Dipolar gases

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Outline

Motivation

Why are we interested in dipolar gases?

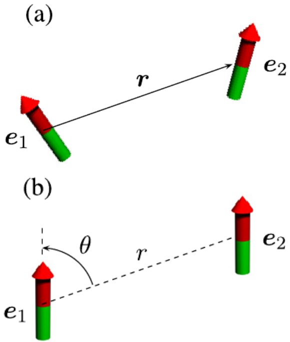
- 1995: Bose-Einstein condensation in diluted gases $\rightarrow$ nobel prize 2001 (Cornell, Wieman, Ketterle)
- 2005: Cr-BEC
- better understanding of static and dynamical properties of weakly interacting Bose gases
- strongly correlated systems reached with ultra-cold atoms and/or molecules
- contact-interaction: short-range and isotropic vs. dipole-dipole interaction: long-range and anisotropic
- supersolids

scattering properties

- Normally the interaction potential between two atoms with distance r is the Van-der-Waals potential ($\propto \frac{1}{r^6}$)
- For vanishing collision energy only the s-wave scattering plays an important role
- Ultra-cold regime: characterization of the potential by a pseudopotential with scattering length a and g as the contact interaction strength

$$U_{\text{contact}}(\mathbf{r}) = \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r}) \equiv g\delta(\mathbf{r}) \tag{1}$$

Two-body dipole-dipole interaction



picture from: The physics of dipolar bosonic quantum gases Rep. Prog. Phys. 72, 126401 (2009)

Dipole-dipole interaction can be written as:

$$U_{dd}(\mathbf{r}) = \frac{C_{dd}}{4\pi} \frac{(e_1 \cdot e_2)\, r^2 - 3\,(e_1 \mathbf{r})\,(e_2 \mathbf{r})}{r^5} \quad (2)$$

$$U_{dd}(\mathbf{r}, \mathbf{r}') = \frac{C_{dd}}{4\pi} \frac{1 - 3\cos^2\theta}{r^3} \quad (3)$$

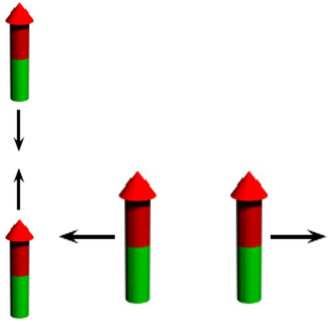
$$C_{dd} = \mu_0 \mu^2$$

(permanent magnetic dipole moment)

$$C_{dd} = \frac{d^2}{\varepsilon_0}$$

(permanent electric dipole moment)

anisotropy



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Dipole-dipole interaction can be written as:

$$U_{dd}(\mathbf{r}, \mathbf{r}') = \frac{C_{dd}}{4\pi} \frac{1 - 3\cos^2\theta}{r^3} \quad (4)$$

$$1 - 3\cos^2\theta = -2 \text{ (attractive)}$$

$$1 - 3\cos^2\theta = 1 \text{ (repulsive)}$$

- 'magic angle' $\rightarrow$ dipole-dipole interaction vanishes

$$\arccos\left(\frac{1}{\sqrt{3}}\right) \simeq 54.7^\circ$$

long-range character

Dipole-dipole interaction has two important properties → anisotropy and **long-range character**

Definition

Long-range character: the integral $\int_{r_0}^{\infty} U(\mathbf{r}) d^{\mathrm{D}} r$ diverges at large distances

- long-range character: not only the density but also the total number of particles have a crucial influence on the energy per particle

$$U(\mathbf{r}) \propto \frac{1}{r^n}$$

- One needs to have $\mathbf{D} \geq \mathbf{n}$ for considering long-range character, in case of the dipole-dipole interaction we consider $n, D = 3 \rightarrow 3 \geq 3$

quantum gas with dipole-dipole interaction

- Realization of quantum gases with dipole-dipole interactions by using particles with electric (much higher coupling!) or magnetic dipole moment
- Typical order of magnitude d for an atomic or molecular system: $d \propto e \cdot a_0$, $\mu \propto \mu_B$
- Ratio of magnetic to electric dipolar coupling:

$$\frac{\mu_0 \mu^2}{d^2/\varepsilon_0} \sim \alpha^2 \sim \frac{1}{137^2} \sim 10^{-4} \tag{5}$$

- In order to define the strength of the dipole-dipole interaction, one use the length:

$$a_{\mathrm{dd}} \equiv \frac{C_{\mathrm{dd}} m}{12\pi\hbar^2} \tag{6}$$

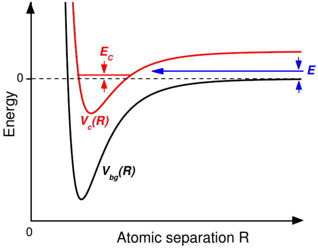
- Ratio of the dipolar length to the s-wave scattering length:

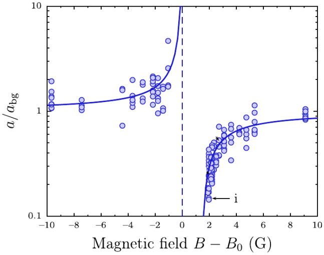
$$\varepsilon_{\mathrm{dd}} \equiv \frac{a_{\mathrm{dd}}}{a} = \frac{C_{\mathrm{dd}}}{3g} \tag{7}$$

Feshbach resonances

- essential tool to control the interaction between atoms in ultra-cold quantum gases
- two atoms colliding at energy E resonantly couple to a molecular bound state with E_C

Tuning of the scattering length a





pictures from: Feshbach resonances in ultracold gases, Rev. Mod. Phys. 82, 1225-1286 (2010) and The

gases used for studying dipole-dipole interaction

- the most famous example: ^{52}Cr
- In the last few years, new systems with dipolar interaction were achieved, e.g.^{168}Er, ^{164}Dy and quantum degenerate dipolar Fermi gases

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

$$\varepsilon_{\mathrm{dd}} \equiv \frac{a_{\mathrm{dd}}}{a} = \frac{C_{\mathrm{dd}}}{3g}$$

Species	Dipole moment
^{52}Cr	$6\mu_{\mathrm{B}}$
^{7}Li	$1\ \mu_{\mathrm{B}}$
^{87}Rb	$1\ \mu_{\mathrm{B}}$
^{164}Dy	$10\ \mu_{\mathrm{B}}$
^{168}Er	$7\ \mu_{\mathrm{B}}$

Gross-Pitaevskii equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + \left(V_{\text{tr}} + \frac{g}{2}|\psi|^2\right)\psi \tag{8}$$

extension of the Schrödinger equation by the interaction term

1. kinetic energy
2. external potential
3. interaction term between particles

time-dependent Gross-Pitaevskii equation

second quantized Hamiltonian in dipole Bose gas:

$$\widehat{H} = \int d\mathbf{r}\widehat{\psi}^{\dagger}(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 - \mu\right]\widehat{\psi}(\mathbf{r}) \tag{9}$$

$$+\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\widehat{\psi}^{\dagger}(\mathbf{r})\widehat{\psi}^{\dagger}(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\widehat{\psi}(\mathbf{r}')\widehat{\psi}(\mathbf{r}) \tag{10}$$

replacement of the short-range interaction by the pseudopotential:

$$\widehat{H} = d\mathbf{r}\widehat{\psi}^{\dagger}(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + \frac{1}{2}g\,|\widehat{\psi}(\mathbf{r})|^2\right]\widehat{\psi}(\mathbf{r}) \tag{11}$$

$$+\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\widehat{\psi}^{\dagger}(\mathbf{r})\widehat{\psi}^{\dagger}(\mathbf{r}')U_d(\mathbf{r}-\mathbf{r}')\widehat{\psi}(\mathbf{r}')\widehat{\psi}(\mathbf{r}) \tag{12}$$

time-dependent Gross-Pitaevskii equation

trapped dipolar Bose gas by the Hamiltonian:

$$\widehat{H} = d\mathbf{r}\,\widehat{\psi}^{\dagger}(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + V_{\mathrm{tr}}(\mathbf{r}) + \frac{1}{2}g\left|\widehat{\psi}(\mathbf{r})\right|^2\right]\widehat{\psi}(\mathbf{r}) \quad (13)$$

$$+\frac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\,\widehat{\psi}^{\dagger}(\mathbf{r})\widehat{\psi}^{\dagger}(\mathbf{r}')U_d(\mathbf{r}-\mathbf{r}')\widehat{\psi}(\mathbf{r}')\widehat{\psi}(\mathbf{r}) \quad (14)$$

with the trapping potential $V_{\mathrm{tr}}(\mathbf{r}) = \frac{m}{2}\left[\omega_\rho^2\left(x^2+y^2\right)+\omega_z^2 z^2\right]$

mean-field approximation

Gross-Pitaevskii equation (GPE)

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + V_{\mathrm{tr}}(\mathbf{r}) + \frac{g}{2}\left|\psi(\mathbf{r},t)\right|^2 \right. \quad (15)$$

$$\left. + \frac{C_{dd}}{8\pi}\int d\mathbf{r}'\frac{1-3\cos^2\theta}{\left|\mathbf{r}-\mathbf{r}'\right|^3}\left|\psi(\mathbf{r}',t)\right|^2\right]\psi(\mathbf{r}) \quad (16)$$

time-dependent Gross-Pitaevskii equation

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stationary non-local Gross-Pitaevskii equation

$$\mu\,\psi_0(\mathbf{r}) = \Bigg[-\frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}\left(\omega_\rho^2\rho^2 + \omega_z^2 z^2\right) \tag{17}$$

$$+\frac{g}{2}\left|\psi_0(\mathbf{r},t)\right| + \frac{C_{dd}}{8\pi}\int d\mathbf{r}'\,\frac{1-3\cos^2\theta}{\left|\mathbf{r}-\mathbf{r}'\right|^3}\left|\psi_0(\mathbf{r}')\right|^2\Bigg]\,\psi(\mathbf{r}) \tag{18}$$

with $\rho^2 = x^2 + y^2$

- Several numerical and approximate methods for the solution of the stationary GPE.
  1. Gaussian ansatz
  2. Thomas-Fermi approximation (neglection of the kinetic energy)

Outline

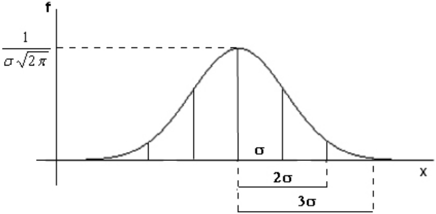
1. Two-body Dipole-dipole interaction
2. Gross-Pitaevskii equation
   - Gaussian ansatz
   - Thomas-Fermi approximation
3. instabilities
   - Phonon
   - Roton

Gaussian ansatz

Gaussian variational ansatz

$$\psi_0(\mathbf{r}) = \sqrt{\frac{N}{\pi^{3/2}\sigma_\rho^2\sigma_z a_{ho}^3}} \exp\left(-\frac{1}{2a_{ho}^2}\left(\frac{r^2}{\sigma_\rho^2}+\frac{z^2}{\sigma_z^2}\right)\right) \qquad (19)$$

with the harmonic oscillator length $a_{\text{ho}} = \sqrt{\frac{\hbar}{m\omega}}$



picture from: www.hanebeck.at

Gaussian ansatz

Together with the Hamiltonian of the trapped dipolar Bose gas, we obtain for the energy:

$$E(\sigma_\rho, \sigma_z) = E_{\text{kin}} + E_{\text{trap}} + E_{\text{int}}$$

$$E_{\text{kin}} = \frac{N\hbar\bar{\omega}}{4}\left(\frac{2}{\sigma_\rho^2} + \frac{1}{\sigma_z^2}\right)$$

$$E_{\text{trap}} = \frac{N\hbar\bar{\omega}}{4\lambda^{2/3}}\left(2\sigma_\rho^2 + \lambda^2\sigma_z^2\right)$$

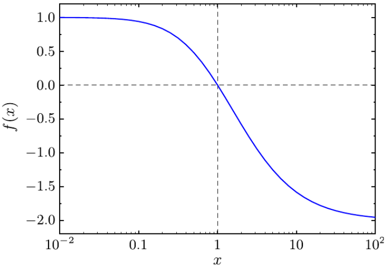
$$E_{\text{int}} = \frac{N^2\hbar\bar{\omega}a_{\text{dd}}}{\sqrt{2\pi}a_{\text{ho}}}\frac{1}{\sigma_\rho^2\sigma_z}\left(\frac{a}{a_{\text{dd}}} - f(\kappa)\right)$$

with the harmonic oscillator length $a_{\text{ho}} = \sqrt{\frac{\hbar}{m\bar{\omega}}}$ corresponding to the trap frequency $\bar{\omega} = \left(\omega_\rho^2\omega_z\right)^{1/3}$

Gaussian ansatz

$$f(\kappa) = \frac{1+2\kappa^2}{1-\kappa^2} - \frac{3\kappa^2 \text{artanh}\left(\sqrt{1-\kappa^2}\right)}{(1-\kappa^2)^{3/2}}$$

$$\text{with } \kappa = \frac{\sigma_\rho}{\sigma_z}$$



picture from: The physics of dipolar bosonic quantum gases Rep. Prog. Phys. 72, 126401 (2009)

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Thomas-Fermi approximation

In this case we neglect the kinetic energy and the GPE reads:

$$\begin{aligned}\mu\,\psi_0(\mathbf{r}) &= \left[\frac{m}{2}\left(\omega_\rho^2\rho^2+\omega_z^2 z^2\right)+\frac{g}{2}\left|\psi(\mathbf{r},\,t)\right|^2\right. \\ &\left.+\frac{C_{dd}}{8\pi}\int d\mathbf{r}'\frac{1-3\cos^2\theta}{\left|\mathbf{r}-\mathbf{r}'\right|^3}\left|\psi_0(\mathbf{r}')\right|^2\right]\psi_0(\mathbf{r})\end{aligned}$$

ansatz for the density profile:

$$\psi_0^2(\mathbf{r}) = n(\mathbf{r}) = n_0\left(1-\frac{\rho^2}{R_x^2}-\frac{z^2}{R_z^2}\right)$$

and the chemical potential:

$$\mu = gn_0\left[1-3\varepsilon_{\mathrm{dd}}f(\kappa)\right]$$

Thomas-Fermi approximation

- case 1: $R_z > R_x$ (prolate) in spheroidal coordinates

$$\phi(\xi,\eta,\varphi) = \frac{R_z^2 - R_x^2}{2} \left[\int_1^{\xi} d\xi' \int_{-1}^{1} d\eta' \left(\xi'^2 - \eta'^2\right) n\left(\xi',\eta'\right) \right.$$

$$\times \sum_{l=0}^{\infty} (2l+1) P_l(\eta) P_l(\eta') Q_l(\xi) P_l(\xi')$$

$$+ \int_{\xi}^{1/\sqrt{1-R_x^2/R_z^2}} d\xi' \int_{-1}^{1} d\eta' \left(\xi'^2 - \eta'^2\right) n(\xi',\eta')$$

$$\left. \times \sum_{l=0}^{\infty} (2l+1) P_l(\eta) P_l(\eta') P_l(\xi) Q_l(\xi') \right]$$

Thomas-Fermi approximation

- case 1: $R_z > R_x$ (prolate) in cartesian coordinates

$$\phi(\mathbf{r}) = \frac{n_0 R_x^2}{192(1-\kappa^2)^2} \left\{ 24\Xi(1-\kappa^2)^2 + 48(1-\kappa^2)(2-\Xi) \times \left(\frac{z}{R_z}\right)^2 - 24(1-\kappa^2)(2-\kappa^2\Xi)\left(\frac{\rho}{R_x}\right)^2 + 8(2\kappa^2 - 8 + 3\Xi)\left(\frac{z}{R_z}\right)^4 + 3[2(2-5\kappa^2)+3\kappa^4\Xi] \times \left(\frac{\rho}{R_x}\right)^4 + 24(2+4\kappa^2-3\kappa^2\Xi)\left(\frac{\rho}{R_x}\right)^2\left(\frac{z}{R_z}\right)^2 \right\}$$

Thomas-Fermi approximation

- case 2: $R_x > R_z$ (oblate) in spheroidal coordinates

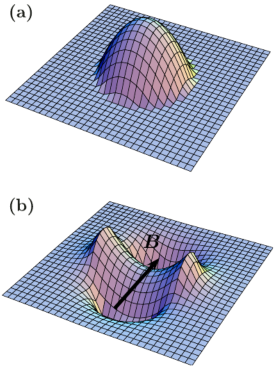
$$\phi(\xi,\eta,\varphi) = \frac{R_x^2 - R_z^2}{2}\left[\int_0^{\xi} d\xi' \int_{-1}^{1} d\eta' \left(\xi'^2 + \eta'^2\right) n\left(\xi',\eta'\right)\right.$$

$$\times i \sum_{l=0}^{\infty} (2l+1) P_l(\eta) P_l(\eta') Q_l(i\xi) P_l(i\xi')$$

$$+ \int_{\xi}^{1/\sqrt{R_x^2/R_z^2 - 1}} d\xi' \int_{-1}^{1} d\eta' \left(\xi'^2 + \eta'^2\right) n(\xi',\eta')$$

$$\left.\times i \sum_{l=0}^{\infty} (2l+1) P_l(\eta) P_l(\eta') P_l(i\xi) Q_l(i\xi')\right]$$

instabilities



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- elongation of the condensate along the polarization axis
- energetically favorable for the cloud to become elongated along the polarization axis

(a) without dipole-dipole interaction
(b) saddle-like mean-field dipolar potential

Outline

scattering properties

- Determination of inelastic scattering properties
- Elementary excitations in dipolar condensates can be described in a better way by using the Fourier transform of the dipole-dipole interaction:

$$\widetilde{U_{dd}}(\mathbf{k}) = C_{dd}\left(\cos^2\alpha - \frac{1}{3}\right) \tag{20}$$

by using the following Fourier transform

$$\widetilde{U_{dd}}(\mathbf{k}) = \int U_{dd}(\mathbf{r})e^{-ikr}d^3r$$

instabilities

- Partially attractive character of the dipole-dipole interaction leads to a stability problem of the dipolar BEC excitation
- spectrum of a homogeneous dipolar condensate:

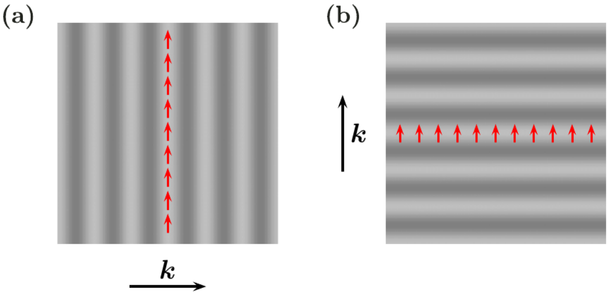
$$\omega = k\sqrt{\frac{n_0}{m}\left[g + \frac{C_{\mathrm{dd}}}{3}\left(3\cos^2\alpha - 1\right)\right] + \frac{\hbar^2 k^2}{4m^2}}$$

together with the definition

$$\varepsilon_{\mathrm{dd}} \equiv \frac{a_{\mathrm{dd}}}{a} = \frac{C_{\mathrm{dd}}}{3g}$$

- metastable for $\varepsilon_{\mathrm{dd}} > 1$
- most unstable situation for $\alpha = \pi/2$

instabilities



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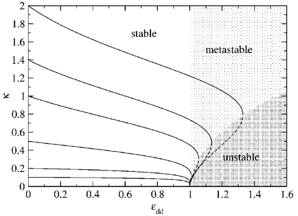
$$\omega = k\sqrt{\frac{n_0}{m}\left[g + \frac{C_{dd}}{3}\left(3\cos^2\alpha - 1\right)\right] + \frac{\hbar^2 k^2}{4m^2}}$$

Thomas-Fermi regime

Another approach with respect to dipolar gases: Thomas-Fermi approximation (neglection of quantum pressure effects)



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- $0 < \kappa < 1$ condensate is prolate
- $\kappa > 1$ condensate is oblate

trap aspect ratio:

$$\lambda = \frac{\omega_z}{\omega_x}$$

- $0 < \lambda < 1$ trap is prolate
- $\lambda > 1$ trap is oblate

$$\kappa(\varepsilon_{dd} = 0) = \lambda$$

instabilities, Gaussian ansatz

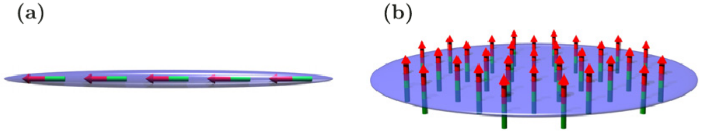
- stabilization by trapping a BEC for small atom numbers

$$\frac{N|a|}{a_{\text{ho}}} \leq 0.58$$

$$a_{\text{ho}} = \sqrt{\hbar/m\omega}$$

- For BEC with dipolar interactions, one can confine the atoms more strongly in the direction of the dipoles alignment.

(a) prolate (cigar-shaped) trap, unstable condensate
(b) oblate (pancake-shaped) trap, stable condensate



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instabilities

variational method to get an idea of the value of $a_{crit}(\lambda)$ by using a Gaussian ansatz – so one can get an expression for the energy:

$$E(\sigma_\rho, \sigma_z) = E_{kin} + E_{trap} + E_{int} \tag{21}$$

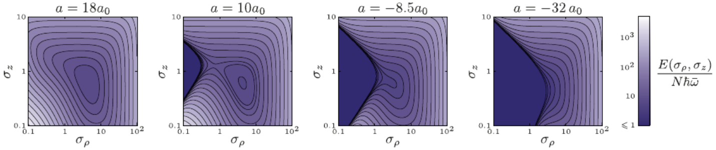
$$E_{kin} = \frac{N\hbar\bar{\omega}}{4}\left(\frac{2}{\sigma_\rho^2} + \frac{1}{\sigma_z^2}\right)$$

$$E_{trap} = \frac{N\hbar\bar{\omega}}{4\lambda^{2/3}}\left(2\sigma_\rho^2 + \lambda^2\sigma_z^2\right)$$

$$E_{int} = \frac{N^2\hbar\bar{\omega}a_{dd}}{\sqrt{2\pi}a_{ho}}\frac{1}{\sigma_\rho^2\sigma_z}\left(\frac{a}{a_{dd}} - f(\kappa)\right)$$

instabilities

- minimization of the energy equation with respect to σ_ρ and σ_z leads then to the critical value $a_{\text{crit}}(\lambda)$ (stability threshold)
- For N = 20000, $\lambda = 10$ and different values for a, we get a contour plot of E as a function of σ_ρ and σ_z from the Gaussian ansatz. In this case, the critical value reads $a_{\text{crit}}(10) = -8.5a_0$



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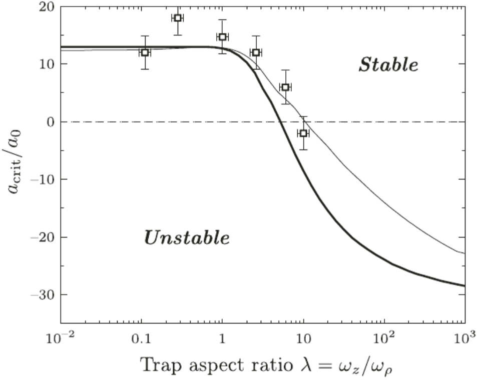
instabilities

Stability diagram of a dipolar condensate in the plane (dots and errorbars are experimental results):



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excitations of the system

- Instabilities in dipolar gases due to excitations in the system (even in the pancake traps)
- gas feels the 3D nature of the dipolar interactions (e.g. their partially attracticve character)

+++

'roton-maxon' instability

- infinite pancake trap with dipoles along z perpendicular to the trap plane
- roton-maxon effects occurs in the Thomas-Fermi limit in the z-direction
- momentum dependence of the dipole-dipole interactions

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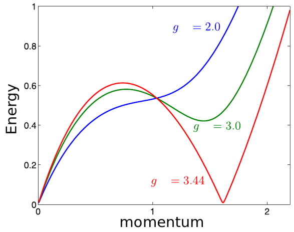

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with increasing g the 'roton gap' decreases and vanishes for a critical particle density

- Roton instability in the Thomas-Fermi regime due to experiences of the system with the 3D partially attractive nature of dipolar forces
- Attractive contact interactions leads to roton instability already in the quasi-2D regime

summary and outlook

- New effects by studying the dipole-dipole interaction due to anisotropy and long-range character
- Gross-Pitaevskii equation for calculations, Gaussian ansatz and Thomas-Fermi approximation
- Instabilities, form of the condensate, minimization of the energy to get $a_{\text{crit}}(\lambda)$, roton-maxon instability
- Beside BEC, atomic degenerate Fermi gases (Fermi superfluidity in the weak interaction limit by BCS theory)
- BEC-BCS crossover in the limit of strong correlations

Acknowledgement

Thank you for your attention!

Acknowledgement

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