Droplets and Supersolids
novel physics of dipolar Bose-Einstein condensates

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Quantum & Kinetic Problems: Modeling, Analysis, Numerics & Applications
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Outline

- Dipolar BECs and the GPE
- Droplets, quantum fluctuations and the extended GPE
- 2D Droplet crystals
- Some numerical considerations for the DDI
- Supersolids
Bose-Einstein condensates (BECs)

- A macroscopic number of Nano-Kelvin atoms occupying a single quantum state
- Condensate described by the mean-field Gross-Pitaevskii equation (GPE)

**Gross-Pitaevskii Theory:**

**Stationary states:**

\[ \mu \psi_0 = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} - g |\psi_0|^2 \right] \psi_0 \]

**Dynamics:**

\[ i\hbar \frac{\partial \Psi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} + g |\Psi|^2 \right] \Psi \]

**Energy:**

\[ E[\Psi] = \int d\mathbf{r} \Psi^* \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} + \frac{1}{2} g |\Psi|^2 \right] \Psi \]

**Norm:**

\[ N[\Psi] = \int d\mathbf{r} |\Psi|^2 \]

Contact interaction determined by the s-wave scattering length

\[ U(\mathbf{r}) = g \delta(\mathbf{r}) \]

First experiments 1995, Nobel Prize 2001
Dipolar (Magnetic) atoms

- Recently atoms with large magnetic moments have been cooled to into BECs

New Feature!

Dipole-Dipole Interactions (DDIs)
long-ranged & anisotropic

Dy the most magnetic atom
10× more magnetic than Rb
i.e. 100× magnetic interaction

Interactions in Dipolar BECs

DDI has an attractive part (head to tail attraction)

When $g_{dd} > g_s$ the system can be unstable to collapse

I.e. when $\epsilon_{dd} \equiv \frac{g_{dd}}{g_s} > 1$ (dipole dominant regime)
classical collapse analog
Observation of droplets

Observation of a stable droplet crystal

- Lifetime > 100’s ms
- ~1000 atoms per droplet
- ~3 micron spacing
- peak density > 5x10^20 m^-3
- \( a_{dd} \gtrsim 1.4a_s \)

Not predicted by meanfield theory

(pre-print appeared 20-Aug 2015)

Supersolid?

- spontaneous breaking of translational symmetry (crystalline order)
- phase coherence across the crystal

Abstract:

“Although our observations do not probe superfluidity in the structured states, if the droplets establish a common phase via weak links, then our system is a very good candidate for a supersolid ground state.”

Q: But why are there stable droplets?
Interaction driven collapse

two-body energy density $E_{2B} = \frac{1}{2} g_{2B} n^2$

unstable with attractive interaction $g_{2B} < 0$
Interaction **arrested** collapse

two-body energy density $E_{2B} = \frac{1}{2} g_{2B} n^2$

**unstable** with attractive interaction $g_{2B} < 0$

Add **repulsive** higher order interaction

How can a higher order interaction arise in a dilute gas?
Quantum Fluctuations

\[ \frac{E}{V} = \frac{1}{2} g_s n^2 \left[ 1 + \frac{128}{15 \sqrt{\pi}} \sqrt{n a_s^3} \right] \]

mean-field energy

quantum ("LHY") corrections

\[ E_{LHY} = V \frac{64}{15} g_s \sqrt{\frac{a_s^3}{\pi}} n^{5/2} \]

For a dipolar condensate:

\[ E_{LHY} = V \frac{64}{15} g_s \sqrt{\frac{a_s^3}{\pi}} \left( 1 + \frac{3}{2} \epsilon_{dd} \right) n^{5/2} \]

Lima and Pelster, PRA 84, 041604 (2011)
Lima and Pelster, PRA 86, 063609 (2012)

chemical potential correction:

\[ \mu_{LHY} = \frac{\partial E_{LHY}}{\partial N} = \frac{32}{3} g_s \sqrt{\frac{a_s^3}{\pi}} \left( 1 + \frac{3}{2} \epsilon_{dd} \right) n^{3/2} \]

\[ \equiv \gamma_{QF} n^{3/2} \]

This correction term is key to understanding the physics of the dipole dominated regime

Extended GPE Theory (eGPE)

Generalised Gross-Pitaevskii equation for evolution of the condensate field

\[ i\hbar \frac{\partial \psi}{\partial t} = \left[H_{\text{sp}} + \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}')|\psi(\mathbf{r}')|^2 + \gamma_{\text{QF}}|\psi|^3 \right] \psi \]

Condensate evolution

- Single particle Hamiltonian
  - kinetic energy
  - trap potential
- Two-body interactions
  - contact term
  - dipole-dipole term

Growing list of applications including theory and experiment

H. Saito, JPSJ 85, 053001 (2016).
F. Wächtler and L. Santos, PRA 93, 061603 (2016).
**Basic droplet physics**

**Magnetostriiction:** Dipolar interaction tuned by system geometry

Ave. interaction for a filament of dipoles

\[ g_{2B} \sim g_s - g_{dd} = g_s (1 - \epsilon_{dd}) \]

negative for \( \epsilon_{dd} > 1 \)

**Meanfield energy**

\[ E_{\text{int}} \sim \frac{1}{2} g_{2B} n^2 + \frac{2}{5} \gamma_{QF} n^{5/2} \]

Negative, therefore unstable!

Do we need a trap potential?

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Lima et al., PRA 2011
Ferrier-Barbut et al., PRL 2017
Chomaz et al., PRX 2016
Wächtl er et al., PRL 2016
Bisset et al., PRA 2016

…..
How can we make a self-bound droplet?

- Starting point: a prolate trapped dipolar BEC, $\varepsilon_{dd} \sim 1$ ($a_s = 130 a_0$)
  - Add quantum/thermal fluctuations
  - Reduce $a_s$ (to make droplet) and turn off trap (~5 ms)
  - Process must be fast enough that loss isn’t too important
Phase diagram path: $a_s$ quench and trap removal

**Circles:** stability boundary obtained from EGPE solution

**Lines:** from variational solution using ansatz

$$\psi_{\text{var}}(x) = N e^{-\sum_{\alpha} x_{\alpha}^2/\sigma_{\alpha}^2}$$
Self-bound droplets of a dilute magnetic quantum liquid

Matthias Schmitt, Matthias Wenzel, Fabian Böttcher, Igor Ferrier-Barbut & Tilman Pfau

Nature 539, 259–252 (10 November 2016) | doi:10.1038/nature20126
Received 25 July 2016 | Accepted 29 September 2016 | Published online 09 November 2016
2D Droplet Crystals

...bringing back the trap
Ground states in an pancake trap

- $^{164}$Dy atoms in fat pancake trap $(\omega_\rho, \omega_z)/2\pi = (60,300)\text{Hz}$

- Fix $a_s = 70 a_0$, i.e. $\epsilon_{dd} = \frac{g_{dd}}{g_s} \approx 1.86$

- Increase atom number $N$

Baillie & Blakie, PRL 2017

Also see striped phase study in elongated geometry — Wenzel et al., PRA 2017
Free space filaments — Cinti et al., PRL 2017
Confining droplets

• Without trap: a single large droplet is energetically preferred

• With tight trap (or big enough $N$): multiple droplets preferred
Stationary states in a trap

$^{164}$Dy atoms, $a_s = 70a_0$, $(\omega, \omega_z) = 2\pi \times (60, 300)$ Hz varying $N$

(j) $\nu = 19$, $N = 200 \times 10^3$

\[ i\hbar \frac{\partial \psi}{\partial t} = \left[ H_{sp} + \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') |\psi(\mathbf{r}')|^2 + \gamma_{QF} |\psi|^3 \right] \psi \]
Stationary states in a trap

\( \nu = 0, \ N = 1 \times 10^3 \)  
\( \nu = 1, \ N = 3.98 \times 10^3 \)  
\( \nu = 2, \ N = 10 \times 10^3 \)  
\( \nu = 3, \ N = 15.8 \times 10^3 \)  
\( \nu = 4, \ N = 22.4 \times 10^3 \)  
\( \nu = 5, \ N = 30.2 \times 10^3 \)  
\( \nu = 6, \ N = 35.5 \times 10^3 \)  
\( \nu = 7, \ N = 39.8 \times 10^3 \)  
\( \nu = 19, \ N = 200 \times 10^3 \)

Dy-164 \( a_s = 70a_0 \), trap: radial=60Hz, axial=300Hz
Stationary state energies

Dy-164 $a_s = 70a_0$, trap: radial=60Hz, axial=300Hz

Dashed line: analytic theory for up to 7 droplets
Variational Model

- $\nu$-droplets at COM variational positions $\mathbf{d}_j$ in the plane of the trap

- Each droplet a Gaussian of the form $\psi_{\text{var}}(\mathbf{x}) = \mathcal{N} e^{-\sum \alpha x_{\alpha}^2/\sigma_{\alpha}^2}$ where the widths $\sigma$ are variational parameters (decouple from the $\mathbf{d}_j$)

- Energy of array: $E_L = \frac{m\omega^2N}{2\nu} \sum_{j=1}^{\nu} |\mathbf{d}_j|^2 + \frac{3g_{dd}N^2}{8\pi\nu^2} \sum_{k\neq j}^{\nu} \frac{1}{|\mathbf{d}_j - \mathbf{d}_l|^3}$
Variational Predictions

- For $\nu \leq 7$ $E_L$ is minimized for droplets at vertices of a regular polygon (with central droplet for $\nu = 6, 7$)
- Analytic results for droplet positions and lattice energy
Properties/Issues

- Phase coherence between droplets destroyed
- Cannot be made with *obvious* adiabatic pathways
- Discontinuous transition - small droplets nucleate

Supersolid?
Numerical considerations (Challenges)
The DDI is singular and has to be treated carefully.

Several approaches discussed in the literature

We employ the convolution theorem to evaluate the DDI and utilise a truncated k-space interaction kernel

\[ \Phi_D(x) = \int dx' U_{dd}(x - x') |\psi(x')|^2 = \mathcal{F}^{-1} \left\{ \tilde{U}_{dd}(k) \mathcal{F} \{ |\psi(x)|^2 \} \right\} \]

\[ U_{dd}(r) \sim \frac{1 - 3 \cos^2 \theta}{r^3} \]

\[ \tilde{U}_{dd}(k) \sim 3 \cos^2 \theta_k - 1 \]

Less badly behaved, but still not good

For droplets it may difficult to have 2SF of accuracy on a reasonable grid choice without a truncated potential

Ronen et al; Lu et al., Jiang et al.; Bao et al., Antoine et al.,
Kernel truncation

Obtain $k$-space kernel from Fourier transform of $U_{dd}(r)$ restricted to a finite region

Spherical truncation

$$
\tilde{U}_{dd}^{\text{sph}}(k) = \left(1 + 3 \frac{\cos R k}{R^2 k^2} - 3 \frac{\sin R k}{R^3 k^3}\right) \tilde{U}_{dd}^\infty(k)
$$

Axial truncation

$$
\tilde{U}_{dd}^{\text{cut}}(k) = \tilde{U}_{dd}^\infty(k) + 3e^{-Zk}[\sin^2 \theta_k \cos(Zk_z) - \sin \theta_k \cos \theta_k \sin(Zk_z)]
$$

Cylindrical truncation

Independent radial and axial cutoffs
Has to be numerically calculated

Gaussian Test

\[ \psi_G = \sqrt{\frac{8N}{\pi^{3/2} \sigma^2} e^{-2(\rho^2/\sigma^2 + z^2/\sigma^2^2)}} \]

<table>
<thead>
<tr>
<th>Gaussian Widths</th>
<th>Number of points</th>
<th>Grid ranges</th>
<th>No Truncation</th>
<th>Spherical Truncation</th>
<th>Cylindrical Truncation</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\sigma_\rho, \sigma_z)/a_{dd})</td>
<td>((N_\rho, N_z))</td>
<td>((R, Z)/a_{dd})</td>
<td>(E_D (\tilde{U}_{\text{bare}}))</td>
<td>(E_D (\tilde{U}_{\text{sph}}))</td>
<td>(E_D (\tilde{U}_{\text{cyl}}))</td>
</tr>
<tr>
<td>(1,10)</td>
<td>(25,25)</td>
<td>(3,30)</td>
<td>-1.8</td>
<td>-1.3</td>
<td>-9.3</td>
</tr>
<tr>
<td>(1,10)</td>
<td>(25,25)</td>
<td>(4,40)</td>
<td>-2.0</td>
<td>-1.7</td>
<td>-15.0</td>
</tr>
<tr>
<td>(1,10)</td>
<td>(250,25)</td>
<td>(40,40)</td>
<td>-5.1</td>
<td>-15.1</td>
<td>-15.1</td>
</tr>
<tr>
<td>(2,1)</td>
<td>(50,25)</td>
<td>(12,4)</td>
<td>-1.7</td>
<td>-1.6</td>
<td>-15.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\log_{10}) absolute relative error.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For Gaussian Dipole energy evaluated analytically \(E_D = \frac{1}{2} \int d\mathbf{r} \Phi_D(\mathbf{r}) |\psi_G|^2\)

Test of numerics by sampling Gaussian on a grid and evaluating DDI energy

**Discretisation:** Bessel quadrature for radial coordinates, Fourier quadrature for \(z\)-coordinates, Fourier-Hankel transform used to evaluate \(\Phi_D\).

Ronen et al., PRA (2006)
Finding EGPE stationary solutions

Minimize GP energy functional iteratively subject to normalization constraint using:

- Gradient flow (imaginary time)
- Conjugate Gradient technique
- Newton-Krylov methods

Time scale dependent on complexity of ground state landscape: **seconds to days/weeks**

Bohn group (JILA), Bao group (Singapore), Antoine group (France), …

Currently we extensively use a Backwards-Forward Euler gradient flow
Supersolids
- Axially-elongated dipolar BEC
- Dipoles along a tightly confined direction
- Dominant dipole interactions
- System is **not** quasi-1D
Interactions and Excitations

Effect $k_z$-space interaction

Accounting for contact interaction
$k$-independent interaction
Tuneable using Feshbach resonances

Q: What happens after the roton softens?

A: Supersolidity

Bogoliubov spectrum:
\[
\epsilon(k) = \sqrt{\epsilon_0(k) \left[ \epsilon_0(k) + 2n\tilde{U}(k) + 3\gamma_{QF}n^{3/2} \right]}
\]

Santos et al., PRL 2003
Chomaz et al., Nat. Phys. 2018
Three Experiments!

- Tanzi et al. PRL 122 (2019)
- Bottcher et al., PRX 9 (2019)
- Chomaz et al., PRX 9 (2019)
- Natale et al., PRL 123 (2019)
- Tanzi et al., Nature 574 (2019)
- Guo et al., Nature 574 (2019)
Simpler theory

- From EGPE set $\Psi(x) = \psi_0(z)\chi_\sigma(\rho)$ with $\chi_\sigma(\rho) = e^{-(\eta x^2 + y^2/\eta)/2l_0^2}/\sqrt{\pi l_0}$.

- Reduces to effective 1D form for stationary states $\mu \psi_0 = \mathcal{L}_z \psi_0$ where

\[
\mathcal{L}_z = \mathcal{E}_\sigma - \frac{\hbar^2}{2m} \frac{d^2}{dz^2} + \frac{1}{2} m \omega_z^2 z^2 + \Phi_z(z) + g_{QF} |\psi_0|^3
\]

\[
\mathcal{E}_\sigma(l_0, \eta) = \frac{1}{4} \left[ \frac{\hbar^2}{ml_0^2} \left( \eta + \frac{1}{\eta} \right) + ml_0^2 \left( \frac{\omega_x^2}{\eta} + \omega_y^2 \eta \right) \right]
\]

Single particle transverse energy

Two-body interactions

\[
\mathcal{F}_z^{-1} \left\{ \tilde{U}_z(k) \mathcal{F}_z \{ |\psi_0|^2 \} \right\}
\]

with

\[
\tilde{U}_z(k) = \int \frac{dk_\rho}{(2\pi)^2} \tilde{U}(k) \left| \mathcal{F}_\rho \{ |\chi(\rho)|^2 \} \right|^2
\]

Key point is that for $\eta = 1$ Gaussian choice $\tilde{U}_z$ has simple analytic form

\[
\tilde{U}_\sigma(k) = \frac{g_s}{2\pi l_0^2} + \frac{g_{dd}}{4\pi l_0^2} \left[ 1 + \frac{3}{2} k^2 l_0^2 \exp \left( \frac{1}{2} k^2 l_0^2 \right) \text{Ei} \left( -\frac{1}{2} k^2 l_0^2 \right) \right],
\]

We have developed a excellent approximation for $\eta \neq 1$ (Blakie et al. in prep)

Deuretzbacher et al., PRA 2010
Sinha et al., PRL 2007
How well does this do in the experimental regime?

Infinite tube and uniform case
i.e. $\omega_z = 0$ & before supersolid
$\Psi(x) = \psi_0(z)\chi(\rho) \rightarrow \sqrt{n}\chi(\rho)$

Example: Infinite tube of $^{164}$Dy
$n = 2.5 \times 10^3 \mu m^{-1}$, $\omega_\rho = 2\pi \times 150$ Hz,

1/e density contours in transverse plane
$\epsilon_{dd} = 1.1$
$\epsilon_{dd} = 1.4$

Roton softening benchmark:
3D EGPE $a_s = 92.5\ a_0$
Our 1D theory $a_s = 91.6\ a_0$
Contrast of density modulations
\[ C = \frac{n_{\text{max}} - n_{\text{min}}}{n_{\text{max}} + n_{\text{min}}} \]

Phase diagram (uniform along z case)

Solution \( \Psi(x) = \psi_0(z)\chi(\rho) \) in single unit cell

Example: Infinite tube of \(^{164}\text{Dy}\)
\[ n = 2.5 \times 10^3 \mu m^{-1}, \quad \omega_\rho = 2\pi \times 150 \text{Hz}, \]

Continuous and discontinuous transitions!
Excitations in the modulated phase

In the reduced zone scheme

More deeply into the modulated phase

Conclusions

• Overview of recent work in dipolar BECs
• Critical role of a higher order nonlinearities arising form quantum fluctuations
• Novel Ground states
  ➞ Droplet states
  ➞ Droplet crystals
  ➞ Supersolids