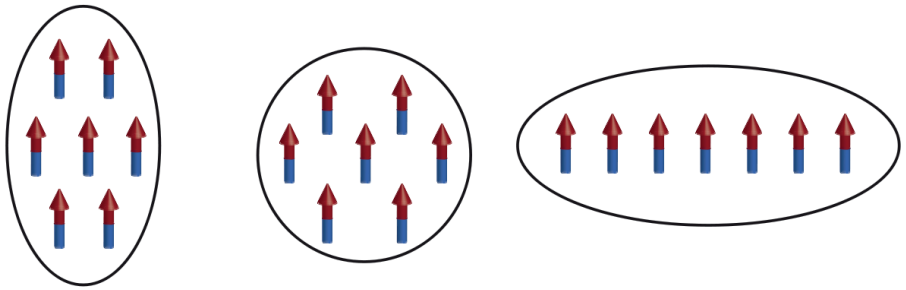
Introduction to dipolar quantum gases



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WHERE?


North Island
Napier
Hastings
Wanganui
Palmerston North
Masterton
Porirua
Wellington
Kahurangi National Park
Nelson
Blenheim
New Zealand
Greymouth
Rangiora
Christchurch
Ashburton
Mount Aspiring National Park
Timaru
Waimate
Oamaru
Fiordland National Park
Dunedin
Gore
Invercargill

Outline

- **Aim:** Provide a basic introduction to physics of quantum degenerate dipolar gases for people working in ultra-cold atomic physics

Focus will be on polarized magnetic gases, but some electric dipole results will be presented.

Why Dipoles?

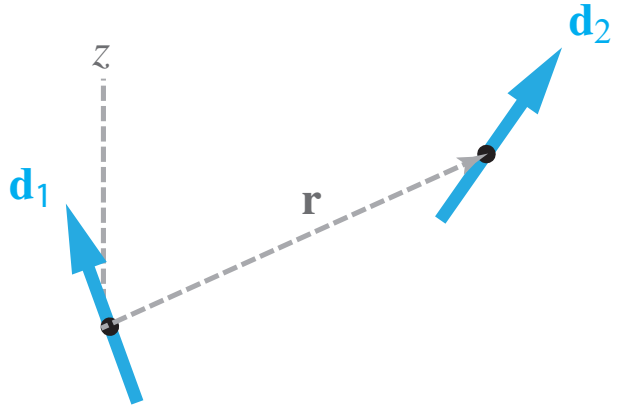
Contents

Useful review articles

- *The physics of dipolar bosonic quantum gases,* T Lahaye, C Menotti, L Santos, M Lewenstein, and T Pfau, Rep. Prog. Phys. **72** 126401 (2009).
- *Condensed Matter Theory of Dipolar Quantum Gases,* M. A. Baranov, M. Dalmonte, G. Pupillo, P. Zoller, Chemical Reviews **112**, 5012 (2012).
- *Spinor Bose–Einstein condensates*, Y.Kawaguchi and M. Ueda, Phys. Rep. **520**, 253 (2012).

1 Dipole-Dipole Interaction (DDI)

General (non-polarized) case



$$U_{\mathrm{dd}}(\mathbf{r}) = \frac{C_{\mathrm{dd}}}{4\pi}\left(\frac{\hat{\mathbf{d}}_1\cdot\hat{\mathbf{d}}_2 - 3(\hat{\mathbf{d}}_1\cdot\hat{\mathbf{r}})(\hat{\mathbf{d}}_2\cdot\hat{\mathbf{r}})}{r^3}\right) = \sum_{\nu,\nu'=x,y,z}\hat{d}_{1\nu}Q_{\nu\nu'}\hat{d}_{2\nu'}$$

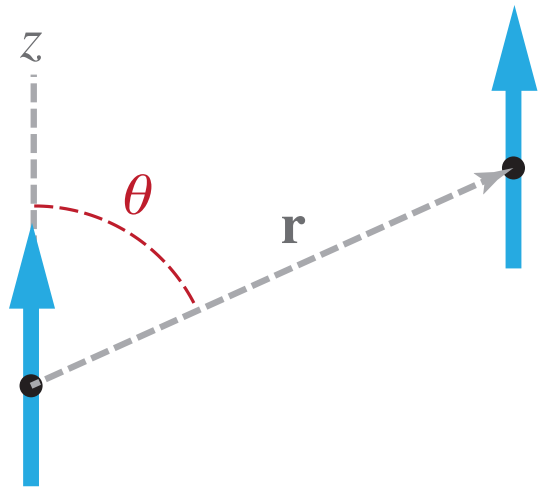
where $Q_{\nu\nu'} = (\delta_{\nu\nu'} - 3\hat{r}_\nu\hat{r}_{\nu'})/r^3$ is traceless tensor, hats denote unit vectors.

- $C_{\mathrm{dd}} = \mu_0\mu_m^2$ for permanent magnetic dipoles of moment μ_m
- $C_{\mathrm{dd}} = d^2/\epsilon_0$ for permanent electric dipoles of moment d.

See Kawaguchi and Ueda [Phys. Rep. 2012] for more details of spinor-dipolar systems.

Polarized case

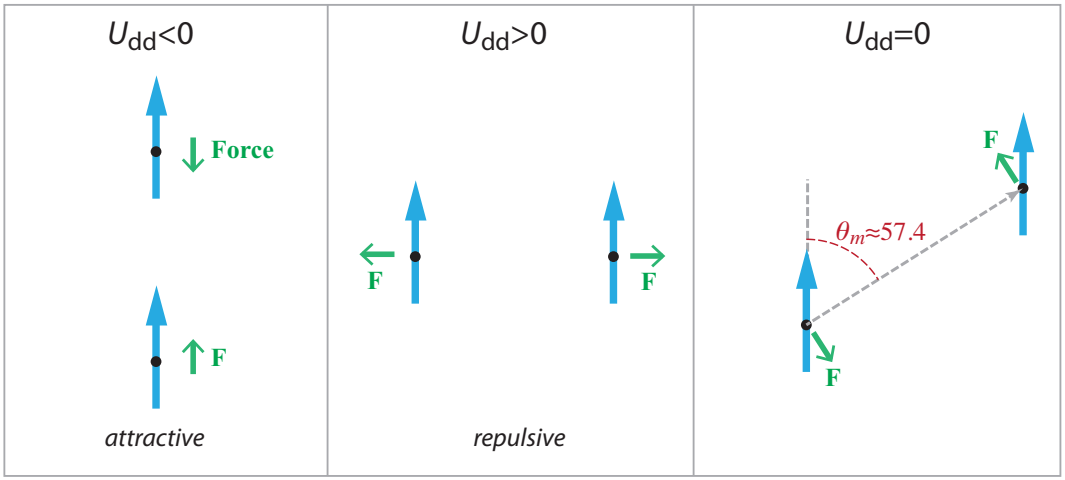
Dipoles polarized in a strong external field along z



Potential simplifies to:

$$U_{\mathrm{dd}}(\mathbf{r}) = \frac{C_{\mathrm{dd}}}{4\pi}\left(\frac{1-3\cos^2\theta}{r^3}\right).$$

Anisotropy of the DDI



- ***Anisotropic*** angular dependence [$\sim$ $\overbrace{Y_{20}(\theta)}^{\text{spherical harmonic}}$ $\sim$ $\overbrace{P_2(\cos(\theta))}^{\text{Legendre polynomial}}$]*:*
  - E.g. Attractive for $\theta = 0$ (i.e. head-to-tail)
  - E.g. Repulsive for $\theta = \frac{\pi}{2}$ (i.e. side-by-side)
  - $U_{\rm dd} = 0$ at the magic angle $\theta_m = \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) \simeq 54.7°$.
- The force is non-central (i.e. not along $\hat{\mathbf{r}}$)

$$\mathbf{F}_{\rm dd} = \frac{3C_{\rm dd}}{4\pi}\left[\hat{\mathbf{r}}\left(\frac{1-3\cos^2\theta}{r^4}\right) - \hat{\boldsymbol{\theta}}\left(\frac{\sin 2\theta}{r^4}\right)\right].$$

Is the DDI long ranged?

Test extensiveness of chemical potential (or energy per particle) of a large uniform system in D dimensions using

$$I_t = \int_{r_{\min}}^{\infty} dr\, r^{D-1} U_{\rm int}(r),$$

with $r_{\min}$ some short distance cutoff. For a long-ranged interaction I_t will diverge as $r \to \infty$.

Neglecting anisotropy in DDI:

- $D = 3$, non-extensive (long ranged)
- $D = 1, 2$ extensive (short ranged).

Note there are alternative definitions of “long-ranged”.

Conservation of angular momentum?

Two particles in free space with total angular momentum $\mathbf{L} = \mathbf{x}_1 \times \mathbf{p}_1 + \mathbf{x}_2 \times \mathbf{p}_2$, and internal forces due to DDIs $\mathbf{F} = \mathbf{F_1} = -\boldsymbol{\nabla}_1 U_{\mathrm{dd}}(\mathbf{r})$ $(= -\mathbf{F}_2)$

$$\dot{\mathbf{L}} = (\mathbf{x}_1 - \mathbf{x}_2) \times \mathbf{F} \neq 0$$

since $\mathbf{F}$ non-central.

Reason: The polarizing field breaks rotational invariance.

In general we must consider **both** orbital and spin angular momentum, i.e.

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

Scattering: partial wave phase shifts

The scattering amplitude is determined by the phase shifts $\delta_l = \delta_l(k)$

$$f(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l}-1)P_l(\cos\theta).$$

For a potential that decreases as $1/r^n$ for large r:

$$\delta_l \sim k^{2l+1} \quad \text{if } l < (n-3)/2$$
$$\delta_l \sim k^{n-2} \qquad \text{otherwise}$$

For $n > 3$, notably van der Waals ($n = 6$), s-wave dominates as $k \to 0$ with $\delta_0 \sim k$.

- Can replace true interaction potential by isotropic *pseudo-potential* $g\delta(\mathbf{r})$ with $g = 4\pi a\hbar^2/m$ where a is the s-wave scattering length ($\lim_{k\to 0}\delta_0 = -ak$).

For $n = 3$, all $\delta_l \sim k$ as $k \to 0$, i.e. all partial waves contribute.

Anisotropy of DDI induces couplings between different partial waves, and spin is not conserved (dipolar relaxation).

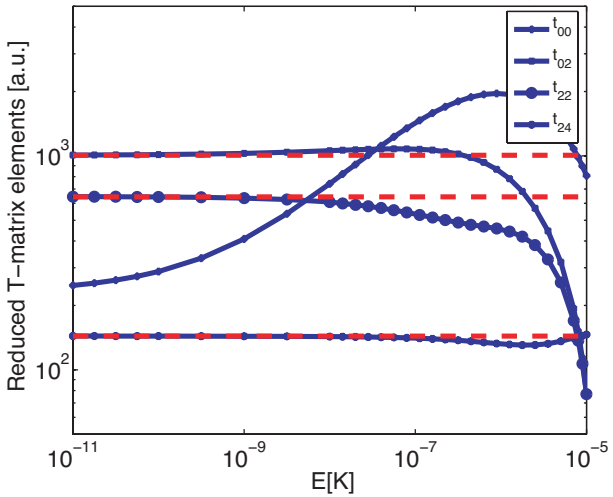
Dipolar Pseudo-Potential

Yi and You [PRA 2001] have shown that the low energy scattering of bosonic particles is described with a pseudo-potential[1]

$$U_{\rm int}(\mathbf{r}) = g\delta(\mathbf{r}) + U_{\rm dd}(\mathbf{r}).$$

I.e. Born scattering amplitude $f_{\rm B}(\hat{\mathbf{k}}_f, \hat{\mathbf{k}}_i) \propto \int d\mathbf{r}\, e^{i(\mathbf{k}_i - \mathbf{k}_f)\cdot\mathbf{r}} U_{\rm int}(\mathbf{r})$ reproduces the exact one.

Short-ranged effects are included in g, which also depends on the dipole moment.[2]



Ronen et al., PRA **74**, 033611 (2006)

Comparison of exact calculations for reduced T-matrix elements (solid) $t_{ll'} \equiv \frac{T_{l0}^{l'0}(k)}{2k}$ against Born results (dashed).

[1] Not too large dipoles and away from shape resonances.

[2] **Note:** Also see work by Derevianko, Wang, and Bohn.

Inelastic scattering and loss

Important inelastic 2-body processes:

- *spin-exchange* (conserves S)
- *dipolar relaxation* (doesn't conserve S)

Maximally polarized states cannot have spin-exchange.

Dipolar relaxation (DR)- the spin of one of the colliding atoms is flipped (allowed as DDI does not conserve S but only $J = L + S$). The cross-section for this $\sigma_{\rm DR} \sim$(dipole moment)^3.

Loss rate $\beta_{\rm DR} \sim 2\langle \sigma_{\rm DR} v_{\rm rel} \rangle_{\rm therm}$

$$\frac{dn}{dt} \sim -\beta_{\rm DR} n^2.$$

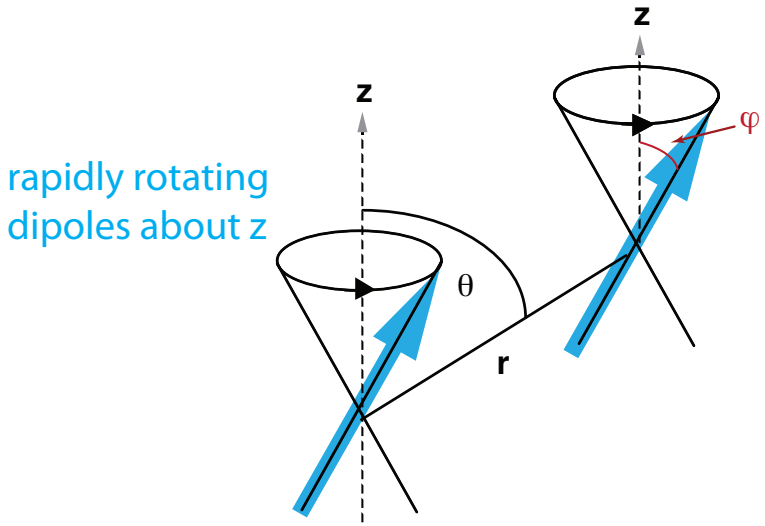
For ^{52}Cr $\beta_{\rm DR} = 4 \times 10^{-12}$cm^{3}s^{-1} at $B = 1G$ [Hensler et al. Appl. Phys. B (2003)][3].

3-body recombination is another important process. For Cr near a Feshbach resonance the rate was found to be $L_3 \sim 2 \times 10^{-40}$m^6/s [PRL **101**, 080401 (2008)] c.f. ^{87}Rb with $L_3 \sim 2 \times 10^{-41} m^6/s$ [Appl. Phys. B **69**, 257 (1999)], where $\dot{n} = -L_3 n^3$.

[3] This rate is more than 2 orders of magnitude higher than for Na, Rb

Controlling interactions

- Feshbach resonances controlling the s-wave interaction have been demonstrated in the atomic dipolar systems (Cr, Er, Dy).
- Tuning the DDI proposed by Giovanazzi et al. [PRL **89**, 130201 (2002)]: rotate the polarizing field (tilted at angle φ to z) at a frequency Ω that satisfies $\omega_{\mathrm{Larmor}} \gg \Omega \gg \omega_{\mathrm{trap}}$



Averaging the interaction over $T = 2\pi/\Omega$ gives

$$\overline{U_{\mathrm{dd}}} = \frac{C_{\mathrm{dd}}}{4\pi}\left(\frac{1-3\cos^2\theta}{r^3}\right)\overbrace{\left(\frac{3\cos^2\varphi-1}{2}\right)}^{-\frac{1}{2}\to 1} = \alpha U_{\mathrm{dd}}, \qquad \alpha \in [-\tfrac{1}{2}, 1].$$

2 Systems

Atoms & molecules

Heteronuclear molecules in low rovibrational states can have large electric dipoles

- Electric dipoles typically given in **debye** $1\mathrm{D} \approx 3.335 \times 10^{-30}\,\mathrm{Cm} \approx 0.39 e a_0$
- Diatomic molecules typically have moments up to $\sim 10\,\mathrm{D}$ (i.e. a few $e a_0$)
- Ground states are rotationally symmetric in lab frame and external E-field ($\sim 10^4\,\mathrm{Vcm}^{-1}$) is needed to orient in lab frame

Magnetic dipoles atoms such as Cr, Er, Eu, Dy,... have a large ground state magnetic moment

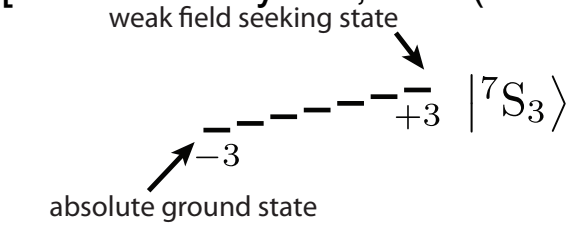
- Alkali atoms have $\mu_m \sim \mu_B$
- Dy (most magnetic atom) has $\mu_m = 10\mu_B$.

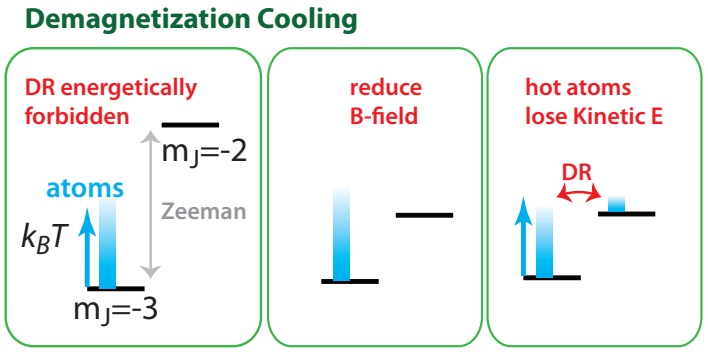
Other systems: **Rydberg atoms, Light induced dipoles (not discussed here)**

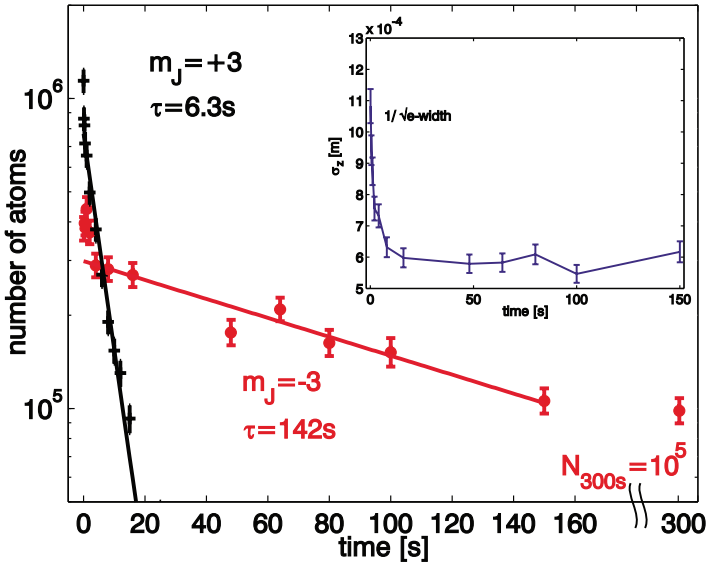
First Dipolar Quantum Gas: Pfau group Stuttgart (2005)

Chromium-52 has 6 valence shell electrons with parallel spin alignment [Ar]3d^5 4s^1 with ground electronic state $^7S_3$ i.e. $J = 3, S = 3, L = 0$, also $I = 0$.

- MOT limited by dipolar relaxation (DR). Pump to $m_J = -3$ and evaporate in optical dipole trap.
- Variation: Use DR to perform lossless cooling (limited to recoil temperature) [see Nat. Phys. 2, **765** (2006)].







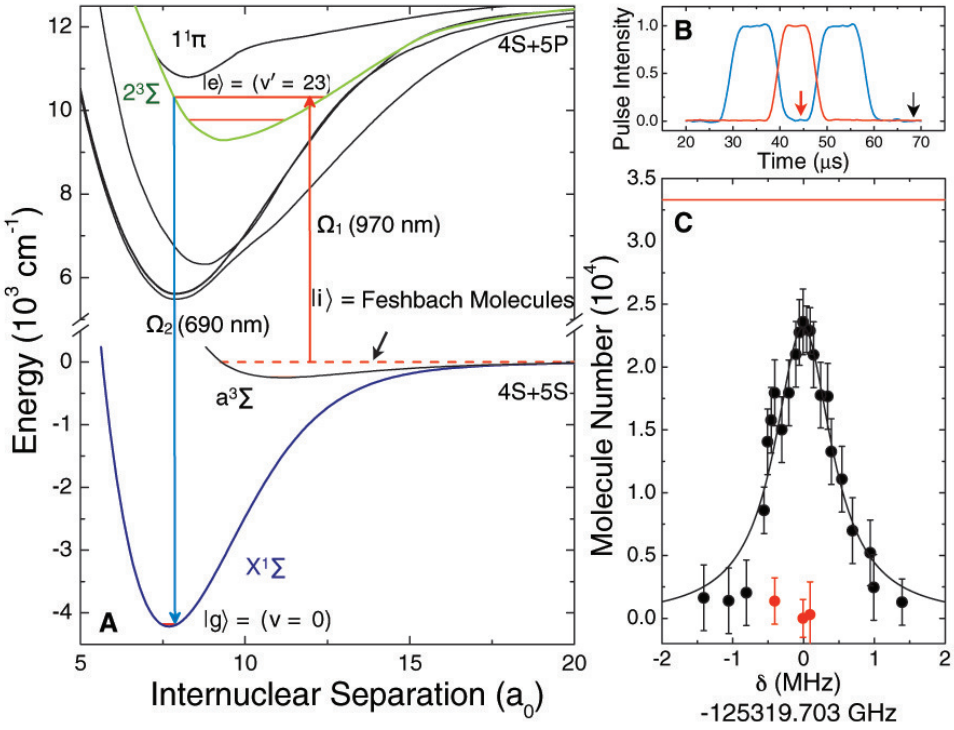
[from PRL 94, 160401 (2005)]

Degenerate Polar molecules: a *holy grail*

Polar molecules have much larger dipoles than atoms $d \sim ea_0$ whereas for magnetic atoms $\mu_m \sim \mu_B$

$$\frac{C_{\rm dd}^{(\rm mag)}}{C_{\rm dd}^{(\rm elec)}} = \frac{\mu_0 \mu_m^2}{d^2/\epsilon_0} \sim \alpha^2 \sim 10^{-4}$$

Variety of techniques being pursued: buffer gas cooling, Stark deceleration, ... most success to date with bi-Alkali's [^{87}Rb^{40}K: JILA group, Science **322,** 231 (2008)]



Cold dipolar gases: experimental milestones

year	system	group	
2005	BEC ^{52}Cr	Stuttgart	
2007	BEC ^{52}Cr	Paris	
2008	Fermi ^{40}K^{87}Rb ($T \sim 2\,T_F$)	Boulder	
2010	Bose ^{41}K^{87}Rb	Tokyo	
2011	BEC ^{164}Dy	Illinois$\rightarrow$Stanford	
2012	DFG ^{161}Dy ($T \sim 0.2\,T_F$)	Illinois$\rightarrow$Stanford	Also BEC of ^{162}Dy as coolant
2012	BEC ^{168}Er	Innsbruck	
2013	DFG ^{167}Er ($T \sim 0.2\,T_F$)	Innsbruck	

DFG = degenerate fermi gas

Interaction Parameters

Convenient to introduce a length scale for the DDI roughly comparable to the s-wave scattering length for the contact interaction: the *dipole length*

$$a_{\rm dd} \equiv \frac{C_{\rm dd} m}{12\pi\hbar^2},$$

Another important figure of merit is the ratio of the dipole to contact interactions

$$\epsilon_{\rm dd} \equiv \frac{a_{\rm dd}}{a} = \frac{C_{\rm dd}}{3g}.$$

A particle with $\epsilon_{\rm dd} > 1$ is referred to as being *dipole dominated.*

Species	μ_m or d	$a_{\rm dd}$	a	$\epsilon_{\rm dd}$
^{87}Rb	$1\,\mu_B$	$0.7\,a_0$	$100\,a_0$	0.007
^{52}Cr	$6\,\mu_B$	$16\,a_0$	$100\,a_0$	0.16
^{168}Er	$7\,\mu_B$	$67\,a_0$	$\sim 175\,a_0$	~ 0.38
^{164}Dy	$10\,\mu_B$	$130\,a_0$	$\sim 100\,a_0$	~ 1.3
^{40}K^{87}Rb	$0.6\,\mathrm{D}$	$3700\,a_0$	$\sim 100\,a_0$	~ 37

3 Semiclassical Theory of Normal Dipolar Gases

Consider spin polarized system! Nice system for learning about the effects of DDIs on quantum gases.

Introduction to semiclassical theory

Basic idea: Wigner distribution function $W(\mathbf{R}, \mathbf{k})$ gives the number of particles in the phase space volume about $\mathbf{R}$ and $\mathbf{k}$. The Wigner function relates to the one-particle density matrix as

$$G(\mathbf{R}, \mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} W(\mathbf{R}, \mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}.$$

Note $G(\mathbf{x}, \mathbf{x}') = \langle \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}') \rangle$, but have transformed to $\mathbf{R} = \frac{1}{2}(\mathbf{x} + \mathbf{x}')$, $\mathbf{r} = \mathbf{x} - \mathbf{x}'$.
From W we can get the position and momentum densities

$$\begin{aligned} n(\mathbf{R}) &= \int \frac{d\mathbf{k}}{(2\pi)^3} W(\mathbf{R}, \mathbf{k}) = G(\mathbf{R}, \mathbf{0}) \\ \tilde{n}(\mathbf{k}) &= \int \frac{d\mathbf{R}}{(2\pi)^3} W(\mathbf{R}, \mathbf{k}) \end{aligned}$$

Such a semi-classical description is applicable to the normal part of a Bose gas at $k_B T \gg \hbar\omega_{\rm trap}$ and to a normal Fermi gas if $E_F \gg \hbar\omega_{\rm trap}$.

Thermodynamic information can be extracted using

$$S = -\int \frac{d\mathbf{x}\, d\mathbf{k}}{(2\pi)^3} \left\{ W(\mathbf{x},\mathbf{k}) \ln W(\mathbf{x},\mathbf{k}) + [1 - W(\mathbf{x},\mathbf{k}) \ln[1 - W(\mathbf{x},\mathbf{k})] \right\}$$

The density-density correlations can be treated using Hartree-Fock (Wick) factorization

$$G^{(2)}(\mathbf{x},\mathbf{x}') = \langle \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x}) \rangle = \overbrace{n(\mathbf{x}) n(\mathbf{x}')}^{\text{Hartree/direct}} + \overbrace{\eta |G^{(1)}(\mathbf{x},\mathbf{x}')|^2}^{\text{Fermi/exchange}} ,$$

with $\eta = +1$ for bosons, and $\eta = -1$ for fermions.

For the case of a trap $V(\mathbf{x}) = \frac{1}{2} m \omega_\rho^2 (\rho^2 + \lambda^2 z^2)$ the energy functional is

$$E = \int d\mathbf{k} \frac{\hbar^2 k^2}{2m} \tilde{n}(\mathbf{k}) + \int d\mathbf{R}\, V(\mathbf{R}) n(\mathbf{R}) + \frac{1}{2} \int d\mathbf{R} \int d\mathbf{r} U_{\rm int}(\mathbf{r}) \left[n(\mathbf{x}) n(\mathbf{x}') + \eta |G^{(1)}(\mathbf{x},\mathbf{x}')|^2 \right] ,$$

All of the above terms can be obtained from W. Progressing any further requires some model for W (or procedure to determine W by minimizing E).

Hartree treatment of $T = 0$ Fermions

Goral et al [PRA **63,** 033606 (2001)] considered $T = 0$ Fermions and chose a *Thomas-Fermi* ansatz

$$W(\mathbf{R}, \mathbf{k}) = \theta([6\pi^2 n(\mathbf{R})]^{2/3} - k^2),$$

where θ is Heaviside's unit step function and noting $k_F = (6\pi^2 n)^{1/3}$. This gives

$$E = \int d\mathbf{R} \left\{ \overbrace{\frac{\hbar^2}{m}\frac{[6\pi^2 n(\mathbf{R})]^{5/3}}{20\pi^2}}^{\text{kinetic energy}} + \overbrace{V(\mathbf{R})n(\mathbf{R})}^{\text{potential energy}} \right\} + \frac{1}{2}\int d\mathbf{R} \int d\mathbf{r} U_{\rm dd}(\mathbf{r}) n(\mathbf{R}+\frac{1}{2}\mathbf{r}) n(\mathbf{R}-\frac{1}{2}\mathbf{r})$$

Using that $g = 0$ for Fermions. Note the exchange vanishes (see why later!) and E only depends on the position density.

Important Integral

Consider the Gaussian ansatz

$$n(\mathbf{r}) = \frac{N\nu^{3/2}}{\pi^{3/2}\sigma_\rho^2\sigma_z a_{\rm ho}^3}\exp\left[-\frac{\nu}{a_{\rm ho}^2}\left(\frac{\rho^2}{\sigma_\rho^2}+\frac{z^2}{\sigma_z^2}\right)\right],$$

where the dimensionless widths are $\{\sigma_\rho, \sigma_z\}$, and $a_{\rm ho} = \sqrt{\hbar/m\bar{\omega}}$ with $\bar{\omega} = \sqrt[3]{\omega_x\omega_y\omega_z}$, and ν is a dimensionless parameter. The direct interaction is

$$\begin{aligned} E_D &= \frac{1}{2}\int d\mathbf{x}\int d\mathbf{x}'\, V_{\rm dd}(\mathbf{x}-\mathbf{x}')n(\mathbf{x})n(\mathbf{x}') \\ &= -\frac{N^2\nu^{3/2}\hbar\bar{\omega}}{\sqrt{2\pi}}\frac{a_{\rm dd}}{a_{\rm ho}}\frac{1}{\sigma_\rho^2\sigma_z} f\left(\sigma_\rho/\sigma_z\right), \end{aligned}$$

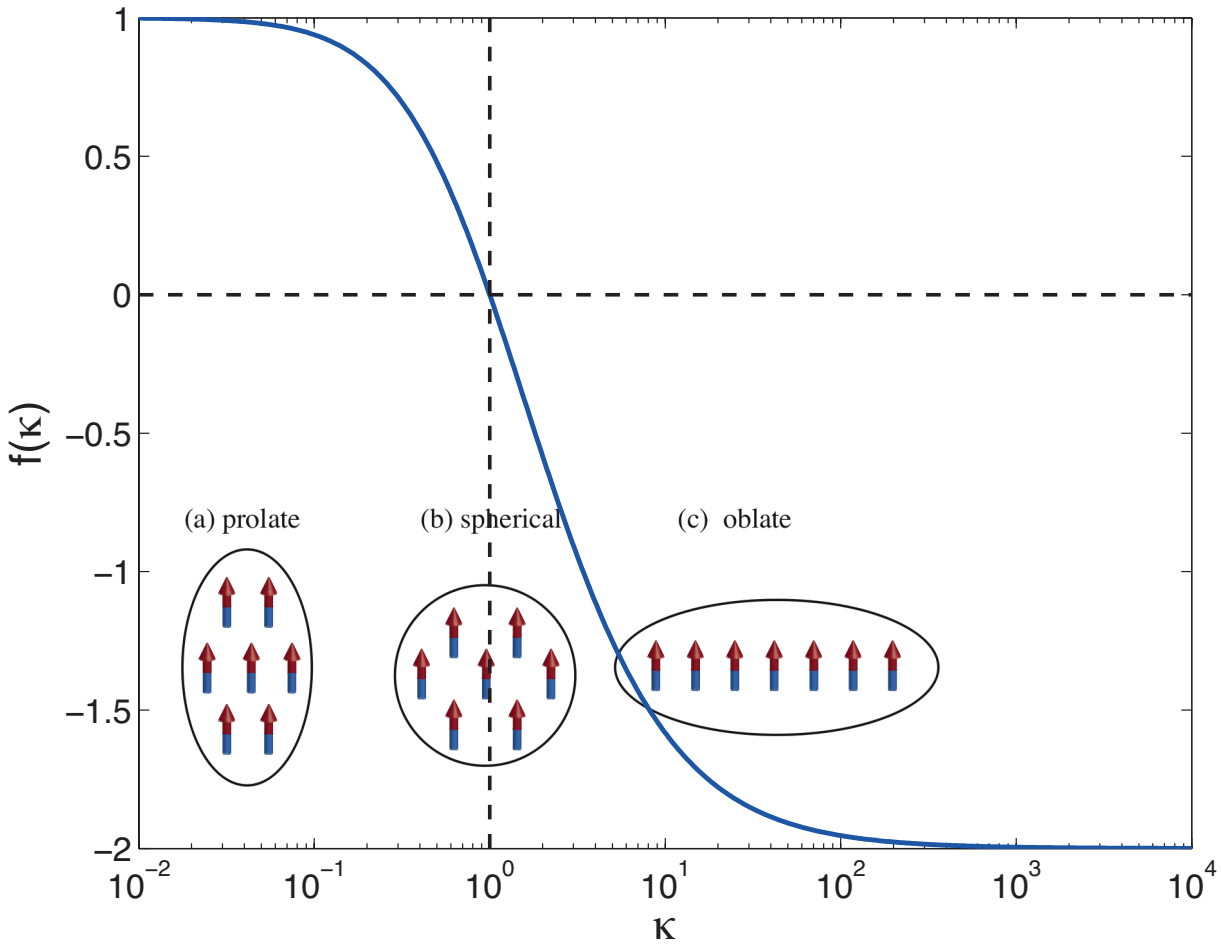
where

$$f(\kappa) = \frac{1+2\kappa^2}{1-\kappa^2} - \frac{3\kappa^2 {\rm arctanh}\sqrt{1-\kappa^2}}{(1-\kappa^2)^{3/2}},$$

with $f(0) = 1$, $f(1) = 0$, and $f(\infty) = -2$.

Behaviour of direct interaction

- $E_D > 0$ for oblate densities ($\sigma_\rho/\sigma_z > 1$)
- $E_D < 0$ for prolate densities ($\sigma_\rho/\sigma_z < 1$)



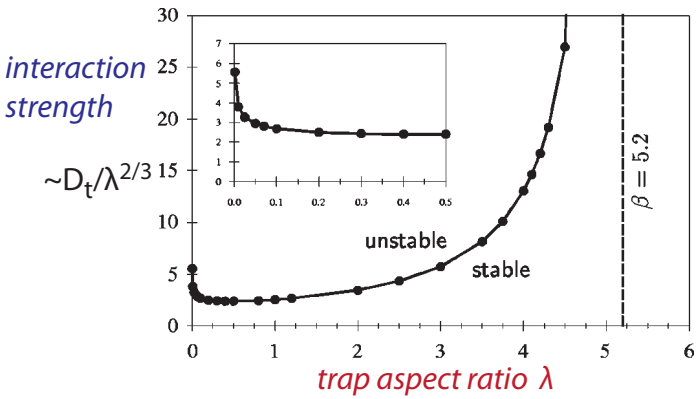
Energy functional

$$E = \overbrace{0.6742\hbar\bar{\omega}\frac{N^{5/3}\nu}{(\sigma_\rho^2\sigma_z)^{2/3}}}^{\text{kinetic}} + \overbrace{\frac{N\hbar\bar{\omega}}{4\nu\lambda^{2/3}}(2\sigma_\rho^2+\sigma_z^2\lambda^2)}^{\text{trap}} - \overbrace{\frac{N^2\nu^{3/2}\hbar\bar{\omega}}{\sqrt{2\pi}}\frac{a_{\rm dd}}{a_{\rm ho}}\frac{1}{\sigma_\rho^2\sigma_z}f\left(\sigma_\rho/\sigma_z\right)}^{\text{DDI}}$$

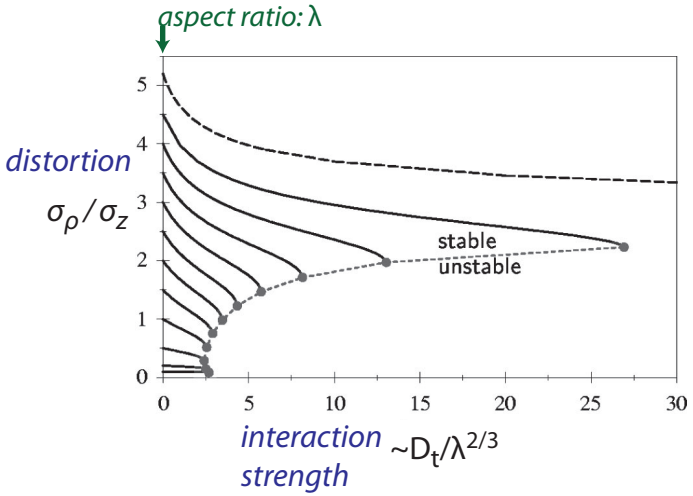
where we have used $\frac{3^{19/6}(\pi/2)^{1/3}}{5^{5/2}} \approx 0.6742$. Setting $\nu = N^{-1/3}$ makes the kinetic and trap terms go as $N^{4/3}$, while the interaction term is $N^{3/2}$. Thus

$$\frac{E}{N^{4/3}\hbar\bar{\omega}} = 0.6742\frac{1}{(\sigma_\rho^2\sigma_z)^{2/3}} + \frac{1}{4\lambda^{2/3}}(2\sigma_\rho^2+\sigma_z^2\lambda^2) - \frac{D_t}{\sqrt{2\pi}\sigma_\rho^2\sigma_z}f\left(\sigma_\rho/\sigma_z\right)$$

setting $D_t = N^{1/6}a_{\rm dd}/a_{\rm ho}$.



[Adapted from PRA **63**, 033606 (2001)]



Magnetostriction

Spatial distortion from interactions is a form of electro-/magneto-striction. System always elongates along direction dipoles are polarized.

Wikipedia: "*Magnetostriction (cf. electrostriction) is a property of ferromagnetic materials that causes them to change their shape or dimensions during the process of magnetization. . . . The effect was first identified in 1842 by James Joule when observing a sample of iron.*"

Exchange interactions? (i.e. including Fock)

Why is the exchange energy zero in the Hartree calculation?

Observation by Miyakawa et al [PRA **77** 061603 (2008)] was that we need to allow for momentum space to distort.

The exchange interaction can be written as:

$$E_E = \frac{\eta}{2}\int \frac{d\mathbf{x}d\mathbf{k}d\mathbf{k}'}{(2\pi)^6}\tilde{U}_{\rm dd}(\mathbf{k}-\mathbf{k}')W(\mathbf{x},\mathbf{k})W(\mathbf{x},\mathbf{k}'),$$

where $\tilde{U}_{\rm dd}(\mathbf{k}) = \frac{1}{3}C_{\rm dd}(3\cos^2\theta_{\mathbf{k}}-1)$ is the Fourier transform of $U_{\rm dd}(\mathbf{r})$.

As a simple example, consider a homogeneous system of volume $\mathcal{V}$ with

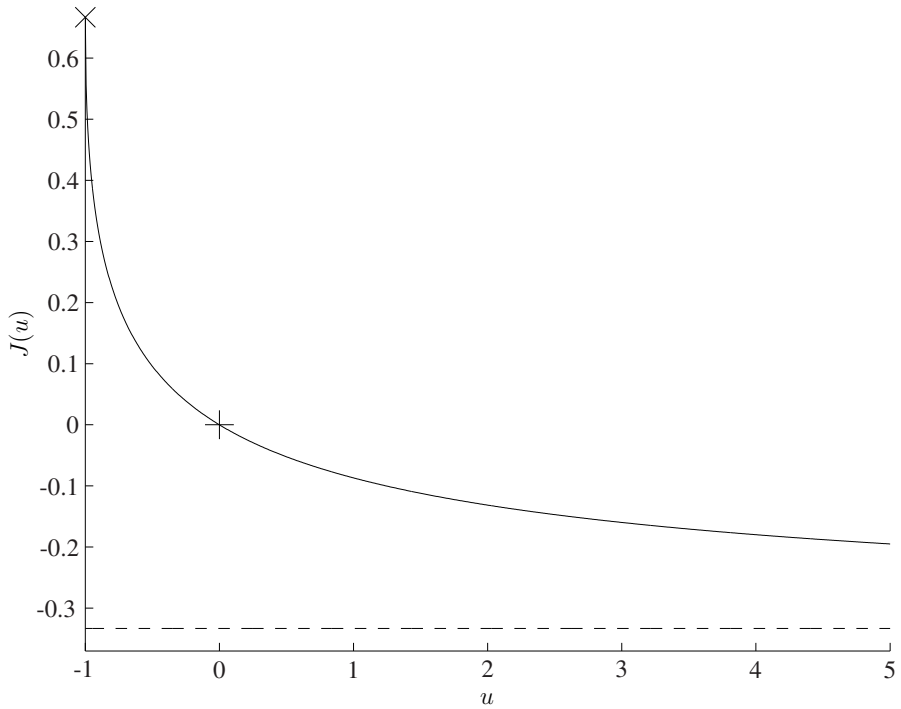
$$W(\mathbf{x},\mathbf{k}) = \theta([6\pi^2 n]^{2/3} - \frac{1}{\alpha}k_\rho^2 - \alpha^2 k_z^2),$$

where α parameterizes the momentum distortion. In this case the direct energy is zero and

$$E_E = -\frac{C_{\rm dd}\mathcal{V}}{2}J(\alpha^3-1)n^2, \qquad \text{(taken } \eta\text{=-1)}$$

where

$$J(u) = \frac{1}{u}\left[\sqrt{1+u}\frac{\sinh^{-1}\sqrt{u}}{\sqrt{u}} - 1\right] - \frac{1}{3}$$



In this case the exchange interactions compete against the kinetic energy (which itself prefers $\alpha = 1$)

$$E_{\text{kin}} = \frac{\mathcal{V}}{5} E_F n \left(\frac{1}{\alpha^2} + 2\alpha \right),$$

leading to a value of $\alpha \leq 1$ i.e. momentum distribution distorts along k_z: momentum space magnetostriction.

HF vs F and Observations:

- Miyakawa treatment can be extended to trapped system ($T = 0$, [see PRA **77** 061603 (2008)]) are predicts both momentum and spatial distortion.
- HF treatment does not prediict $\lambda_{\rm crit} \approx 5$ above which the system is stable.

Direct interactions	$\rightarrow$ position space distortion
Exchange interactions	$\rightarrow$ momentum space distortion

To explore quantum statistical effects need to go to $T \neq 0$ to apply theory to a normal Bose gas for comparison.

General ($T \neq 0$) Semiclassical Treatment

Hartree-Fock semiclassical treatment is[4]

$$\begin{aligned} W(\mathbf{x},\mathbf{k}) &= \frac{1}{e^{[\epsilon(\mathbf{x},\mathbf{k})-\mu]/k_BT}-\eta} \\ \epsilon(\mathbf{x},\mathbf{k}) &= \frac{\hbar^2k^2}{2m}+V(\mathbf{x})+2gn(\mathbf{x})+\Phi_D(\mathbf{x})+\eta\Phi_E(\mathbf{x},\mathbf{k}) \end{aligned}$$

where $g = 0$ for Fermions and we have introduced the direct and exchange interaction terms

$$\begin{aligned} \Phi_D(\mathbf{x}) &= \int \frac{d\mathbf{x}'d\mathbf{k}'}{(2\pi)^3}U_{\rm dd}(\mathbf{x}-\mathbf{x}')W(\mathbf{x}',\mathbf{k}') = \int d\mathbf{x}'\, U_{\rm dd}(\mathbf{x}-\mathbf{x}')n(\mathbf{x}'), \\ \Phi_E(\mathbf{x},\mathbf{k}) &= \int \frac{d\mathbf{k}'}{(2\pi)^3}\tilde{U}_{\rm dd}(\mathbf{k}-\mathbf{k}')W(\mathbf{x},\mathbf{k}') \end{aligned}$$

These equations have to be solved self-consistently for the Wigner function.

[4] Obtained variationally by minimizing the free energy. Also assuming a quadratic Hamiltonian (HF) and constraining the total number of atoms.

General Hartree theory

Obtained by neglecting the exchange dipolar term (but keep Fock for contact). In this case

$$\epsilon(\mathbf{x},\mathbf{k}) = \frac{\hbar^2 k^2}{2m} + V_{\rm eff}(\mathbf{x})$$

with

$$V_{\rm eff}(\mathbf{x}) = V(\mathbf{x}) + 2gn(\mathbf{x}) + \Phi_D(\mathbf{x})$$

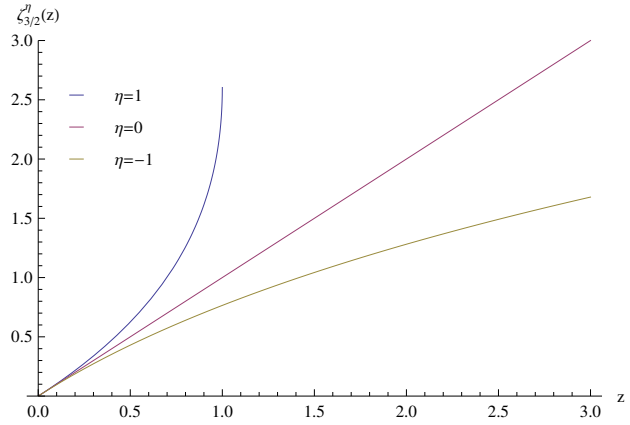
The simple k-dependence allows us to integrate for density

$$n(\mathbf{x}) = \int \frac{d\mathbf{k}}{(2\pi)^3} W(\mathbf{x},\mathbf{k}) = \frac{1}{\lambda_{\rm dB}^3}\zeta_{3/2}^{\eta}\left(e^{[\mu - V_{\rm eff}(\mathbf{x})]/k_B T}\right)$$

where $\lambda_{\rm dB} = h/\sqrt{2\pi m k_B T}$ and

$$\begin{aligned}\zeta_{\alpha}^{\eta}(z) &= \sum_{j=1}^{\infty} \eta^{j-1} z^j / j^{\alpha} \\ &= \frac{1}{\Gamma(\alpha)} \int_0^{\infty} \frac{t^{\alpha-1}}{e^t/z - \eta} dt.\end{aligned}$$

is the polylogarithm function [aka Bose ($\eta = 1$) or Fermi ($\eta = -1$) functions and



polylogrithm functions

Thus the Hartree solution can be obtained via $n(\mathbf{x})$ [i.e. we don't need $W(\mathbf{x}, \mathbf{k})$].

Notes

- For $T = 0$ Fermions we have

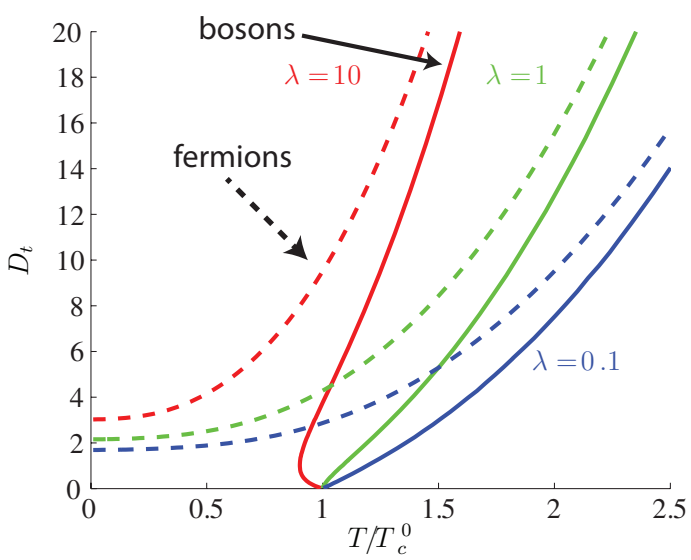
$$W(\mathbf{x}, \mathbf{k}) = \theta[\mu - \epsilon(\mathbf{x}, \mathbf{k})] \rightarrow \text{basis of variational treatments}$$

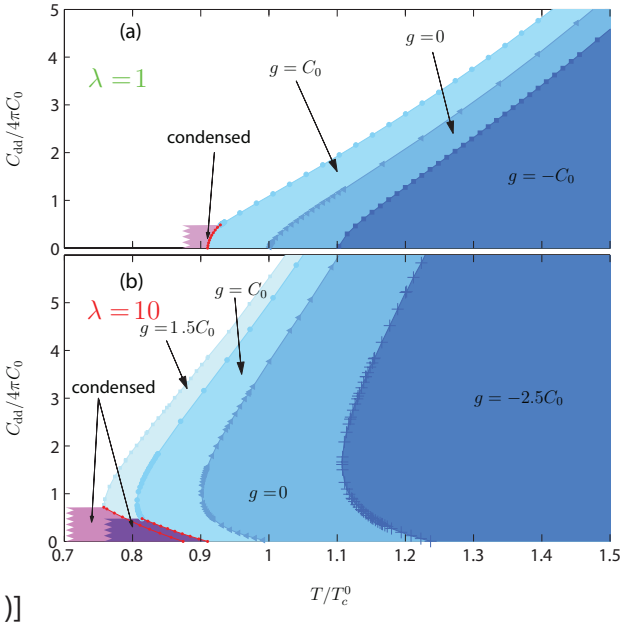
- $\Phi_D(\mathbf{x})$ is most easily calculated using the convolution theorem

$$\Phi_D(\mathbf{x}) = \mathcal{F}^{-1}\left\{\tilde{U}_{\mathrm{dd}}(\mathbf{k})\mathcal{F}\{n(\mathbf{x})\}\right\}$$

Hartree results

- Stability boundaries strikingly different for bosons and fermions
- Saturated Bose gas is fragile
- Double valued instability line emerges for bosons in pancake traps.





[From Bisset et al., PRA 83, 061602(R) (2011)]

General Hartree-Fock theory

HF calculations for trapped system are demanding but are tractable.

Simple characterization of magneto-striction effects is through the rms widths

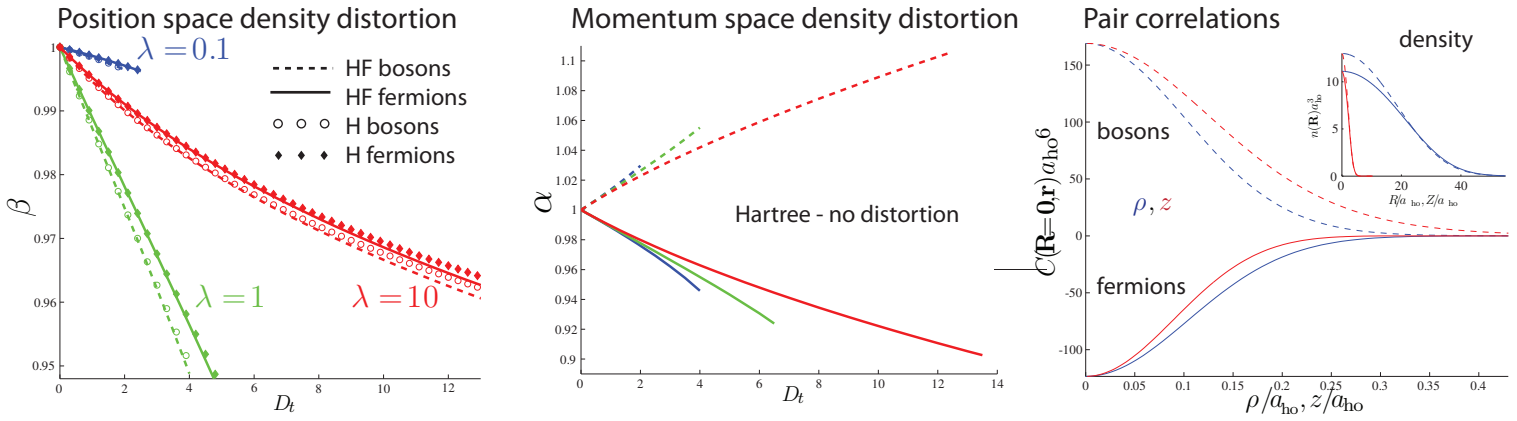
$$\sigma_\nu = \left[\frac{1}{N} \int \frac{d\mathbf{x} d\mathbf{k}}{(2\pi)^3} \nu^2 W(\mathbf{x}, \mathbf{k}) \right]^{1/2},$$

with momentum and position space density distortions defined as

$$\alpha \equiv \frac{\sigma_{k_x}}{\sigma_{k_z}}, \qquad \beta \equiv \frac{1}{\lambda} \frac{\sigma_x}{\sigma_z},$$

Also consider the pair correlation function

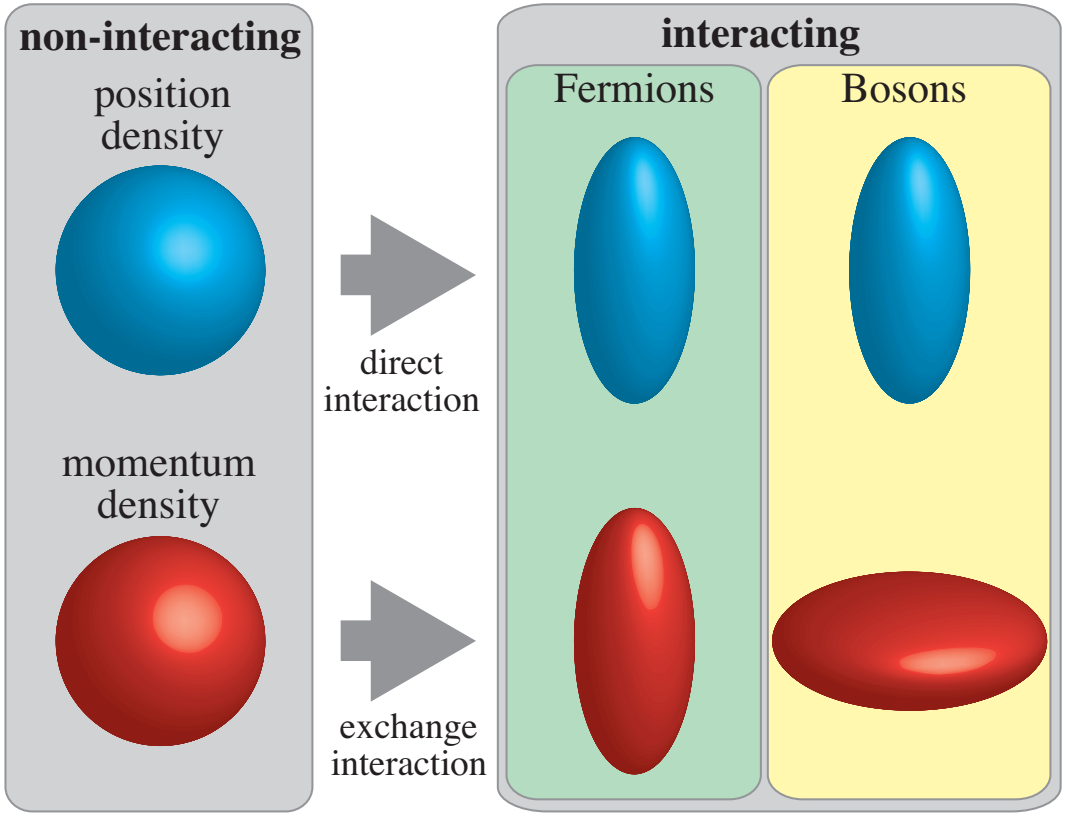
$$C(\mathbf{R}, \mathbf{r}) = G^{(2)}(\mathbf{R}, \mathbf{r}) - n(\mathbf{R} + \frac{1}{2}\mathbf{r}) n(\mathbf{R} - \frac{1}{2}\mathbf{r}) = \eta \left| \int \frac{d\mathbf{k}}{(2\pi)^3} W(\mathbf{R}, \mathbf{k}) e^{i\mathbf{k}\cdot r} \right|^2$$



[Adapted from Baillie et al., PRA **86**, 023605 (2012)]

Hartree vs. Fock Observations (part 2):

Direct interactions	$\rightarrow$ position space distortion **(prolate)**
Exchange interactions	$\rightarrow$ momentum space distortion: bosons — oblate; fermions — prolate



Extensions and other work

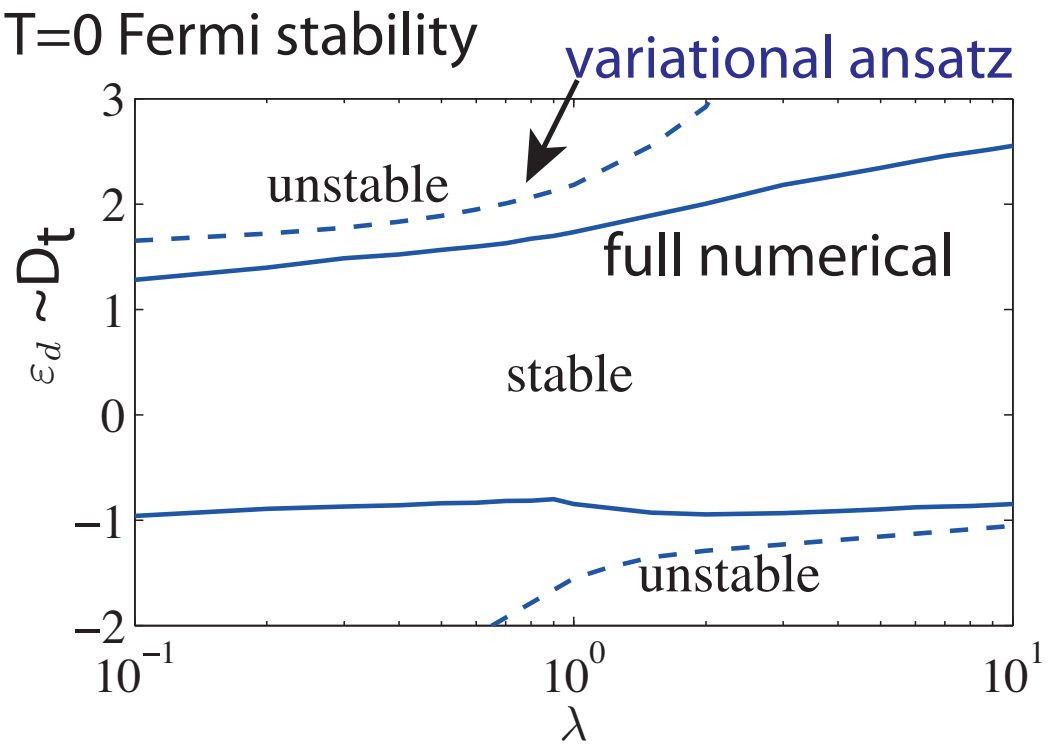
- Simplified variational treatments for trapped systems at finite T (see work by Nikuni and coworkers), and multicomponent systems [Bienias, PRA **88**, 043604 (2013)]

- Possible to use semiclassical theory to consider excitations and expansion dynamics [e.g. T Sogo et al., NJP **11,** 055017 (2009)]

- Much simpler to implement: a local HF theory [Baillie et al PRA **86**, 041603 (2012)] based on idea of a local momentum distortion:

$$\epsilon(\mathbf{x},\mathbf{k}) = \frac{\hbar^2}{2m}\left[\kappa_\rho(\mathbf{x})k_\rho^2 + \kappa_z(\mathbf{x})k_z^2\right] + V_{\rm eff}(\mathbf{x}).$$

Variational vs full calculations: what next?



[From Zhang PRA 80, 053614 (2009)]

$T = 0$ trapped fermions with pure DDIs

4 Dipolar Bose-Einstein Condensates

Gross-Pitaevskii equation (GPE)

From the usual GPE equation the replacement $g\delta(\mathbf{r}) \rightarrow g\delta(\mathbf{r}) + U_{\rm dd}(\mathbf{r})$ gets us the non-local (dipolar) GPE:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + (V + g|\psi|^2 + \Phi_{\rm dd})\psi$$

where $\Phi_{\rm dd}(\mathbf{x}) = \int d\mathbf{x}'\, U_{\rm dd}(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x}')|^2$ (c.f. Φ_D). The condensate wave function ψ is normalized to N.

With time-independent form (for ground states) of

$$\mu\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + (V + g|\psi|^2 + \Phi_{\rm dd})\psi,$$

where μ is the chemical potential. Validations of the dipolar GPE against diffusion Monte-Carlo were performed by Bohn, Blume and co-workers (also see Astrakharchik).

Condensate energy functional

The condensate energy functional is

$$E[\psi] = \int d\mathbf{x}\, \psi^*(\mathbf{x}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + \frac{1}{2}g|\psi(\mathbf{x})|^2 + \frac{1}{2}\Phi_{\rm dd}(\mathbf{x}) \right] \psi(\mathbf{x})$$

The time-independent GPE can be derived by minimizing E subject to the normalization constraint

$$N = \int d\mathbf{x}|\psi(\mathbf{x})|^2,$$

which introduces μ as a Lagrange multiplier.

Note both E and N are constants of motion under evolution with the time-dependent GPE [unless $V = V(\mathbf{x}, t)$].

Thomas-Fermi (TF) ground state

Contact case:

The TF solution, valid for $Na/a_{\rm ho} \gg 1$ where interactions dominate, is obtained by neglecting the kinetic energy. Has an inverted parabola form:

$$|\psi|^2_{\rm TF} = \begin{cases} \frac{\mu - V}{g}, & \text{for } \mu > V \\ 0 & \text{otherwise} \end{cases}$$
$$\rightarrow \; n_{\rm peak}\left(1 - \frac{x^2}{R_x^2} - \frac{y^2}{R_y^2} - \frac{z^2}{R_z^2}\right)$$

with $n_{\rm peak} = \mu/g = 15N/8\pi R_x R_y R_z$, and the TF *radius* $R_x = \sqrt{2\mu/m\omega_x^2}$ etc.

Dipolar case:

O'Dell and coworkers showed [PRL **92**, 250401 (2004); also see van Bijnen et al PRA (2010)] that despite the nonlocal potential $\Phi_{\rm dd}$, the **dipolar TF solution is of the same parabolic form!** However, the TF radii are not as simply related to the trap as in the contact case.

Dipolar TF solution: $\Phi_{\rm dd}$

Key point: for a density of parabolic form $\Phi_{\rm dd}$ is quadratic in (x, y, z).

For the cylindrical case $R_\rho = R_x = R_y$ and let $\kappa \equiv R_\rho/R_z$ be the TF anisotropy (c.f. trap anisotropy $\lambda = \omega_z/\omega_\rho$). For the inverted parabola form $|\psi|^2_{\rm TF}$**:**

$$\Phi^{\rm in}_{\rm dd}(\mathbf{x}) = \frac{n_{\rm peak} C_{\rm dd}}{3}\left[\frac{\rho^2}{R_\rho^2} - \frac{2z^2}{R_z^2} - f(\kappa)\left(1 - \frac{3}{2}\frac{\rho^2 - 2z^2}{R_\rho^2 - R_z^2}\right)\right], \quad \text{valid inside condensate}$$

where $f(\kappa)$ [$= \frac{1+2\kappa^2}{1-\kappa^2} - \frac{3\kappa^2 \operatorname{arctanh}\sqrt{1-\kappa^2}}{(1-\kappa^2)^{3/2}}$] was introduced earlier.

Outside the condensate (i.e. where $\rho^2/R_\rho^2 + z^2/R_z^2 > 1$) the asymptotic expression for large distances $|\mathbf{x}|$ is basically that of an N atom dipole:

$$\Phi^{\rm out}_{\rm dd}(\mathbf{x}) = \frac{N C_{\rm dd}}{4\pi|\mathbf{x}|^3}\left[\overbrace{\left(1 - 3\cos^2\theta\right)}^{\text{giant dipole}} + \overbrace{\frac{R_\rho^2 - R_z^2}{|\mathbf{x}|^2}\left(\frac{9}{14} - \frac{45}{7}\frac{z^2}{|\mathbf{x}|^2} + \frac{15}{2}\frac{z^4}{|\mathbf{x}|^4}\right)}^{\text{shape dependent higher multipole}} + O\left(\frac{R_\rho, R_z}{|\mathbf{x}|}\right)^4\right],$$

Dipolar TF solution: μ and R

The TF solution is then obtained by solving

$$\mu = V(\mathbf{x}) + g|\psi(\mathbf{x})|^2_{\rm TF} + \Phi_{\rm dd}(\mathbf{x}).$$

Solving for the constant terms gives the chemical potential

$$\mu = g n_{\rm peak}[1 - \epsilon_{\rm dd} f(\kappa)].$$

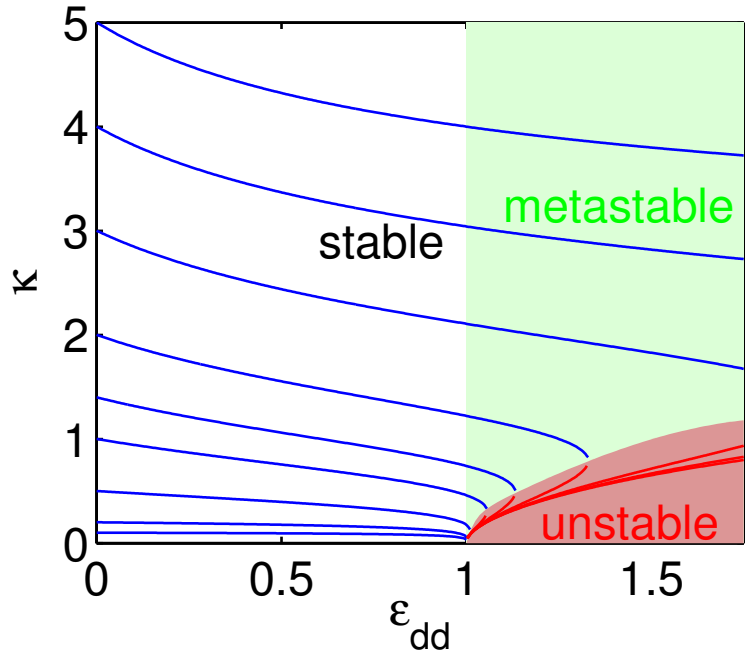
Solving for ρ^2 and z^2 terms gives

$$R_\rho = \left[\frac{15gN\kappa}{4\pi m\omega_\rho^2}\left\{1 + \epsilon_{\rm dd}\left(\frac{3\kappa^2 f(\kappa)}{2(1-\kappa^2)} - 1\right)\right\}\right]^{1/5},$$

and hence $R_\rho = \kappa R_z$, where κ is given by a solution of the transcendental equation

$$3\kappa^2\left[\frac{\epsilon_{\rm dd} f(\kappa)}{1-\kappa^2}\left(\frac{\lambda^2}{2} + 1\right) - 1\right] + (\epsilon_{\rm dd} - 1)(\kappa^2 - \lambda^2) = 0.$$

Stability of TF solution



- For $\epsilon_{\rm dd} < 1$ there is a single stable solution (global minimum)
- For $\epsilon_{\rm dd} > 1$ there is a global minimum with $\kappa = 0$ (needle shaped solution).
  - For $\lambda < \lambda_{\rm crit} = 5.17$ then there is a finite $\epsilon_{\rm dd}^{\rm crit}$ below which there is a metastable (local min) and unstable (saddle pt) solutions.
    - At $\epsilon_{\rm dd} = \epsilon_{\rm dd}^{\rm crit}$ a quadrupolar mode goes soft.
  - For $\lambda > \lambda_{\rm crit}$, then $\epsilon_{\rm dd}^{\rm crit} = \infty$

Other TF properties

Must be cautious applying this theory beyond $\epsilon_{\rm dd} = 1$:

- For $\epsilon_{\rm dd} > 1$ phonon instabilities can occur (see Bogoliubov treatment later)
  - Also, short wavelength roton instabilities can occur (see roton discussion later)
- The energy of a cylindrical parabolic state $|\psi|^2_{\rm TF}$ for any R_ρ and R_z is (neglecting kinetic)

$$E = \overbrace{\frac{N}{14\lambda^{2/3}}\hbar\bar{\omega}\left(2\frac{R_\rho^2}{a_{\rm ho}^2} + \lambda^2\frac{R_z^2}{a_{\rm ho}^2}\right)}^{\text{trap}} + \overbrace{\frac{15N^2\hbar\bar{\omega}}{7}\frac{a_{\rm ho}^3}{R_\rho^2 R_z}\left(\frac{a}{a_{\rm ho}} - \frac{a_{\rm dd}}{a_{\rm ho}}f(\kappa)\right)}^{\text{contact+DDIs}}$$

Hydrodynamic description of dynamics

- Hydrodynamics description following [Castin & Dum, PRL **77**, 5315 (1996)]. Noting that the wavefunction can be written as

$$\psi = \sqrt{n} e^{i\phi}$$

with velocity field

$$\mathbf{v} = \frac{\hbar}{m} \boldsymbol{\nabla} \phi,$$

the dynamics of the system in the TF regime [i.e. time dependent GPE neglecting the quantum pressure term $-\hbar^2 \nabla^2 \sqrt{n}/2m\sqrt{n}$] is

$$\begin{aligned} \frac{\partial n}{\partial t} &= -\boldsymbol{\nabla} \cdot (n\mathbf{v}), \qquad \text{continuity eq.} \\ m\frac{\partial \mathbf{v}}{\partial t} &= -\boldsymbol{\nabla} \left(\frac{mv^2}{2} + V + gn + \Phi_{\rm dd} \right) \qquad \text{Euler eq.} \end{aligned}$$

Scaling solutions to the hydrodynamic equations

A class of *scaling* solutions are given by:

$$
\begin{aligned}
n(\mathbf{x},t) &= n_0(t)\left[1-\frac{x^2}{R_x^2(t)}-\frac{y^2}{R_y^2(t)}-\frac{z^2}{R_z^2(t)}\right], \\
\mathbf{v}(\mathbf{x},t) &= \frac{1}{2}\boldsymbol{\nabla}[\alpha_x(t)x^2+\alpha_y(t)y^2+\alpha_z(t)z^2],
\end{aligned}
$$

where $n_0(t) = 15N/[8\pi R_x(t)R_y(t)R_z(t)]$, and $\alpha_j = \dot{R}_j/R_j$. Substituting the scaling solution into the continuity and Euler equations yields the solutions

$$
\begin{aligned}
\ddot{R}_x &= -\omega_x^2(t)R_x + \frac{15Ng}{4\pi m R_x R_z}\left[\frac{1}{R_x^2}-\epsilon_{\rm dd}(t)\left(\frac{1}{R_x^2}+\frac{3}{2}\frac{f(R_x/R_z)}{R_x^2-R_z^2}\right)\right], \\
\ddot{R}_z &= -\omega_z^2(t)R_z + \frac{15Ng}{4\pi m R_x^2}\left[\frac{1}{R_z^2}+2\epsilon_{\rm dd}(t)\left(\frac{1}{R_z^2}+\frac{3}{2}\frac{f(R_x/R_z)}{R_x^2-R_z^2}\right)\right],
\end{aligned}
$$

where $\omega_j(t)$ allows the description of time-dependent traps (modulation or switch off), similarly the DDI could be changed in time [via $\epsilon_{\rm dd}(t)$].

Gaussian Solution

Another useful approach is to set

$$\psi = \sqrt{\frac{N}{\pi^{3/2}\sigma_\rho^2\sigma_z a_{\rm ho}^3}}\exp\left[-\frac{1}{2a_{\rm ho}^2}\left(\frac{\rho^2}{\sigma_\rho^2}+\frac{z^2}{\sigma_z^2}\right)\right],$$

so that $|\psi|^2$ corresponds to our Gaussian ansatz used earlier with $\nu = 1$.
Evaluating the energy functional we obtain

$$E = \overbrace{\frac{N\hbar\bar{\omega}}{4}\left(\frac{2}{\sigma_\rho^2}+\frac{1}{\sigma_z^2}\right)}^{\text{kinetic}} + \overbrace{\frac{N\hbar\bar{\omega}}{4\lambda^{2/3}}(2\sigma_\rho^2+\lambda^2\sigma_z^2)}^{\text{trap}} + \overbrace{\frac{N^2\hbar\bar{\omega}}{\sqrt{2\pi}\sigma_\rho^2\sigma_z}\left(\frac{a}{a_{\rm ho}}-\frac{a_{\rm dd}}{a_{\rm ho}}f(\sigma_\rho/\sigma_z)\right)}^{\text{contact + DDIs}}.$$

This approach can be extended to dynamics by making the widths $\{\sigma_\rho, \sigma_z\}$ time-dependent variational parameters and by introducing associated variational phases.

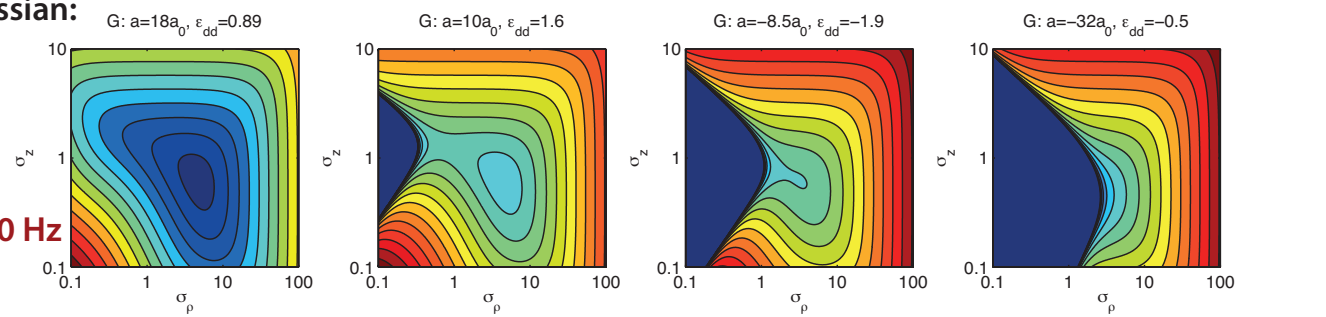
writing: $\dfrac{2E}{N\hbar\bar{\omega}} = \dfrac{1}{2}\left(\dfrac{2}{\sigma_\rho^2}+\dfrac{1}{\sigma_z^2}\right) + \dfrac{1}{2\lambda^{2/3}}(2\sigma_\rho^2+\lambda^2\sigma_z^2) + \sqrt{\dfrac{2}{\pi}}\dfrac{N}{\sigma_\rho^2\sigma_z}\dfrac{a}{a_{\rm ho}}\left(1-\epsilon_{\rm dd}f(\sigma_\rho/\sigma_z)\right),$

shows that for $Na/a_{\rm ho} \gg 1$ and $\epsilon_{\rm dd} > 1$ then global minimum is a needle solution with $\sigma_\rho \to 0$ ($E \to -\infty$).

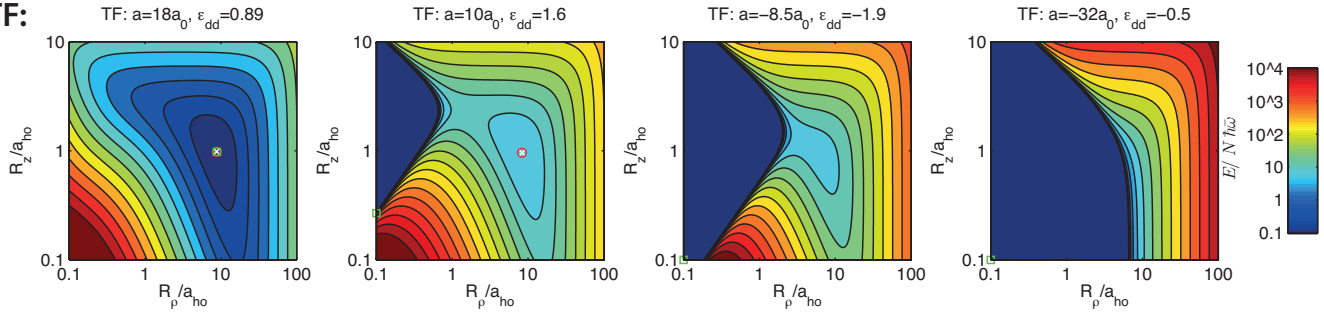
Trapped condensate stability: experimental comparison

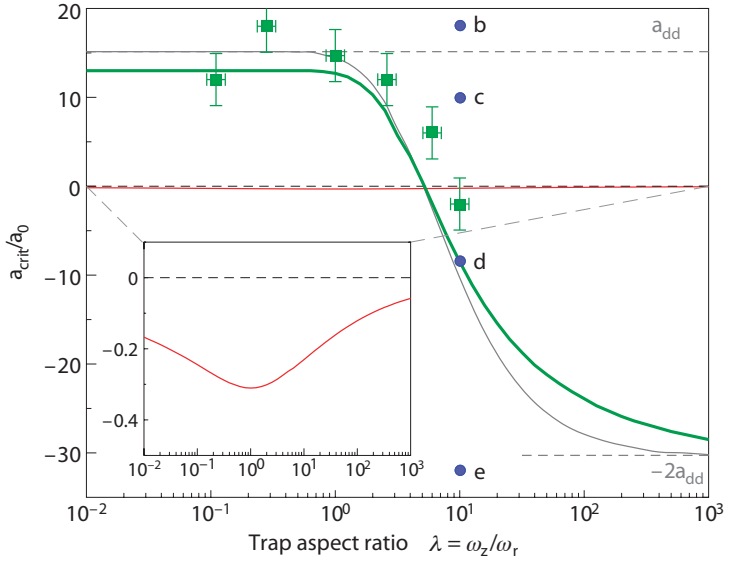
Gaussian:

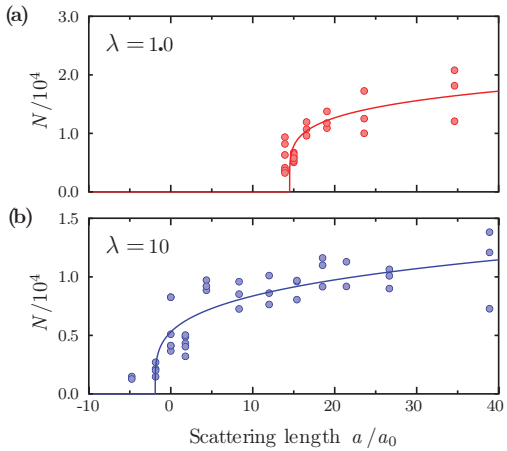
Cr-52:
$a_{dd}=16a_0$,
$\lambda=10$,
N=20e3,
$\bar{\omega}=2\pi\times800$ Hz



TF:







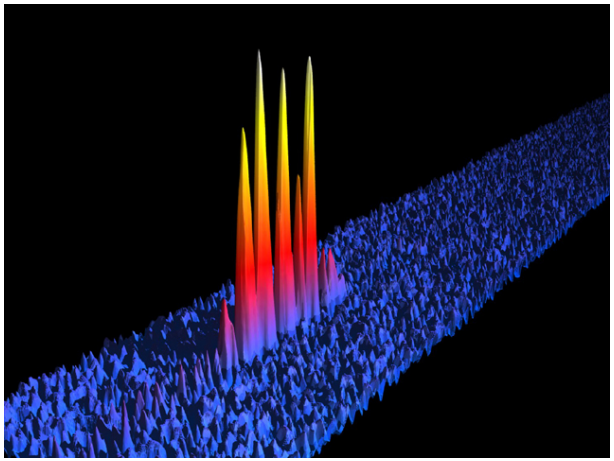
[From Nature Phys. 4, 218 (2008

Solitons

What is a soliton?

Wikipedia: *"...a self-reinforcing solitary wave (a wave packet or pulse) that maintains its shape while it travels at constant speed."*

A **dark soliton** is a localized absence of atoms (dip) in the atomic field, observed in condensates with $a > 0$. Dark solitons are constrained to propagate in the nonlinear medium (the condensate!). In contrast a **bright soliton** is a localized wave packet that can occur for a quasi-1D condensate with $a < 0$.



Train of bright solitons in ^{7}Li produced in a quasi-1D wave guide with attractive contact interactions. K.E. Strecker, G. Partridge, A.G. Truscott , and R.G. Hulet, "Formation and Propagation of Matter Wave Soliton Trains", Nature (2002)

Bright solitons in dipolar BECs

A novel prediction for dipolar condensates is the existence of 2D bright solitons [Pedri et al PRL (2005)].

Consider the Gaussian energy functional in the **absence of radial confinement**

$$E = \frac{N\hbar\omega_z}{4}\left(\frac{2}{\sigma_\rho^2}+\frac{1}{\sigma_z^2}\right)+\frac{N\hbar\omega_z}{4}\sigma_z^2+\frac{N^2\hbar\omega_z}{\sqrt{2\pi}\sigma_\rho^2\sigma_z}\left(\frac{a}{a_z}-\frac{a_{\rm dd}}{a_z}f(\sigma_\rho/\sigma_z)\right),$$

with σ_ρ, σ_z the widths in units of $a_z=\sqrt{\hbar/m\omega_z}$.

Consider the case where the z-confinement is *strong,* so that we can take $\sigma_z\approx 1$. We then get

$$E(\sigma_\rho) = \frac{N\hbar\omega_z}{4}\left(\frac{2}{\sigma_\rho^2}\right)+\frac{N^2\hbar\omega_z}{\sqrt{2\pi}\sigma_\rho^2}\left(\frac{a}{a_z}-\frac{a_{\rm dd}}{a_z}f(\sigma_\rho)\right)+\text{const.}$$

For **pure contact interactions** both kinetic and interactions terms scale as $E\sim\sigma_\rho^{-2}$, i.e. monotonic in σ_ρ, and depending on the value of Na, $E(\sigma_\rho)$ ether increases with σ_ρ (collapse instability) or decreases (expansion instability). Thus 2D solitons are not stable.

Quasi-2D condition for a bright soliton

With dipolar interactions a minimum can occur in $E(\sigma_\rho)$. Writing it as

$$E(\sigma_\rho) = \frac{N}{2}\hbar\omega_z \frac{1 + Aa - Aa_{\rm dd} f(\sigma_\rho)}{\sigma_\rho^2},$$

with $A = \frac{N}{a_z}\sqrt{\frac{2}{\pi}}$, we clearly need $E(\sigma_\rho \to 0) \to +\infty$ (to avoid collapse), i.e. [using $f(0) = 1$]

$$1 + A(a - a_{\rm dd}) > 0$$

But we also need $E(\infty) = 0^-$ to have a local minimum. Given $f(\infty) \to -2$, this means

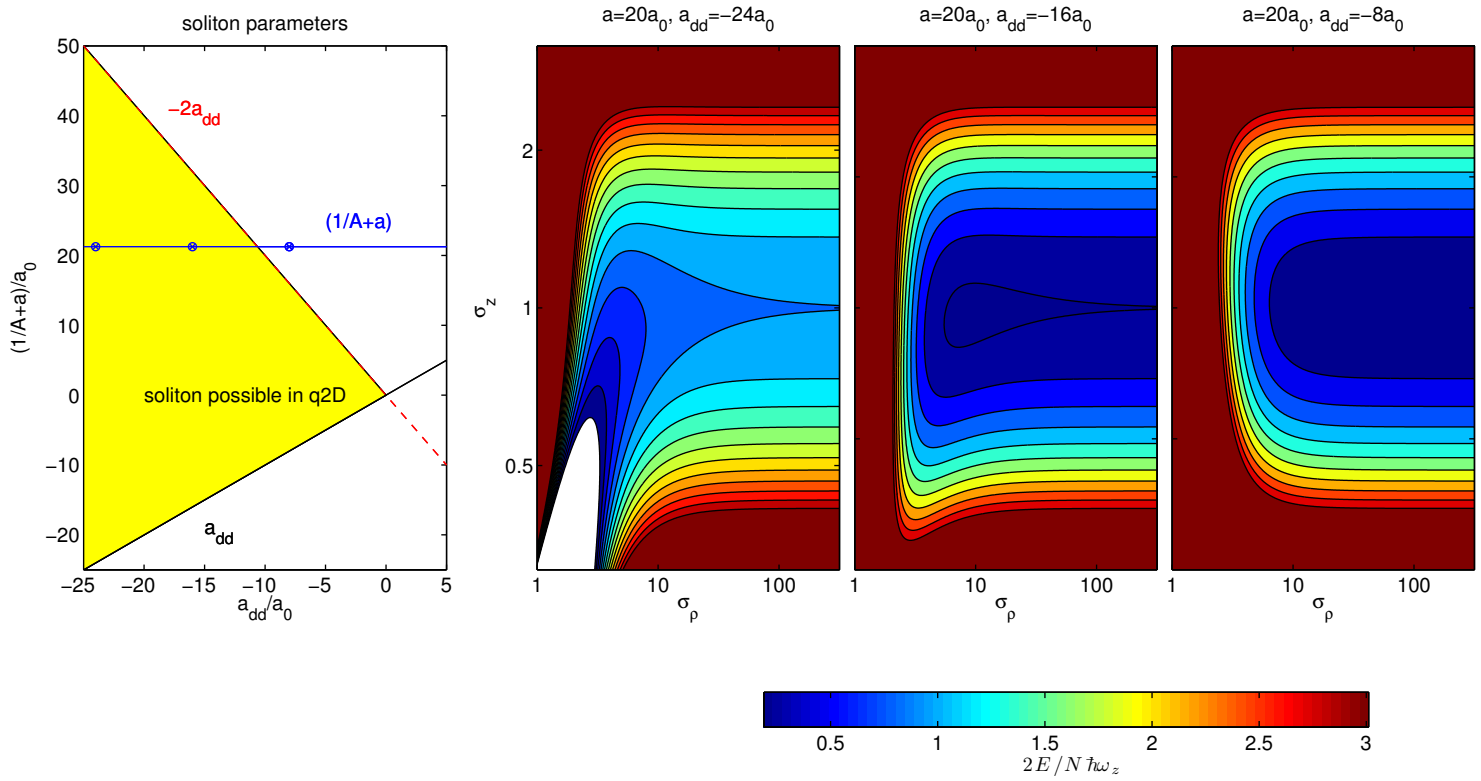
$$1 + A(a + 2a_{\rm dd}) < 0$$

Combined conditions:

$$a_{\rm dd} < \frac{1}{A} + a < -2a_{\rm dd},$$

This is only satisfied for $a_{\rm dd} < 0$, i.e. **negatively tuned dipoles.**

Example and 3D breakdown

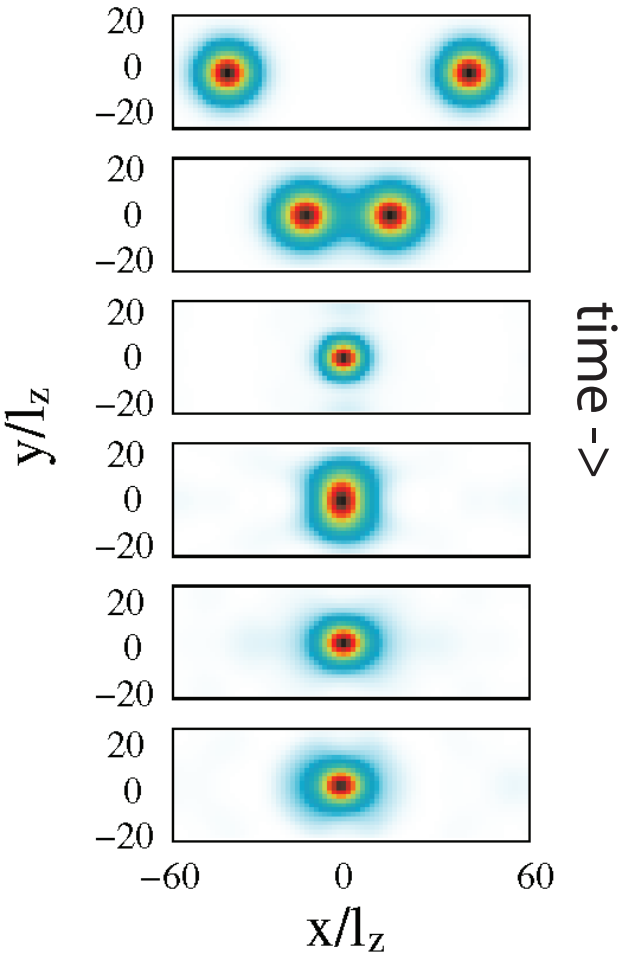


Example parameters for $a = 20\,a_0$ and $N = 10,000$ atoms with $\omega_z = 2\pi \times 700\text{s}^{-1}$.

Left: Parameters and quasi-2D conditions

Right 3 subplots: Gaussian energy function for 3 parameter sets.

Inelastic collision of two bright dipolar solitons



[From Pedri etal., PRL 2005]

Inelastic collision of solitons: quasi-2D simulation from Pedri et al., PRL (2005).

Full numerical solution of time independent GPE

A number of groups have performed full numerical calculations for the time-dependent and time-independent GPE with DDIs. We briefly review an important technique:

Cylindrical solution technique:

Seminal work by Ronen and coworkers [PRA 2006] demonstrated an accurate and efficient method for solving the dipolar GPE and Bogoliubov excitations in a cylindrical harmonic trap. Two important innovations in that work are:

1. It is necessary to take Fourier transforms to evaluate $\Phi_{\rm dd}(\mathbf{x}) = \mathcal{F}^{-1}\{\tilde{U}_{\rm dd}(\mathbf{k})\mathcal{F}\{n(\mathbf{x})\}\}$ (z transformed separately). Consider the function $F(\boldsymbol{\rho}) = e^{im\phi}f(\rho)$ with Fourier transform

$$\begin{aligned}
\tilde{f}(k_\rho,\phi_k) &= \mathcal{F}\{F\} = \int_0^\infty d\rho\,\rho\int_0^{2\pi} d\phi e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{im\phi}f(\rho) \\
&= \int_0^\infty d\rho\,\rho\int_0^{2\pi} d\phi\, e^{ik_\rho\rho\cos(\phi-\phi_k)+im\phi}f(\rho) \\
&= i^{-m}e^{im\phi_k}\int_0^\infty d\rho\,\rho\,2\pi J_m(k_\rho\rho)\,f(\rho) = 2\pi i^{-m}e^{im\phi_k}\mathcal{H}_m\{f(\rho)\}
\end{aligned}$$

where $\mathcal{H}_m\{f(\rho)\} \equiv \int_0^\infty d\rho\,\rho\,J_m(k_\rho\rho)\,f(\rho)$ is the *Hankel transform* of order m.

This can be implemented a using a Bessel quadrature.

2. Cutoff interaction potential. The k-space interaction $\tilde{U}_{\rm dd}(\mathbf{k}) = \frac{1}{3}C_{\rm dd}(3\cos^2\alpha - 1)$ is much nicer than in r-space. However the long range nature of the interaction causes phantom interactions with aliased copies of the condensate $\rightarrow$ slow convergence with grid extent. Can remedy by *cutting-off* the interaction:

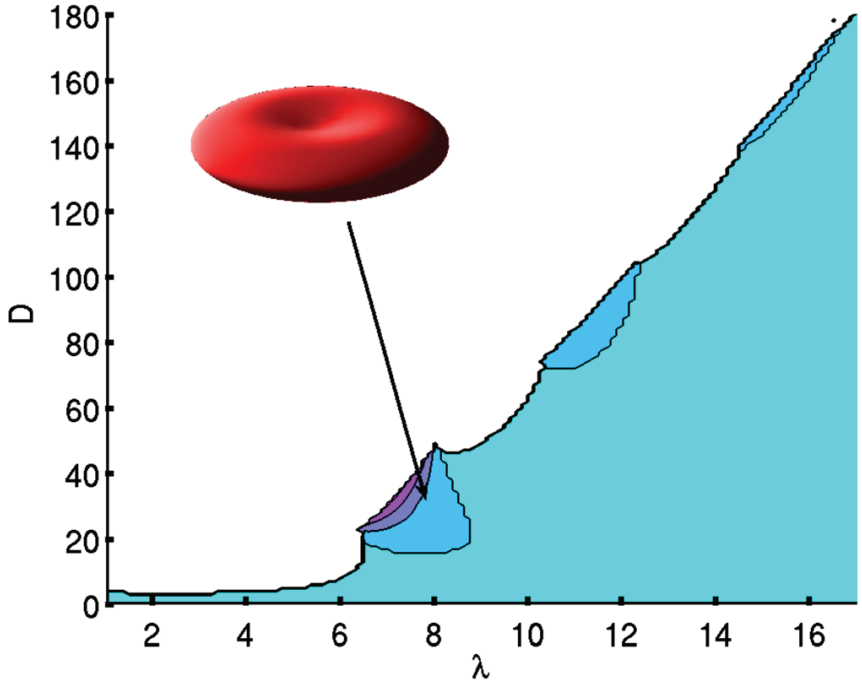
$$U^R_{\rm dd}(\mathbf{r}) \equiv \begin{cases} \frac{C_{\rm dd}}{4\pi}\frac{1-3\cos^2\theta}{r^3}, & r < R \\ 0, & \text{otherwise} \end{cases}$$

where R is the system size (e.g. grid extent). Fortunately this has an analytic transform:

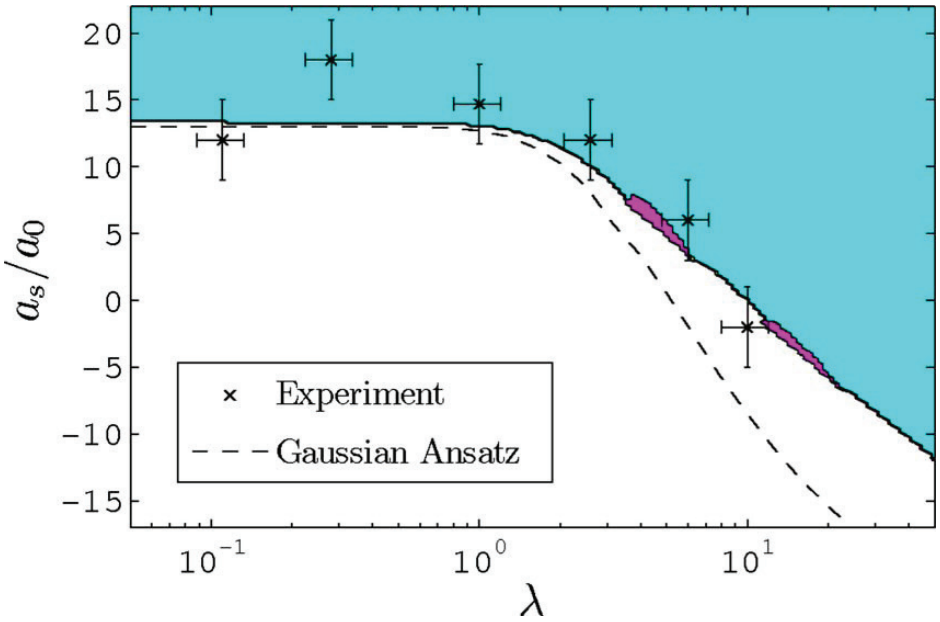
$$\tilde{U}^R_{\rm dd}(\mathbf{k}) = \tilde{U}_{\rm dd}(\mathbf{k}) \times \left[1 + 3\frac{\cos(Rk)}{R^2k^2} - 3\frac{\sin(Rk)}{R^3k^3}\right].$$

More general, e.g. cylindrical cutoffs Lu et al [PRA 2010], are beneficial for highly anisotropic systems.

GPE calculations: stability



[From Ronen PRL (2007)]

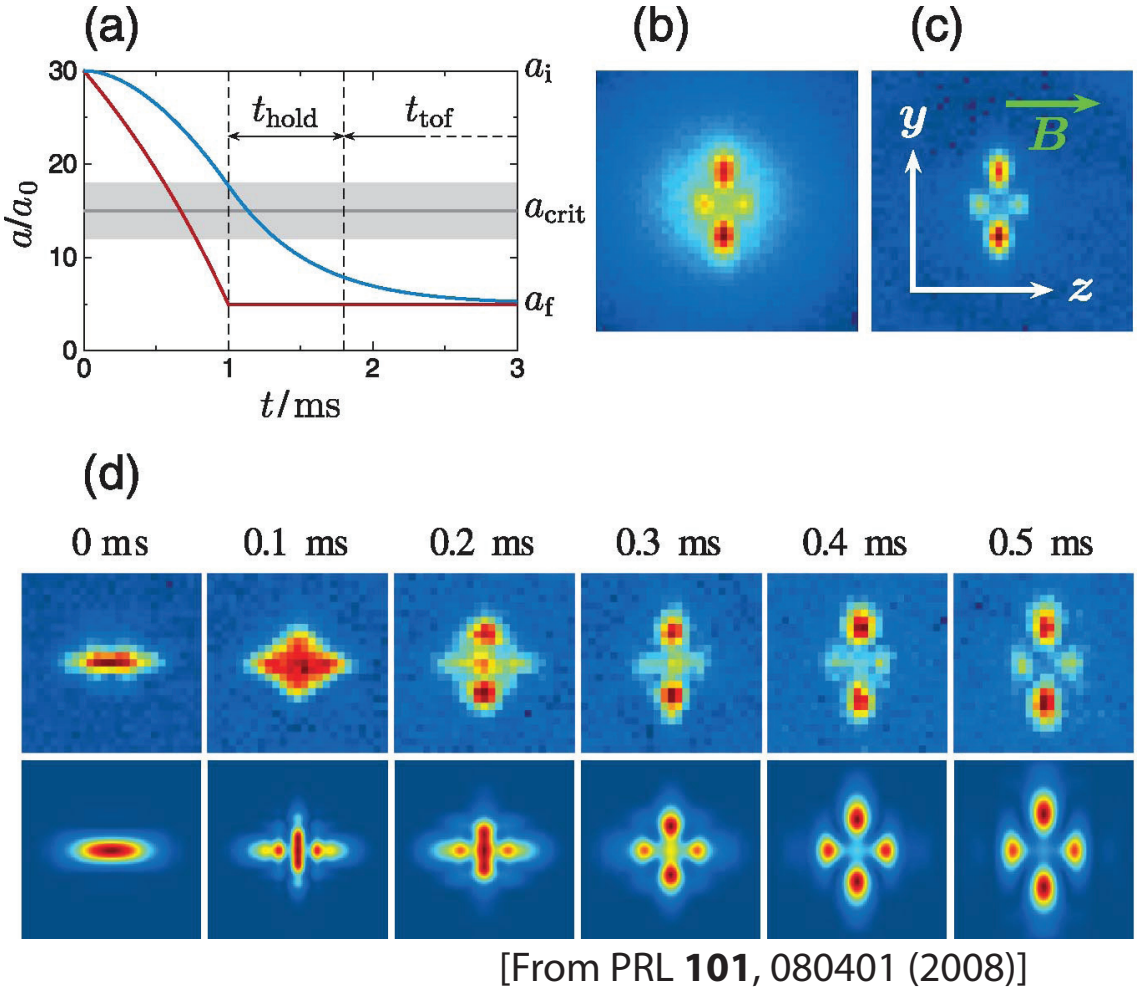


[From Wilson PRA (2009)]

LEFT: Stability diagram of a purely dipolar condensate (stable regions shaded). $D = 3Na_{\rm dd}/a_\rho$, with $a_\rho = \sqrt{\hbar/m\omega_\rho}$.

RIGHT: GPE stability diagram for parameter regime of Koch et al experiment.

Expts & GPE calculations: collapse dynamics



[From PRL **101**, 080401 (2008)]

(a) Feshbach ramp of a. (b), (c) samples images after $t_{\mathrm{hold}} = 0.4$ ms, in (c) the thermal cloud is subtracted. (d) (upper) experimental results; (lower) GPE simulations including 3-body loss. Experiments for Cr-52 in a nearly spherical trap with $\bar{\omega} \sim 2\pi \times 500$ Hz, $N \approx 20 \times 10^3$.

5 Bogoliubov theory for a dipolar condensate

Manybody Hamiltonian

For a uniform system in d-dimensions with volume $V = L^d$ the bosonic field is

$$\hat{\psi}(\mathbf{x}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{x})\hat{a}_{\mathbf{k}}, \quad \text{where} \quad \phi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}},$$

and the manybody Hamiltonian is

$$\begin{aligned}
\hat{H} &= \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x}) \frac{-\hbar^2\nabla^2}{2m} \hat{\psi}(\mathbf{x}) + \frac{1}{2}\int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')U_{\rm int}(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x}), \\
&= \sum_{\mathbf{k}} \epsilon_k^0 \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \tilde{U}_{\rm int}(\mathbf{k}_1 - \mathbf{k}_3)\, \hat{a}_{\mathbf{k}_1}^\dagger \hat{a}_{\mathbf{k}_2}^\dagger \hat{a}_{\mathbf{k}_3}\hat{a}_{\mathbf{k}_4}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4},
\end{aligned}$$

where $\epsilon_k^0 = \hbar^2 k^2/2m$, $\tilde{U}_{\rm int}(\mathbf{k}) = g + \tilde{U}_{\rm dd}(\mathbf{k})$.

Quadratic Hamiltonian for condensed system

Assuming a condensate we set $\hat{a}_0,\, \hat{a}_0^\dagger \to \sqrt{N_0}$. Substituting this into the Hamiltonian and only keeping terms of order N_0^2 and N_0 , the interaction part becomes

$$\hat{H}_{\rm int} \approx \frac{1}{2V}\left[N_0^2 \tilde{U}_{\rm int}(0) + N_0 \sum_{\mathbf{k}\neq\mathbf{0}} \left\{ \overbrace{\tilde{U}_{\rm int}(0)\left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}\right)}^{\text{Direct}} + \tilde{U}_{\rm int}(\mathbf{k}) (\overbrace{\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}}^{\text{Exchange}} + \overbrace{\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger + \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}}}^{\text{Pair Excitation}}) \right\} \right]$$

To consider states of fixed total number we use $N \approx N_0 + \frac{1}{2}\sum_{\mathbf{k}\neq\mathbf{0}} \left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}\right)$, to replace $N_0 \to N$, which gives

$$\hat{H}_{\rm int} \approx \frac{1}{2V}\left[N^2 \tilde{U}_{\rm int}(0) + N \sum_{\mathbf{k}\neq\mathbf{0}} \left\{ \tilde{U}_{\rm int}(\mathbf{k}) \left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}\right) + \tilde{U}_{\rm int}(\mathbf{k}) \left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger + \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}}\right) \right\} \right],$$

i.e. cancelling the direct interaction term. Setting $n = N/V$ we have

$$\hat{H} = \frac{N^2 \tilde{U}_{\rm int}(0)}{2V} + \frac{1}{2}\sum_{\mathbf{k}\neq\mathbf{0}} \left[\left(\epsilon_k^0 + n\tilde{U}_{\rm int}(\mathbf{k})\right) \left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}\right) + n\tilde{U}_{\rm int}(\mathbf{k}) \left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger + \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}}\right) \right],$$

Diagonalizing quadratic Hamiltonian

The quasiparticle transformations $\hat{a}_{\mathbf{k}} = u_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} - v_{\mathbf{k}}\hat{\alpha}^{\dagger}_{-\mathbf{k}}$, with inverse transformation $\hat{\alpha}_{\mathbf{k}} = u_{\mathbf{k}}\hat{a}_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^{\dagger}_{-\mathbf{k}}$. Require $u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 1$ to ensure the transformation is canonical (i.e. $[\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}^{\dagger}_{\mathbf{k}}] = 1$).

$$\begin{aligned}
\hat{H} \;=\; & \tfrac{1}{2}\tilde{U}_{\rm int}(0)n^2V + \sum_{\mathbf{k}\neq 0}\left[\left(\epsilon^0_k + n\tilde{U}_{\rm int}(\mathbf{k})\right)v^2_{\mathbf{k}} - n\tilde{U}_{\rm int}(\mathbf{k})u_{\mathbf{k}}v_{\mathbf{k}}\right] \\
& + \tfrac{1}{2}\sum_{\mathbf{k}\neq 0}\left[\left(\epsilon^0_k + n\tilde{U}_{\rm int}(\mathbf{k})\right)\left(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}\right) - 2n\tilde{U}_{\rm int}(\mathbf{k})u_{\mathbf{k}}v_{\mathbf{k}}\right]\left(\hat{\alpha}^{\dagger}_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}^{\dagger}_{-\mathbf{k}}\hat{\alpha}_{-\mathbf{k}}\right) \\
& + \tfrac{1}{2}\sum_{\mathbf{k}\neq 0}\left[n\tilde{U}_{\rm int}(\mathbf{k})\left(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}\right) - 2\left(\epsilon^0_k + n\tilde{U}_{\rm int}(\mathbf{k})\right)u_{\mathbf{k}}v_{\mathbf{k}}\right]\left(\hat{\alpha}^{\dagger}_{\mathbf{k}}\hat{\alpha}^{\dagger}_{-\mathbf{k}} + \hat{\alpha}_{\mathbf{k}}\hat{\alpha}_{-\mathbf{k}}\right).
\end{aligned}$$

The last off-diagonal term can be eliminated by choosing $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ to satisfy

$$n\tilde{U}_{\rm int}(\mathbf{k})\left(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}\right) = 2\left(\epsilon^0_k + n\tilde{U}_{\rm int}(\mathbf{k})\right)u_{\mathbf{k}}v_{\mathbf{k}}.$$

Taking $u_{\mathbf{k}} = \cosh\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sinh\theta_{\mathbf{k}}$ [ensures $u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 1$] and solving above Eq:

$$\tanh 2\theta_{\mathbf{k}} = \frac{n\tilde{U}_{\rm int}(\mathbf{k})}{\epsilon^0_k + n\tilde{U}_{\rm int}(\mathbf{k})}.$$

Using $\cosh(\theta) = \sqrt{\frac{1}{2}[\cosh 2\theta - 1]}$, $\cosh 2\theta = \cosh[\operatorname{arctanh}(x)] = \frac{1}{\sqrt{1-x^2}}$ with $x = n\tilde{U}/[\epsilon + n\tilde{U}]$ etc., we get

$$v_{\mathbf{k}}^2 = u_{\mathbf{k}}^2 - 1 = \frac{1}{2}\left(\frac{\epsilon_k^0 + n\tilde{U}_{\rm int}(\mathbf{k})}{\epsilon_{\mathbf{k}}} - 1\right),$$

where

$$\epsilon_{\mathbf{k}} = \sqrt{\left(\epsilon_k^0 + n\tilde{U}_{\rm int}(\mathbf{k})\right)^2 - \left(n\tilde{U}_{\rm int}(\mathbf{k})\right)^2}.$$

Thus we have the Bogoliubov description of the excitations:

$$\epsilon = \sqrt{\epsilon_k^0\left(\epsilon_k^0 + 2n\tilde{U}_{\rm int}(\mathbf{k})\right)}, \tag{1}$$

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(\frac{\epsilon_k^0 + n\tilde{U}_{\rm int}(\mathbf{k})}{\epsilon_{\mathbf{k}}} + 1\right)}, \tag{2}$$

$$v_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(\frac{\epsilon_k^0 + n\tilde{U}_{\rm int}(\mathbf{k})}{\epsilon_{\mathbf{k}}} - 1\right)}\,\mathrm{sign}(\tilde{U}_{\rm int}(\mathbf{k})) \tag{3}$$

Note: Assuming stable, i.e. $\epsilon_k^0 + n\tilde{U}_{\rm int}(k) > 0$, we have $\theta_k > 0$ for repulsive interactions, $\theta_{\mathbf{k}} = 0$ for non-interacting and $\theta_k < 0$ for attractive interactions.

In the Bogoliubov basis the quadratic Hamiltonian is diagonal

$$\hat{H} = \frac{1}{2}\tilde{U}_{\rm int}(0)n^2V - \tfrac{1}{2}\sum_{\mathbf{k}\neq\mathbf{0}}\left(\epsilon_k^0 + n\tilde{U}_{\rm int}(\mathbf{k}) - \epsilon_{\mathbf{k}}\right) + \tfrac{1}{2}\sum_{\mathbf{k}\neq 0}\epsilon_{\mathbf{k}}\left(\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^\dagger\hat{\alpha}_{-\mathbf{k}}\right).$$

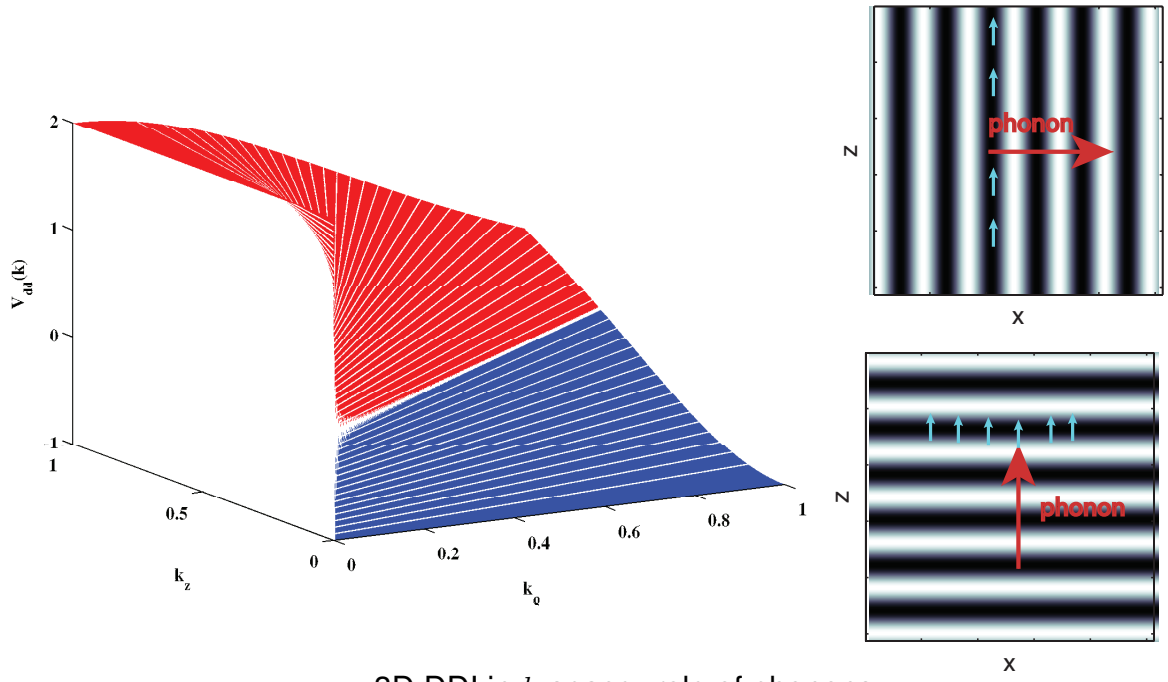
- These results all revert to the usual contact case if we replace $\tilde{U}_{\rm int}(\mathbf{k}) \to g$.
- This can be generalized to the trapped case and solved using the techniques discussed for the GPE (e.g. see Ronen et al., PRA (2006)).

Stability of a uniform 3D dipolar BEC

A necessary for condition for stability is that the system is dynamically and thermodynamically stable. The requires that all ϵ are real and positive.

For a BEC with DDIs $\tilde{U}_{\rm int}(\mathbf{k}) = \tilde{U}_{\rm int}(\theta_{\mathbf{k}})$ and we need to concern ourselves with $\theta_{\mathbf{k}} = \pi/2$ where $\tilde{U}_{\rm int} = g(1-\epsilon_{\rm dd})$ [cf. $\theta_{\mathbf{k}} = 0$ where $\tilde{U}_{\rm int} = g(1+2\epsilon_{\rm dd})$]. The Bogoliubov spectrum is real and positive if $\tilde{U}_{\rm int} \geq 0$, i.e.

$$\epsilon_{\rm dd} \leq 1, \quad \text{(stabilty condition 3D uniform)}$$



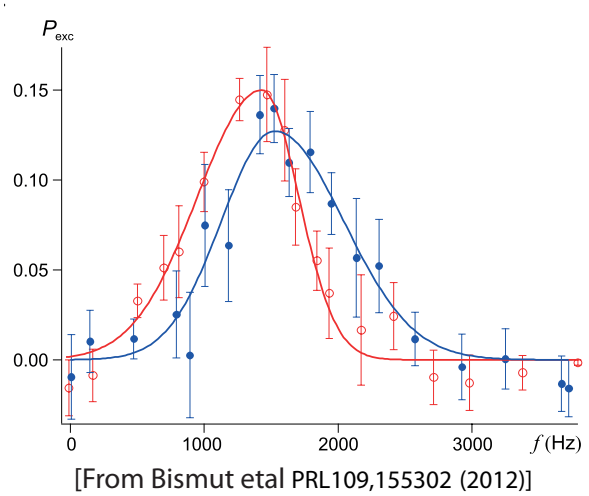
3D DDI in k-space: role of phonons.

Speed of sound

In the 3D uniform system ($\epsilon_{\rm dd} < 1$) the excitation spectrum is linear (phonon like) for small k. However the slope, and hence the speed of sound c is *anisotropic*.

$$c_\rho = \lim_{k_\rho \to 0} \frac{\epsilon(k_\rho, k_z = 0)}{k_\rho} = c_0\sqrt{1-\epsilon_{\rm dd}},$$
$$c_z = \lim_{k_z \to 0} \frac{\epsilon(k_\rho = 0, k_z)}{k_z} = c_0\sqrt{1+2\epsilon_{\rm dd}},$$

where $c_0 = \sqrt{gn/m}$ is the speed of sound for the contact interactions alone.



[From Bismut etal PRL109,155302 (2012)]

Bragg spectroscopy at fixed momentum transfer (•) along z, (○) along x.

6 Quasi-2D System

Quasi-2D interaction

Assume tight confinement along z provided by $V = \frac{1}{2}m\omega_z^2 z^2$ and assume the condensate and excitations can all be taken as

$$\psi \sim \psi(\boldsymbol{\rho})\sqrt{n_{\rm ho}(z)},$$

where $n_{\rm ho}(z) = \frac{1}{l_z\sqrt{\pi}}e^{-z^2/l_z^2}$ is the oscillator ground state density, with $l_z = \sqrt{\hbar/m\omega_z}$. The tight direction can be integrated out to give a quasi-2D interaction:

$$\tilde{U}_{q2D}(\mathbf{k}_\rho) = \int dk_z\, \tilde{U}_{\rm int}(\mathbf{k})[\tilde{n}_{\rm ho}(k_z)]^2.$$

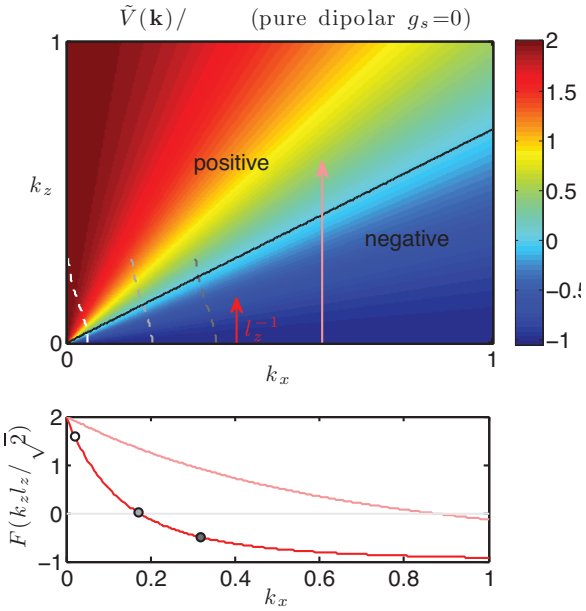
to obtain [e.g. see Pedri PRL (2005)]

$$\tilde{U}_{q2D}(\mathbf{k}_\rho) = \frac{g}{\sqrt{2\pi}l_z} + \frac{g_{\rm dd}}{\sqrt{2\pi}l_z}F\left(\frac{1}{\sqrt{2}}k_\rho l_z\right),$$

with $F(q) = 2 - 3\sqrt{\pi}qe^{q^2}\mathrm{erfc}(q)$ and introducing $g_{\rm dd} = \frac{C_{\rm dd}}{3}$.

Momentum dependence of Quasi-2D interaction

Limits $F(0) = 2$, $F(\infty) = -1$



3D $\rightarrow$ quasi-2D DDI in k-space

A uniform quasi-2D condensate of density n has chemical potential [neglecting z confinement energy]

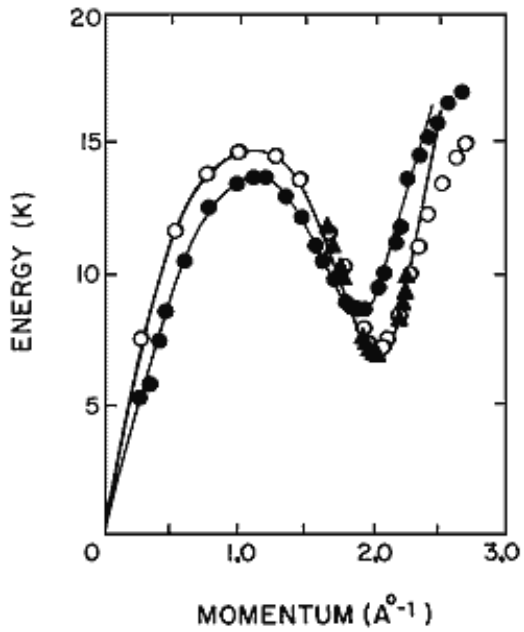
$$\mu_{q2D} = n\tilde{U}_{q2D}(0) = n[g + 2g_{\rm dd}]/\sqrt{2\pi}l_z$$

Note: for $g_{\rm dd} > 0$ the long wavelength interaction is repulsive and the system *appears* stable even for $g = 0$. However, need to carefully look at $k_\rho > 0$.

Rotons

What is a roton?

The "roton minimum" is the local minimum observed in the excitation spectrum of superfluid Helium.



The excitation spectrum of superfluid He at two pressures at $T = 1.1$ K. Dots, SVP, open circles, 25.3 atm, Henshaw and Woods [Proc. 7th Int. Conf. on LTP, (1961)]; triangles, 1.25 K, 24.26 atm, [Dietrich et al. PRA (1972)]

Rotons in a quasi-2D dipolar condensate

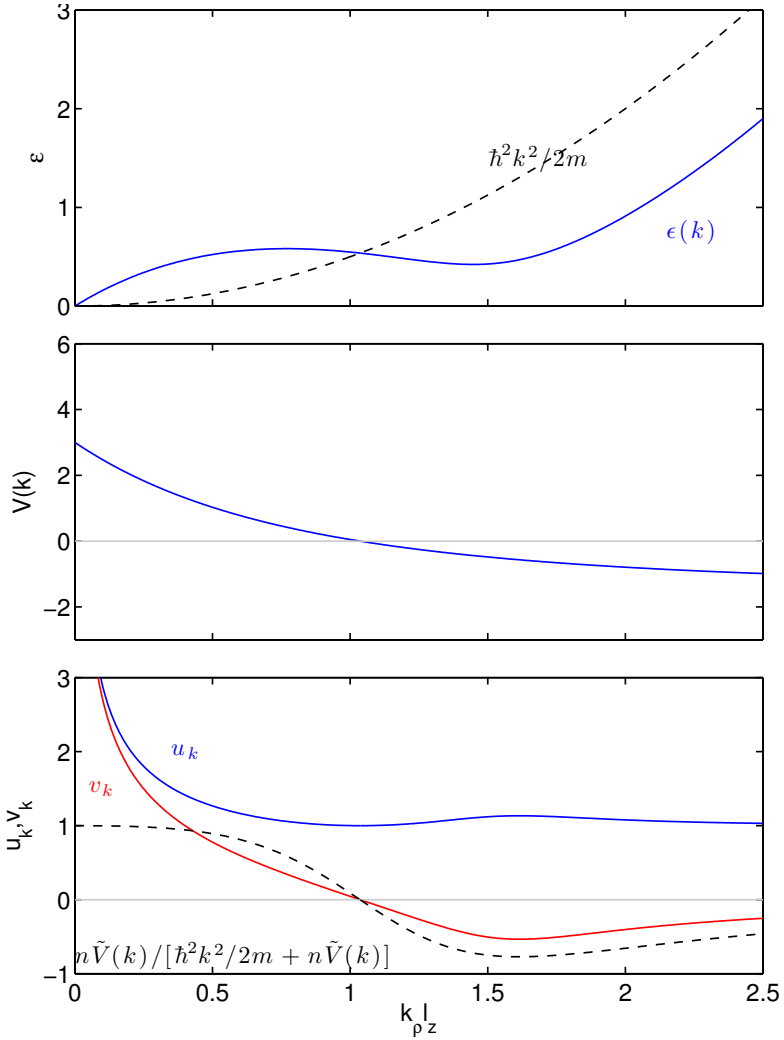
Immediate consequence of the k-dependence (high k attractiveness) of the quasi-2D interaction is that the dispersion relation is modified. This can allow a *roton*-like excitation to emerge: first predicted by Santos et al [PRL 2003] (also earlier work by O'Dell on light induced dipoles).

The Bogoliubov theory derived immediately applies to 2D if there is a condensate [or can be adapted to quasi-condensates, see Mora & Castin PRA (2003)]. The dispersion relation is

$$\epsilon(\mathbf{k}_\rho) = \sqrt{\frac{\hbar^2 k_\rho^2}{2m}\left\{\frac{\hbar^2 k_\rho^2}{2m} + 2n\tilde{U}_{q2D}(\mathbf{k}_\rho)\right\}}.$$

Roton example

For appropriately values of g, $C_{\rm dd}$ and n, the spectrum has a finite-k local minimum:

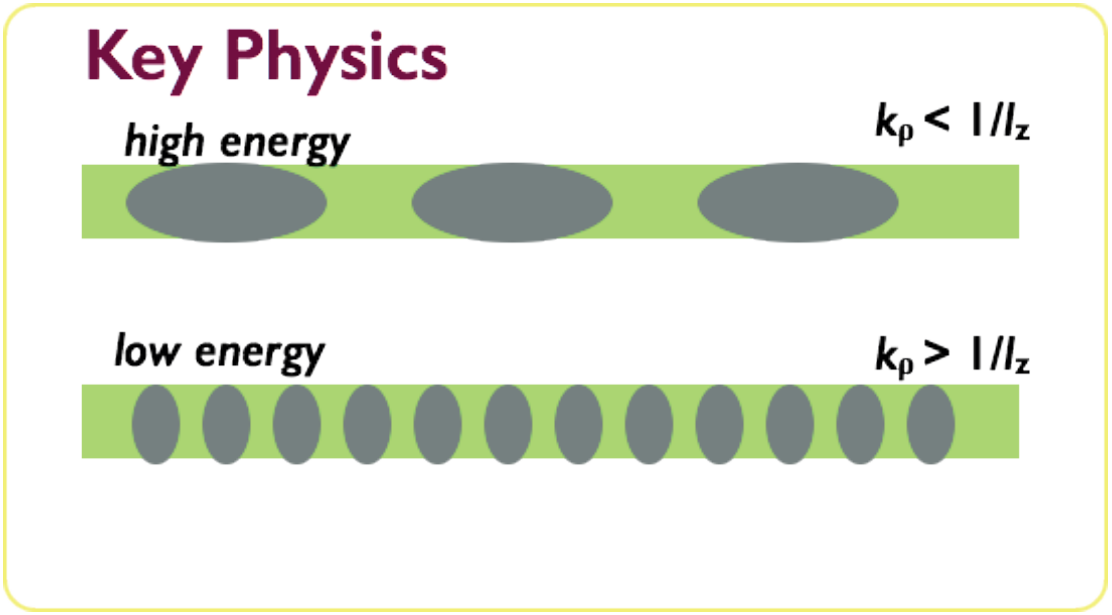


Roton dispersion relation, k-space interaction and Bogoliubov amplitudes. Parameters: $g = 0$, $ng_{\rm dd} = 1.5\hbar\omega_z$.

Careful: Is quasi-2D Valid?

Why do interactions lower the energy at high k?

Excitations of wavelength shorter than l_z create prolate density modulations that lower the DDI energy.



Density Fluctuations

It is interesting to consider the Fourier transformed density operator.
Using that the field operator is $\hat{\psi}(\mathbf{x}) = \sum_{\mathbf{k}} \frac{1}{\sqrt{A}} e^{i\mathbf{k}\cdot\mathbf{x}} \hat{a}_{\mathbf{k}}$ and $\hat{n}(\mathbf{x}) = \hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{x})$, the Fourier transformed density operator

$$\hat{n}_{\mathbf{q}} = \int d\mathbf{x}\, e^{-i\mathbf{q}\cdot\mathbf{x}} \hat{n}(\mathbf{x}) = \sum_{\mathbf{k}} \hat{a}^{\dagger}_{\mathbf{k}-\mathbf{q}} \hat{a}_{\mathbf{k}},$$

with $\hat{n}^{\dagger}_{\mathbf{q}} = \hat{n}_{-\mathbf{q}}$. For a condensed Bose gas

$$\hat{n}_{\mathbf{q}} \approx n\delta_{\mathbf{q0}} + \sqrt{n}(\hat{a}^{\dagger}_{\mathbf{q}} + \hat{a}_{-\mathbf{q}}),$$

the density fluctuation

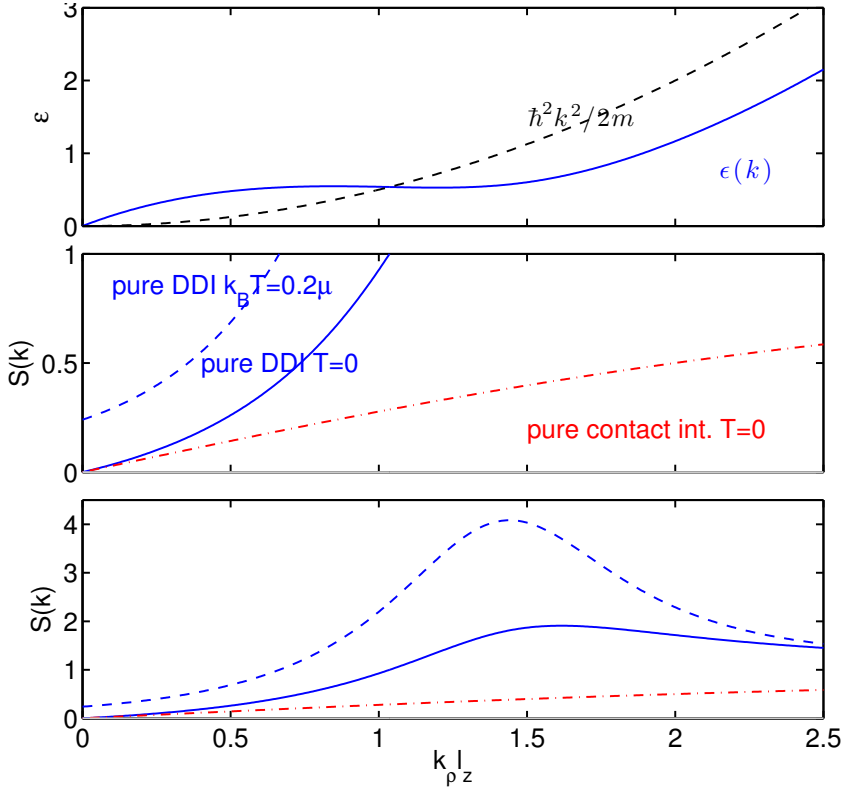
$$\delta\hat{n}_{\mathbf{q}} = \hat{n}_{\mathbf{q}} - \langle \hat{n}_{\mathbf{q}} \rangle \approx \sqrt{n}(u_{\mathbf{q}} - v_{\mathbf{q}})(\hat{\alpha}^{\dagger}_{\mathbf{q}} + \hat{\alpha}_{-\mathbf{q}}).$$

Static structure factor

The density fluctuations are characterized by the static structure factor

$$S(\mathbf{q}) = \frac{1}{N}\langle \delta\hat{n}^\dagger_{\mathbf{q}} \delta\hat{n}_{\mathbf{q}}\rangle \approx (u_{\mathbf{q}} - v_{\mathbf{q}})^2 \langle \hat{\alpha}_{\mathbf{q}}\hat{\alpha}^\dagger_{\mathbf{q}} + \hat{\alpha}^\dagger_{\mathbf{q}}\hat{\alpha}_{\mathbf{q}}\rangle = \frac{\hbar^2 q^2}{2m\,\epsilon(\mathbf{q})} \coth\left[\frac{\epsilon(\mathbf{q})}{2k_B T}\right],$$

Here we have used $\langle \hat{\alpha}^\dagger_{\mathbf{q}}\hat{\alpha}_{\mathbf{q}}\rangle = [e^{\epsilon(\mathbf{q})/k_B T} - 1]^{-1}$. Note $S(\mathbf{q}\to 0) = \frac{k_B T}{\mu}$ [compressibility].



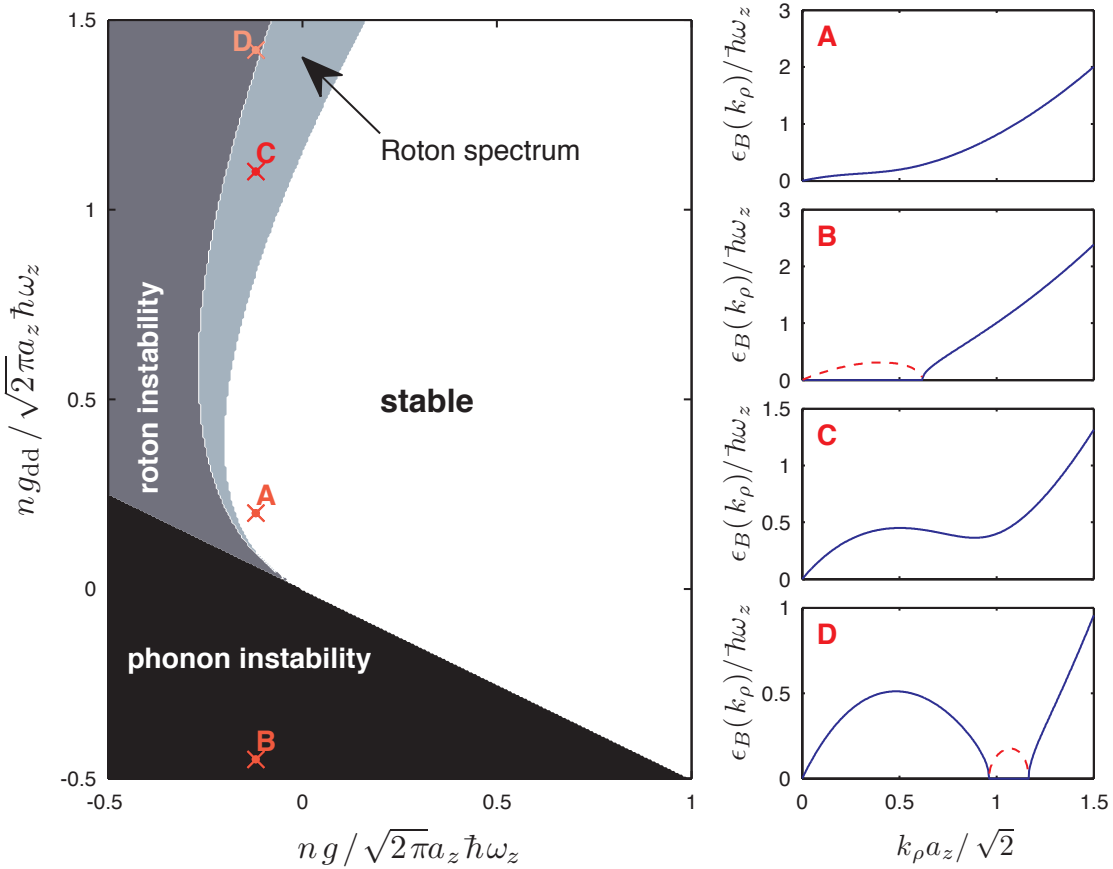
Roton dispersion relation, k-space interaction and Bogoliubov amplitudes.

Stability in 2D

Two ways that the system can become dynamically unstable

Phonon unstable: energy of $k \to 0$ mode becomes imaginary. Occurs when $\mu_{q2D} < 0$, i.e. $g < -2g_{\rm dd}$.

Roton unstable: energy of $k > 0$ (typically $k \sim 1/l_z$) mode becomes imaginary.



Stability and roton phase diagram. Example dispersion relations (dashed parts are imaginary).

Summary

Main topicscovered in my lectures:

- Basic features of the DDI, systems and experiments
- Semiclassical analysis of normal Bose + Fermi gases: direct/exchange and magnetostriction
- Dipolar BECs: Thomas-Fermi; bright solitons in 2D; stability.
- Bogoliubov theory; stability and sound.
- Quasi-2D regime - rotons and fluctuations.