Microscopic Description of Anisotropic Quantum Bose Dipoles in 2D

A. Macia, F. Mazzanti, J. Boronat
in collaboration with R.E. Zillich, D. Hufnagl and G.E. Astrakharchik

Departament de Física i Enginyeria Nuclear
Universitat Politècnica de Catalunya
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Outline

- The dipolar interaction
- Low density regime and universal properties
  - Building a trial wave function
- High density regime and the effect of the anisotropy
  - Density Response Function
  - The phase diagram
The Dipolar Interaction

The general form of the interacting potential between two dipoles \( p_1 \) and \( p_2 \) is

\[
V_{dd}(\mathbf{r}) = \frac{C_{dd}}{4\pi} \left[ \hat{p}_1 \cdot \hat{p}_2 - \frac{3(\hat{p}_1 \cdot \mathbf{r})(\hat{p}_1 \cdot \mathbf{r})}{r^3} \right]
\]

There are 2 types of dipolar interactions:

- **Magnetic dipoles**: Typical example: \(^{52}\text{Cr}\)
- **Electric dipoles**: Essentially polar molecules

<table>
<thead>
<tr>
<th>Species</th>
<th>Dipole moment</th>
<th>( a_{dd} )</th>
<th>( \varepsilon_{dd} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{87}\text{Rb})</td>
<td>( 1.0 \mu_B )</td>
<td>0.7 ( a_0 )</td>
<td>0.007</td>
</tr>
<tr>
<td>(^{52}\text{Cr})</td>
<td>( 6.0 \mu_B )</td>
<td>16 ( a_0 )</td>
<td>0.16</td>
</tr>
<tr>
<td>KRb</td>
<td>0.6 D</td>
<td>( 2.0 \times 10^3 a_0 )</td>
<td>20</td>
</tr>
<tr>
<td>ND(_3)</td>
<td>1.5 D</td>
<td>( 3.6 \times 10^3 a_0 )</td>
<td>36</td>
</tr>
<tr>
<td>HCN</td>
<td>3.0 D</td>
<td>( 2.4 \times 10^4 a_0 )</td>
<td>240</td>
</tr>
</tbody>
</table>

\( C_{dd} = \mu_0 \mu^2 \)
\( C_{dd} = d^2/\varepsilon_0 \)

\( a_{dd} = \frac{mC_{dd}}{12\pi \hbar^2} \quad : \text{dipolar length} \)

What really matters is the ratio of dipolar to contact lengths:

\( \varepsilon_{dd} = \frac{a_{dd}}{a} \)

The Dipolar Interaction

The general form of the interacting potential between two dipoles \( p_1 \) and \( p_2 \) is

\[
V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi} \left[ \hat{p}_1 \cdot \hat{p}_2 - 3(\hat{p}_1 \cdot \hat{r})(\hat{p}_1 \cdot \hat{r}) \right]
\]

Interaction Features:

- **Long ranged** compared to common interactions in Condensed Matter which typically have Van der Waals tails

\[
\text{Dipolar : } V_{dd}(r \to \infty) \approx \frac{1}{r^3} \quad \text{Van der Waals : } V(r \to \infty) \approx \frac{1}{r^6}
\]

- Diverges at the origin as \( 1/r^3 \) at \( r=0 \)

Not realistic as in real systems the complete interaction has an additional standard Lenard-Jones-like potential with an infinitely repulsive Hard Core near the origin
It is anisotropic

Simple Cases:

- Repulsion: $\frac{1}{r^3}$
- Attraction: $\frac{1}{r^3}$

Twice as attractive: $-\frac{2}{r^3}$

Twice as repulsive: $\frac{2}{r^3}$
It is anisotropic and depends on the dimensionality of the space. Assuming a fully polarized system:

**In 3D**

\[ V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi} \left[ 1 - 3 \cos^2 \theta \right] \frac{1}{r^3} \]

**In 1D**

Different pairs have different angles \( \theta \) and the interaction varies with the angle and the distance. Critical angle \( \theta_c = 54^\circ 7 \)

\[ V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi} \left[ 1 - 3 \sin^2 \theta \right] \frac{1}{r^3} \]

Very similar expression to the 3D case. But a very important difference!

For fixed polarization angle \( \theta \), \( 1 - 3 \cos^2 \theta \) is a constant. This acts as a renormalization of \( C_{dd} \) and the system behaves as if all dipoles were polarized perpendicularly to the line. Critical angle \( \theta_c = 35^\circ 3 \)
In 2D

\[ V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi} \left[ \frac{1 - 3\lambda^2 \cos^2 \theta}{r^3} \right] \]

Looks similar to the 3D case but it is in fact different

\( \{r, \theta\} \) are IN PLANE spherical coordinates

\[ \lambda = \sin \alpha \quad \alpha : \text{Polarization angle} \]

Now for a polarized system, \( \lambda \) becomes a constant.

We can then use \( \lambda \) as an expansion parameter to see how the anisotropy enters in the wave function of the system.

The interaction \( V_{dd}(r) \) depends on \( \lambda \) and the system properties change when \( \lambda \) varies. The special case \( \lambda = 0 \) is the simplest to analyze and we take it as the reference case to start with.
The Dipolar Interaction

The dipolar coupling is much higher in the electric case

\[ \frac{\mu_0 \mu^2}{d^2/\varepsilon_0} \sim \frac{1}{4} \alpha^2 \sim 10^{-5} \]

\( \alpha \): fine structure constant

It is clearly possible to see dipolar effects! \(^{52}\text{Cr}\) close to a Feshbach resonance

\[ a = a_{bg} \left( 1 - \frac{\Delta}{B - B_0} \right) \]

\( a_{bg} \): background scattering length
\( B_0 \): resonance magnetic field
\( \Delta \): resonance width

\[ a \to 0 \text{ when } B \to B_0 + \Delta \]

Dipolar effects are then enhanced

\[ \Delta \sim 1.7 \text{G} \]
\[ B_0 = 589 \text{ G} \]

T. Lahaye et al.
Tuning the Interaction in magnetic systems

**Magnetic dipoles:** external fields allow tuning the strength and sign of the dipolar interaction

A static field in the z direction together with a fast rotating field in the XY plane induce a dipolar moment

\[
d(t) = p \left[ \hat{e}_z \cos \phi + \left( \hat{e}_x \cos(\Omega t) + \hat{e}_y \sin(\Omega t) \right) \right] \sin \phi
\]

with \( \phi \) determined by the ratio of the amplitudes of the static and rotating fields.

When \( \Omega \) is large enough, particles feel an average interaction

\[
\langle V_d(r) \rangle = \frac{p^2}{r^3} \left( 1 - 3 \cos^2 \theta \right) a(\phi)
\]

This technique allows reversal of the sign in the dipole-dipole interaction as well as its cancellation at the critical angle

\[\cos^2 \phi_c = 1/3 \quad \rightarrow \quad 54.7^\circ\]
Tuning the Interaction in electric systems

**Electric dipoles:** mostly talking about polar molecules.

Electric fields mix internal rotational states of the molecule and that induces a new electric moment that varies with the field. These can be very large!

\[
H = \sum_{i=1}^{N} \left[ \frac{\mathbf{p}_i^2}{2m} + V_{\text{trap}}(\mathbf{r}_i) + H_{\text{int}}^{(i)} - \mathbf{d}_i \cdot \mathbf{E} \right] + \sum_{i<j} V_{d\!d}(\mathbf{r}_i - \mathbf{r}_j)
\]

External fields mix internal rotational states that increase \( \mathbf{d}_i \)
and that in turn enhances \( V_{d\!d}(\mathbf{r}) \)

The effective potential creates an attractive component at short distances that induces collapse in head-to-tail configurations.

**Solution:** tightly trap along the Z direction.
Weakly Interacting Systems and Universal Regime

Dilute systems are dominated by two-body correlations.
System in gaseous phase

**Mean interparticle distance**

\[
d = \rho^{-1/3} \text{ large}
\]

**Low-Energy two-body processes**

\[
E = \frac{\hbar^2 k^2}{2m} \rightarrow \tan \delta_l(k) \sim k^{2l+1}
\]

only s-wave scattering (l=0)

\[
\cot \delta_l = -\frac{1}{ka} + \frac{1}{2}kr_0 + \cdots
\]

\(a = \text{scattering length}\)

only the s-wave scattering length is relevant when \(ka \to 0\)

Universal Regime at \(T=0\):

\[
x = \rho a^3 \to 0 \quad ka \to 0
\]

...but what about dipoles, with a (nearly, in 2D) long-range interactions?
**Diffusion Monte Carlo**

Schrödinger Eq. in imaginary time for the *mixed* distribution \( f(R; \tau) = \psi_T(R)\Psi(R; \tau) \) with: \( \psi_T = \) variational wave function used for Importance Sampling

\[
- \frac{\partial f(R; \tau)}{\partial \tau} = - \frac{\hbar^2}{2m} \nabla^2 f(R; \tau) + \frac{\hbar^2}{2m} \vec{\nabla} \left( \vec{F} f(R; \tau) \right) + [E_L(R) - f(R; \tau)] f(R, \tau)
\]

**A₁**: isotropic diffusion  
**A₂**: Drift term  
**A₃**: Branching term

\[
- \frac{\partial}{\partial \tau} f(R; \tau) = [A_1 + A_2 + A_3] f(R; \tau)
\]

**Formal solution**:  
\[
f(R; \tau + \Delta \tau) = \int dR' G(R, R'; \tau) f(R'; \tau)
\]

\[
\rightarrow G(R, R'; \tau) = \langle R | e^{-H\Delta \tau} | R' \rangle = 2\text{nd. order Chin approx.}
\]

Repeated iteration of this scheme finally yields \( f(R; \tau \rightarrow \infty) \rightarrow \psi_T(R)\Psi_0(R) \)

\[
\rightarrow \text{We NEED a GOOD trial wave function for this scheme to work well}
\]
The 2-body problem

The Hamiltonian for the relative motion of two dipoles becomes

\[ H = -\frac{\hbar^2}{2\mu r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{\hat{L}^2}{2\mu r^2} + \frac{C_{dd}}{4\pi} \left[ \frac{1 - 3\lambda^2 \cos^2 \theta}{r^3} \right] \]

written in terms of the angular momentum operator and its orthogonal basis

\[ \hat{L}^2 = -\hbar^2 \frac{\partial^2}{\partial \theta^2} \]

The eigenstates of H can be expanded in that basis

\[ \Psi_0(\vec{r}) = \sum_{m=0}^{\infty} \varphi_m(r) \cos(m\theta) \]

However:

\[ [\hat{H}, \hat{L}^2] \neq 0 \]

Parity symmetry considerations under \( \vec{r} \rightarrow -\vec{r} \) rule out modes

**BOSONS:** \( \hat{P}\Psi_0 = +\Psi_0 \)

**Odd modes:** FERMIONS

\[ \Psi_0(\vec{r}) = \sum_{m=0}^{\infty} \varphi_m(r) \cos(m\theta) \]

**Even modes:** BOSONS

only **EVEN** modes

\[ m = 0, 2, 4, \ldots \]
Solution of the Zero Energy Two-Body problem

Expand the wave function in partial waves

Each separate mode satisfies the equation

Finally rearrange terms to find the following Modified Bessel’s Equation with general solution

Boundary condition

1/r^3 diverges at r=0 and the contribution to the potential energy would diverge

Boundary condition

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General Anisotropic case ($\lambda \neq 0$)

Separate explicitly the anisotropic part of the interaction

$$-
\n\nabla^2 \Psi + \left[ \frac{1 - 3\lambda^2 \cos^2 \theta}{r^3} \right] \Psi = 0 \quad \rightarrow \quad -\n\n\nabla^2 \Psi + \frac{1}{r^3} \Psi = \frac{3\lambda^2 \cos^2 \theta}{r^3} \Psi$$

and solve

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + \Psi_p(\vec{r})$$

Particular solution

Homogeneous: ($\lambda = 0$) solution

The homogeneous problem is isotropic and so we know

$$\Psi_h(\vec{r}) = K_0 \left( \frac{2}{\sqrt{r}} \right)$$

The particular solution can be built from the exact Green's function, and the complete solution of the problem becomes

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + 3\lambda^2 \int d\vec{s}_1 \, G(\vec{r}, \vec{s}_1) \frac{\cos^2 \theta_1}{s_1^{13}} \Psi(\vec{s}_1)$$

and solve by iteration to get the different orders in $\lambda^2$

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + 3\lambda^2 \int d\vec{s}_1 \, G(\vec{r}, \vec{s}_1) \frac{\cos^2 \theta_1}{s_1^{13}} \Psi_h(\vec{s}_1) +$$

$$+ (3\lambda^2)^2 \int d\vec{s}_1 \int d\vec{s}_2 \, G(\vec{r}, \vec{s}_1) G(\vec{s}_1, \vec{s}_2) \frac{\cos^2 \theta_1}{s_1^{13}} \frac{\cos^2 \theta_2}{s_2^{13}} \Psi_h(\vec{s}_2) + \cdots$$
General Anisotropic case ($\lambda \neq 0$)

The Green’s function is the solution of the problem

$$\left[ -\nabla^2 + V_{dd}(\vec{r}) \right] G(\vec{r}, \vec{s}) = -\delta(\vec{r} - \vec{s})$$

and we expand it in partial waves

$$G(\vec{r}, \vec{r}) = \frac{1}{2\pi} g_0(r, r') + \frac{1}{\pi} \sum_{m=1}^{\infty} g_m(r, r') \cos [m(\theta - \theta')]$$

where $g_m(r, r')$ is the Green’s function of each separate mode, which reads

$$g_m(r, s) = \begin{cases} 2 K_{2m} \left( \frac{2}{\sqrt{r}} \right) I_{2m} \left( \frac{2}{\sqrt{s}} \right) & \text{if } r < s \\ 2 I_{2m} \left( \frac{2}{\sqrt{r}} \right) I_{2m} \left( \frac{2}{\sqrt{s}} \right) & \text{if } r > s \end{cases}$$

Upon substitution on the expression of the solution one can see how the different modes couple with increasing orders in $\lambda$

$$\Psi(\vec{r}) = \Psi_n(\vec{r}) + 3\lambda^2 \int d\vec{r} \frac{\cos^2 \theta'}{r'^3} \left[ \frac{1}{2\pi} g_0(r, r') + \frac{1}{\pi} \sum_{m=1}^{\infty} g_m(r, r') \cos [m(\theta - \theta')] \right] \Psi(\vec{r}')$$
General Anisotropic case ($\lambda \neq 0$)

How does the coupling between different modes appears? We can see this looking at the lowest order in $\lambda^2$

Order $\lambda^0$: only $m=0$ (isotropic)

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) = K_0 \left( \frac{2}{\sqrt{r}} \right)$$

Order $\lambda^2$: the coupling induces the coupling to the $m=2$ mode

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + 3\lambda^2 \int d\vec{r}^{\prime} \frac{\cos^2 \theta^\prime}{r^{\prime} 3} \left[ \frac{1}{2\pi} g_0(r, r^{\prime}) + \frac{1}{\pi} \sum_{m=1}^{\infty} g_m(r, r^{\prime}) \cos \left[ m \left( \theta - \theta^{\prime} \right) \right] \right] \Psi_h(\vec{r}^{\prime})$$

developing

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + \frac{3\lambda^2}{2} \int d\vec{r}^{\prime} \frac{1 + \cos(2\theta^\prime)}{r^{\prime} 3} \left[ \frac{1}{2\pi} g_0(r, r^{\prime}) + \frac{1}{\pi} \sum_{m=1}^{\infty} g_m(r, r^{\prime}) \cos \left[ m \left( \theta - \theta^{\prime} \right) \right] \right] \Psi_h(\vec{r}^{\prime})$$

$$m = 0$$

$$m = 2$$
General Anisotropic case ($\lambda \neq 0$)

In this way to order $\lambda^2$ the wave function couples the $m=0$ mode to $m=0$ and $m=2$

$$\Psi(\vec{r}) = \psi_{00}(r) + \lambda^2 \left[ \psi_{02}(r) + \psi_{22}(r) \right] \cos(2\theta)$$

Plug it back into the general equation and obtain the contribution to order $\lambda^4$

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + \frac{3\lambda^2}{2} \int d\vec{r}' \frac{1 + \cos(2\theta')}{r'^3} \left[ \frac{1}{2\pi} g_0(r, r') + \frac{1}{\pi} \sum_{m=1}^{\infty} g_m(r, r') \cos [m (\theta - \theta')] \right] \Psi(\vec{r}')$$

two cosine terms couple state $m$ to states $m$

$$\begin{align*}
\lambda^0 & : \psi_{00}(r) \\
\lambda^2 & : \psi_{02}(r), \psi_{22}(r) \\
\lambda^4 & : \psi_{04}(r), \psi_{24}(r) \\
\lambda^6 & : \psi_{06}(r), \psi_{26}(r), \psi_{44}(r), \psi_{46}(r), \psi_{66}(r)
\end{align*}$$

three cosine terms couple state $m$ to states $m \pm 2$

coupling scheme
Contribution of the different modes

The anisotropy is there, but the coupling to modes $m \geq 4$ is very weak.
Scattering length

The exact Schrödinger equation for the m=0 mode $\psi_0(r)$ reads

$$-\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \psi_0(r)}{\partial r} \right) + \frac{1}{r^3} \psi_0(r) = \frac{3\lambda^2}{2r^3} \left[ \psi_0(r) + \psi_2(r) \right]$$

At large distance $r \gg 1$ we know $\psi_0(r) \gg \psi_2(r)$ and therefore the previous equation is well approximated by

$$-\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \psi_0(r)}{\partial r} \right) + \frac{1}{r^3} \left( 1 - \frac{3\lambda^2}{2} \right) \psi_0(r) = 0$$

Change variables $x = r/(1 - 3\lambda^2/2)$ to find

$$-\frac{1}{x} \frac{\partial}{\partial x} \left( x \frac{\partial \psi_0(x)}{\partial x} \right) + \frac{1}{x^3} \psi_0(x) = 0 \quad \text{same as } \lambda = 0 !$$

so the solution at large distances reads

$$\varphi_0(r) \approx K_0 \left( 2 \sqrt{\frac{1 - 3\lambda^2/2}{r}} \right) \approx \frac{1}{2} \ln \left( \frac{r}{a_\lambda} \right)$$

Scattering length

$$a_\lambda = e^{2\gamma} \left( 1 - \frac{3\lambda^2}{2} \right)$$
Scattering length as a function of the polarization angle $\lambda = \sin(\alpha)$

Exact result for $\lambda = 0$

$$a(\lambda = 0) = e^{2\gamma} \sim 3.17$$

Approximation for $\lambda \neq 0$

$$a(\lambda) = a(0) \left(1 - \frac{3\lambda^2}{2}\right)$$
The Many-Body problem

**Many-Body Hamiltonian**

\[
H = -\frac{1}{2} \sum_{j=1}^{N} \nabla_j^2 + \sum_{i<j} \frac{1 - 3\lambda^2 \cos^2 \theta_{ij}}{r_{ij}^3}
\]

Isotropic interactions at low densities follow a universal curve describing the energy per particle as a function of the gas parameter \( x = na^2 \)

\[
\left( \frac{2ma^2}{\hbar^2} \right) \left( \frac{E}{N} \right) = \frac{4\pi x}{|\ln(x)|} \left[ 1 + O(\ln(x)) \right]
\]

In isotropic systems and for a given interaction, \( a=\text{cte.} \) and the density fixes the value of the gas parameter \( x \).

In the anisotropic dipolar case considered, a given value of \( x \) can be obtained from different densities and polarization angles since \( a = a(\lambda) \)

\[
a_{\lambda} = e^{2\gamma} \left( 1 - \frac{3\lambda^2}{2} \right)
\]

Keeping \( x \) fixed and varying \( \lambda \) means varying the density accordingly

Many-Body energies can be obtained by means of variational methods (HNC, VMC) or exact ones (DMC)
The Many-Body problem

Two-Body wave function compared with optimal HNC/0 Jastrow factor

**Optimal HNC**

\[ \Psi = \prod_{i<j} f(\vec{r}_{ij}) \]

\[ \frac{\delta E}{\delta f} = 0 \]

**Phonons in 2D**

\[ f(r) = e^{u_2(r)} \]

\[ u_2(r) = -\frac{c}{r} \]

\[ \alpha = 0.6 \]

\[ \chi = 0.01 \]
The Many-Body problem

Universal Energy per particle.
Scaled energies

\[ \tilde{E} = \left( \frac{2ma^2}{\hbar^2} \right) \left( \frac{E}{N} \right) \]

Pair Distribution Function

Low densities
Universal regime

Intermediate densities
Microscopic Description of Anisotropic Quantum Bose Dipoles in 2D

Static Structure Factor

Low densities
Universal regime

Intermediate densities

\[ \alpha = 0.4 \quad x = 10^{-3} \]
\[ \alpha = 0.6 \quad x = 10^{-3} \]

\[ nr_0^2 = 1 \]
\[ \alpha = 0.4 \]
\[ nr_0^2 = 1 \]
\[ \alpha = 0.6 \]
Condensate Fraction

The condensate fraction is obtained from the asymptotic behavior of the m=0 mode of the Off-Diagonal One-Body Density Matrix

\[
\rho_1(r_1, r'_1) = N \frac{\int dr_2 \cdots r_N \Psi_0(r_1, r_2, \ldots, r_N) \Psi_0(r'_1, r_2, \ldots, r_N)}{\int dr_1 dr_2 \cdots r_N \Psi_0^2(r_1, r_2, \ldots, r_N)}
\]

\[x = 0.05\]

Momentum Distribution

\[
\rho_1(r_{11'}) = FT[n(k)]
\]

\[n_0 = \lim_{r_{11'} \to \infty} \frac{1}{\rho} \rho_1(r_{11'})\]

Bogoliubov (universal) prediction

\[n_0(x) = 1 - \frac{1}{|\ln x|}\]
Density Response and System Instabilities

Pancake geometry: harmonic confinement along the Z direction


In the Gross-Pitaevskii framework the authors described a roton-instability associated with the quantity

\[ \beta = \frac{g}{g_d} \]

coupling constant of the effective dipolar coupling constant

Below a critical value \( \beta_c \) depending on the density and trap confinement leads to the roton collapse

\[ \frac{\pi p^2}{3} \]
Density Response Function in CBF Approximation

\[ S(q, \omega) \] is the Imaginary part of the Density-Density response induced by a time-dependent perturbation

\[
S(q, \omega) = -\frac{1}{\pi} \text{Im} \chi(k, \omega) \equiv -\frac{1}{\pi} \text{Im} \left[ \frac{\delta \rho_1(k, \omega)}{\rho_0 U_{\text{ext}}(k, \omega)} \right]
\]

with a time-dependent variational wave function

\[
\Psi = \frac{1}{\sqrt{N(t)}} e^{\delta U(t)} e^{-iE_0 t/\hbar} \Psi_0
\]

and time-dependent correlations

\[
\delta U(t) = \sum_j \delta u(r_j; t) + \sum_{i<j} \delta u_2(r_i, r_j; t) + \cdots
\]

minimize the action

\[
\delta S = \delta \int_0^t dt \langle \Psi | H - i \frac{\partial}{\partial t} | \Psi \rangle
\]

Lowest order: setting \( \delta u_n = 0 \ \forall n > 1 \) leads to the Feynman approximation

\[
S(k, \omega) = S(k) \delta(\omega - \epsilon_F(k)) \quad \epsilon_F(k) = \frac{\hbar^2 k^2}{2m}
\]
Density Response Function in CBF Approximation

Keeping $\delta u_2$ improves over Feynmann. Use continuity equations for the one- and two-particle densities and currents to isolate $\delta u_1$ and $\delta u_2$ in terms of one- and two-body density fluctuations.

Disregarding triplet correlations one arrives at

$$\chi(k, \omega) = \frac{S(k)}{\hbar \omega - \epsilon_F(k) - \Sigma(k, \omega)} - \frac{S(k)}{\hbar \omega + \epsilon_F(k) + \Sigma^*(k, \omega)}$$

with the Self-Energy

$$\Sigma(k, \omega) = \frac{1}{2} \int \frac{dp \ dq}{(2\pi)^3 \rho} \frac{\delta(k + p + q)}{\hbar \omega - \epsilon_f(p) - \epsilon_F(q)} |V_3(k; p, q)|^2$$

and the two-phonon coupling vertex

$$V_3(k; p, q) = \frac{\hbar^2}{2m} \sqrt{\frac{S(p)S(q)}{S(k)}} \left[ k \cdot p X(p) + k \cdot q X(q) - k^2 u_3(k; p, q) \right]$$

in terms of $S(k)$ ONLY through

$$X(q) = 1 - \frac{1}{S(q)}$$
Density Response Function in CBF Approximation

2D dipoles polarized perpendicular to the plane ($\lambda = 0$)

F. Mazzanti, R.E. Zillich, G.E. Astrakharchik and J. Boronat
Phys. Rev. Lett. 102, 110405 (2009)
System Instabilities in the phase diagram
Can we determine transition lines in the phase diagram?

In Optimized HNC theory one can tell when solutions can no longer be found. Castillejo et al. showed that when the lowest eigenvalue of the Hessian is non-positive, the system becomes unstable against infinitesimal fluctuations in $g(r)$.

$$K(r, r') = \frac{\partial^2 E[g]}{\delta \sqrt{g(r)} \delta \sqrt{g(r')}}$$

...still this is an approximate result as HNC solutions become less accurate at larger densities.
Variational Path Integral (VPI)
also called Path Integral Ground State (PIGS)

Start from the Time Evolution Operator in imaginary time

\[ G = e^{iHt} = \{ it \to \tau \} \longrightarrow e^{-\tau H} \]

Devise a Variational Wave function |\( \Phi \rangle \) not orthogonal to the true ground state, (may not be completely trivial). The closest to the exact ground state, the better.

The iterated action of \( G \) on |\( \Phi \rangle \) becomes

\[
G^n |\Phi\rangle = \left[e^{-H\tau}\right]^n \left[a_0 |\Psi_0\rangle + a_1 |\Psi_1\rangle + \cdots \right] \\
= a_0 e^{-\tau E_0^n} |\Psi_0\rangle + a_1 e^{-\tau E_1^n} |\Psi_1\rangle + \cdots \longrightarrow a_0 e^{-\tau E_0^n} |\Psi_0\rangle 
\]

... and thus all excited states contributions are killed, yielding a wave function proportional to the actual ground state.

|\( \longrightarrow \) a key ingredient is a good representation of \( G \) that ensures fast convergence |
Variational Path Integral (VPI)

S. Chin derived a One-Parameter family of propagator representations that are exact up to fourth order in time. Our choice is:

\[ e^{\epsilon H} = e^{\epsilon V/6} e^{\epsilon T/2} e^{2\epsilon \tilde{V}/3} e^{\epsilon T/2} e^{\epsilon V/6} \]

The iteration of the propagator leads to the single-particle chains of the simulation.

Bose symmetry is taken into account by the symmetry of the variational model \( |\Phi\rangle \)

Central bead
exact ground state at both sides

The tilde potential
\[ \tilde{V} = V + \frac{\hbar^2}{m} \frac{u_0}{v_2} \left( \sum_j \nabla_j V \right)^2 \]

brings a characteristically new contribution not present in other, simpler approximations like the primitive.
Static Structure Factor and Stripe Phase Formation

When do the stripes form?

... at large densities & close to the critical angle
Microscopic Description of Anisotropic Quantum Bose Dipoles in 2D

Static Structure Factor and Stripe Phase Formation

$n=128$
$\alpha=0.58$

$n=200$
$\alpha=0.58$
Pair Distribution Function and the Stripe Phase

Stripes can be clearly seen in the Pair Distribution function $g(r)$

$n = 128$, $\alpha = 0.58$

$n = 256$, $\alpha = 0.61$
A new **Stripe Phase** develops when the density increases for a large enough polarization angle $\alpha$ because:

- side-by-side dipoles interact through $\frac{1}{r^3}$ forces
- head-to-tail dipoles interact through $\frac{1 - 3\lambda^2}{r^3}$ forces
Many different phases in Optical Lattices

Extended Bose-Hubbard models predict a rich phase diagram in 2D dipolar systems on the lattice

\[ H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + V \sum_{i<j} \frac{n_i n_j}{r_{ij}^3} - \mu \sum_i n_i \]

B. Capogrosso-Sansone et al.  
_PRL_ **104**, 125301 (2010)
The Stripe Phase and the Dynamic Response

... the roton minimum in the Y direction drops to zero

... and a strongly marked second roton seems to develop

$n = 128$
Maximum of $S(k_x, k_y)$
Evolution with the density and tilting angle

Gas-Solid transition
Use $\frac{S(0, k)}{N_p}$ as the order parameter

Gas-Stripe transition
A hint at the Phase Diagram

What do we have in this region?

(At this point) we can’t decide where does the stripe phase ends and where the solid forms...

...work in progress
Stripes-Solid transition (?)
Static Structure factor along the $X$ direction

A new peak reveals crystaline order, or is it a quirk of the simulation induced by finite size effects?

Work in progress !!!
Thank you very much :)