Roton spectroscopy in a harmonically trapped dipolar Bose-Einstein condensate

P. B. Blakie, D. Baillie, and R. N. Bisset
Jack Dodd Centre for Quantum Technology, Department of Physics, University of Otago, Dunedin, New Zealand.

We study a harmonically trapped Bose-Einstein condensate with dipole-dipole interactions in a regime where a roton spectrum emerges. We show that the roton spectrum is clearly revealed in the static and dynamic structure factors which can be measured using Bragg spectroscopy. We develop and validate a theory based on the local density approximation for the dynamic structure factor.

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A variety of atomic species with large magnetic dipoles have been cooled to the quantum degenerate regime in which a Bose-Einstein condensate (BEC) forms [1]. The key feature of these gases is that the particles interact via a dipole-dipole interaction (DDI) that is long-ranged and anisotropic [2]. A fascinating prediction is that when such a BEC is tightly confined in the direction that the dipoles are polarized, a roton-like spectrum can emerge [3]. A number of theoretical proposals for detecting roton features have been made including sensitivity to external perturbations [4], depression in the critical velocity [5, 6], and signatures in density fluctuations [7] (c.f. [8]). However, to date there has been no experimental evidence for roton properties in dipolar BECs [9].

In this paper we study a dipolar BEC confined in a quasi-two-dimensional (quasi-2D) harmonic trap. We vary contact and dipole interaction parameters over a wide range and characterize the emergence of a roton through the static and dynamic structure factors. These quantities closely relate to the observable for Bragg spectroscopy [10, 11], and thus are readily measured in experiments. We note that Bragg spectroscopy has emerged as a flexible tool for investigating ultra-cold gases and has been applied to resonant Bose [12] and Fermi [13] gases, quasi-1D Bose gases [14], and vortices in BECs [15]. Recently the first application of Bragg spectroscopy to a dipolar BEC has been made [16] in a nearly spherical trap, and used to demonstrate an anisotropic speed of sound.

Our calculations for the structure factors are based on solving the non-local Gross-Pitaevskii equation (GPE) for the condensate and the Bogoliubov de-Gennes (BdG) equations for the quasi-particle excitations. Our calculations are fully three-dimensional (3D), i.e. we do not make the quasi-2D approximation in which an ansatz for the condensate shape in the tightly confined direction is assumed (this approximation has been shown to be surprisingly inaccurate in the regime of interest [17]). We finish by developing a local density approximation (LDA) theory that provides a reasonably accurate description of our full theory. We emphasize that the regime of our study is appropriate to current experiments with magnetic dipoles. We refer the reader to Ref. [18] for a discussion of the true-2D regime that might be realized in future polar-molecule experiments.

The DDI potential between a pair of dipolar atoms is

$$U_{dd}(r) = \frac{3g_{dd}}{4\pi} \frac{1 - 3\cos^2 \theta}{|r|^3},$$

(1)

where $g_{dd} = \mu R^2_m/3$, $\mu_m$ is the dipole strength, and $\theta$ is the angle between the dipole separation $r$ and the polarization axis, which we take to be the $z$ direction. The atoms also interact via a contact interaction of strength $g = 4\pi a h^2/m$ with $a$ the s-wave scattering length. We take the atoms to be confined in a cylindrically symmetric trap $U(x) = \frac{1}{2} m \omega_z^2 \rho^2 + \lambda^2 z^2$ of aspect ratio $\lambda = \omega_z/\omega_x$. Here we consider tight axial confinement ($\omega_z \gg \omega_x$) to produce a quasi-2D trap favorable for the emergence of rotons.

It is useful to review the properties of a homogeneous dipolar gas (i.e. with $\omega_\rho = 0$), which admits a simple analytic treatment under the quasi-2D approximation (assuming a Gaussian mode structure along the tight direction). In this case the tight direction can be integrated out and the Fourier transform of the in-plane interaction potential is [3]

$$\bar{V}_{2D}(k_{\rho}) = \bar{g} + g_{dd} F_{\perp}(k_{\rho} \alpha_z/\sqrt{2}),$$

(2)

where $F_{\perp}(x) = 2 - 3\sqrt{\pi} x e^2 x e^{2x} \text{erfc}(x)$, $\bar{g} = g/\sqrt{2\pi} \alpha_z$ and $g_{dd} = g_{dd}/\sqrt{2\pi} \alpha_z$ are the 2D interaction parameters, with

![FIG. 1. (color online) Stability phase diagram and related excitation properties of quasi-2D uniform dipolar BEC. White and light-grey regions indicate where the BEC is dynamically stable. In the light-grey and black regions the system is dynamically unstable. This can arise from modes at zero momentum (phonon instability – black region) or finite momentum (roton instability – dark grey region) developing imaginary parts. Subplots A-D show cases of the spectrum (3), with the real (solid line) and imaginary (dashed line) parts shown.](image-url)
\[ a_z = \sqrt{\hbar/m_\omega z} \] the z-confinement length scale. For a condensate of areal density \( n \) the Bogoliubov dispersion relation for in-plane modes (i.e. no z excitation) is

\[ \epsilon_\ell(k_\rho) = \sqrt{\epsilon(k_\rho)^2 + 2\epsilon(k_\rho)n\tilde{V}_{2D}(k_\rho)}, \]

where \( \epsilon(k_\rho) = \hbar^2 k_\rho^2/2m \). In Fig. 1 we show the generic features of the quasi-2D system as the dipolar and contact interaction parameters are varied. Notably, the system can become unstable through a phonon or roton instability where \( k_\rho \to 0 \) (case B) or \( k_\rho \sim 1/a_z \) (case D) modes, respectively, soften and develop imaginary eigenvalues. Within the stable region we have indicated a sub-region where the dispersion relation has a roton feature i.e. a local minimum at finite \( k_\rho \) (case C).

We now turn to our main concern, a fully 3D calculation of the trapped system. To do this we numerically solve the non-local GPE for the unit normalized condensate orbital \( \psi_0(x) \) and chemical potential \( \mu \), and then diagonalize the BdG equations for the quasi-particle excitations \{\( u_j(x), v_j(x) \)\}, with respective energies \( \epsilon_j \) [19]. Our numerical method, similar to Ref. 20, utilizes the cylindrical symmetry by employing a Fourier-Hankel representation to separate the GPE and BdG equations into a set of 2D problems specified by the angular quantum number \( m_z = 0, \pm 1, \pm 2, \ldots \) [e.g. \( u_j(x) = u_j(\rho, z) e^{im_z \phi} \)]. We also use a cylindrically cutoff of the interaction potential [1] to improve numerical convergence [21].

The results we present focus on a trap with \( \lambda = 40 \), although we find qualitatively similar behavior for \( \lambda \gtrsim 10 \). We have chosen \( \lambda = 40 \) as being sufficiently tight for the roton to emerge at a reasonably large \( k \) value, yet is an aspect ratio that is readily achievable in experiments (e.g. [22]). For convenience we introduce \( D = 3Ngm/4\pi\hbar^2 a_\rho \) and \( C = N/m/4\pi\hbar^2 a_\rho \) as dimensionless parameters for the dipolar and contact interactions, respectively, with \( a_\rho = \sqrt{\hbar/m_\omega \rho} \) and \( N \) the number of condensate atoms.

In Fig. 2(a) we show the excitation spectrum of \( m_z = 0 \) modes for \( C = 0 \) as a function of \( D \). For \( D \gtrsim 400 \) we observe that high-lying quasi-particle modes begin to rapidly decrease in energy as \( D \) increases. We identify the softening of these highly excited modes (i.e. modes with many radial nodes) as the manifestation of the roton spectrum in the trapped gas. This interpretation is supported by other studies of the trapped system in which the quasi-particle spectrum was approximately mapped onto a dispersion relation [23] (also see \( k \) defined below). At \( D \approx 730 \) the first of these roton (quasi-particle) modes hits zero energy and develops an imaginary part, signaling the onset of a dynamical instability. We note that modes with \( |m_z| > 0 \) exhibit similar trends to the \( m_z = 0 \) results shown in Fig. 2(a).

The condensate orbital and the density perturbations associated with two quasi-particle modes are indicated in Fig. 2(b)-(d). Notably the roton mode [Fig. 2(d)] is localized near the center of the condensate and has a short wavelength. Following [23] we assign a wavevector to the modes according to \( \bar{k} = \sqrt{(k_\rho^2)/\rho} \), and find that for this mode \( \bar{k} = 6.45/a_\rho \), similar to the inverse \( z \) confinement length \( 1/a_z \approx 6.3/a_\rho \).

The dynamic structure factor for a \( T = 0 \) BEC is [11],

\[ S(k, \omega) = \sum_j \int dx [u_j^*(x) + v_j^*(x)] e^{ik \cdot x} \psi_0(x) \] \[ \sum_j \left| \langle \delta(\omega - \epsilon_j) \right|, \]

where \( \omega_j \equiv \epsilon_j/\hbar \). It is worth noting that Bragg spectroscopy measures the imaginary part of the response function \( \text{Im} [\chi(k) \omega)] = -\frac{n}{\pi} [S(k, \omega) - S(-k, -\omega)] \) [24], and to leading order this is only sensitive to the zero-temperature dynamic structure factor. Thus our results should be applicable to regimes with a discernible non-condensate fraction. Cor-

FIG. 2. (color online) (a) Spectrum of \( m_z = 0 \) quasi-particle modes demonstrating the roton-softening. (b)-(d) Contour plots of modes at \( D = 700 \). (b) Condensate density. (c) and (d) give the density perturbations associated with two quasi-particle modes indicated in Fig. 2(b)-(d). Results for \( \lambda = 40 \) and \( C = 0 \).
reactions beyond leading order will require a finite temperature extension of the theory (e.g. see [25]).

Integrating \( S(k, \omega) \) over frequency yields the static structure factor \( S(k) = \int d\omega S(k, \omega) \), which also relates to the Fourier transform of the pair correlation function \( f_1 \). For the uniform system \( S(k) \) directly gives the dispersion relation through the Bijn-Feynman formula \( S(k) = \epsilon(k) / \epsilon_B(k) \).

Here we restrict our attention to evaluating the structure factors for radial wavevectors \( k = k \rho \), since the roton modes exhibit non-trivial structure in-plane [see Fig. 2(d)], and from hereon will denote these with scalar arguments, i.e. \( S(k, \omega) \), \( S(k) \). For a given value of \( k \) the numerical evaluation of \( S(k, \omega) \) requires including modes up to a maximum energy \( \epsilon_{\text{max}} \) with \( \epsilon_{\text{max}} \geq \hbar^2 k^2 / 2m \). In practice we check that sufficiently many modes are included by ensuring that the \( f \)-sum rule, \( \int_0^\infty d\omega \omega S(k, \omega) = \hbar k^2 / 2m \), is satisfied. For the \( k \) values we consider here \( (k \lesssim 20 / a_\rho) \) we typically use \( \geq 10^4 \) modes in our calculations.

We present results for \( S(k) \) in Fig. 2(e) for various values of the dipole interaction strength. The suppression of \( S(k) \) as \( k \to 0 \) reveals the low-energy phonon spectrum of the system (see [10]). A significant peak in \( S(k) \) at \( k_{\text{peak}} \sim 6.5 / a_\rho \) forms for interaction values of \( D > 400 \), which corresponds to where the high energy modes begin to rapidly descend in the spectrum [see Fig. 2(a)]. Appealing to the Bijn-Feynman formula we identify a significant peak in the static structure factor with the appearance of a roton feature in the excitation spectrum. This identification is useful because it corresponds to a practical experimental observable and does not depend upon any \textit{ad hoc} scheme for assigning a dispersion relation to the excitations of the trapped system.

In Fig. 3 we characterize the behavior of \( S(k) \) over a broad range of contact and dipole parameters where the BEC is dynamically stable. We show where a peak in \( S(k) \) emerges and characterize its height [Fig. 3(a)] and wavevector \( (k_{\text{peak}}) \) [Fig. 3(b)]. Our results show that the roton character of the spectrum is generally enhanced [i.e. height of peak in \( S(k) \)] increases] at fixed dipole strength by decreasing (i.e. making more negative) the contact interaction strength, although the value of \( k_{\text{peak}} \) tends to decrease as this happens.

In Fig. 3 we also indicate the boundary upon which the BEC becomes dynamically unstable. Because the cloud is tightly confined in the \( z \) direction the repulsive character of the DDI (due to side-by-side dipoles) dominates and hence the DDI partially stabilizes the BEC against collapse from a negative value of the contact interaction. Similar observations, for gases with smaller trap aspect ratio, were presented in Ref. [21]. There are regions near the boundary where the condensate develops a bi-concave density profile with a local minimum in the BEC density at trap centre [3][26]. We do notice any signature of the bi-concave BEC in \( S(k) \).

![Figure 3](https://example.com/figure3.png)

**Figure 3.** (color online) Characterization of the roton properties of a \( \lambda = 40 \) trapped dipolar BEC using \( S(k) \). (a) Peak value of \( S(k) \). (b) Peak wavevector \( k_{\text{peak}} \) (none shown when \( \max[S(k)] < 1.05 \)). Circles mark the parameters of states analyzed in Fig. 2(e). Grey boundary line indicates when the system is unstable due to excited modes softening, with black segments indicating that the BEC is in a bi-concave state at the boundary (see [3]).

In Fig. 4(a) we show \( S(k, \omega) \) for indicated values of \( D \). A Gaussian of width \( \Delta \omega = 0.5 \omega_\rho \) is used to smooth the \( \delta \)-functions in \( S(k, \omega) \). The solid black and grey lines are the mean response \( \omega(\omega) \) obtained from GPE based and quasi-2D approximation LDA calculations, respectively [see text and below]. White ellipse in (f) identifies a roton response feature. LDA calculations of \( S(k, \omega) \) for the parameters in (f) are shown in (f1) and (f2). (f1) GPE based LDA approach of Eq. (6), (f2) quasi-2D approximation LDA approach (see text). The mean response \( \omega(\omega) \equiv \int d\omega \omega S(k, \omega) / S(k) \) is shown for each result. Other parameters: \( C = 0 \) and \( \lambda = 40 \).

![Figure 4](https://example.com/figure4.png)

**Figure 4.** (color online) (a)-(f) \( S(k, \omega) \) for indicated values of \( D \). A Gaussian of width \( \Delta \omega = 0.5 \omega_\rho \) is used to smooth the \( \delta \)-functions in \( S(k, \omega) \). The white dashed line shows the free particle dispersion \( \epsilon(\omega)/\hbar \). The solid black and grey lines are the mean response \( \omega(\omega) \) obtained from GPE based and quasi-2D approximation LDA calculations, respectively [see text and below]. White ellipse in (f) identifies a roton response feature. LDA calculations of \( S(k, \omega) \) for the parameters in (f) are shown in (f1) and (f2). (f1) GPE based LDA approach of Eq. (6), (f2) quasi-2D approximation LDA approach (see text). The mean response \( \omega(\omega) \equiv \int d\omega \omega S(k, \omega) / S(k) \) is shown for each result. Other parameters: \( C = 0 \) and \( \lambda = 40 \).

Because the frequency dependence of the system response is most directly measured in Bragg spectroscopy experiments it is also worth discussing the behavior of the dynamic structure factor. In Figs. 4(a)-(f) we show \( S(k, \omega) \) for the same cases considered in Fig. 2(e). In the vicinity of the roton wavevector [i.e. \( k \sim 6.5 / a_\rho \)] the frequency response is quite broad and dips down sharply towards zero frequency for \( D \geq 700 \). The discernible response feature indicated with an ellipse in Fig. 4(f) is due to the roton mode identified in Fig. 2(d) (but also has contributions from similar modes with \( |m_z| > 0 \)).
For the case of BECs with contact interactions a successful analytic approximation for \(S(k, \omega)\) has been developed using the Thomas-Fermi approximation for the condensate and treating the excitations within LDA \([11]\). We have found that the main issue in extending this type of analysis to the tightly confined dipolar BEC arises from the sensitive dependence of the in-plane DDI potential \([\text{c.f. Eq. (2)}]\) upon the shape of the condensate in the \(z\) direction. For this reason we use the GPE solution itself as the basis for calculating \(S(k, \omega)\) using an LDA treatment of the excitations, thus avoiding the need to numerically solve for the BdG equations. We note that generalized mode treatments, e.g. Ref. \([17]\), could also be used.

We define a locally varying in-plane interaction potential

\[
\hat{V}_{2D}(k_{\rho}, \rho) = \int \frac{dk_z}{\pi \mu^2(\rho)} \left[ g + \hat{U}_{dd}(k_{\rho}, k_z) \right] \left| \hat{n}(k_{\rho}, \rho) \right|^2, \tag{5}
\]

where \(n(\rho) = \int dz |\psi(\rho, z)|^2\) is the areal density, \(\hat{n}(k_{\rho}, \rho)\) is the \(z\)-Fourier transform of the condensate density, and \(\hat{U}_{dd}(k_{\rho}, k_z) = -\omega_0 k_{\rho, z} / k_0^2 - 1\) is the Fourier transform of \(U_{dd}(r)\). The \(\rho\) dependence of \(\hat{V}_{2D}(k_{\rho}, \rho)\) accounts for the changing \(z\) profile of the condensate as \(\rho\) varies. Note that in the limit of vanishing interactions, where the \(z\) shape of the condensate is a Gaussian (independent of \(\rho\), \(\hat{V}_{2D}(k_{\rho}, \rho)\) reduces to the analytic result in Eq. \(\text{(2)}\)).

We construct \(S(k, \omega)\) treating the in-plane excitations with the LDA, i.e. summing over the parts of the BEC at various densities \([11]\).

\[
S_{\text{LDA}}(k, \omega) = \int d\rho \pi \rho \frac{n(\rho) \epsilon(\rho) \epsilon_B(k_{\rho}, \rho)}{\epsilon_B(k_{\rho}, \rho)} \delta(\omega - \epsilon_B(k_{\rho}, \rho)/h), \tag{6}
\]

where \(\epsilon_B(k_{\rho}, \rho) = \sqrt{\epsilon(k_{\rho})^2 + 2\epsilon(k_{\rho}) n(\rho) \hat{V}_{2D}(k_{\rho}, \rho)}\). In Figs. \(\text{(f1)}\) and \(\text{(f2)}\) we compare our GPE based LDA \([6]\) against LDA calculation using the quasi-2D approximation [this only differs by the replacement \(\hat{V}_{2D}(k_{\rho}, \rho) \rightarrow \hat{V}_{2D}(k_{\rho})\) in Eq. \(\text{(6)}\)]. This comparison reveals the sensitivity of \(S(k, \omega)\) to the \(z\) shape of the condensate. In the inset to Fig. \(\text{(f3)}\) we compare the full numerical calculations of \(S(k)\) against the GPE based LDA, and find good agreements until \(D \gtrsim 700\) where the roton modes approach zero energy.

Finally, we relate the dimensionless parameters of our calculations to current experimental systems. A value of \(D \sim 700\) for \(\omega_0 = 2\pi \times 40 \text{ s}^{-1}\) would require a condensate with \(N = \{64.3, 4.1, 8.1\} \times 10^4\) atoms for \(\{^{52}\text{Cr}, \ 164\text{Dy}, \ 168\text{Er}\}\), respectively. The value of \(D\) can be adjusted by changing the radial confinement, atom number or dipolar strength \([27]\). Our results demonstrate [see Fig. \(\text{(3)}\)] that instead, for fixed dipole strength, the roton spectrum can be accessed by making the \(s\)-wave scattering length negative (e.g. see \([28]\)].

In conclusion we have explored the excitation properties of a quasi-2D dipolar BEC in terms of the dynamic and static structure factors. Our results show that clear and direct signatures for the roton spectrum will emerge in the structure factors and should be readily observable with Bragg spectroscopy in current experiments. We have constructed an approximate LDA theory for \(S(k, \omega)\) which we have validated against the full theory. Future work will consider the extension to a set of quasi-2D traps realized with an optical lattice \([17, 29]\).

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