



The Abdus Salam  
International Centre for Theoretical Physics



SMR 1666 - 25

**SCHOOL ON QUANTUM PHASE TRANSITIONS  
AND  
NON-EQUILIBRIUM PHENOMENA IN COLD ATOMIC GASES**

**11 - 22 July 2005**

***Dipolar gases: Theory***

Presented by:

**Luis Santos**

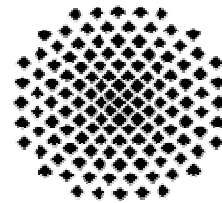
University of Stuttgart, Germany

Trieste, 21<sup>th</sup> July 2005

# Dipolar gases: theory

Luis Santos

Universität Stuttgart



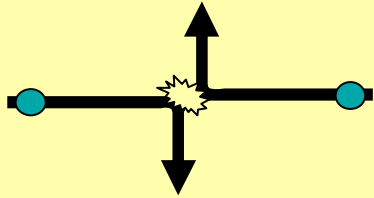
**CO.CO.MAT**

CONTROL OF QUANTUM CORRELATIONS IN TAILORED MATTER  
SFB/TR 21 – STUTTGART, ULM, TÜBINGEN

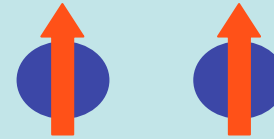
# Outline of the talk

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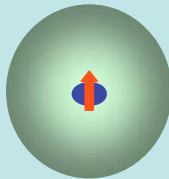
1. The role of the interactions



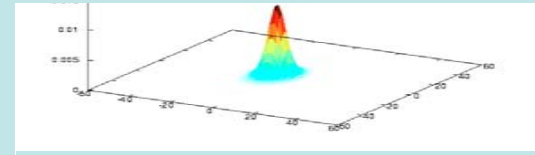
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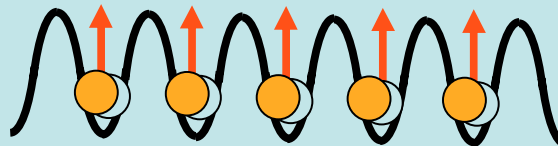
3. Ground-state and stability of a  
dipolar BEC



4. Nonlocal nonlinearity.  
Multidimensional solitons



5. Dipolar gases in optical  
lattices

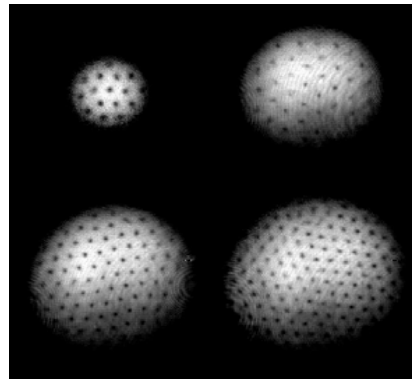


## The role of the interactions

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Ultra cold gases are very dilute, with typical densities lower than  $10^{14}$  atoms/cm<sup>3</sup>

But the interparticle interactions play a crucial role in the properties of ultra cold gases, as e.g. **superfluidity**



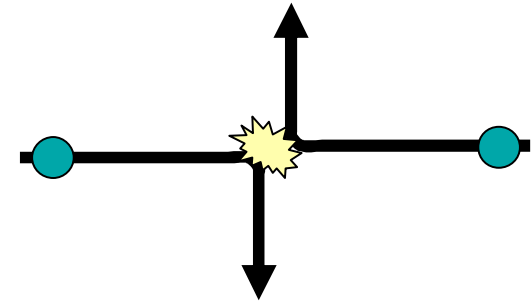
See lectures of S.  
Stringari and A. Fetter

[Raman et al., PRL  
87, 210402 (2001)]

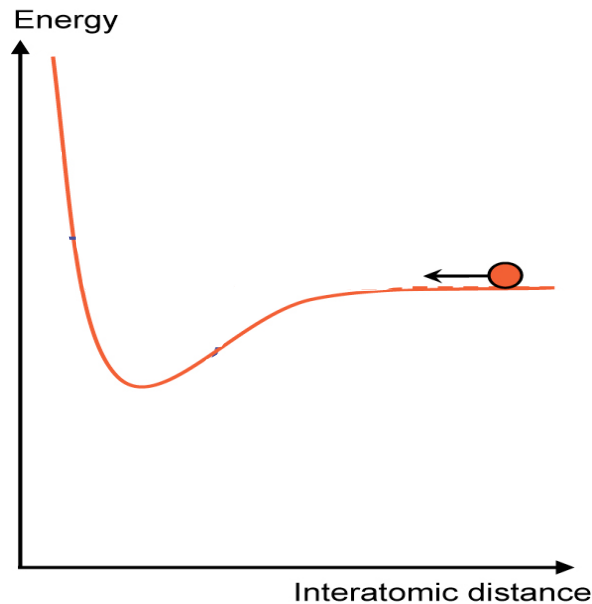
# The role of the interactions

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In typical experiments the atoms interact via short-range isotropic interactions

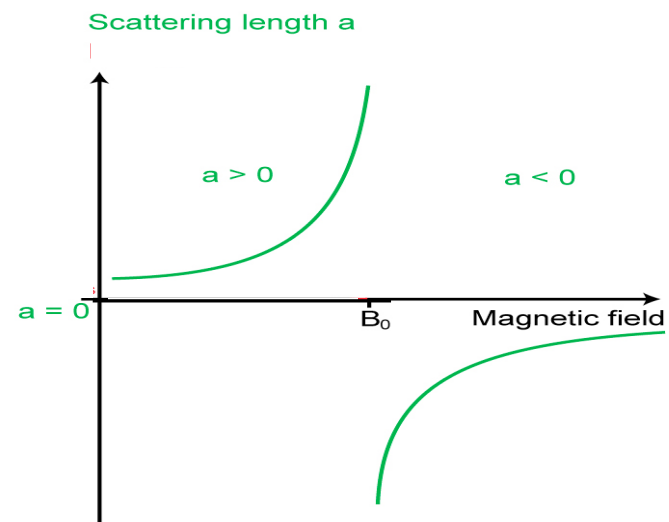
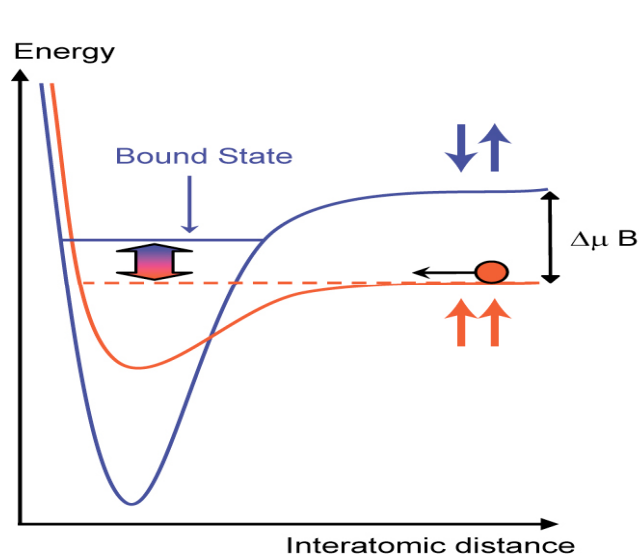


The interaction between ultracold atoms is determined by the s-wave scattering length “a”



$$V(\vec{r} - \vec{r}') \approx \frac{4\pi\hbar^2 a}{m} \delta(\vec{r} - \vec{r}')$$

# The role of the interactions



[Tiesinga et al, PRA **47**, 4114 (1993); Inouye et al., Nature **392**, 151 (1998)]

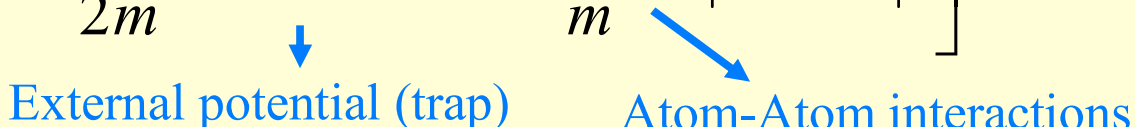
## The role of the interactions

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At low Temperatures the BEC physics is given by a nonlinear Schrödinger equation with local cubic nonlinearity

### Gross-Pitaevskii equation

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \left[ -\frac{\hbar^2 \nabla^2}{2m} + U(r,t) + \frac{4\pi\hbar^2 a N}{m} |\Psi(r,t)|^2 \right] \Psi(r,t)$$



External potential (trap)      Atom-Atom interactions

The stability of the BEC depends very much on the sign of  $a$

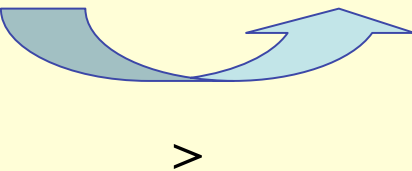
$a > 0$   
Repulsive interactions  
STABLE

$a < 0$   
Attractive interactions  
UNSTABLE IN  $d > 1$

## The role of the interactions

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But...a trapped attractive gas can be stable!

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \left[ -\frac{\hbar^2 \nabla^2}{2m} + U(r,t) + \frac{4\pi\hbar^2 a N}{m} |\Psi(r,t)|^2 \right] \Psi(r,t)$$


The zero-point oscillation compensates the attraction

$$\frac{4\pi\hbar^2 a}{m} n < \hbar\omega$$

Critical number of particles

[Bradley et al., PRL **78**, 985 (1997)]



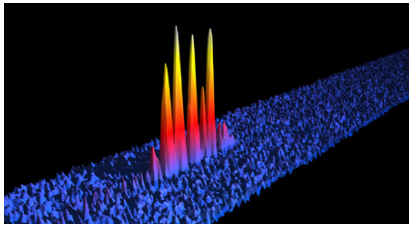
# The role of the interactions

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Due to the interactions, **BEC physics is intrinsically nonlinear**

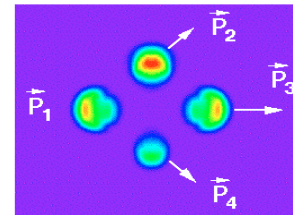
## Bright solitons

[Strecker et al., Nature **417**, 150 (2002) ]  
[Khaykovich et al., Science **296**, 1290 (2002)]



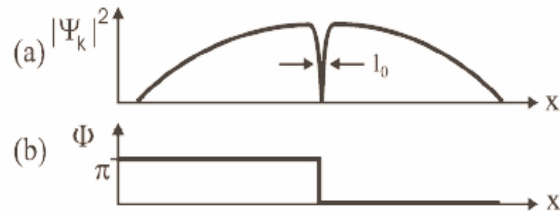
## Four-wave mixing

[Deng et al., Nature **398**, 218 (1999)]



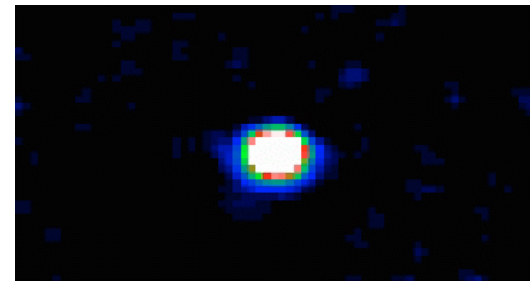
## Dark Solitons

[Burger et al, PRL **83**, 5198 (1999)]  
[Denschlag et al., Science **287**, 97 (2000)]



## Condensate collapse

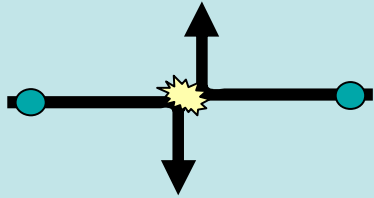
[E. A. Donley et al. Nature **412**, 295 (2001)]



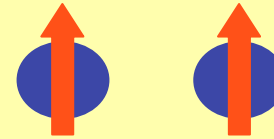
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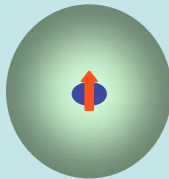
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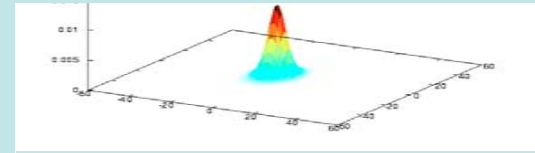
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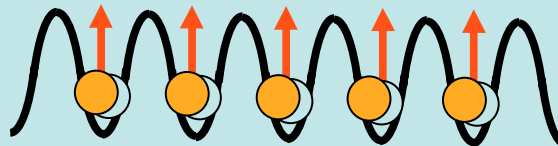
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Multidimensional solitons



5. Dipolar gases in optical lattices



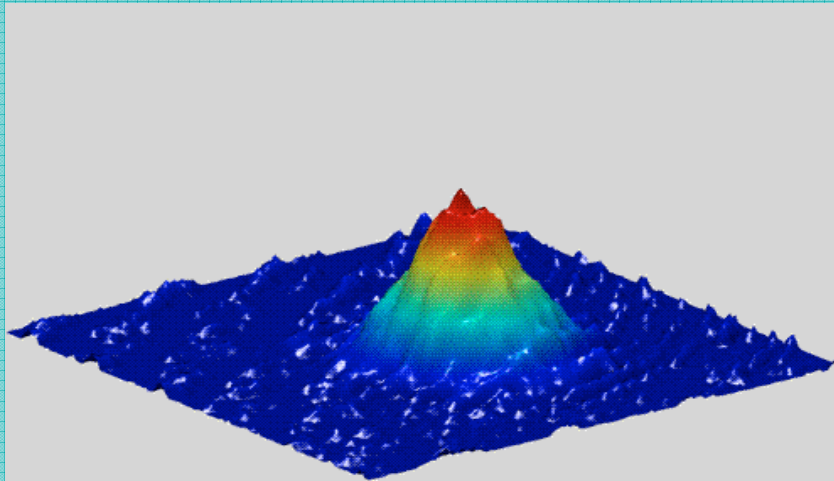
# Dipolar gases. The dipole-dipole interaction

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Recent experimental developments have opened a novel research area in cold gases: the analysis of dipolar gases

## BEC in Chromium atoms

[Griesmaier et al., PRL **94**, 160401 (2005)]



Chromium has a large magnetic moment,  $\mu=6\mu_B$

See lecture of Jürgen Stuhler

# Dipolar gases. The dipole-dipole interaction

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Atoms with large magnetic moment

Cooling and trapping of polar molecules

[Bethlem and Meijer, Int. Rev. Phys. Chem. **22**, 73 (2003)]

Feshbach resonances in binary mixtures

[Stan et al. PRL **93**, 143001 (2004); Inouye et al., PRL **93**, 183201 (2004); Petrov et al., cond-mat/0502010]

Photoassociation of polar molecules in optical lattices

[Jaksch et al., PRL **89**, 040402 (2002); Damski et al., PRL **90**, 110401 (2003); Rom et al., PRL **93**, 073200 (2004)]

Laser induced dipole-dipole interaction

[O'Dell et al., PRL **84**, 5687 (2000)]

Rydberg atoms

[Jaksch et al., PRL **85**, 2208 (2000)]

# Dipolar gases. The dipole-dipole interaction

Dipole-dipole interaction

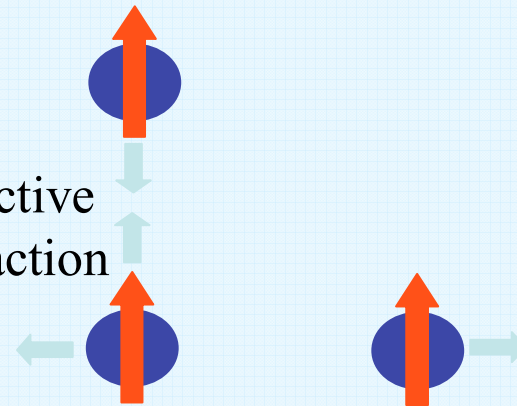


$$V(\vec{r}) = \frac{d^2}{r^3} (1 - 3 \cos^2 \theta)$$

The interaction is anisotropic  
(partially attractive and partially  
repulsive!)

Long-range interaction

Attractive  
interaction



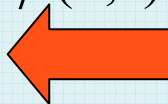
Repulsive interaction

The condensate properties are critically determined  
by the trap geometry

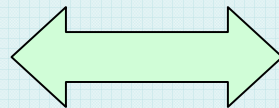
## Dipolar gases. The dipole-dipole interaction

At low temperatures the physics of a dipolar BEC is given by a nonlocal nonlinear Schrödinger equation

### Nonlocal NLSE

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left\{ \begin{aligned} &-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) + g |\psi(\vec{r}, t)|^2 + \\ &+ g_d \int d\vec{r}' \frac{(1 - 3 \cos^2 \theta)}{|\vec{r} - \vec{r}'|^3} |\psi(\vec{r}', t)|^2 \end{aligned} \right\} \psi(\vec{r}, t)$$


$$g \propto a$$



$$g_d \propto d^2$$

Resemblances to

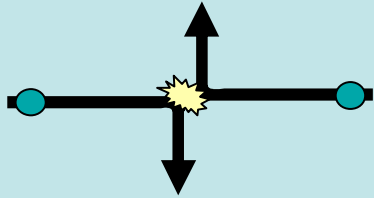
plasma physics [Litvak et al., Sov. J. Plasma Phys. **1**, 60 (1975)]

physics of nematic liquid crystals [Conti et al., PRL **91**, 073901 (2003)]

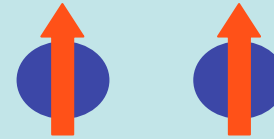
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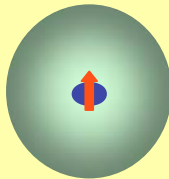
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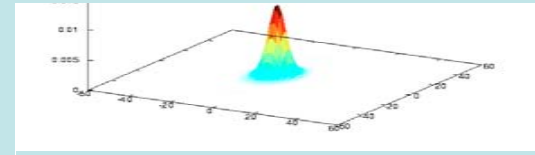
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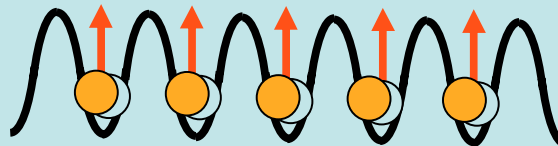
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# Ground-state and stability of a dipolar BEC

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Let's assume that there is no local interaction:  $g=0$

Homogeneous space (no trap)

Like for  $a < 0$  the system is unstable

Dispersion law for elementary excitations

$$E(k) = \sqrt{E_k^2 + \frac{8\pi}{3} g_d n_0 (3 \cos \theta_k - 1) E_k}$$

Trapped case

Like for  $a < 0$  a stable condensate can be found under certain conditions

Contrary to  $a < 0$  the sign and value of the mean dipole-dipole interaction is strongly modified by the trapping potential



# Ground-state and stability of a dipolar BEC

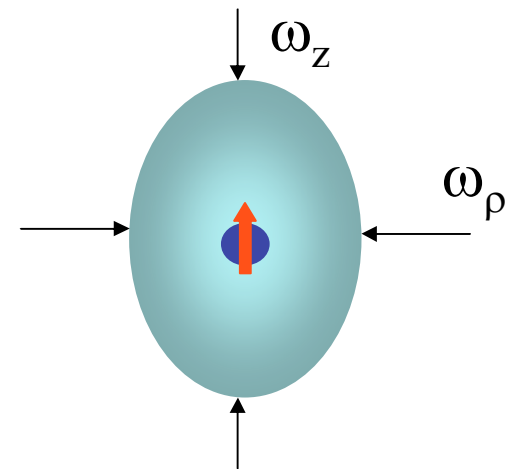
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[Yi and You, PRA **61**, 041604 (2000); Góral et al., PRA **61**, 051601 (2000); Santos et al., PRL **85**, 1791 (2000)]

Cylindrical trap: axis in the dipole direction

Trap frequencies  $\omega_\rho$  and  $\omega_z$

Trap aspect ratio  $\sqrt{\omega_\rho / \omega_z}$

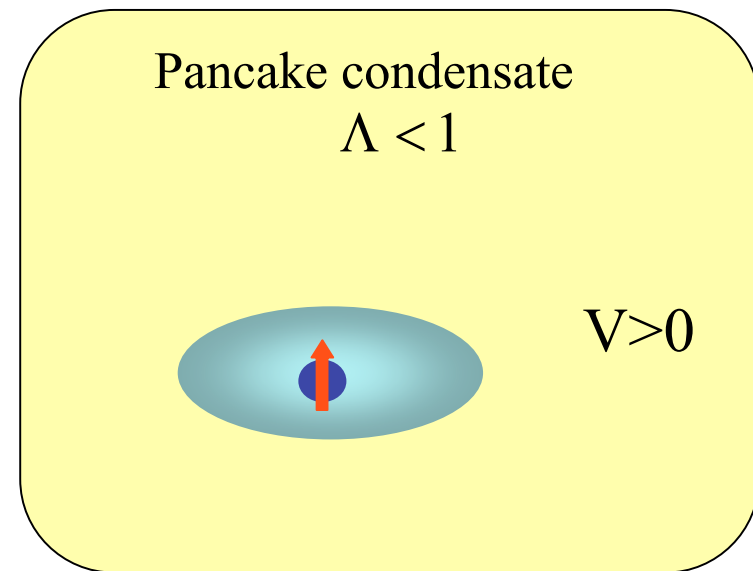
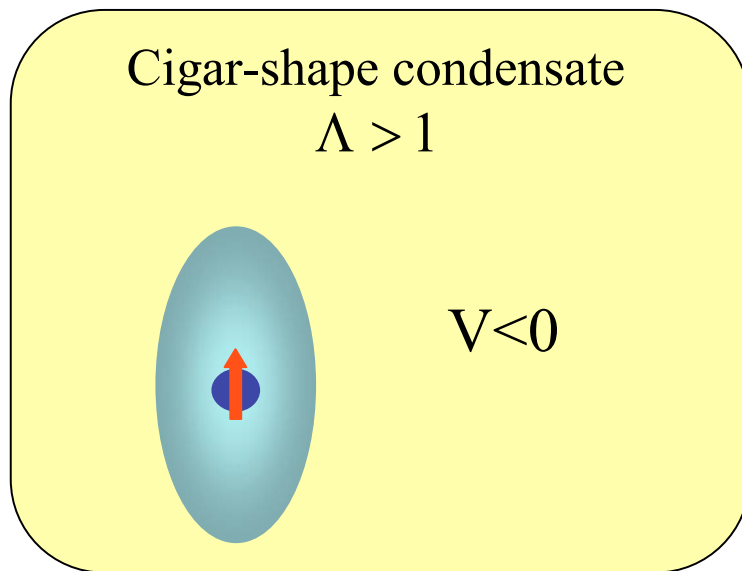


# Ground-state and stability of a dipolar BEC

## Mean dipole-dipole interaction

$$V = g_d \int d\vec{r}' \frac{1 - 3 \cos^2 \theta}{|\vec{r} - \vec{r}'|^3} |\psi(\vec{r}')|^2 |\psi(\vec{r})|^2$$

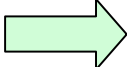
$$\psi(\rho, z) \propto \exp\left[-\frac{1}{2L_z^2}(\Lambda^2 \rho^2 + z^2)\right] \quad V = V_0 \frac{1}{1 - \Lambda^2} \left[ 2 - \Lambda^2 - \frac{3\Lambda \tanh^{-1}(\sqrt{\Lambda^2 - 1} / \Lambda)}{\sqrt{\Lambda^2 - 1}} \right]$$


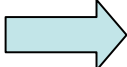


$$\Lambda = L_z / L_\rho$$

# Ground-state and stability of a dipolar BEC

Cigar-shape traps ( $\omega_z < \omega_\rho$ )

$V < 0$   **Attractive gas**

$\hbar\omega_z \ll |V| \ll \hbar\omega_\rho$    $|V| < \hbar\omega_\rho$    $|V| > \hbar\omega_\rho$   
**Bright-soliton-like BEC**      3D Attractive gas      **Collapse**

Eventually collapse occurs for  $\sqrt{\omega_\rho / \omega_z} > 0.41$

Pancake-shape traps with  $\sqrt{\omega_\rho / \omega_z} < 0.41$

$V > 0$  and grows with  $g_d$   **Repulsive gas**

$\hbar\omega_\rho \ll V \ll \hbar\omega_z$    $V > \hbar\omega_z$   
**Quasi2D** : Bose Gas with repulsive interaction. Radially Thomas-Fermi      3D Thomas-Fermi

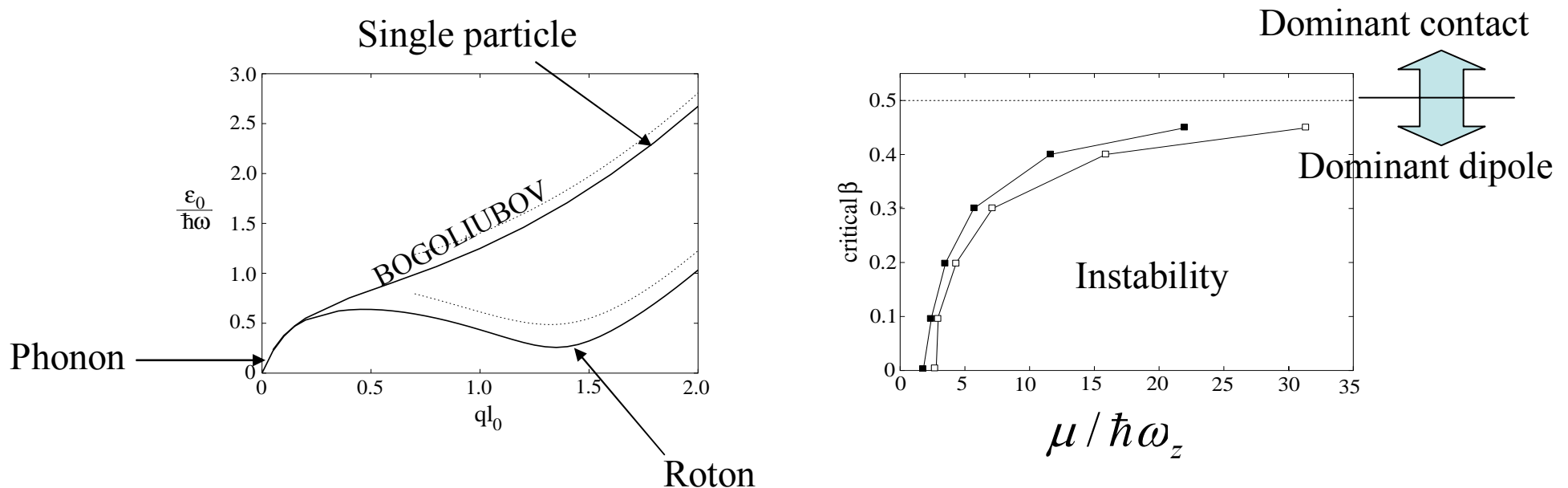
[O'Dell et al., PRL **92**, 250401 (2004)]

# Ground-state and stability of a dipolar BEC

[O'Dell et al., PRL **90**, 110402 (2003); Santos et al., PRL **90**, 250403 (2003)]

What happens if  $\sqrt{\omega_\rho / \omega_z} < 0.41$

The dispersion law acquires a roton-maxon character for sufficiently large dipole-dipole interactions

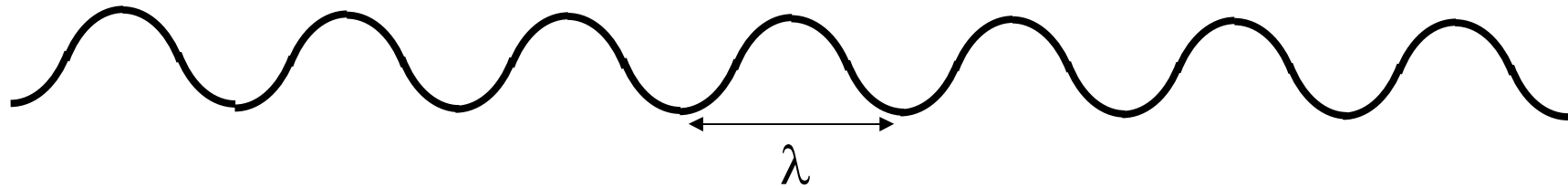


The gas becomes eventually unstable unstable when the roton touches zero

# Ground-state and stability of a dipolar BEC

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Why do we see a roton in a dipolar gas?



$\lambda \gg l_z$

$\langle V_{dip} \rangle_\lambda > 0$

2D Excitations

$\lambda < l_z$

$\langle V_{dip} \rangle_\lambda < 0$

3D Excitations

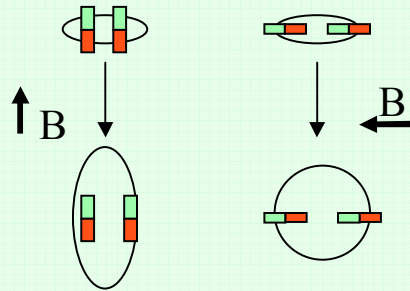


# Ground-state and stability of a dipolar BEC

## Expansion

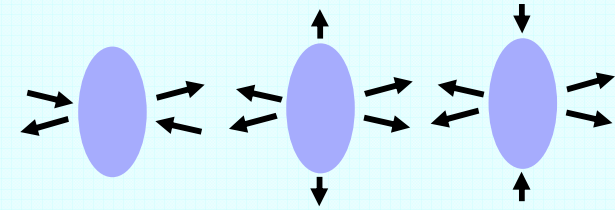
[Góral and Santos, PRA **66**, 023613 (2002);  
Yi and You, PRA **67**, 045601 (2003);  
Giovannazzi *et al.*, J. Opt. B **5**, 208 (2003)]

**See talk of Jürgen Stuhler**



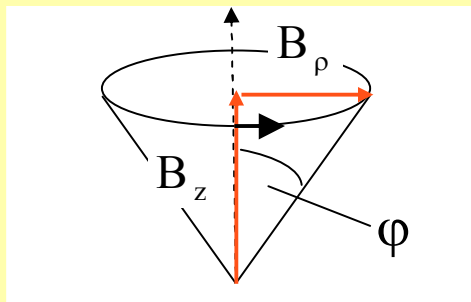
## Low-lying excitations

[Yi and You, PRA **66**, 013607 (2002);  
Góral and Santos, PRA **66**, 023613 (2002)]

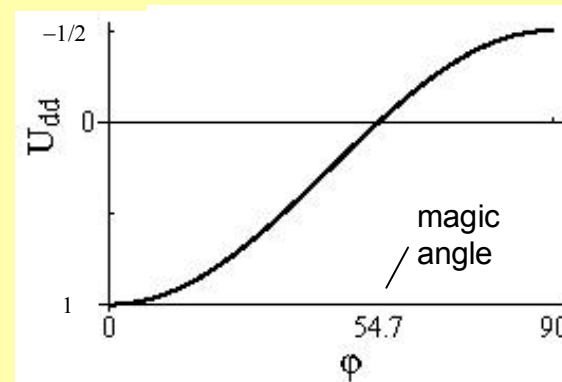


## Tunability

[Giovannazzi *et al.*, PRL **89**, 130401 (2002)]



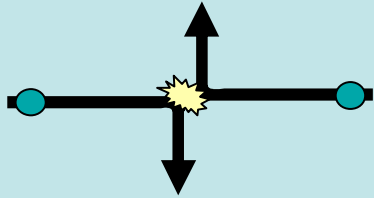
$$V_d(\vec{r}) = \frac{\mu_0 \mu^2}{4\pi} \underbrace{\left( \frac{3 \cos^2 \varphi - 1}{2} \right)}_{\text{magic angle}} \left( \frac{1 - 3 \cos^2 \theta}{r^3} \right)$$



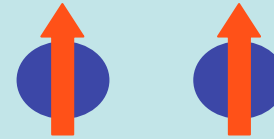
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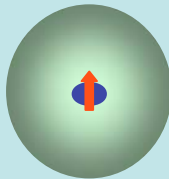
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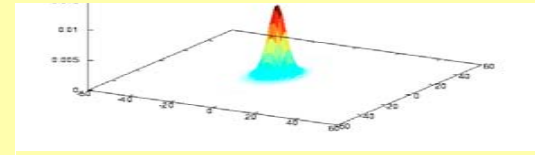
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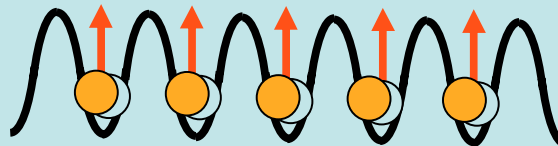
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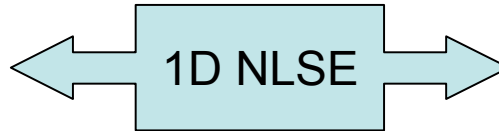


# Nonlocal nonlinearity. Multidimensional solitons

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„Standard“-BEC physics is described by a NLSE with local cubic nonlinearity

**Dark Solitons ( $a > 0$ )**



1D NLSE

**Bright solitons ( $a < 0$ )**

[Zakharov & Shabat., JETP **34**, 62 (1972)]

Continuous solitons become unstable in 2D and 3D

## Periodic potentials: BEC in Optical Lattices

**Gap Solitons**: Bright solitons with  $a > 0$

[Eiermann et al., PRL **92**, 230401 (2004)]

Multidimensional **discrete solitons**  
in periodic potentials but they **do not move**

[Fleischer et al., Nature **422**, 147 (2003)]

2D (3D) mobile solitons are possible combining 1D  
(2D) lattices with one uniform direction.

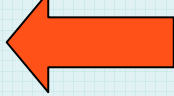
[Baizakov et al., PRA **70**, 053613 (2004)]

But **the motion is only in 1D.**

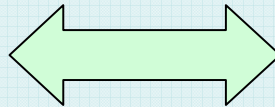


# Nonlocal nonlinearity. Multidimensional solitons

## Nonlocal NLSE

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left\{ \begin{array}{l} \frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) + g |\psi(\vec{r}, t)|^2 + \\ + g_d \int d\vec{r}' \frac{(1 - 3 \cos^2 \theta)}{|\vec{r} - \vec{r}'|^3} |\psi(\vec{r}', t)|^2 \end{array} \right\} \psi(\vec{r}, t)$$


$$g \propto a$$



$$g_d \propto d^2$$

Nonlocal nonlinearity is also observed in disparate physical systems

### Plasma physics

[Litvak et al., Sov. J. Plasma Phys. **1**, 60 (1975)]

### Photorefractive materials

[Shin et al., PRL **78**, 130401 (2002)]

### Nematics

[Peccianti et al., Nature **432**, 733 (2004)]

# Nonlocal nonlinearity. Multidimensional solitons

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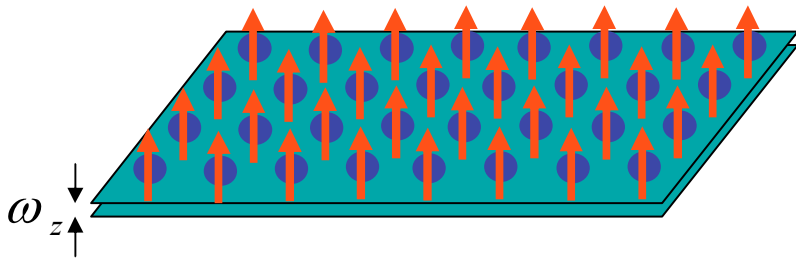
Very active research field in non linear physics

Nonlocal nonlinearity can **stabilize** multidimensional solitons

[Bang et al., PRE **66**, 046619 (2002)]

Multidimensional solitons observed e.g. in Nematics

[Peccianti et al., Nature **432**, 733 (2004)]



**Is it possible to observe 2D solitons in dipolar BEC which move truly in 2D?**

[P. Pedri and L. Santos, cond-mat/0503019]

# Nonlocal nonlinearity. Multidimensional solitons

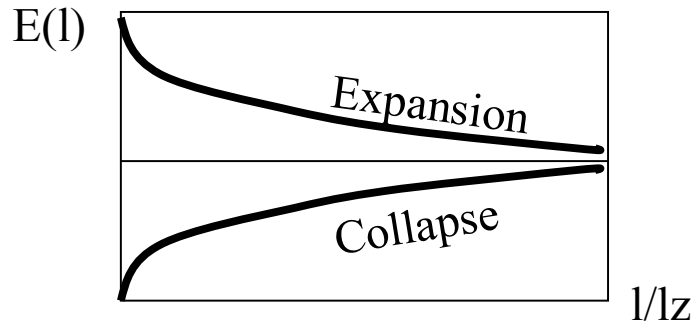
Gaussian Ansatz

$$\psi(\vec{r}) \propto e^{-\rho^2/2l^2} e^{-z^2/2l_z^2}$$

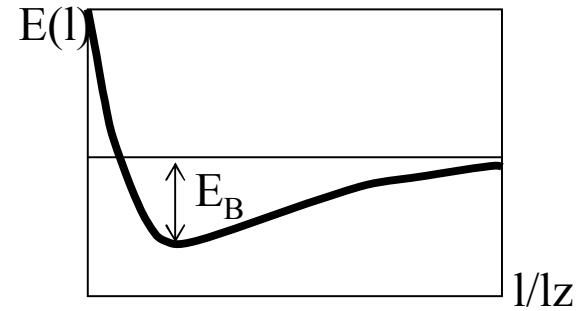
$$E(l) \propto \frac{1}{(l/l_z)^2} \left( 1 + \frac{g}{2(2\pi)^{3/2}} + \frac{g_d}{3\sqrt{2\pi}} f\left(\frac{l}{l_z}\right) \right)$$

$$f(x) = \frac{1}{x^2 - 1} \left[ 2x^2 + 1 - \frac{3x^2 \arctan[\sqrt{x^2 - 1}]}{\sqrt{x^2 - 1}} \right]$$

No dipole



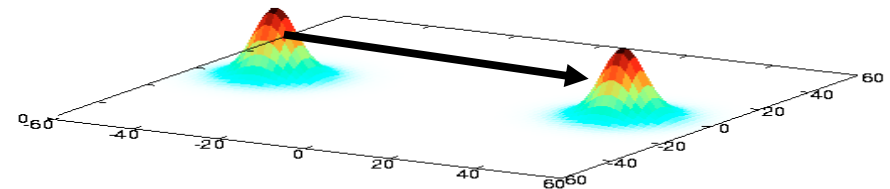
Dipolar gas



Stability condition

$$\frac{g_d}{3\sqrt{2\pi}} < 1 + \frac{g}{2(2\pi)^{3/2}} < \frac{-2g_d}{3\sqrt{2\pi}}$$

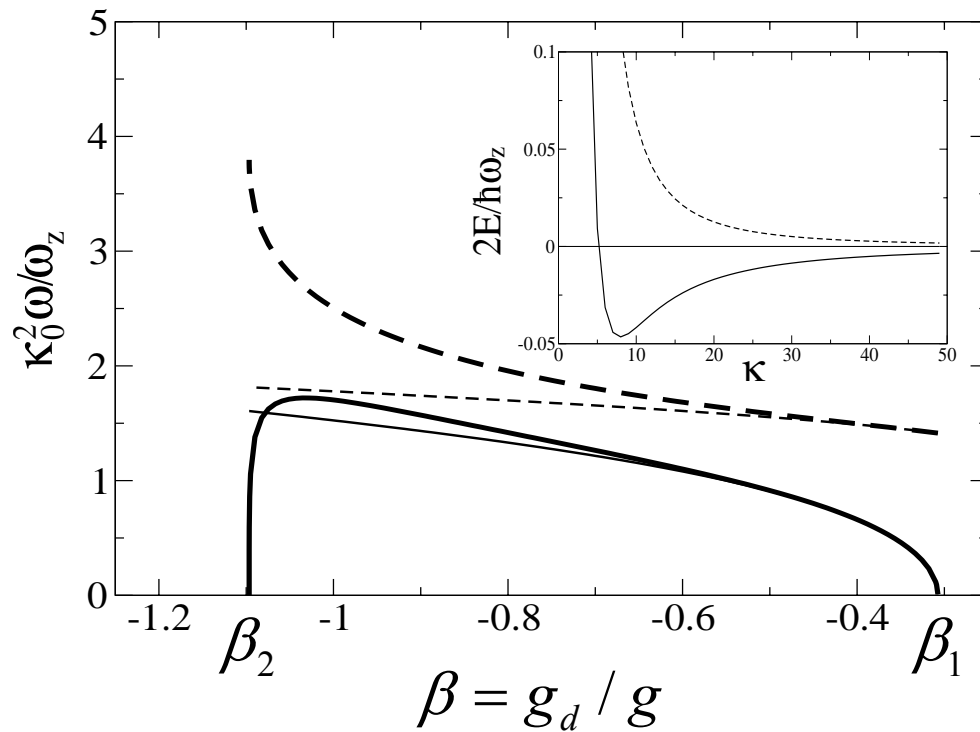
**Truly-2D motion without distortion!!**



We need  $g_d < 0$   $\Rightarrow$  Tunability

# Nonlocal nonlinearity. Multidimensional solitons

## 3D Analysis of the lowest-lying excitations



## Crucial role of the anisotropy

### Stability Window

$$|\beta| > |\beta_1|$$

2D instability against expansion  
for small dipoles

$$|\beta| < |\beta_2|$$

3D instability against collapse  
for large dipoles

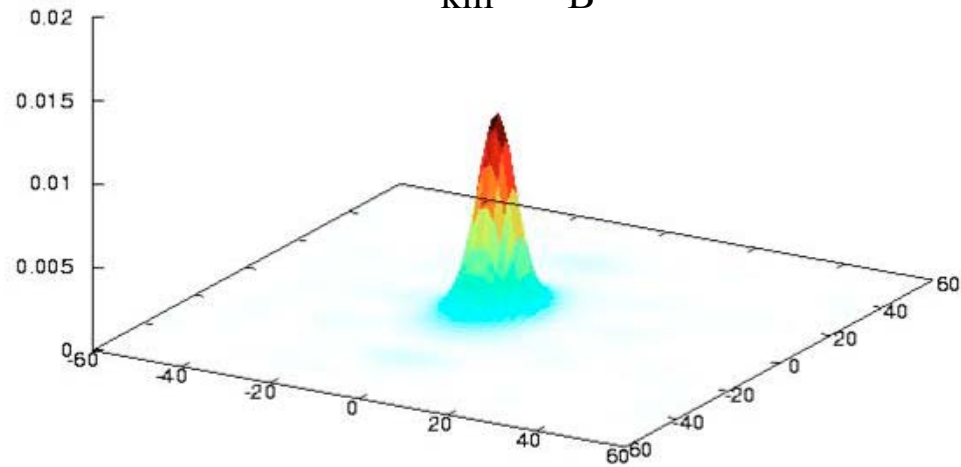
The lowest lying level is always the breathing mode

# Nonlocal nonlinearity. Multidimensional solitons

The 2D Solitons scatter inelastically

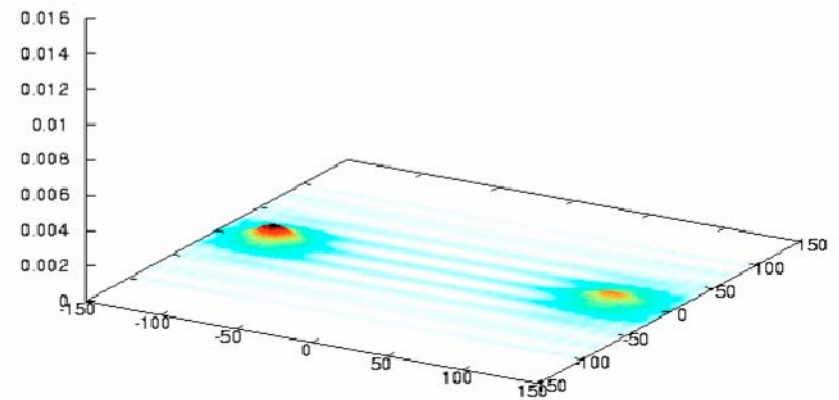
Soliton fusion

$$E_{\text{kin}} < E_B$$



Soliton destruction

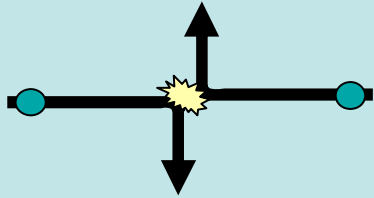
$$E_{\text{kin}} > E_B$$



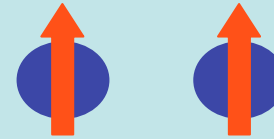
# Outline of the talk

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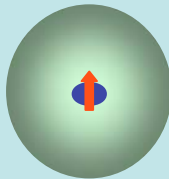
1. The role of the interactions



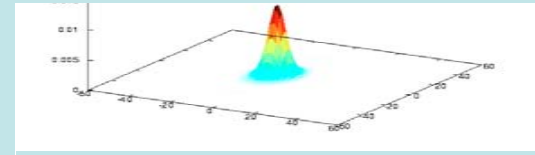
2. Dipolar gases.  
The dipole-dipole interaction



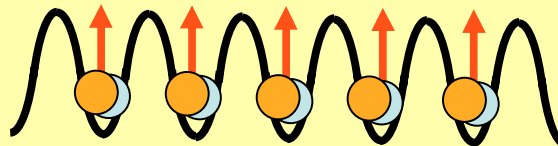
3. Ground-state and stability of a  
dipolar BEC



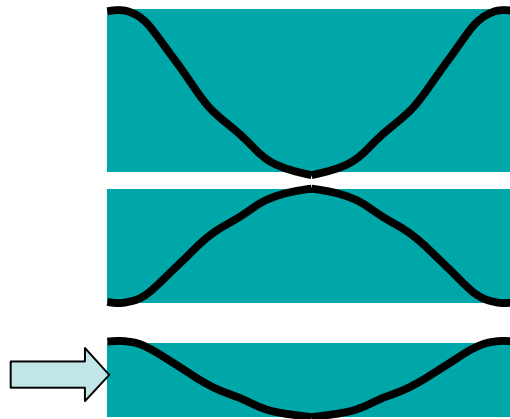
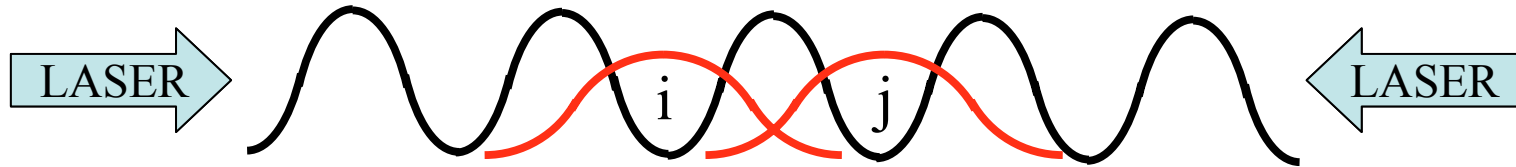
4. Nonlocal nonlinearity.  
Multidimensional solitons



5. Dipolar gases in optical  
lattices



# Dipolar gases in optical lattices

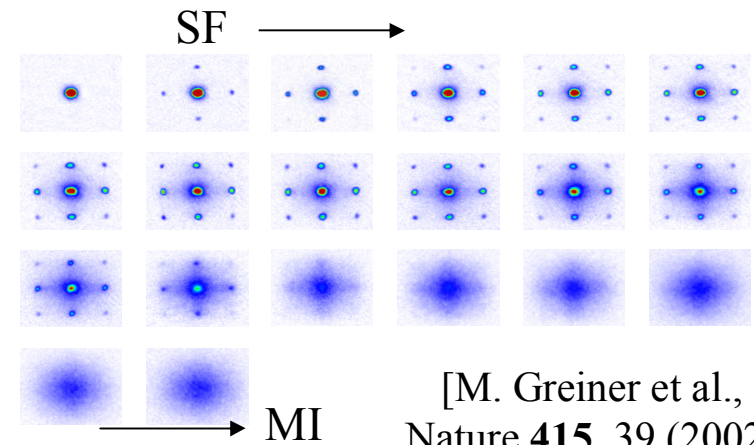
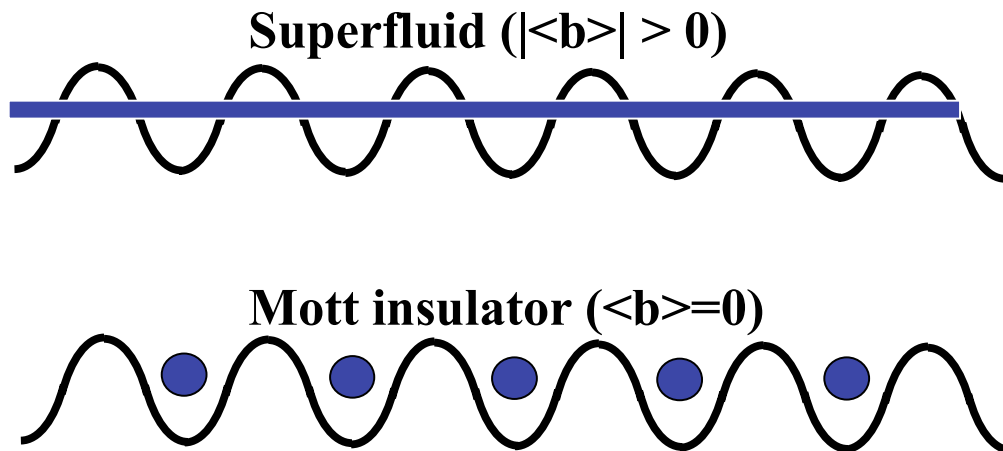


## Short-range interacting bosons in lattices

### Bose-Hubbard Hamiltonian

[Fisher *et al.*, PRB **40**, 546 (1989) ; Jaksch *et al.*, PRL **81**, 3108 (1998)]

$$H = -J \sum_{\langle ij \rangle} (b_i^\dagger b_j + H.c.) + \frac{U_0}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i$$



[M. Greiner *et al.*, Nature **415**, 39 (2002)]

# Dipolar gases in optical lattices

---

## Bose-Hubbard with finite-range interactions

$$H = -J \sum_{\langle ij \rangle} (b_i^\dagger b_j + H.c.) - \mu \sum_i n_i + \frac{U_0}{2} \sum_i n_i (n_i - 1) + \frac{U_1}{2} \sum_{\langle i,j \rangle} n_i n_j + \frac{U_2}{2} \sum_{\langle\langle i,j \rangle\rangle} n_i n_j + \dots$$

### Supersolid

[Andreev and Lishitz, JETP **29**, 1107 (1969); Chester, PRA **2**, 256 (1970); Leggett, PRL **25**, 1543 (1970)]

Superfluidity + periodic modulation of the density

Experiment in Solid Helium [Kim and Chan, Science **305**, 1941 (2004)]

Still a rather controversial issue

[Leggett, Science **305**, 1921 (2004);  
Prokof'ev and Svistunov, PRL **94**, 1555302 (2005)]

In a square lattice, for hard-core bosons ( $U_0 \gg U_1$ ),  
the supersolid phase is unstable against phase separation

[Batrouni and Scalettar,  
PRL **84**, 1599 (2000)]

The supersolid phase can be stabilized for  
softcore bosons ( $U_0 < 4U_1$ )

[Sengupta et al., cond-  
mat/0412338]



# Dipolar gases in optical lattices

## Bose-Hubbard with dipole-dipole interactions

[K. Góral et al., PRL **88**, 170406 (2002)]

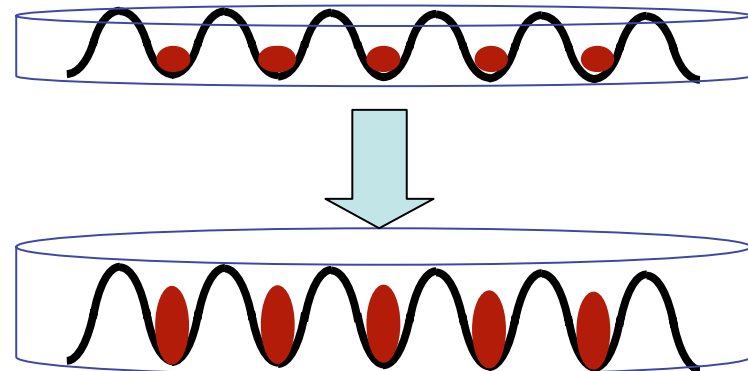
$$J = -\int w^*(\vec{r} - \vec{r}_i) \left[ \frac{-\hbar^2}{2m} \nabla^2 + V_{latt}(\vec{r}) \right] w(\vec{r} - \vec{r}_j) d^3\vec{r} \quad \leftarrow \text{Tunneling}$$

Interaction energy  $\rightarrow U_m = \int |w^*(\vec{r} - \vec{r}_i)|^2 V_{int}(\vec{r} - \vec{r}') |w(\vec{r} - \vec{r}_j)|^2 d^3\vec{r}' d^3\vec{r}$

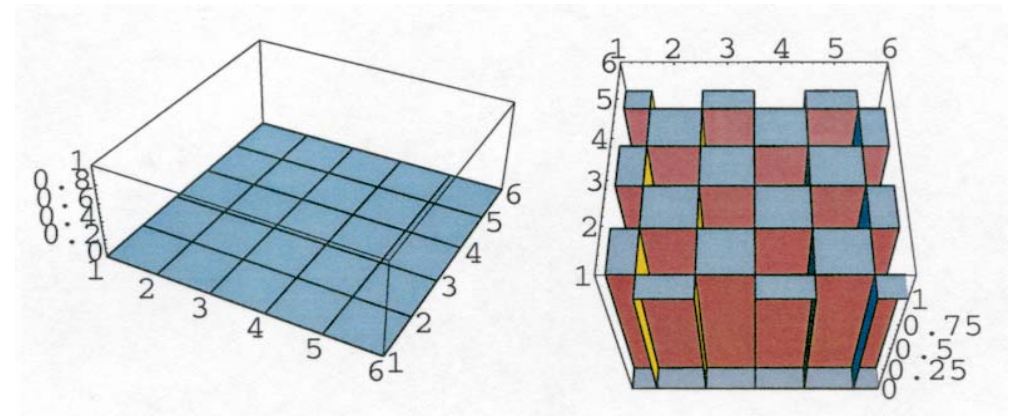
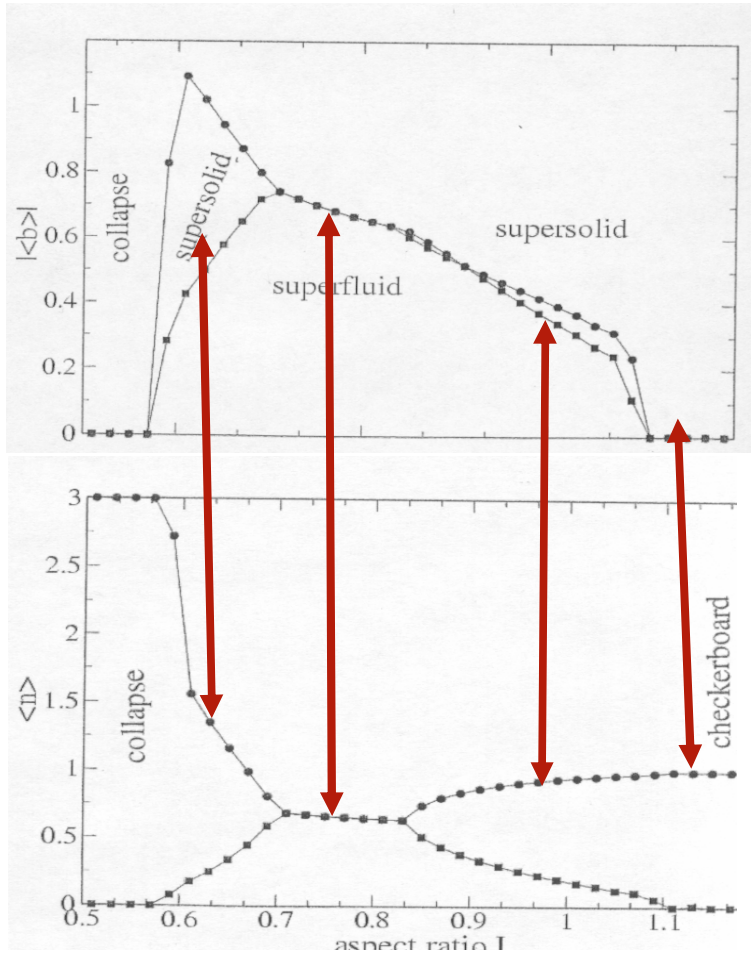
$$V_{int}(\vec{r}) = \frac{g_d}{r^3} (1 - 3 \cos^2 \theta) + g\delta(\vec{r}) \quad \rightarrow U_m = U_m^{(d)} + U_m^{(c)}$$

Let  $a > 0$  ( $U_0^{(c)} > 0$ ) and a dipole oriented perpendicular to a 2D lattice ( $U_{m>0}^{(d)} > 0$ )

Changing the transversal confinement changes the  $U_m$  coefficients.  
In particular  $U_1/U_0$ , this allows an easy control of the quantum phases



# Dipolar gases in optical lattices



- Similar control by changing the angle between dipole and lattice plane

- Gutzwiller Ansatz, up to 80x80 sites

$$|\Psi\rangle = \prod_i \sum_{n_i} f(i, n_i) |n_i\rangle_i$$

# Dipolar gases in optical lattices

## Creation of a dipolar lattice gas in 3 stages

[Jaksch et al., PRL **89**, 040402 (2002); Damski et al., PRL **90**, 110401 (2003)]

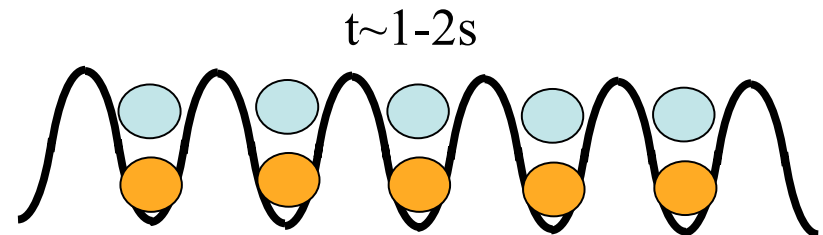
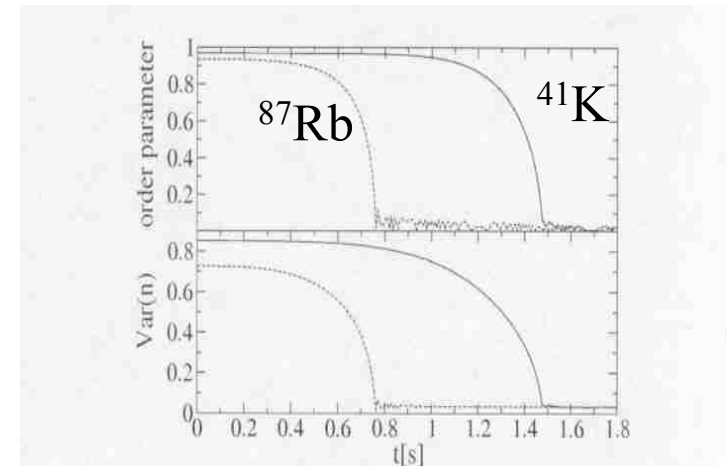
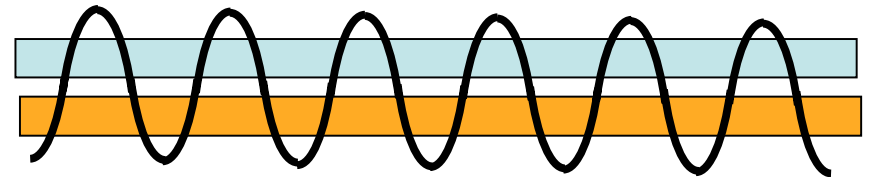
### 1) Adiabatic growing of the lattice

- Two trapped atomic species  
In particular  $^{87}\text{Rb}$ - $^{41}\text{K}$
- 2-species BH Hamiltonian:

$$H = \sum_{\langle ij \rangle} [J_a a_i^\dagger a_j + J_b b_i^\dagger b_j] + U_{ab} \sum_i n_{ai} n_{bi} + \frac{1}{2} \sum_i [U_{0a} n_{ai} (n_{ai} - 1) + U_{0b} n_{bi} (n_{bi} - 1)]$$

- We consider miscibility:  
Eventually Feshbach res.
- Dynamical Gutzwiller Ansatz

[Jaksch et al., PRL **89** 040402 (2002)]



# Dipolar gases in optical lattices

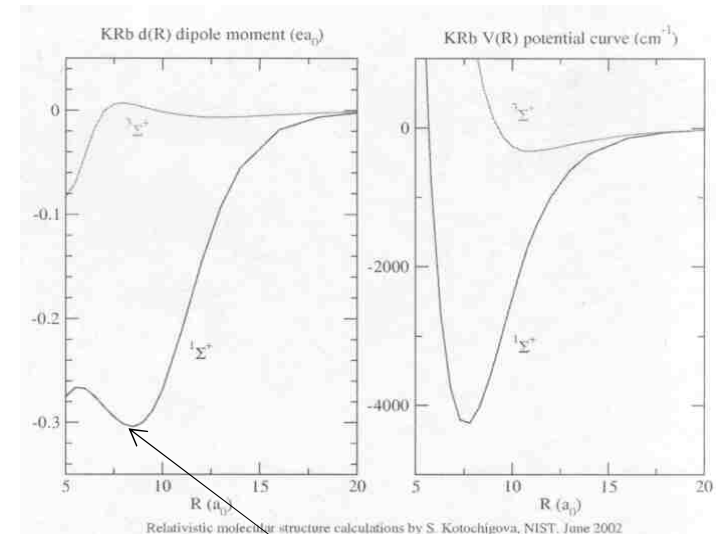
## 2) In-site molecule formation

- Two possible routes:

1) Two-color Raman photoassociation to make ground-state  $^1\Sigma^+$  or  $^3\Sigma^+$  dimers.

2) Use a pulse of microwave radiation to adiabatic pass from a free-free state to a bound one.

- A succession of Raman pulses transfer to the  $v=0$  state
- For the  $^1\Sigma^+$   $v=0$  level,  $d=0.76$  D has been predicted for RbK

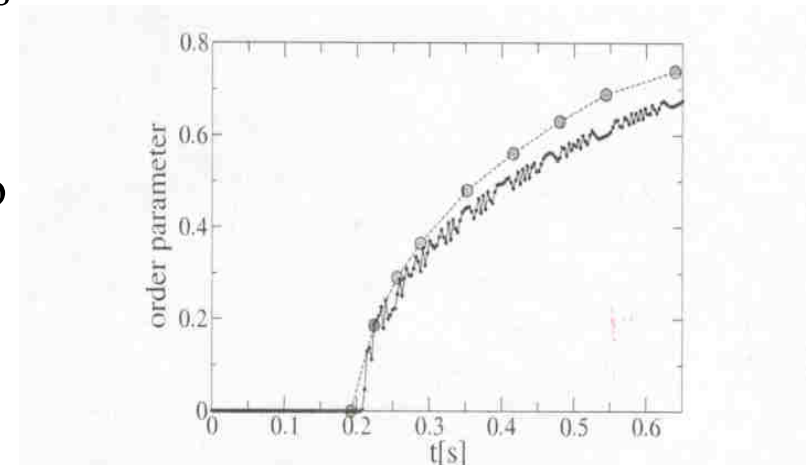
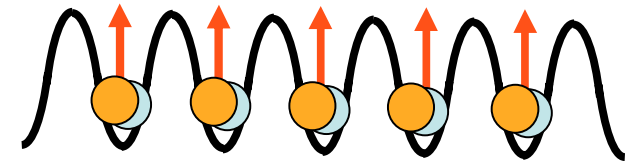


0.76 Debyes

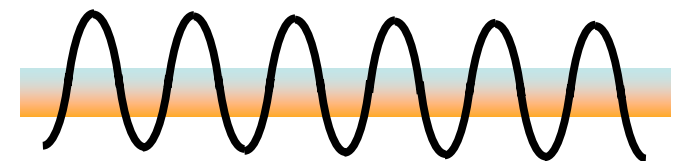
# Dipolar gases in optical lattices

## 3) Adiabatic melting

- After the formation: Molecular Mott Applications to QC [Brennen *et al.*, PRL **82**, 1060 (1999); DeMille, PRL **88**, 067901]
- Melting dynamics : Gutzwiller Ansatz taking into account the dip-dip interact.
- Two stages in the melting:
  - 1) Reduce the lattice potential:  $U_0/J$  decreases
  - 2) Reduce the transversal confinement: The anisotropy of the dip-dip helps to further reduce  $U_0$



$t \sim 1$  s

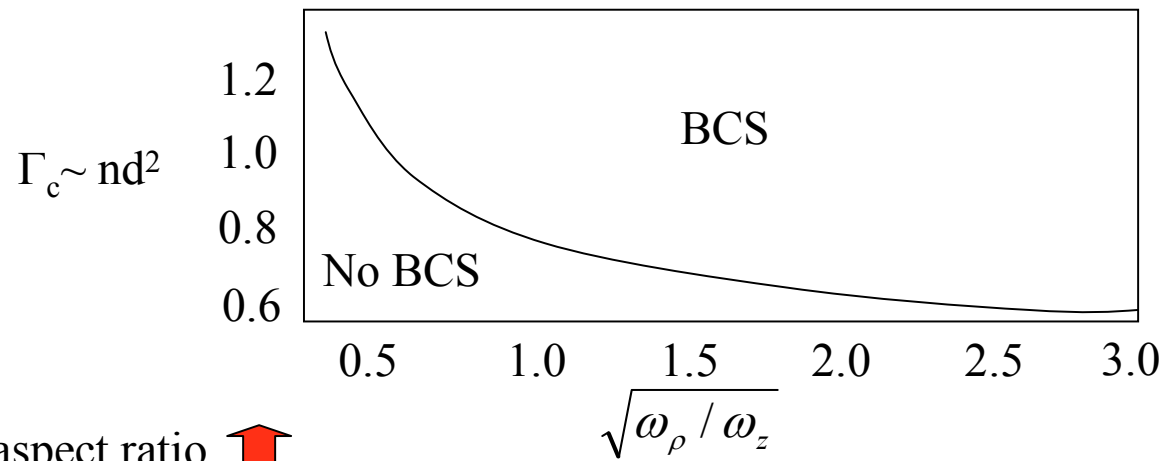



# Other interesting developments in dipolar gases

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## Fermionic dipolar gases

[Baranov et al., PRA **66**, 013606 (2002); Baranov et al., PRL **92**, 250403 (2004)]



Critical trap aspect ratio   
(once more!)

# Other interesting developments in dipolar gases

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## Rapidly-rotating dipolar gases

[Baranov et al., PRL **94**, 070404 (2005); Rezayi et al., cond-mat/0507064]

**Lecture of Nigel Cooper tomorrow**

## Dipolar effects in spinor condensates

[Pu et al., PRL **87**, 140405 (2001); Yi and You, PRL **93**, 040403 (2004)]

## Quantum information applications

[Brennen et al., PRL **82**, 1060 (1999); Jaksch et al., PRL **85**, 2208 (2000); DeMille et al., PRL **88**, 067901 (2002)]

# People

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P. Pedri  
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M. Lewenstein

S. Kotochigova  
P. Julienne

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