moreover, the depth of this minimum is controlled by the strength of the dipolar interaction (proportional to the square of the dipole moment and the density). If this interaction is large enough, the roton minimum can become degenerate with the ground state.

In experiments, however, the gas is confined, leading to a discrete excitation spectrum rather than a continuous dispersion relation. Nevertheless, signatures of the roton excitation have been identified in calculations with fully three-dimensional trap geometries [2]. Certain excitations exhibit nodal structures on the same length scale as the free rotons. Moreover, the excitation energies of these modes drop rapidly as the dipolar interaction strength increases. We note that the first dipolar BECs (DBECs) have already been created using atomic ^{52}Cr [3–6] while molecular BECs (promising far larger dipoles and tunable dipole moments) are the target of active experimental work.

In this Letter we explore another aspect of roton physics that may be observable in dipolar gases. It has previously been suggested that boundaries in superfluid ^{4}He, including vortex cores, should give rise to radial density oscillations whose length scale is characteristic of the roton wavelength [7–9]. More recently, calculations of vortex states in a DBEC in a highly oblate trap have exhibited similar radial structures [10], raising the question of the relation between these structures and rotons in this system. (Progress has also been made in the understanding of the vortex state in a DBEC in the Thomas-Fermi regime. However, in this regime the vortex does not manifest a radial ripple [11,12].)

Our objective in the present work is to explore this relationship. Whereas the complete description of superfluid He is complicated by strong interactions, this is not the case in a DBEC, where the gas is dilute enough that a mean-field approach should work quite well [13]. Indeed, we find that the main effect generating the radial density oscillations is the perturbation caused by the centrifugal potential of the vortex state. This perturbation contaminates the ground state with the lowest-lying excited state, which, in the limit of strong interactions, is the roton excitation. We demonstrate this effect by applying a perturbation theory to the nonlinear mean-field equations; the perturbative approach is in good agreement with our full numerical calculations.

At very low temperatures, N bosons trapped in an external potential $U(\mathbf{r})$ may be described within mean-field theory by the nonlocal Gross-Pitaevskii equation (GPE):

$$\Big[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + (N-1)\int d\mathbf{r}'\Psi^*(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\Psi(\mathbf{r}')\Big]\Psi(\mathbf{r}) = \mu\Psi(\mathbf{r}), \quad (1)$$

where $\Psi(\mathbf{r})$ is the condensate wave function (with unit norm), $\mathbf{r}$ is the distance from the trap center, m is the boson's mass, and $V(\mathbf{r}-\mathbf{r}')$ is the two-particle interaction potential. We consider the case of a cylindrical harmonic trap, for which the external potential is $U(\mathbf{r}) = \frac{1}{2}m\omega_\rho^2(\rho^2 + \lambda^2 z^2)$, where $\lambda = \omega_z/\omega_\rho$ is the trap aspect ratio. The interaction potential has the form [14]

$$V(\mathbf{r} - \mathbf{r}') = \frac{4\pi\hbar^2 a_s}{m}\delta(\mathbf{r} - \mathbf{r}') + d^2\frac{1 - 3\cos^2\theta}{|\mathbf{r} - \mathbf{r}'|^3}, \quad (2)$$

where a_s is the s-wave scattering length, d is the dipole moment, and θ is the angle between the vector $\mathbf{r} - \mathbf{r}'$ and the dipole axis. The first term in $V(\mathbf{r} - \mathbf{r}')$ is the familiar contact potential, while the second term is the long-range anisotropic dipole-dipole potential. This potential describes interactions of dipoles that are polarized along the trap axis, as could be achieved in an experiment by applying a strong external field. For the sake of illuminating purely dipolar effects, we set $a_s = 0$ in this work, a limit that can potentially be achieved experimentally in ^{52}Cr [15].

Because of the azimuthal symmetry of both the trapping potential and the dipole-dipole potential, the ground state solutions of Eq. (1) may be written in the form $\Psi(\mathbf{r}, t) = \psi(\rho, z)e^{ik\varphi}$, where k is the quantum number representing the projection of orbital angular momentum about the trap's axis [16]. The $k = 0$ solutions of Eq. (1) correspond to rotationless BECs, while the $k = 1$ solutions correspond to BECs with singly quantized vortices. The radial structure of the vortex is the same as that of a rotationless BEC in a trap with a central potential representing the centrifugal force: indeed, by inserting the vortex form written above into Eq. (1), one obtains

$$\left\{-\frac{\hbar^2}{2m}\nabla_\rho^2 - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{\hbar^2 k^2}{2m\rho^2} + \frac{1}{2}m\omega_\rho^2(\rho^2 + \lambda^2 z^2) + (N-1) \times \int d\mathbf{r}'\psi^*(\rho', z')V(\mathbf{r} - \mathbf{r}')\psi(\rho', z')\right\}\psi(\rho, z) = \mu\psi(\rho, z). \quad (3)$$

The centrifugal potential $\hbar^2 k^2/2m\rho^2$ is responsible for the vortex core (i.e., vanishing density at $\rho = 0$).

Following the systematic mapping of the structure and stability of $k = 0$ DBECs in oblate traps [2], here we undertake to characterize the structure and stability of a $k = 1$ vortex in DBECs. To characterize the dipolar interaction strength we introduce the dimensionless parameter $D = (N - 1)\frac{md^2}{\hbar^2 a_{\rm ho}}$, where $a_{\rm ho} = \sqrt{\hbar/m\omega_\rho}$ is the radial harmonic oscillator length. The DBEC possesses dynamic stability when all of the excited-state Bogoliubov–de Gennes (BdG) eigenenergies are real-valued. As was found for $k = 0$ condensates in Ref [2], we find that for the vortex state there also exists, at any finite aspect ratio, a critical value of $D = D_{\rm crit}$ above which the $k = 1$ DBEC is dynamically unstable to small perturbations, while below it the vortex is dynamically stable. We assume that the trap itself is nonrotating, so that the vortex is not the lowest energy state and therefore is not thermodynamically stable. However, here we are interested in the question of the dynamical stability, which is relevant for a closed system at $T = 0$.

We find $D_{\rm crit}$ for various trap aspect ratios by solving the linearized BdG equations, as was done in Ref. [17]. Figure 1 illustrates the regions of dynamical stability for $k = 1$ and $k = 0$ DBECs at trap aspect ratios that are relevant to this Letter. We concentrate here on a specific region in parameter space where we find ripples in the DBEC density profiles, as illustrated in the insets. Whereas previously the ripple was reported for a trap with aspect ratio $\lambda \sim 100$ and required the existence of a negative scattering length [10], we find that vortices with ripple structure exist also at milder trap aspect ratios of $\lambda \sim 17$ and with purely dipolar interactions ($a_s = 0$).

It is natural to hypothesize that the appearance of the ripple in the vortex structure is related to a roton mode which is excited by the centrifugal potential of Eq. (3). This raises the interesting question, could such a ripple also be observed in the ground (nonvortex) state of DBEC perturbed by an external potential at the center of the trap? Such a perturbation may be realized experimentally by applying a blue-detuned laser along the trap axis, taking the form $U'(\mathbf{r}) = A\exp(-\rho^2/2\rho_0^2)$, where A is the height of the Gaussian and ρ_0 is its width.

For sufficiently oblate traps, $k = 0$ DBECs exhibit radial density oscillations in the presence of such Gaussian potentials. Figure 2 illustrates the radial profiles of $k = 0$ DBECs in a harmonic trap with aspect ratio $\lambda = 17$ and with a Gaussian potential having $A = \hbar\omega_\rho$ and $\rho_0 = 0.2a_{\rm ho}$. To give a concrete example, for ^{52}Cr atoms in a

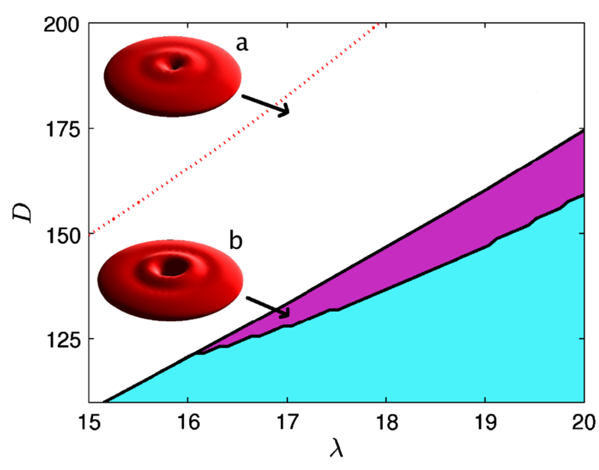

FIG. 1 (color online). The red (thin) dotted line marks the maximum dipole strength, for a given trap aspect ratio λ, below which a rotationless ($k = 0$) DBEC is dynamically stable. The colored regions represent the dynamically stable region for a $k = 1$ DBEC, while the pink (darker) region is where radial oscillations with local minima are observed. The inset (a) is an isodensity surface plot of a $k = 0$ DBEC perturbed by a small Gaussian potential centered on the trap axis, while the inset (b) is an isodensity surface plot of a $k = 1$ DBEC. The presence of radial oscillations is clear in both cases.

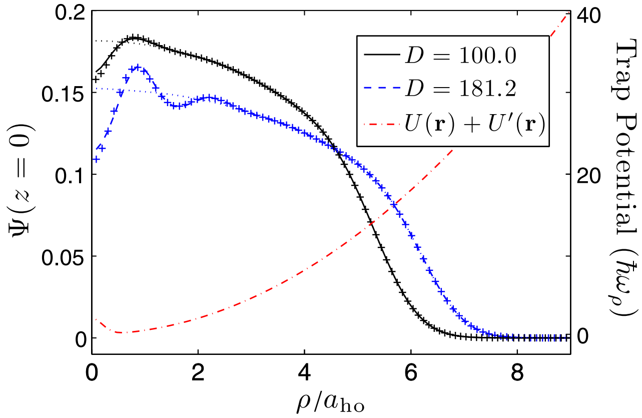

FIG. 2 (color online). Radial profiles of the $k = 0$ DBEC subject to the perturbing potential $U'(\mathbf{r}) = \hbar\omega_\rho \exp[-\rho^2/2(0.2a_{\rm ho})^2]$ in a trap with aspect ratio $\lambda = 17$. The red dash-dotted line represents the trapping potential at $z = 0$, the black solid line represents the radial profile of the DBEC at $D = 100$, and the blue dotted line represents the radial profile at $D = 181.2$, near the point of dynamic instability for the $k = 0$ DBEC. The "+" signs represent the perturbation theory results and the thin dotted lines represent the unperturbed radial profiles at the corresponding dipole strengths.

harmonic trap with radial frequency $\omega_\rho = 2\pi \times 100$ Hz, this translates to having a beam width of $\rho_0 = 280$ nm. In this trap, an interaction strength of $D = 181.2$, very near the point on instability for a $k = 0$ DBEC in a trap with the above aspect ratio, may be achieved with $\sim$104 000 ^{52}Cr atoms. It is seen that in this case even a small Gaussian perturbation makes a dramatic change in the DBEC density profile. The radial oscillations near $D_{\rm crit}$ are much more pronounced than for a smaller DBEC with $D = 100$. This is suggestive of the roton presence in this structure, since the roton is expected to emerge with increasing dipolar interaction strength (i.e., increasing density for a fixed dipole moment) [1,9,17]. As was shown in Ref. [2], the roton mode undergoes a significant decrease in energy with increase in D until it achieves zero energy at $D_{\rm crit}$, marking the point of dynamical instability for the $k = 0$ condensate. Beyond this $D_{\rm crit}$, the roton energy is purely imaginary. Examining the nature of the roton itself within BdG theory tightens up its relationship with the observed structure discussed above.

For a $k = 0$ condensate, the coupled BdG equations reduce to a single equation, given by

$$\tilde{G}\tilde{F}|f\rangle = \omega^2|f\rangle. \tag{4}$$

Here, $\tilde{G} = P(G - \mu)P$ and $\tilde{F} = P(F - \mu)P$, where $P = I - |\Psi\rangle\langle\Psi|$ is the projection operator into the space orthogonal to ground state wave function $|\Psi\rangle$. Also, $G = H_0 + C$ and $F = H_0 + C + 2X$, where H_0 is the zero-interaction Hamiltonian, C describes a direct interaction, and X describes an exchange interaction between the Bogoliubov quasiparticle with eigenvector $|f\rangle$ and the condensate. All of these operators are defined as in Ref. [17]. The eigenvector $|f\rangle$ is given by $|f\rangle = |u\rangle + |v\rangle$, where $\{u, v\}$ are the familiar Bogoliubov eigenfunctions. The ω appearing on the right-hand side of Eq. (4) is the energy eigenvalue corresponding to $|f\rangle$.

In Eq. (4), it is understood that the linear space on which $\tilde{F}$ and $\tilde{G}$ act, and to which $|f\rangle$ belongs, is orthogonal to $|\Psi\rangle$. Thus, we eliminate a nonphysical solution with eigenvalue zero [18]. The justification for working in this reduced linear space is that it can be shown that all physical excitations obey $\langle f|\Psi\rangle = 0$ [16].

It seems natural to assume that the roton mode dominates the structure of the perturbed DBEC near instability because its energy is much lower than the energies of the other BdG modes. To explicitly demonstrate this, one needs to formulate a perturbation theory of the nonlinear GPE with respect to external potential perturbation.

To do so, we begin by writing a perturbation to the trapping potential as $U \to U + U'$, where U' is the small perturbation. The response of the condensate wave function to this perturbation is then $|\Psi\rangle \to |\Psi\rangle + |\Psi'\rangle$. We insert these expressions into Eq. (1), linearize in the primed quantities, and obtain the equation

$$\tilde{F}|\Psi'\rangle = -PU'|\Psi\rangle. \tag{5}$$

To solve Eq. (5), we introduce a basis defined by the eigenvalue equation

$$\tilde{F}|\varphi_n\rangle = \varepsilon_n|\varphi_n\rangle \tag{6}$$

and use its eigenfunction solutions to expand $|\Psi'\rangle$ in the $|\varphi_n\rangle$ basis. Plugging these expansions back into Eq. (5) and working to first order gives the expression for the wave function perturbation,

$$|\Psi'\rangle = -\sum_n \frac{\langle\varphi_n|U'|\Psi\rangle}{\varepsilon_n}|\varphi_n\rangle. \tag{7}$$

This derivation involves the use of the orthogonality condition $\langle\Psi'|\Psi\rangle = 0$ and the fact that $\langle\varphi_n|\Psi\rangle = 0$. The final expression is formally identical to that of the usual perturbation theory of the linear Schrödinger equation.

The connection between the BdG roton mode and the perturbative modes is clear in the limit that the roton mode becomes degenerate with the ground state. In this limit, the roton energy ω goes to zero. In Eq. (4), this means that $\tilde{G}\tilde{F}$ has eigenvalue zero. Now, note that the operator G is positive semidefinite. (Its lowest eigenvalue is zero, with eigenfunction $|\Psi\rangle$. This is indeed the ground state, since $|\Psi\rangle$ is nodeless). Accordingly, the operator $\tilde{G}$ that, by definition, acts on the linear space orthogonal to $|\Psi\rangle$ is positive definite. It then follows that any solution of $\tilde{G}\tilde{F}|f_{\rm roton}\rangle = 0$ must also satisfy $\tilde{F}|f_{\rm roton}\rangle = 0$. Thus, $|\varphi_0\rangle = |f_{\rm roton}\rangle$ is a solution of Eq. (6) with eigenvalue $\varepsilon_0 = 0$. Since $|\Psi'\rangle$ is written as an expansion in $|\varphi_n\rangle$ with weights proportional to $1/\varepsilon_n$, the eigenfunction $|\varphi_0\rangle$ with eigenvalue $\varepsilon_0 \sim 0$ makes a contribution to $|\Psi'\rangle$ that

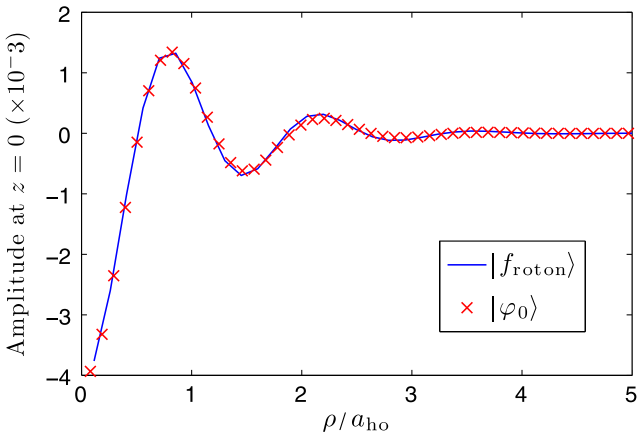

FIG. 3 (color online). Radial profiles of excitations on a rotationless DBEC with dipole strength $D = 181.2$ in a trap with aspect ratio $\lambda = 17$. The solid blue line represents the BdG roton mode while the red marks represent the F-operator eigenfunction with eigenvalue μ, $|\varphi_0\rangle$.

strongly overwhelms the contributions of the other eigenfunctions. Thus, in the limit that the roton energy goes to zero, $|\Psi'\rangle$ is dominated by the BdG roton mode $|f_{\rm roton}\rangle$.

To show that $|\varphi_0\rangle$ becomes identical to BdG roton mode $|f_{\rm roton}\rangle$ when the roton energy goes to zero, Fig. 3 shows the radial profiles of both of these excited modes for a rotationless DBEC with dipole strength $D = 181.2$ in a trap with aspect ratio $\lambda = 17$, which is very near the point of instability. Additionally, Fig. 2 illustrates the accuracy with which this perturbation theory predicts the wave function of a DBEC when perturbed by a Gaussian potential, as discussed earlier in this Letter.

Recall that the $k = 1$ solution of the GPE gave rise to a centrifugal potential in the radial part of Eq. (3). This potential is constant along the trap axis and decreases quickly in the radial direction. So, just as the Gaussian potential perturbs the DBEC and gives rise to ripples on its density profile, we expect similar behavior for trapped DBECs with a centrifugal potential, i.e., DBECs with vortex structure. To treat the centrifugal potential with our perturbation theory, we introduce a radial cutoff that is chosen to be much smaller than the spatial extent of the vortex core itself. We find that for large λ there is good agreement between our perturbation theory and the results of our exact calculations. Just as is the case for a Gaussian perturbing potential, the roton mode is responsible for the rich structure observed in the $k = 1$ vortex state of a DBEC close to instability.

In conclusion, we have developed a perturbation theory for the GPE and have applied it to DBECs perturbed both by thin Gaussian potentials centered on the trap axis and by centrifugal potentials. This theory allows us to relate the radial oscillations observed on the exact ground state profiles of perturbed DBECs to the roton mode observed in the BdG spectrum of rotationless DBECs. For ^{52}Cr and the trap parameters discussed in this Letter, the length scale of the oscillations is $\sim 2\ \mu$m. This is in comparison to the length scale of the predicted ripple in the ^{4}He vortex, which is of the order of 1 Å, and has not been resolved experimentally up to now.

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[1] L. Santos, G. V. Shlyapnikov, and M. Lewenstein, Phys. Rev. Lett. **90**, 250403 (2003).
[2] S. Ronen, D. C. E. Bortolotti, and J. L. Bohn, Phys. Rev. Lett. **98**, 030406 (2007).
[3] A. Griesmaier, J. Werner, S. Hensler, J. Stuhler, and T. Pfau, Phys. Rev. Lett. **94**, 160401 (2005).
[4] J. Stuhler, A. Griesmaier, T. Koch, M. Fattori, T. Phau, S. Giovanazzi, P. Pedri, and L. Santos, Phys. Rev. Lett. **95**, 150406 (2005).
[5] T. Koch, T. Lahaye, J. Metz, B. Frohlich, A. Griesmaier, and T. Pfau, Nature Phys. **4**, 218 (2008).
[6] T. Lahaye, T. Koch, B. Frohlich, M. Fattori, J. Metz, A. Griesmaier, S. Giovanazzi, and T. Pfau, Nature (London) **448**, 672 (2007).
[7] D. Bohm and B. Salt, Rev. Mod. Phys. **39**, 894 (1967).
[8] T. Regge, J. Low Temp. Phys. **9**, 123 (1972).
[9] F. Dalfovo, Phys. Rev. B **46**, 5482 (1992).
[10] S. Yi and H. Pu, Phys. Rev. A **73**, 061602(R) (2006).
[11] D. H. J. O'Dell and C. Eberlein, Phys. Rev. A **75**, 013604 (2007).
[12] R. M. W. van Bijnen, D. H. J. O'Dell, N. G. Park, and A. M. Martin, Phys. Rev. Lett. **98**, 150401 (2007).
[13] D. C. E. Bortolotti, S. Ronen, J. L. Bohn, and D. Blume, Phys. Rev. Lett. **97**, 160402 (2006).
[14] S. Yi and L. You, Phys. Rev. A **61**, 041604(R) (2000).
[15] J. Werner, A. Griesmaier, S. Hensler, A. Simoni, E. Tiesinga, J. Stuhler, and T. Pfau, Phys. Rev. Lett. **94**, 183201 (2005).
[16] L. P. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Oxford University, New York, 2003).
[17] S. Ronen, D. C. E. Bortolotti, and J. L. Bohn, Phys. Rev. A **74**, 013623 (2006).
[18] C. Huepe, L. S. Tuckerman, S. Métens, and M. E. Brachet, Phys. Rev. A **68**, 023609 (2003).