Eur. Phys. J. D **31**, 439–445 (2004)
DOI: 10.1140/epjd/e2004-00146-7

THE EUROPEAN
PHYSICAL JOURNAL D

Instabilities and the roton spectrum of a quasi-1D Bose-Einstein condensed gas with dipole-dipole interactions

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Received 26 August 2004

Abstract. We point out the possibility of having a roton-type excitation spectrum in a quasi-1D Bose-Einstein condensate with dipole-dipole interactions. Normally such a system is quite unstable due to the attractive portion of the dipolar interaction. However, by reversing the sign of the dipolar interaction using either a rotating magnetic field or a laser with circular polarization, a stable cigar-shaped configuration can be achieved whose spectrum contains a 'roton' minimum analogous to that found in helium II. Dipolar gases also offer the exciting prospect of tuning the depth of this 'roton' minimum by directly controlling the interparticle interaction strength. When the minimum touches the zero-energy axis the system is once again unstable, possibly to the formation of a density wave.

PACS. 03.75.Hh Static properties of condensates; thermodynamical, statistical and structural properties. – 03.75.Kk Dynamic properties of condensates; collective and hydrodynamic excitations, superfluid flow – 71.45.Lr Charge-density-wave systems

1 Introduction

Ultra-cold gases of atoms which interact with long-range anisotropic dipole-dipole interactions have been the subject of a number of theoretical analyses over the past few years [1–10]. The very recent advent of Bose-Einstein condensation of molecules [11] has renewed interest in the investigation of quantum gases with dipolar interactions since molecules can potentially possess large dipole moments. One of the novel properties that has been predicted for gaseous Bose-Einstein condensates (BECs) with dipole-dipole interactions is a 'roton' minimum in the excitation spectrum [12,13], a feature which is absent in the usual case of repulsive short-range *s*-wave interactions, and seems to originate in the long-range and partially attractive nature of dipolar interactions.

The 'roton' minimum can be interpreted with the help of Feynman's formula for the dispersion relation for excitations of energy E and momentum $\hbar k$ of a Bose liquid [14]

$$E(k) = \frac{\hbar^2 k^2}{2mS(k)} \tag{1}$$

where m is the atomic mass. This remarkable formula relates the excitation spectrum to the two-particle correlation properties as encapsulated in the static structure factor $S(k)$, which is the Fourier transform of the pair correlation function. A peak in $S(k)$ due to strong two-particle correlations can lead to a minimum in the energy spectrum. The most famous example of a roton minimum (and the system for which the name was first coined, by Landau) is helium II where the roton minimum occurs at wavelengths coinciding with the average interparticle separation. The roton minimum in helium II has often been regarded as indicating that the superfluid is very close to crystallization [15–17] since the ordering of atoms on a crystal lattice would lead to a corresponding peak in $S(k)$. However, many questions concerning this superfluid to density-wave transition remain difficult to answer, essentially because liquid helium is a strongly correlated system. Our aim in this paper is to explore an analogous 'roton' spectrum in a quasi-1D BEC with dipole-dipole interactions. The tunability of the various parameters (interaction strength, density, effective dimensionality, etc.) controlling these relatively simple quantum gases gives the exciting possibility of varying the depth of the roton minimum and hence explore the onset of this zero-temperature phase transition.

2 Dipole-dipole interactions in a Bose-Einstein condensate

The long-range part of the interaction between two dipoles separated by $\mathbf{r}$, and aligned by an external field along a unit vector $\hat{\mathbf{e}}$, is given by

$$U_{\mathrm{dd}}(\mathbf{r}) = \frac{C_{\mathrm{dd}}}{4\pi}\, \hat{\mathrm{e}}_i \hat{\mathrm{e}}_j \frac{(\delta_{ij} - 3\hat{r}_i\hat{r}_j)}{r^3}. \tag{2}$$

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Dipoles induced by an electric field $\mathbf{E} = E\hat{\mathbf{e}}$ have a coupling $C_{\mathrm{dd}} = E^2\alpha^2/\epsilon_0$, where α is the static polarizability, and ϵ_0 the permittivity of free space. For atoms with a magnetic dipole moment d_m aligned by a magnetic field $\mathbf{B} = B\hat{\mathbf{e}}$, one has $C_{\mathrm{dd}} = \mu_0 d_m^2$, where μ_0 is the permeability of free space. The isotropic short-range part of the interatomic interactions is modelled by a pseudo-potential, $U_{\mathrm{s}}(\mathbf{r}) = (4\pi a_{\mathrm{s}}\hbar^2/m)\delta(\mathbf{r}) \equiv g\delta(\mathbf{r})$, where g incorporates the quantum aspects of low-energy scattering via the s-wave scattering length, a_{s}. In order to apply Bogoliubov (perturbation) theory to a BEC one generally needs to use such an effective- or pseudo-potential rather than the bare interaction [19]. In what follows we shall assume, however, that the dipole-dipole interaction can be treated within the Born approximation, which corresponds to the Fourier transform of the bare potential (2). The Born approximation has been shown by Yi and You [1] to work reasonably well for the long-range dipole-dipole interaction, but see Derevianko's work [6] for corrections, which can be substantial [7].

The basic quantity that then enters the Bogoliubov theory is the Fourier transform of the total effective interaction, $\widetilde{U}_{\mathrm{tot}}(\mathbf{k}) = \int \mathrm{d}^3\mathrm{r} \exp[-\mathrm{i}\mathbf{k}\cdot\mathbf{r}]\{g\delta(\mathbf{r}) + U_{\mathrm{dd}}(\mathbf{r})\}$,

$$\widetilde{U}_{\mathrm{tot}}(\mathbf{k}) = g\left[1 + \varepsilon_{\mathrm{dd}}\,\hat{\mathrm{e}}_i\hat{\mathrm{e}}_j\left(3\hat{k}_i\hat{k}_j - \delta_{ij}\right)\right] \tag{3}$$

where $\varepsilon_{\mathrm{dd}}$ is a dimensionless measure of the strength of the dipolar interactions relative to the s-wave scattering

$$\varepsilon_{\mathrm{dd}} \equiv \frac{C_{\mathrm{dd}}}{3g}. \tag{4}$$

The definition includes a factor of 3 because for a homogeneous system (no confining trap) one finds instabilities when $\varepsilon_{\mathrm{dd}} \geq 1$ [2,5,10]. This can be seen directly from the Bogoliubov dispersion for phonon-like density perturbations in a homogeneous dipolar BEC [2]

$$E_{\mathrm{B}} = \sqrt{\left(\frac{\hbar^2k^2}{2m}\right)^2 + 2gn\left\{1 + \varepsilon_{\mathrm{dd}}\left(3\cos^2\theta - 1\right)\right\}\frac{\hbar^2k^2}{2m}} \tag{5}$$

where n is the density. This dispersion relation (5) can become imaginary when $\varepsilon_{\mathrm{dd}} > 1$, indicating an instability. The interactions enter the dispersion in the second term under the square root via the effective potential (3). The dispersion (5) relation has an angular dependence (θ is the angle between the momentum of the phonon and the external polarizing field) which further illustrates the richness of dipolar systems in comparison to the non-dipolar case.

Santos et al. [13] considered the case of a quasi-2D *pancake*-shaped BEC, where the dipoles are aligned (by an external static field) along the symmetry axis of the trap. They predicted that the analogous expression to (5) gives a roton minimum in the excitation spectrum. In this paper, however, we want to see if a roton minimum can be achieved in the quasi-1D case where the condensate is *cigar* shaped, being tightly confined in the radial $(x - y)$ plane, say, and very elongated along the axial (z) direction. At first sight this seems unlikely because the anisotropy of the dipole-dipole interaction means that the quasi-1D and -2D cases are very different. Two dipoles lying side-by-side in the radial plane are repulsive, whilst two lying end-to-end along the axial direction are attractive so, broadly speaking, a pancake shaped BEC tends to be more stable since the mean-field energy is more positive (repulsive) than that of a cigar-shaped BEC. Indeed, an infinite quasi-1D BEC with only dipole-dipole interactions (no repulsive s-wave short range interactions) is unstable to density perturbations, as we shall see. Therefore we shall employ a special trick and *reverse* the sign of the dipole-dipole interaction (see also [5]). Two methods for achieving the reversed dipole-dipole interaction will be reviewed in the next section. With the sign of the dipole-dipole interactions reversed, two dipoles lying end-to-end along the axial direction are now repulsive and in this way an infinite quasi-1D dipolar BEC can be stabilized somewhat against collapse induced by density perturbations.

In our previous work on the possibility of a roton spectrum in a BEC [12] we took the case of laser-induced dipole-dipole interactions [18], which on top of the static interactions of equation (2), also have a very long-range component ($1/r^2$, or even $1/r$, depending on the polarization direction) arising from retardation effects due to the finite wavelength of the laser radiation. In principle this is a very general scheme since one can benefit from the large polarizability of atoms/molecules close to an electronic transition. The disadvantage of laser-induced dipole-dipole interactions, in atomic systems at least, is the unavoidable presence of spontaneous emission which heats the sample. In molecular systems one may be able to circumvent spontaneous emission problems somewhat by using transitions in the infra-red or even microwave regions where spontaneous emission rates are low and the long wavelength of the radiation allows one to have many particles in an 'interaction volume' (given by $\lambda^3_{\mathrm{laser}}$). In [20] we discussed how a BEC with light-induced dipole-dipole interactions is unstable to the formation of a density wave. The periodicity of the modulation is determined by the wavelength of the laser light and in one interpretation can be understood in terms of the back-scattered light interfering with the incident light to form an optical grating which the atoms then minimize their energy in by trying to sit predominantly in the wells. In this paper we are interested in the case of static dipole-dipole interactions. Although at first sight there are many similarities between the two cases, in the light-induced case the optical wavelength provides the fundamental (classical) scale in the problem whereas here the parameters we must form a length scale from are C_{dd}, n, m and $\hbar$.

3 Reversing the sign of the dipole-dipole interaction

(i) In the case of magnetic dipoles the sign of the dipole-dipole interaction (2) can be reversed by rapidly rotating a component of the external magnetic field in the radial plane [5], similarly to a well-known technique from solid state NMR. The magnetic field should have the form

$$\mathbf{B}(t) = B\left\{\cos\phi\hat{\mathbf{z}} + \sin\phi\left[\cos(\Omega t)\,\hat{\mathbf{x}} + \sin(\Omega t)\,\hat{\mathbf{y}}\right]\right\} \tag{6}$$

which is a combination of a static magnetic field directed along z, and a field rotating at frequency Ω in the perpendicular radial plane. The frequency should be such that the dipoles practically do not move during the time Ω^{-1}, but their moments adiabatically follow the external field $\mathbf{B}(t)$. This corresponds to the condition $\omega_{\text{Larmor}} \gg \Omega \gg \omega_r,\ \omega_z$, where $\omega_r,\ \omega_z$ are the radial and axial trapping frequencies, respectively. Under these conditions the particles experience a time-averaged interaction whose form is exactly the same as equation (2) except for being multiplied by $\left(3\cos^2\phi - 1\right)/2$. By varying the angle ϕ this factor can be continuously changed between $-1/2$ to 1, giving the possibility to reverse the sign of the interaction. At the so-called 'magic angle' of $\phi_M = 54.7°$ the dipolar interaction averages to zero. This technique can be adapted to the case of heteronuclear molecules polarized by a rotating electric field. (ii) For dipoles induced by the electric field of a very long wavelength laser propagating along the z-direction, then one obtains a reversed dipolar interaction when the laser is circularly polarized. In the static limit the laser induced dipole-dipole interaction gives

$$C_{\text{dd}} = I\alpha^2/(c\epsilon_0^2) \tag{7}$$

where I is the laser intensity and c is the speed of light. For a laser with wavevector $\mathbf{q} = \hat{\mathbf{z}}\omega/c$, then application of the identity $\hat{e}_i^{*(\pm)}(\mathbf{q})\hat{e}_j^{(\pm)}(\mathbf{q}) = \frac{1}{2}[(\delta_{ij} - \hat{q}_i\hat{q}_j) \pm \mathrm{i}\epsilon_{ijk}\hat{q}_k]$, where $+(-)$ corresponds to left (right) circular polarizations, leads to the interaction

$$U_{\text{dd}}^{\text{circ}}(\mathbf{r}) = -\frac{1}{2}\frac{I\alpha^2(0)}{4\pi c\epsilon_0^2}\frac{\left(1 - 3\cos^2\theta\right)}{r^3} \tag{8}$$

where θ is angle the interparticle separation vector $\mathbf{r}$ makes with the z-axis. We see that the sign of the interaction has been reversed and multiplied by one half, corresponding to the maximal change possible in the magnetic case. In order to keep the notation as simple as possible, whenever reversed dipolar interactions are used in the rest of this paper C_{dd} will be taken to include the multiplying prefactors (such as 1/2).

4 Quasi-1D ansatz

The dipole-dipole energy functional of the gas is given by

$$H_{\text{dd}} = \frac{1}{2}\iint \mathrm{d}^3r\,\mathrm{d}^3r'\,n(\mathbf{r})\,U_{\text{dd}}(\mathbf{r}-\mathbf{r}')\,n(\mathbf{r}') \tag{9}$$

$$= \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\,\widetilde{n}(\mathbf{k})\,\widetilde{U}_{\text{dd}}(\mathbf{k})\,\widetilde{n}(-\mathbf{k}) \tag{10}$$

where $n(\mathbf{r})$ and $\widetilde{n}(\mathbf{k})$ are the number density and its Fourier transform (F.T.), respectively. The F.T. of the dipole-dipole potential is given in (3).

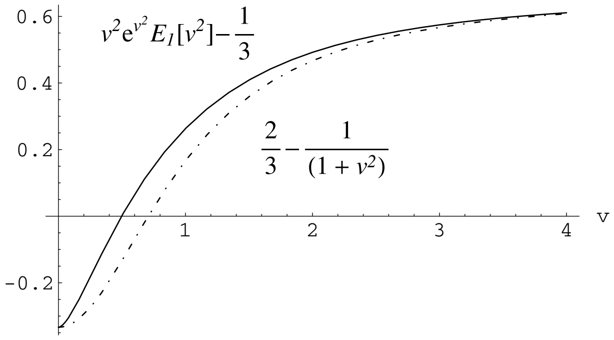

Fig. 1. Solid curve: effective 1D dipolar potential $\widetilde{U}_{\text{dd}}^z(v)$, in momentum space in units of $C_{\text{dd}}/(2\pi w_x^2)$. Dot-dashed curve: a simple approximation (as given in Eq. (16)).

Assuming an harmonic radial trapping $V_{\text{trap}} = (1/2)m\omega_x^2(x^2+y^2)$ with $\hbar\omega_x$ larger or equal to the mean-field energy, we make a Gaussian ansatz for the radial part of the number density profile

$$n(\mathbf{r}) = (\pi w_x^2)^{-1} n^z(z)\exp\left[-(x^2+y^2)/w_x^2\right] \tag{11}$$

$$\widetilde{n}(\mathbf{k}) = \widetilde{n}^z(k_z)\exp[-(k_x^2+k_y^2)w_x^2/4] \tag{12}$$

where w_x is the characteristic radial width and N is the total number of atoms in the sample. The axial density profile $n^z(z)$ is normalized to N, and its F.T. is $\widetilde{n}^z(k_z)$. Upon inserting the Gaussian ansatz into the dipolar energy functional, and taking the polarization direction of the dipoles to be in the axial (z) direction the H_{dd} reduces to

$$H_{\text{dd}} = \frac{1}{2}\iint \mathrm{d}z\,\mathrm{d}z'\,n^z(z)U_{\text{dd}}^z(z-z')n^z(z') \tag{13}$$

$$= \frac{1}{2}\int \frac{\mathrm{d}k_z}{2\pi}\,\widetilde{n}^z(k_z)\widetilde{n}^z(-k_z)\widetilde{U}_{\text{dd}}^z(k_z) \tag{14}$$

which defines $\widetilde{U}_{\text{dd}}^z(k_z)$ as the F.T. of the effective one-dimensional dipole-dipole potential. One finds that

$$\widetilde{U}_{\text{dd}}^z(k_z) = \frac{C_{\text{dd}}}{2\pi w_x^2}\left(\frac{k_z^2 w_x^2}{2}\exp[k_z^2 w_x^2/2]\,E_1[k_z^2 w_x^2/2] - \frac{1}{3}\right) \tag{15}$$

where $E_1[x] = \int_x^\infty \mathrm{d}t\,\exp[-t]/t$ is the exponential integral [21]. In an analogous fashion, the effective 1D s-wave contact interaction in momentum space is given by $\widetilde{U}_{\text{s}}^z = 2\hbar^2 a_{\text{s}}/(m w_x^2)$.

In order to give a qualitative impression of what the effective 1D potential looks like in coordinate space we note that an analytically simple approximation to $\widetilde{U}_{\text{dd}}^z$ is given by (see Fig. 1)

$$\widetilde{U}_{\text{dd}}^z(k_z) \approx \frac{C_{\text{dd}}}{2\pi w_x^2}\left(\frac{2}{3} - \frac{1}{k_z^2 w_x^2/2 + 1}\right). \tag{16}$$

Upon transforming back into coordinate space, the $1/(k_z^2 w_x^2/2 + 1)$ term gives an exponential contribution to the effective coordinate-space 1D potential $U^z_{\text{tot}}(z) = \int(\mathrm{d}k_z/2\pi)\exp[\mathrm{i}k_z z]\,\widetilde{U}^z_{\text{tot}}(k_z)$, i.e.

$$U^z_{\text{tot}}(z) = \frac{g}{2\pi w_x^2}\Bigg(\{2\varepsilon_{\text{dd}}+1\}\,\delta(z) - \frac{3\varepsilon_{\text{dd}}}{\sqrt{2}w_x}\exp\left[-\sqrt{2}z/w_r\right]\Bigg). \quad (17)$$

5 Bogoliubov excitation spectrum for a quasi-1D dipolar BEC

The Bogoliubov dispersion relation for excitations in a homogeneous nearly ideal BEC is

$$E_{\text{B}}^2 = c^2p^2 + (p^2/2m)^2 \quad (18)$$

where for a quasi-1D system, with a Gaussian radial profile of peak density $n(0)$, one has $c^2 = \pi n(0)w_x^2\widetilde{U}^z_{\text{tot}}/m$. For the linear parts of the spectrum c plays the role of the speed of sound. It is useful to write the Bogoliubov relation in terms of the following dimensionless quantities

$$\bar{k}_z = \frac{k_z w_x}{\sqrt{2}} \quad (19)$$

$$\bar{\mu} = \frac{gn(0)}{\hbar^2/(mw_x^2)} \quad (20)$$

$$\bar{E}_{\text{B}} = \frac{E_{\text{B}}}{\hbar^2/(mw_x^2)}. \quad (21)$$

$\bar{k}_z$ is the wavenumber scaled by the inverse radial size, w_x, of the condensate radial wave function ansatz. The Bogoliubov dispersion relation becomes

$$\bar{E}_{\text{B}}^2 = \bar{\mu}\left(3\varepsilon_{\text{dd}}\left\{\bar{k}_z^2\exp[\bar{k}_z^2]E_1[\bar{k}_z^2] - \frac{1}{3}\right\} + 1\right)\bar{k}_z^2 + \bar{k}_z^4. \quad (22)$$

When $\varepsilon_{\text{dd}} > 1$ one finds that the Bogoliubov energy becomes imaginary for a range of momenta, see Figure 2, indicating an instability due to density perturbations. If there are no repulsive s-wave interactions ($\varepsilon_{\text{dd}} \to \infty$) to counterbalance the attractive portion of the dipolar interactions then there is an instability even for vanishingly small dipole-dipole coupling strength in this infinite 1D case. In an actual experiment the trapping potential along the axial direction can stabilize the BEC somewhat, in an analogous fashion to the case of a negative s-wave scattering length [22].

However, as pointed out earlier, the stability properties of the condensate can be dramatically changed by reversing the sign of the dipolar interaction. Figure 3 shows the Bogoliubov excitation spectrum in the case of negative ε_{dd}. In contrast to liquid helium, where one only has control over macroscopic thermodynamic variables such as temperature and pressure, in an atomic or molecular BEC considerable control can be exerted over microscopic quantities such as the interparticle interactions. A well-known example is tuning the s-wave scattering length using a Feshbach resonance [23]. Similarly, in a system of atoms or molecules with a permanent magnetic or electric dipole, one can envisage an experiment at a fixed value of $\bar{\mu}$ and adiabatically changing the dispersion relation by adjusting ε_{dd} via the angle of the rotating external field. Alternatively, for dipoles induced by an electric field one can imagine slowly changing the field strength. Within the current model we find that as ε_{dd} is increased in magnitude below zero (made more negative), first an inflection point appears in the dispersion relation and then a fully fledged roton minimum as shown in Figure 3. As $|\varepsilon_{\text{dd}}|$ is increased yet further the roton minimum deepens and eventually touches the zero-energy axis, at which point, following the earlier discussion of helium, we might expect an instability towards a density-wave. The value of the wavenumber when the roton touches the zero-energy

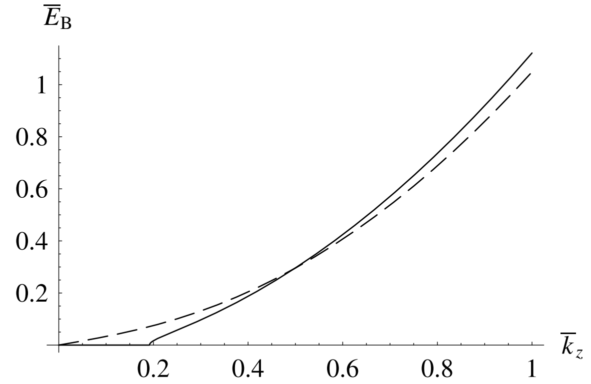

Fig. 2. Bogoliubov dispersion relation for axial excitations in a quasi-1D BEC with $\bar{\mu} = 0.1$. Dashed curve: s-wave contact interactions only ($\varepsilon_{\text{dd}} = 0$). Solid curve: dipole-dipole plus s-wave contact interactions, $\varepsilon_{\text{dd}} = 2$. For $\bar{k}_z < 0.19$ the Bogoliubov energy for the dipolar case is imaginary. In general, whenever $\varepsilon_{\text{dd}} > 1$ the spectrum is imaginary at long wavelengths, indicating an instability to density perturbations.

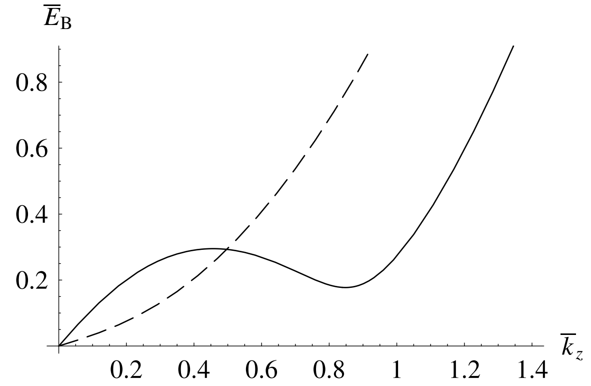

Fig. 3. 'Roton' minimum in the Bogoliubov dispersion relation for axial excitations in a quasi-1D dipolar BEC with $\bar{\mu} = 0.1$. Dashed curve: s-wave contact interactions only ($\varepsilon_{\text{dd}} = 0$). Solid curve: reversed dipole-dipole plus s-wave contact interactions, $\varepsilon_{\text{dd}} = -13$.

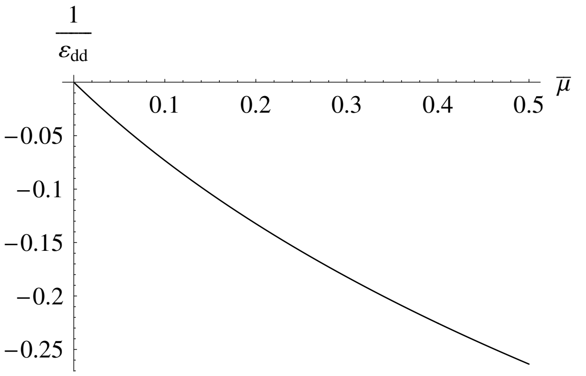

Fig. 4. The critical value of $1/\varepsilon_{\rm dd}(= 3g/C_{\rm dd})$ when the roton minimum touches the zero-energy axis plotted as a function of $\bar{\mu} = gn(0)/(\hbar^2/mw_x^2)$ in an infinite quasi-1D dipolar BEC.

axis is found to be

$$(\bar{k}_z^{\rm crit})^2 = -\frac{\bar{\mu}}{2}\,(2\varepsilon_{\rm dd}+1) - \frac{1}{2}\sqrt{\bar{\mu}^2(2\varepsilon_{\rm dd}+1)^2 + 4\bar{\mu}(\varepsilon_{\rm dd}-1)}. \qquad (23)$$

The particular values of the dimensionless chemical potential $\bar{\mu}$, which is representative of the density, and the dipolar interaction strength, as represented by $\varepsilon_{\rm dd}$, at which this instability occurs obey the transcendental equation

$$3\bar{\mu}\varepsilon_{\rm dd}\left(\bar{k}_z^{\rm crit}\right)^2 \exp\left[(\bar{k}_z^{\rm crit})^2\right] E_1\left[(\bar{k}_z^{\rm crit})^2\right] = \bar{\mu}(\varepsilon_{\rm dd}-1) - \left(\bar{k}_z^{\rm crit}\right)^2. \qquad (24)$$

By substituting equation (23) into (24), one can numerically obtain the relationship between $\varepsilon_{\rm dd}$ and $\bar{\mu}$ at the instability. The results are shown in Figure 4.

In the case of pure dipolar interactions (no s-wave) the point at which the roton touches the zero-energy axis can be reduced to a single number

$$\frac{n(0)C_{\rm dd}}{\hbar^2/(mw_r^2)} \approx -3.6. \qquad (25)$$

In this limiting case the wavelength associated with the roton minimum is given by $\lambda_{\rm roton} = \sqrt{3}\pi\hbar/\sqrt{mn(0)C_{\rm dd}}$, which sets the scale for the density-wave that we expect to form.

6 Effect of axial trapping upon the roton instability

Up till now we have discussed the idealized case of an infinite quasi-1D cylindrical BEC. We now want to move closer to the possible experimental situation where the trap is in fact 3D, but is still assumed to be highly elongated and have cylindrical symmetry. The ansatz for the condensate density may now be taken as a 3D Gaussian

$$n(\mathbf{r}) = \frac{N}{\pi^{3/2}w_x^2w_z}\exp\left[-(x^2+y^2)/w_x^2 - z^2/w_z^2\right]. \qquad (26)$$

Using this ansatz, the contribution of the dipole-dipole interactions to the total energy is found to be given by the expression [1,5,10]

$$H_{\rm dd} = -\frac{N^2C_{\rm dd}}{12\pi\sqrt{2\pi}}\frac{f(\kappa)}{w_x^2w_z} \qquad (27)$$

where $\kappa = w_x/w_z$ is the aspect ratio of the trapped BEC and

$$f(\kappa) = \frac{1+2\kappa^2}{1-\kappa^2} - \frac{3\kappa^2\tanh^{-1}\sqrt{1-\kappa^2}}{(1-\kappa^2)^{3/2}}. \qquad (28)$$

Assuming that the large extension of the trap in the axial direction means that the system is in the Thomas-Fermi limit for that direction (i.e. the zero-point kinetic energy due to the axial trapping can be ignored relative to the trap potential and interaction energies — see [10] for a discussion of the Thomas-Fermi limit for dipolar gases) then the total energy functional, scaled by the transverse trapping energy, is approximately

$$\frac{H_{\rm tot}}{N\hbar\omega_x} \approx \frac{1}{2}\left(\bar{w}_x^2 + \frac{1}{\bar{w}_x^2}\right) + \frac{\lambda}{4}\bar{w}_z^2 - \frac{\eta}{\sqrt{2\pi}}\,(\varepsilon_{\rm dd}-1)\,\frac{1}{\bar{w}_x^2\bar{w}_z} \qquad (29)$$

where $\lambda = \omega_z/\omega_x$ is the aspect ratio of the trap, $\bar{w}_x = w_x/l_x$ is radial size of the BEC scaled by the oscillator length of the trap $l_x = \sqrt{\hbar/(m\omega_x)}$, and $\bar{w}_z = w_z/l_z$ is the corresponding axial quantity. The first terms in brackets on the rhs are the radial energy due to the trap and zero-point kinetic energy, respectively. The next term is the axial trapping energy and the last term is the total interaction energy, being the sum of the s-wave and dipolar contributions. In order to obtain this simple expression for $H_{\rm tot}$ we have expanded $f(\kappa)$ for small κ and retained only the first term. We have also used the quantity $\eta = Na_s/l_z$ which is a key interaction strength parameter known from regular BECs with contact interactions [24]: when η is large the system is in the Thomas-Fermi regime.

Minimising $H_{\rm tot}$ with respect to variations of the condensate radii gives equations for the equilibrium values of these quantities. One finds

$$\lambda\eta^2\left(\varepsilon_{\rm dd}-1\right)^2 = \frac{\pi}{2}\frac{\left(\bar{w}_x^4-1\right)^3}{\bar{w}_x^2} \qquad (30)$$

$$\frac{2}{\sqrt{2\pi}}\eta\left(\varepsilon_{\rm dd}-1\right)\frac{1}{\bar{w}_z} = 1-\bar{w}_x^4. \qquad (31)$$

Solving these equations gives the condensate radii as a function of the various parameters. Figure 5 illustrates the dependence of the radius on the parameter combination $|\eta(\varepsilon_{\rm dd}-1)|\sqrt{\lambda}$. From Figure 5 one sees that, all other things being equal, the radial size increases as the dipolar interaction strength is increased: the cigar becomes fatter. It is useful to note that equations (30) and (31) allow us to

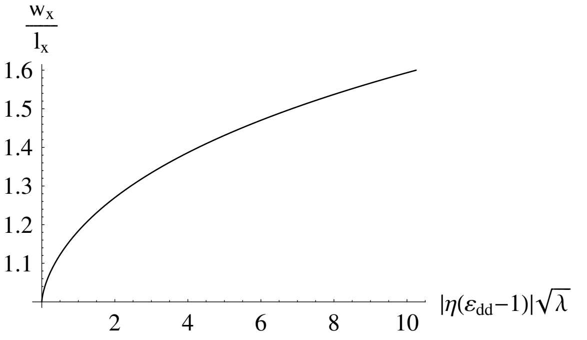

Fig. 5. Dependence of the radial size w_x of a cigar-shaped dipolar condensate in a 3D trap upon the system parameters.

write the total energy functional and the actual chemical potential of the BEC in the trap (defined as $\mu = [H_{\rm kin} + H_{\rm trap} + 2H_s + 2H_{\rm dd}]/N$) solely in terms of the radius

$$\frac{H_{\rm tot}}{N\hbar\omega_x} = \frac{5\bar{w}_x^4 - 1}{4\bar{w}_x^2} \tag{32}$$

$$\frac{\mu}{N\hbar\omega_x} = \frac{7\bar{w}_x^4 - 5}{4\bar{w}_x^2}. \tag{33}$$

The solutions of equations (30) and (31) minimise the total energy functional in the 2D parameter space spanned by the radii $\bar{w}_x$ and $\bar{w}_z$ for particular fixed values of λ, η and $\varepsilon_{\rm dd}$. Providing the minimum is a global one they correspond to the lowest energy solutions one can obtain from *scaling* variations. Perturbations about these equilibrium values should result in stable oscillations which physically correspond to monopole and quadrupole shape oscillations. If, for new values of λ, η and $\varepsilon_{\rm dd}$, the minimum in this $(\bar{w}_x, \bar{w}_z)$ parameter space becomes only a local minimum, or a saddle, then the system is now either only metastable, or unstable, respectively, to scaling perturbations. The roton instability is in principle, however, an independent type of instability due essentially to local density perturbations (phonons) in the same spirit as the instability we first noted in equation (5) for a homogeneous system and developed in Section 5. for an infinite cylinder. Local density perturbations are not captured by the simple $(\bar{w}_x, \bar{w}_z)$ parameter space and so must in general be considered in addition to instabilities arising from scaling perturbations. Scaling instabilities in trapped dipolar gases have been extensively discussed before [1–3,5,10]. Our main purpose here is to highlight the local density instability connected with the roton minimum touching the zero energy axis.

We therefore now wish to calculate how the roton instability point (defined by the roton minimum touching the zero-energy axis) depends upon $\varepsilon_{\rm dd}$ and the value of the chemical potential in a cigar-shaped 3D trap. In Figure 4 we indicate how $\varepsilon_{\rm dd}$ depends on $\bar{\mu}$ at the instability. For the case of a 3D trap $\bar{\mu}$ is not the best quantity to consider since it depends upon the density which is itself a non-trivial function of $\varepsilon_{\rm dd}$ via equations (30, 31). In fact one can show

$$\bar{\mu} = \frac{gn(0)}{\hbar^2/(mw_r^2)} = \frac{4}{\sqrt{\pi}}\frac{\eta}{\bar{w}_z} = 2\sqrt{2}\frac{1-\bar{w}_x^4}{\varepsilon_{\rm dd}-1}. \tag{34}$$

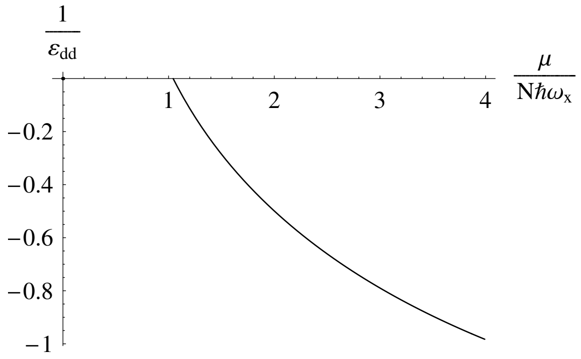

Fig. 6. The critical value of $1/\varepsilon_{\rm dd}$ when the roton minimum touches the zero-energy axis plotted as a function of the chemical potential μ in a very elongated 3D trap.

For the 3D trap we therefore prefer to illustrate the critical value of $\varepsilon_{\rm dd}$ in terms of the true chemical potential in the trap μ, as given by equation (33). The result is shown in Figure 6. In the limit that $1/\varepsilon_{\rm dd} \to 0$ we have the case of a purely dipolar BEC with no s-wave interactions. We find that the limiting value of the chemical potential at this point is $\mu/(N\hbar\omega_x) = 1.043$ and the corresponding value of the condensate radius is $\bar{w}_x = 1.093$. These numbers should only be taken as a qualitative guide rather than quantitatively accurate since the BEC is no longer one dimensional when $\mu/(N\hbar\omega_x) \approx 1$, and the effective 1D potential approximation will begin to break down. In particular, one should include radial excitations in order to give a consistent treatment. This is beyond the scope of this largely illustrative paper, but for a pancake-shaped dipolar BEC such a treatment can be found in [13]. Nevertheless, the very simple treatment given here should give the general picture of what to expect.

7 Conclusion and outlook

A infinite quasi-1D dipolar BEC gas would normally be unstable to local density fluctuations if $\varepsilon_{\rm dd} > 1$ on account of the attractive nature of the dipolar interactions along the axis of the trap. However, by reversing the sign of the dipolar coupling using either a rotating polarizing field for permanent dipoles [5], or a very long wavelength circularly polarized laser beam for electrically induced dipoles, one can obtain a stable quasi-1D system. This configuration has the possibility of a 'roton' minimum in its long-wavelength axial excitation spectrum.

This minimum is tunable via parameters such as the dipolar interaction strength and the density. As is suspected to be the case in helium II, we speculate that the roton minimum could be the precursor of a transition to a density wave. The tunability of dipolar gases means that this phase transition could be explored experimentally when quantum gases with significant dipole-dipole interactions are realized. One of the important features of the 1D system discussed in this paper is that the change in the order parameter between a superfluid and a density wave does not seem to involve any fundamental change of symmetry and so the phase transition could be a smooth one of 2nd order. For a pancake or fully 3D system the change in symmetry is more dramatic and these transitions may not be smooth. We believe considerations such as these make dipolar quantum gases very worthwhile systems to study.

We acknowledge financial support from the EPSRC (UK) and the Marie Curie Programme of the European Commission.

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