(Aligned) Dipolar (Bose) gases: Long-range and angle-dependent interactions

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Outline of This Talk

• Introduction:
  ▪ Why are ultracold dipolar gases interesting?
  ▪ What are they?
  ▪ How can they be realized experimentally?

• Three aspects of dipolar systems:
  ▪ Two-body scattering properties.
  ▪ DMC and MF-GP results: How to properly compare results from microscopic many-body and mean-field GP treatments?
  ▪ Mean-field results for double-well potential.

• Summary.
Why are Ultracold Dipolar Systems Interesting?

- Anisotropic and long-range interactions.
- Study of chemistry in ultracold regime (e.g., determination of molecule-molecule scattering lengths, fine-tuning of interaction potentials, ...).
- Sensitive probe of phenomena beyond the standard model of particle physics.
- Free space or harmonic trap: Novel collapse mechanisms and phase diagrams.
- Dipolar gas loaded into optical lattices: Realization of novel condensed matter analogs.
- Quantum computing (polar molecule used as qubit).
Experimental Realization of Dipolar Condensate in 2005: Atomic Chromium

- $^{52}\text{Cr} ([\text{Ar}] 3d^5 4s^1)$: Electron spin of 3, nuclear spin 0, composite boson.
- Magnetic moment of $6\mu_B$ (six times larger than for alkali atoms).
- Still comparatively small magnetic interaction (factor of 36); but isotropic s-wave interaction can be tuned to zero.

Sequence of time of flight images [Lahaye et al., PRL 101, 080401 (2008)]:

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<th>0.2 ms</th>
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Roadmap: Long-Range and Anisotropic

• Two-body scattering:
  ▪ Anisotropy leads to coupling of (many) different partial waves (for identical bosons: \(a_{00}, a_{20}, a_{02}, a_{22}, \ldots\) finite but \(a_{40}, a_{62}, \ldots\) zero).
  ▪ Identical bosons: even \(l\) only [exchange of two particles gives \((-1)^l\)].
  ▪ Long-range nature requires integrating out to large interparticle distances.

• Many-body treatment:
  ▪ Quantum Monte Carlo approaches:
    • Account for all correlations and lead (in principle) to exact results.
    • DMC: Anisotropy needs to be built into guiding function.
    • Homogeneous system: LR tail increases numerical complexity.

• Mean-field treatment:
  • Integro-differential equation.
  • Applicability requires: \(na_{00}^3 \ll 1, nr_c^3 \ll 1\) (SR), \(nD_\ast^3 \ll 1\) (LR).

Long-range potential \(V_{dd}: d^2 (1 - 3\cos^2 \theta) / r^3\)
Two-Body Scattering: How to Get K-Matrix or Phase Shifts?

- \( V(r, \theta) = V_{SR}(r) = \infty \) for \( r < r_c \) and \( V(r, \theta) = V_{dd}(r, \theta) \) for \( r > r_c \).

- Separate off CM motion and express relative Hamiltonian in terms of \( Y_{lm} \) basis.
- Result is \( V(r) \), i.e., coupled radial SE.

- Define log derivative matrix \( y(r) = \frac{u'(r)}{u(r)} \).
- Then \( y'(r) = -[y(r)]^2 + V_{\text{eff}}(r) \), where \( V_{\text{eff}} \) includes potential, angular momentum barrier and energy.

- Propagate \( y(r) \) to large \( r \) using Johnson algorithm and match to \( J - N K \), where \( K_{ll'} = \tan(\delta_{ll'}) \).
- Initial condition at \( r = r_c \): \( y \) diagonal matrix with \( y_{ll} = \infty \), i.e., large.

Scattering of Two Aligned Identical Bosonic Point Dipoles

- LR interaction: \( d^2 \left( 1 - 3 \cos^2 \theta \right) / r^3 \).
- LR dipole length \( D_\ast = md^2/h^2 \) (\( d \): dipole moment).
- Short-range interaction: hard wall at \( b \).
- Notable variation of \( a_{00} \) with \( D_\ast/b \):
  - \( D_\ast << b \) (SR dominated): No s-wave bound states
  - \( D_\ast >> b \) (LR dominated): One s-wave bound state
  - \( D_\ast >> b \) (LR dominated): Two s-wave bound states
Scattering Lengths for Two Aligned Identical Bosonic Point Dipoles

Two types of resonances. Why?

Scattering length \( a_{\|'} \) for each partial wave:

\[
a_{\|'} = \lim_{k \to 0} -\tan[\delta_{\|'}(k)]/k
\]

\( a_{\|'} \) constant as \( E \to 0 \).

\( a_{00} \) depends on SR and LR part of potential.

\( a_{\|'} \propto D_\ast \) for \( l, l' > 0 \) (except near resonance).

[dipole length \( D_\ast = \mu d^2/\hbar^2 \). SR cutoff \( r_c = b \)]
Rationalizing the Results of Coupled Channel Calculation

• Why are \( a_{l''} \) (l or \( l' > 0 \), \(|l-l'|=0,2\)) away from resonance proportional to \( D_\ast \)?
  ▪ First Born approximation applied to \( V_{dd} \) alone (\( r=0 \) to \( \infty \)) gives \( a_{l''} \propto D_\ast \).
  ▪ Corrections due to starting at \( r=r_c \) as opposed to \( r=0 \) scale with \( (r_c/D_\ast)^{|l|+|l'|+1} \).
  ▪ Qualitatively, the finite angular momentum barrier suppresses dependence on SR part of the potential.

• Why is s-wave scattering length \( a_{00} \) modified by long-range \( V_{dd} \) potential?
  ▪ Naively: \( <00|V_{dd}|00> = 0 \), suggesting that there should be no modification of \( a_{00} \) due to \( V_{dd} \)…
  ▪ However, the different partial wave channels are coupled at \( r=r_c \) and decouple only at much larger \( r \).
  ▪ Thus, the 00 channel continues to accumulate phase for \( r>r_c \) through the coupling to 20 and 02 channels.
Understanding Resonances: Adiabatic Potential Curves and WKB Phase

- Diagonalizing Hamiltonian in angular momentum basis for fixed $r$ determines adiabatic potential curves.

- Neglecting coupling/adiabatic correction, WKB phases $\phi_i$ give good prediction for resonance positions. Look for $\phi_i/\pi = \text{integer}$, where $\phi_i = \int_{\text{cl. allowed}} [2\mu V_i(r)/\hbar^2]^{1/2} \, dr$.

see Ticknor and Bohn, PRA 72, 032717 (2005); Roudnev and Cavagnero, arXiv:0806.1982.

$\phi_0$: lowest adiabatic curve only

$\Sigma_i \phi_i$: phase due to all other adiabatic curves
WKB Prediction of Resonance Positions for Two Identical Bosons

Crosses: Potential resonances. No barrier in adiabatic potential curve → broad resonance. WKB phase predicts resonance position accurately.

Squares: Shape resonances. Barrier in adiabatic potential curves → narrow resonance. WKB phase predicts number of resonances roughly correctly.

Kanjilal and Blume, PRA 78, 040703(R) (2008); see also Deb and You, PRA 64, 022717 (2001).
Finite-Range Pseudo-Potential For Two Interacting Dipoles

• Pseudo-potential needs to account for dipole-dependent s-wave scattering length [Yi and You, PRA 61, 041604 (2000)]:

\[
V(\vec{r}, \vec{r}') = \frac{4\pi \hbar^2 a(d)}{m} \delta(\vec{r} - \vec{r}') + d^2 \frac{1 - 3\cos^2 \theta}{|\vec{r} - \vec{r}'|^3}
\]

s-wave scattering (determined by interplay between SR and dipole potential)

Mixing between different partial waves (goes all the way to zero)

• This pseudo-potential works because its scattering amplitudes, calculated in the first Born approximation, agree with the full scattering amplitudes of the model potential.
Mean-Field Gross-Pitaevskii Description of Dipolar Bose Gas

\[
\begin{align*}
  i\hbar \frac{\partial \psi(r, t)}{\partial t} &= \left[ -\frac{\hbar^2}{2M} \nabla^2 + \frac{M\omega^2}{2}(\rho^2 + \lambda^2 z^2) \\
  &+ (N - 1)\left[4\pi\hbar^2 a M \right] |\psi(r, t)|^2 + \int d\mathbf{r}' V_d(\mathbf{r} - \mathbf{r}') |\psi(\mathbf{r}', t)|^2 \right] \psi(r, t)
\end{align*}
\]

Mean-field interaction:
contact s-wave (SR) + dipole-dipole (LR)

Integro-differential equation solved following Ronen et al., PRA 74, 013623 (2006):
Take advantage of cylindrical symmetry and perform Fourier transform in \( z \) and Hankel transform in \( \rho \).

Compare with results from many-body Schroedinger equation that uses model potential (hardwall + \( V_{dd} \)) as input.
Spherical Confinement \((N=10, \ b=0.0137a_{ho})\):

**GP versus Many-Body DMC Energies**

Excellent agreement between GP and DMC many-body energies!

Validation of mean-field treatment!

s-wave induced instability.

Bortolotti, Ronen, Bohn, Blume, PRL 97, 160402 (2006)

GP: \(a=a(d)\), LR=0 (contact potential only)

increasing E-field / dipole moment
Spherical Confinement (N=10, b=0.0137а₀): Size and Aspect Ratio

Structural properties depend on dipole moment!

Aspect ratio Z/X

Size X=√<x²>, Size Z=√<z²>

Instability!

DMC
GP, a(d)

GP, a(d). LR part = 0 (isotropic).
Many-Body Variational Calculation: Nature of the Mechanical Instability

Stability of dipolar Bose gas is due to “potential” barrier; collapse occurs when barrier disappears (→ s-wave Bose gas).

Variational wave function:

\[ \Psi = \prod \Phi(r_i) \prod \varphi(r_{jk}) \]

\[ \exp[-(r^2/2b_{r^2})] \]

Parameter \( b_r \): size.

N=20, \( b=0.0137a_{ho} \).
Using OH mass and $\nu=1\text{kHz}$.

Would be stable even w/o trap, $a(d) > D_*/12\pi$

[e.g., Eberlein et al., PRA 71, 033618 (2005)].

Experiment for fixed $N$:
Sequence of stable and unstable regions.
**N=10: Tuning Interactions By Changing Confining Potential**

**Non-interacting gas:**
- **Spherical:** \((0.5+0.5+0.5)h_\nu = 1.5h_\nu\)
- **Cigar:** \((0.5+0.5+0.05)h_\nu_\rho = 1.05h_\nu_\rho\)
- **Pancake:** \((0.05+0.05+0.5)h_\nu_z = 0.6h_\nu_z\)

**E/N increases with increasing** \(D_\ast\), **and then decreases.**

**E/N first increases with increasing** \(D_\ast\), **and then decreases.**

**DMC**

**GP**
Double-Well Potential Along z-Direction

- **Large $\lambda$:**
  - Two “sheets” of dipoles:
    - Interaction within each sheet predominantly repulsive.
    - Interaction between sheets predominantly attractive.
    - Interplay?
  - Building up a lattice of pancake-shaped dipolar gases.

- **Small $\lambda$:**
  - Analogy between two weakly-coupled superconductors and two-weakly-coupled BECs (barrier ~ weak link).
  - Josephson oscillation and macroscopic quantum self-trapping have been observed for s-wave interactions (Oberthaler group).
  - Can they be observed for dipolar Bose gas?
Mean-Field Gross-Pitaevskii Description of Dipolar Bose Gas

\[ i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \left[ -\frac{\hbar^2}{2M} \nabla^2 + \frac{M \omega^2}{2} \left( \rho^2 + \lambda^2 z^2 \right) + A \exp(-0.5z^2/b^2) + \right. \]

\[ + (N - 1) \left[ \frac{4\pi \hbar^2 a}{M} |\psi(\mathbf{r}, t)|^2 + \int d\mathbf{r}' V_d(\mathbf{r} - \mathbf{r}') |\psi(\mathbf{r}', t)|^2 \right] \]

Mean-field interaction:
contact s-wave (SR) + dipole-dipole (LR) \( V_d = d^2(1-3\cos^2\theta)/r^3 \)

A=0, \( \lambda > 1 \): pancake-shape trap
Effectively (more) repulsive

A=0, \( \lambda < 1 \): cigar-shape trap
Effectively (more) attractive

5 parameters: \((N-1)a, \lambda, (N-1)d^2, A, b\). Here: Fix \((N-1)a, b, A\); vary \(\lambda, (N-1)d^2\).
MF-GP Treatment of Pure Dipolar BEC in Double-Well Trap

"Phase diagram" based on stationary solutions of GP equation (A=12E_z, b=0.2a_z, a_s=0):

Transition from symmetry-preserving (S) to symmetry-breaking (SB) is driven by mean-field interaction.

Add particles

Tighten confinement along ρ

D = d^2(N-1) / (E_z a_z^3)

For Cr and ν_z=10Hz: D=1 → N~1800
**Ground State GP Densities for Aspect Ratio $\lambda=0.3$**

Asad-uz-Zaman and Blume, PRA 80, 053622 (2009).
For a related study, see Xiong, Gong, Pu, Bao, Li, Phys. Rev. A (2009) [this study tunes dipole-dipole interactions by changing axis along which dipoles are aligned]
Excitation Frequencies for Aspect Ratio $\lambda=0.3$

Bogoliubov de Gennes excitation spectrum:

Three distinct regimes as function of $D$:

i) Josephson oscillation.

ii) Self-trapping regime.

iii) Collapse.

Lowest $m=0$ eigenmode:

Population transfer between L and R well

($\text{BdG }$frequency is nearly identical to Josephson oscillation frequency obtained by time evolving initial state with small population imbalance)
Two-Mode Variational Description

• Ansatz: \( \Psi(\rho, z, t) = \psi_L(t)\Phi_L(\rho, z) + \psi_R(t)\Phi_R(\rho, z) \), where

\[ \Phi_{L,R}(\rho, z) \propto \Phi_+(\rho, z) \pm \Phi_-(\rho, z) \]

(\( \Phi_+ \) and \( \Phi_- \) are stationary GP solutions)

\[ \psi_{L,R}(t) = \sqrt{N_{L,R}(t)} \exp[i\theta_{L,R}(t)] \]

• Plugging ansatz into time-dependent GP equation and introducing population difference \( Z(t), Z(t) = N_L(t) - N_R(t) \), and phase difference \( \phi(t), \phi(t) = \theta_R(t) - \theta_L(t) \), leads to classical Hamiltonian that is governed by ratio between “effective interaction energy (U-B)” to “tunneling energy (2T)”.

Bogoliubov de Gennes versus Two-Mode Model Prediction ($\lambda=0.3$)

Two-mode model provides qualitative but not quantitative description. Overlap between amplitudes in left and right well appreciable.

Improved two-mode model [Ananikian and Bergeman, PRA 73, 013604 (2006)] does not lead to improvement.
Ground State Densities for Large Aspect Ratio: $\lambda = 10$

For $A = 0$, “red blood cell” was predicted by Ronen et al., PRL 98, 030406 (2007):
Angular Roton Instability

BdG eigenmodes (density osc.):

(a) $k=0$

(b) $k=2$

(c) $k=1$

(d) $k=3$
Summary

• Aligned dipolar Cr Bose gases with long-range and anisotropic interactions have been condensed.
• Huge progress toward condensing cold molecular sample with large electric dipole moment.
• Two-dipole system shows interesting scattering properties that need to be accounted for in comparisons between mean-field and many-body calculations.
• Effective interactions of aligned dipolar Bose gas can be tuned through variation of external confining potential.
• Rich stability and phase diagram as functions of dipole strength and aspect ratio.
• There’s a lot more to do to fully uncover the physics of dipolar systems!