2D Dipolar Bosons with Non-zero Tilt Angles

Pengtao Shen and Khandker Quader
Department of Physics, Kent State University, Kent, OH 44242, USA
E-mail: quader@kent.edu

Abstract. Recent experimental advances in creating stable dipolar systems, including polar molecules with large electric dipole moments, have led to vigorous theoretical activities. Here we discuss our work on homogeneous 2D dipolar bosons with dipoles oriented at an angle to the direction perpendicular to the confining 2D plane, i.e. for non-zero tilt angles. Using Bogoliubov-de Gennes equations, we obtain T=0 excitation spectrum of the dipolar Bose gas, and explore instabilities at varying tilt angle, density and dipolar coupling. We map out a phase diagram a function of tilt angle, dipole strength and density. We find the development of maxon-roton behavior leading to roton instabilities at large densities for small tilt angles, and at low densities for large tilt angles. The behavior is anisotropic in k-space; accordingly the roton instabilities occur in the \( k_y \) direction, suggestive of inhomogeneity and stripe phase, with density mode becoming soft in the \( y \) direction. Our results compare favorably with existing Quantum Monte Carlo calculations for non-zero tilt angles.

1. Introduction
In recent years, systems with long-range and anisotropic interaction have generated considerable interest. Among these are dipolar interactions between Bosonic atoms or polar molecules. Examples are \( ^{52}Cr \) \cite{1}, \( ^{87}Rb^{133}Cs \) \cite{2}, \( ^{41}K^{87}Pb \), among which RbCS in particular has sizable electric dipole moment \( \simeq 1.28 \) Debye. In general, the electric dipole moments of the polar molecules are substantially larger than the magnetic dipole moments of atoms. The nature of the dipolar interaction can give rise to novel quantum phases. Experimentally, low dimensional cold gas system has been realized by optical trapping. A recent reporting \cite{3} of observation of roton mode in dipolar system provides added motivation for theoretical exploration. Since applied electric field can be used to fix the orientation of 2D dipoles in a system, one of the degrees of freedom in these systems is the tilt angle fixed by the direction of the applied electric field. Much of the work on quasi 2D and other 2D Bose systems has been done for zero tilt angle \cite{4, 5}, except for Quantum Monte Carlo (QMC) calculations \cite{6, 7} on 2D bosons.

While it is possible to realize various kinds of low dimensional systems, here we focus on homogeneous 2D Bose gas at zero temperature, for arbitrary tilt angles. Among our objectives is to test how well mean-field calculations such Hartree-Fock-Bogoliubov (HFB) compare with the findings of QMC calculations. As a background for our work, we first review the Hartree Fock Bogoliubov (HFB) theory in the next section.
2. Background: Hartree Fock Bogoliubov (HFB) theory

The grand canonical Hamiltonian of the interacting Bose gas is given by:

$$\hat{K} \equiv \hat{H} - \mu \hat{N} = \int dr \hat{\psi}^\dagger(r) \left[ -\frac{\nabla^2}{2m} + U_{ex}(r) - \mu \right] \hat{\psi}(r)$$

$$+ \frac{1}{2} \int dr dr' \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r') V(r - r') \hat{\psi}(r) \hat{\psi}(r')$$  \hspace{1cm} (1)

where \(\hat{\psi}(r)\) is the annihilation Bose field operator. The field operator is expanded as: \(\hat{\psi}(r) = \phi_0(r) + \tilde{\psi}(r)\), with \(\phi_0(r) = \langle \hat{\psi}(r) \rangle\) being the condensate wave function and \(\tilde{\psi}(r) = \hat{\psi}(r) - \phi_0(r)\) the fluctuation from the condensate. Substituting the expansion into Eq.(1), the grand canonical Hamiltonian \(\hat{K}\) can be expanded in orders of \(\tilde{\psi}\).

In Bogoliubov approximation, the expansion is taken up to second order of \(\tilde{\psi}\). \(K = K_0 + K_1 + K_2\), where

$$\hat{K}_0 = \int dr \phi_0^\dagger(r) \left[ -\frac{\nabla^2}{2m} + U_{ex}(r) - \mu \right] \phi_0(r)$$  \hspace{1cm} (2)

$$\hat{K}_1 = \int dr \phi_0^\dagger(r) \left[ -\frac{\nabla^2}{2m} + U_{ex}(r) - \mu \right] \tilde{\psi}(r)$$

$$+ \int dr \tilde{\psi}^\dagger(r) \left[ -\frac{\nabla^2}{2m} + U_{ex}(r) - \mu \right] \phi_0(r)$$

$$+ \int dr dr' [\phi_0(r')]^2 \phi_0^\dagger(r) V(r - r') \tilde{\psi}(r)$$

$$+ \int dr dr' [\phi_0(r')]^2 \tilde{\psi}^\dagger(r) V(r - r') \phi_0(r)$$  \hspace{1cm} (3)

$$\hat{K}_2 = \int dr \tilde{\psi}^\dagger(r) \left[ -\frac{\nabla^2}{2m} + U_{ex}(r) - \mu \right] \tilde{\psi}(r)$$

$$+ \int dr dr' [\phi_0(r')]^2 \tilde{\psi}^\dagger(r) V(r - r') \tilde{\psi}(r)$$

$$+ \int dr dr' \phi_0^\dagger(r) \phi_0(r') \tilde{\psi}^\dagger(r') V(r - r') \tilde{\psi}(r)$$

$$+ \frac{1}{2} \int dr dr' [\phi_0(r')]^2 \tilde{\psi}^\dagger(r) \tilde{\psi}(r') V(r - r') \phi_0(r)$$

$$+ \frac{1}{2} \int dr dr' \phi_0^\dagger(r) \phi_0(r') V(r - r') \tilde{\psi}(r) \tilde{\psi}(r')$$  \hspace{1cm} (4)

\(K_1\) has to vanish so as to minimize the grand canonical Hamiltonian, so one obtains the equation

$$\left[ -\frac{\nabla^2}{2m} + U_{ex}(r) + \int dr' [\phi_0(r')]^2 V(r - r') \right] \phi_0(r) = \mu \phi_0(r)$$  \hspace{1cm} (5)

This is the generalized Gross-Pitaevskii equation, which gives the condensate wave function \(\phi_0(r)\).
Combining $K_0$ and $K_2$, and defining $T(r) = -\frac{\nabla^2}{2m} + U_{ex}(r) - \mu$, one obtains the Hartree-Fock-Bogoliubov (HFB) Hamiltonian:

$$\hat{K}_{HFB} = \int dr \phi_0^*(r)T(r)\phi_0(r) + \int dr \bar{\psi}^\dagger(r)\psi(r) + \int dr dr' |\phi_0(r')|^2 \bar{\psi}^\dagger(r)V(r-r')\psi(r) + \int dr dr' \phi_0^*(r)\phi_0(r')\bar{\psi}^\dagger(r')V(r-r')\psi(r) + \frac{1}{2} \int dr dr' \phi_0^*(r)\phi_0(r')V(r-r')\bar{\psi}(r)\psi(r') + \frac{1}{2} \int dr dr' \phi_0^*(r)\phi_0(r')V(r-r')\bar{\psi}(r)\psi(r') \quad (6)$$

Bogoliubov transformation $\bar{\psi}(r) = \sum [u_i(r)\hat{a}_i - v_i^*(r)\hat{a}_i^\dagger]$ diagonalizes the Hamiltonian, with $u_i(r)$ and $v_i(r)$ satisfying the equation

$$\varepsilon_j u_j(r) = (\bar{T}(r) + \int dr' |\phi_0(r')|^2 V(r-r'))u_j(r) + \int dr' V(r-r')\phi_0^*(r)\phi_0(r')u_j(r') + \int dr' \phi_0^*(r)\phi_0(r')V(r-r')u_j(r') \quad (7)$$

$$-\varepsilon_j v_j(r) = (\bar{T}(r) + \int dr' |\phi_0(r')|^2 V(r-r'))v_j(r) + \int dr' V(r-r')\phi_0^*(r)\phi_0(r')v_j(r') + \int dr' \phi_0^*(r)\phi_0(r')V(r-r')v_j(r') \quad (8)$$

In homogenous case, $U_{ex}(r) = 0$; the ground state is $\phi_0(r) = 0$; the condensate density is $\int dr \phi_0^2(r) = n_0$; and $\mu = \int dr' |\phi_0(r')|^2 V(r-r') = n_0 V(q)$. The Bogoliubov transform of the fluctuation is $\bar{\psi}(r) = \sum [e^{-iqr}\hat{a}_q - e^{iqr}\hat{a}_q^\dagger]$ Substituting $\bar{\psi}(r)$ into Eq.(7) and Eq.(8), and Fourier transforming $V(r-r')$, one obtains

$$\varepsilon_q e^{-iqr} = (q^2/2m + V(q)n_0)e^{-iqr} + V(q)n_0 e^{iqr}$$

$$-\varepsilon_q e^{iqr} = (q^2/2m + V(q)n_0)e^{iqr} + V(q)n_0 e^{-iqr} \quad (9)$$

This gives the Bogoliubov spectrum

$$\varepsilon(q) = \sqrt{(q^2/2m)^2 + n_0 V(q) q^2/m} \quad (10)$$

An equivalent result can be derived in the random phase approximation (RPA) approach. If in the Hartree approximation the density-density response is $\chi_0(k, w)$, then the RPA response function is given by:

$$\chi_{RPA}(k, w) = \frac{\chi_0(k, w)}{1 - V_k \chi_0(k, w)} \quad (11)$$
For a free boson system with condensation, and \( n_0 \approx n \),
\[
\chi_0(k, w) = \frac{n_0}{\hbar w - \epsilon_k} - \frac{n_0}{\hbar w + \epsilon_k}
\]
(12)
where \( n_0 \) is the condensate density, and \( \epsilon_k = \hbar^2 k^2 / 2m \) is the free particle kinetic energy. Substitute Eq.(12) into Eq.(11), one can obtain the density-density response function of the interacting boson system with a condensate,
\[
\chi_0(k, w) = \frac{2n_0\epsilon_k}{\hbar^2 w^2 - \epsilon_k^2 - 2n_0 V_k \epsilon_k}
\]
(13)
The pole of the above equation, \( \hbar w = \sqrt{\epsilon_k^2 + 2n_0 V_k \epsilon_k} \), is exactly the Bogoliubov spectrum obtained we in Eq.(10).

3. Dipolar Bosons in 2 dimension
Consider a homogenous system of dipolar bosons in XY plane with tilt angle \( \theta \) which is confined by a harmonic trap in z direction. The projection of the dipole is in x direction.

The 2D dipole-dipole interaction is:
\[
V_{2d}(r) = \frac{d^2}{r^3}(1 - 3\sin^2 \theta \cos^2 \phi)
\]
\[
= \frac{d^2}{r^3}[P_2(\cos \theta) - \frac{3}{2}\sin^2 \theta \cos 2\phi]
\]
(14)
where \( \phi \) is the azimuthal angle relative to x direction, \( \theta \) the tilt angle, and \( d \) strength of the dipolar interaction. The Fourier transform of 2D dipole interaction in momentum space is:
\[
V(q) = \int_0^\infty d^2r V(r)e^{iqr}
\]
(15)
The 2D integral however is divergent in the limit \( r \to 0 \). One way to regularize [8] this is to introduce a short-range cut-off, \( r_c \) in the Fourier transform. The choice of a value for \( r_c \) can be motivated in the case of polar molecules, at least, by taking \( r_c \) to be of the order of the size of the molecule. It typically would be of the order of several Bohr radius, \( a_0 \). Performing the integral \( \int_{r_c}^\infty \), the 2D dipole-dipole interaction (DDI) in momentum space can be written as \( V(q) = V_s + V_l(q) \), with
\[ V_s = 2\pi d^2 \frac{P_2(\cos \theta)}{r_c} \]
\[ V_l(q) = -2\pi d^2 q(\cos^2 \theta - \sin^2 \theta \cos^2 \phi) \]

The short range part of the interaction \( V_s \) depend on the tilt angle \( \theta \): \( V_s \) is positive at small \( \theta \) and becomes negative at large \( \theta \). The long range term, \( V_l(q) \) has linear \( q \) dependence. At zero tilt angle, \( V_l(q) \) is isotropic and negative in all direction. For non-zero tilt angle, \( V_l(q) \) become anisotropic. In x direction, \( V_l(q) \) gets less negative and becomes positive when \( \theta > \pi/4 \). In y direction, it is always negative. As will be seen, interesting consequences of 2D DDI, viz. instabilities of the system, happen when the DDI gets attractive in some direction. Hence, it is most interesting to consider the behavior in the y direction, i.e. \( \phi = \pi/2 \), when the DDI is most attractive. Following standard practice, we define the dipolar interaction length \( a_{dd} = \frac{\hbar^2}{m} \). \( a_{dd} \) can vary from 10\( a_0 \) for magnetic dipoles to 10\(^4\)\( a_0 \) for electric dipoles. On scaling with \( a_{dd} \), we obtain

\[ V(q, \phi) = 2\pi d^2 \left[ \frac{P_2(\cos \theta)}{r_c} - q(\cos^2 \theta - \sin^2 \theta \cos^2 \phi) \right] \]
\[ = 2\pi \frac{\hbar^2}{m} \left[ \frac{a_{dd}}{r_c} P_2(\cos \theta) - q a_{dd}(\cos^2 \theta - \sin^2 \theta \cos^2 \phi) \right] \]
\[ V(q, \phi = \pi/2) = 2\pi d^2 \left[ \frac{P_2(\cos \theta)}{r_c} - q \cos^2 \theta \right] \]
\[ = 2\pi \frac{\hbar^2}{m} \left[ \frac{a_{dd}}{r_c} P_2(\cos \theta) - q a_{dd} \cos^2 \theta \right] \] (17)

4. Spectrum and Stability

Using Eq.(10) in Eq.(16), we can immediately obtain the HFB spectrum. On scaling with the dipolar strength \( a_{dd} \), \( \bar{\varepsilon} = \varepsilon / \bar{m} a_{dd} \), \( \tilde{q} = q a_{dd} \) and \( \tilde{n} = n_0 a_{dd}^2 \), we obtain a spectrum with dimensionless energy and momentum:

\[ \bar{\varepsilon}(\tilde{q}, \phi) = \sqrt{\frac{\tilde{q}^4}{4} + 2\pi \tilde{q}^2 \tilde{n} \left[ \frac{a_{dd}}{r_c} P_2(\cos \theta) - \tilde{q}(\cos^2 \theta - \sin^2 \theta \cos^2 \phi) \right]} \] (18)

The spectrum is anisotropic and spectrum energy in y direction is lower than any other direction.

\[ \bar{\varepsilon}(\tilde{q}, \phi = \pi/2) = \sqrt{\frac{\tilde{q}^4}{4} + 2\pi \tilde{q}^2 \tilde{n} \left[ \frac{a_{dd}}{r_c} P_2(\cos \theta) - \tilde{q} \cos^2 \theta \right]} \] (19)

We can now study the stability of the 2D dipolar Bose gas by considering the above expression for the spectrum.

A. \( \theta < \cos^{-1} \frac{1}{\sqrt{3}} \)

For \( \theta < \cos^{-1} \frac{1}{\sqrt{3}} \approx 0.955 \), the short range interaction is positive and the long range part in y direction is negative. The spectrum is always real and positive at small momentum; see Fig. 2. However, at sufficiently large density, \( n \), a roton-maxon characteristic, reminiscent of that in \(^4\)He, develops in the spectrum. For even larger density, the roton spectra becomes imaginary.
in y direction; this can be seen as “holes” at symmetric ±q region in the 3D plot in Fig. 3; the “holes” signifying that the energy ε is no longer real. The corresponding 2D plot depicts this feature as negative energy for φ = π/2, i.e. the y-direction. At the same time, the spectra in the x-direction remain real, positive. This means the existence of density waves along one direction and not along that perpendicular to it. This can then be taken to imply a transition of the BEC phase to a stripe phase.

B. θ > cos⁻¹ 1/√3

For θ > cos⁻¹ 1/√3 = 0.955, the short range interaction become negative, and as a consequence, the spectrum is imaginary at small momentum. So, the system has long-wavelength (q → 0) instability and hence a collapse of the BEC phase.

![Figure 2](image)

**Figure 2.** Figure showing the spectrum of dipolar Boson with tilt angle θ = 0.4 at scaled density \( \tilde{n} = 100 \). \( a_{dd} \) is taken to be \( 10^4 a_0 \), and \( r_c = 10 a_0 \).

![Figure 3](image)

**Figure 3.** Figure showing the spectrum of dipolar Boson with tilt angle θ = 0.4 at scaled density \( \tilde{n} = 200 \), \( a_{dd} \) is taken to be \( 10^4 a_0 \), and \( r_c = 10 a_0 \).

The set of figures in Fig. 4 are meant to show variation of the energy spectrum \( (\epsilon^2) \) vs \( q_y \) with tilt angle θ, and density n. Variation with respect to density are shown for fixed θ = 0, 0.4, 0.6, 0.9. The last plot in Fig. 4 shows the spectrum for θ = 1.0, which is beyond the critical \( \theta_c = 0.955 \), and hence shows phonon instability. In each of the other figures, with increasing density, the roton minimum deepens till at sufficiently large density, the frequency becomes imaginary, shown as negative \( \epsilon^2 \) in the plots.
5. Phase Diagram
We combine our results above for various tilt angles and densities to obtain a density vs tilt angle phase diagram for a homogeneous 2D dipolar boson system at zero temperature; this is shown as the left side figure in Fig 5. Since one of our goals was to see how a mean-field description compares with Quantum Monte Carlo calculation for a homogeneous 2D Bose gas subject to DDI, on the right hand plot we show phase diagram obtained from a QMC calculation [7]. It is interesting that some of the key features of the QMC phase diagram are captured in our HFB calculation. While the general phase boundary of the BEC phase, the collapse and the stripe phases are in qualitative agreement with the QMC result, we are not able to obtain the solid phase within our HFB approximation; we find the existence of density wave/stripes in the region of the QMC solid phase of high density and smallish tilt angle.

We note that our calculations are done under the assumption that the condensate density \( n_0 \approx n \), which implies that the depletion from the condensate is small. Given that, we have attempted to describe the effect of a finite-range anisotropic dipole-dipole interaction in 2D, by exploring the effect of non-zero tilt angles. Our calculations and results show that in the relatively weakly interacting regime, the roton instability does not occur, and the uniform condensate is stable. As we approach the roton instability as a function of tilt angle \( \theta \) and also...
Figure 5. Scaled density vs tilt angle phase diagram. The left figure is based on our calculation; the right figure is reproduced from Ref. [7]. $\theta$ and $\alpha$ refer to tilt angle discussed in text. In our calculation, critical $\theta$ is determined from $q$-space consideration ($2D$ Fourier-transformed $V(q)$); in Monte-Carlo calculations it is determined from $r$-space $V(r)$. We have chosen $a_{dd}$ to be $10^4a_0$, and $r_c = 10a_0$.

For large enough densities, depletion will start to increase, and at roton instability, depletion will become significant enough that the uniform condensate may not be sustainable. Since the dipolar interaction is anisotropic, it becomes attractive for some direction first, prior to becoming attractive in other directions. In our 2D case with non-zero tilt angle, this occurs first in the $y$-direction. Roton instability at finite momentum results in standing wave. The system exhibits density wave modulations in that direction, resulting in a "stripe phase" behavior.

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