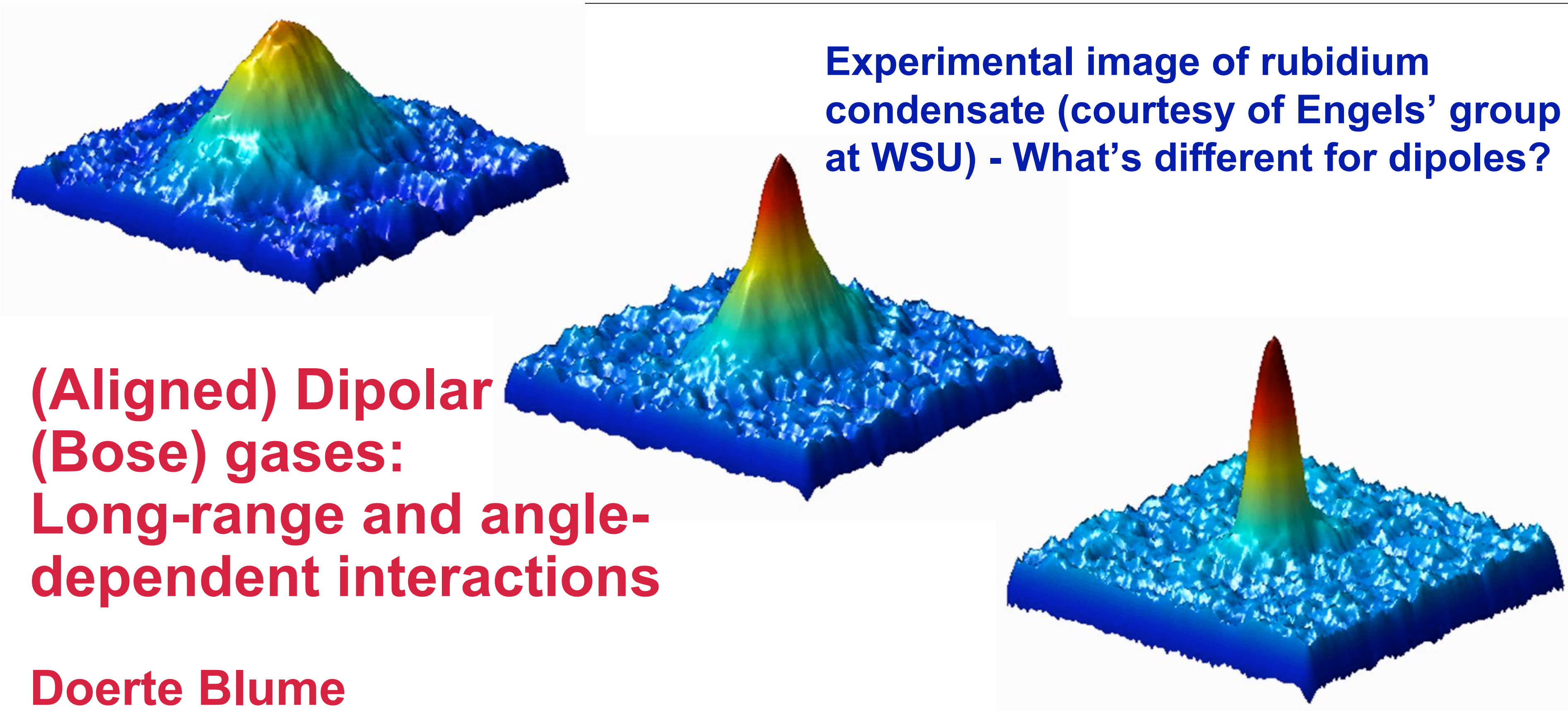

Experimental image of rubidium condensate (courtesy of Engels' group at WSU) - What's different for dipoles?

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

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At JILA: Chris Greene, Javier von Stecher, Seth Rittenhouse, John Bohn, Shai Ronen, Danielle Bortolotti.
At BEC Center in Trento: Stefano Giorgini, Grigori Astrakharchik.

Supported by NSF and ARO.

Outline of This Talk

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

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

- Summary.

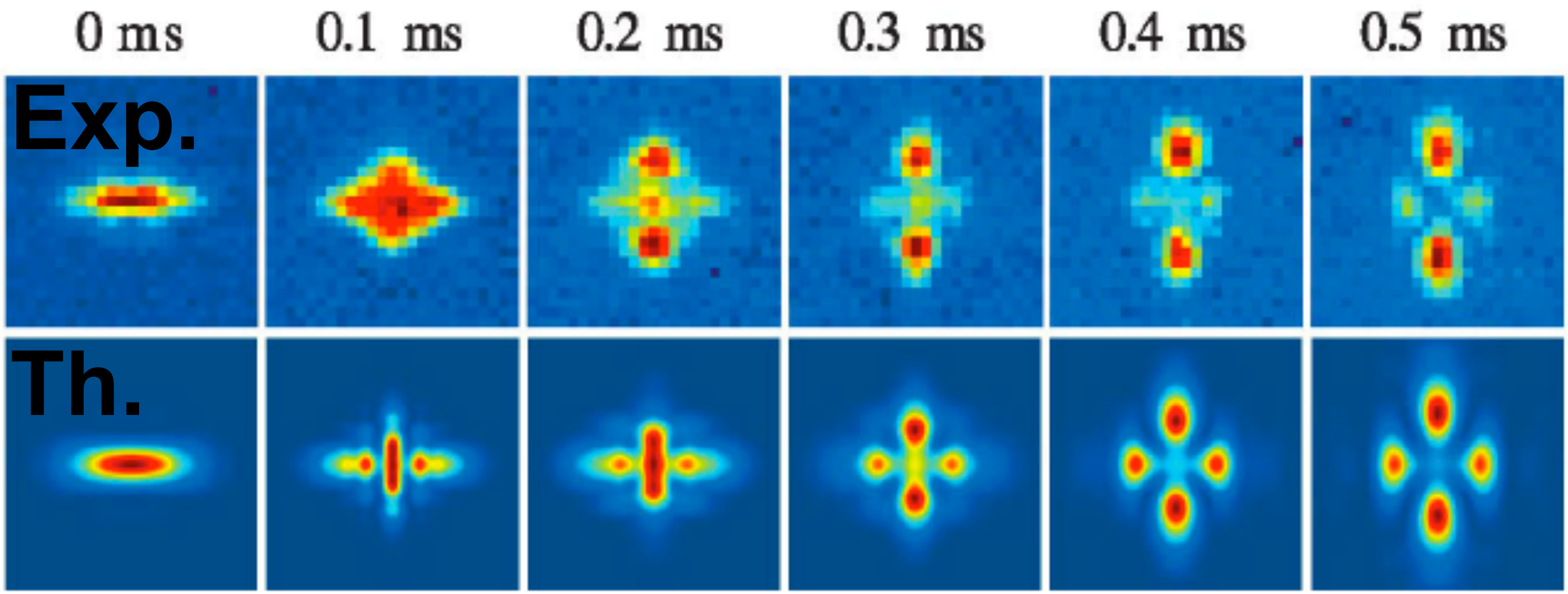
Why are Ultracold Dipolar Systems Interesting?

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

Experimental Realization of Dipolar Condensate in 2005: Atomic Chromium

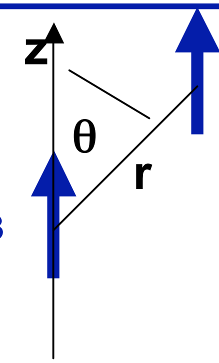
- ^{52}Cr ([Ar]$3d^5 4s^1$): Electron spin of 3, nuclear spin 0, composite boson.
- Magnetic moment of $6\mu_B$ (six times larger than for alkali atoms).
- Still comparatively small magnetic interaction (factor of 36); but isotropic s-wave interaction can be tuned to zero.

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



Roadmap: Long-Range and Anisotropic

Long-range potential V_{dd}: $d^2 (1-3\cos^2\theta) / r^3$



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

- **Many-body treatment:**
  - **Quantum Monte Carlo approaches:**
    - Account for all correlations and lead (in principle) to exact results.
    - DMC: Anisotropy needs to be build into guiding function.
    - Homogeneous system: LR tail increases numerical complexity.
  - **Mean-field treatment:**
    - Integro-differential equation.
    - Applicability requires: $n a_{00}^3 << 1$, $n r_c^3 << 1$ (SR), $n D_*^3 << 1$ (LR).

Two-Body Scattering:
How to Get K-Matrix or Phase Shifts?

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

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

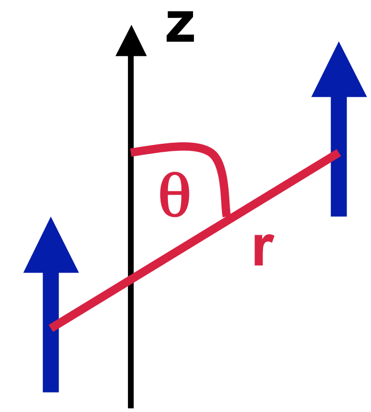
- Define log derivative matrix $\underline{y}(r)=\underline{u}'(r)/\underline{u}(r)$.
- Then $\underline{y}'(r) = -[\underline{y}(r)]^2+\underline{V}_{eff}(r)$, where $\underline{V}_{eff}$ includes potential, angular momentum barrier and energy.

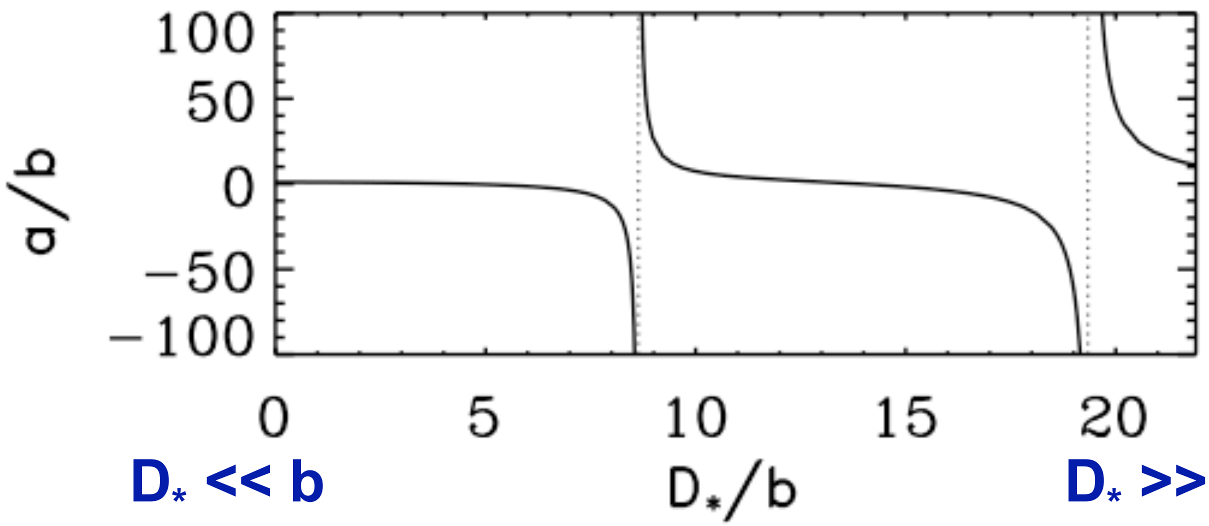
- Propagate $\underline{y}(r)$ to large r using Johnson algorithm and match to $\underline{J} - \underline{N}\ \underline{K}$, where $K_{ll'}=\tan(\delta_{ll'})$.
- Initial condition at $r=r_c$: $\underline{y}$ diagonal matrix with $y_{ll}=\infty$, i.e., large.

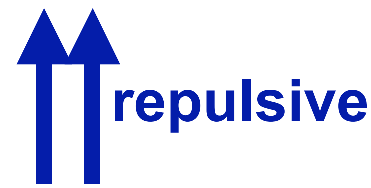
B.R. Johnson, J. Comput. Phys. 13, 445 (1973).

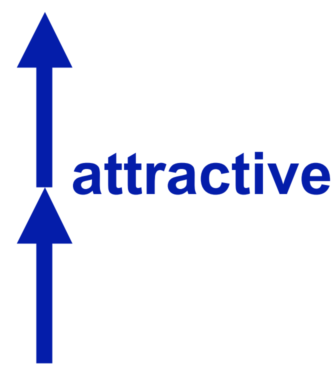
Scattering of Two Aligned Identical Bosonic Point Dipoles

- LR interaction: $d^2 (1-3\cos^2\theta) / r^3$.
- LR dipole length $D_* = md^2/\hbar^2$ (d: dipole moment).
- Short-range interaction: hard wall at b.
- Notable variation of a_{00} with D_*/b!









$D_* \ll b$ (SR dominated)

$D_* \gg b$ (LR dominated)

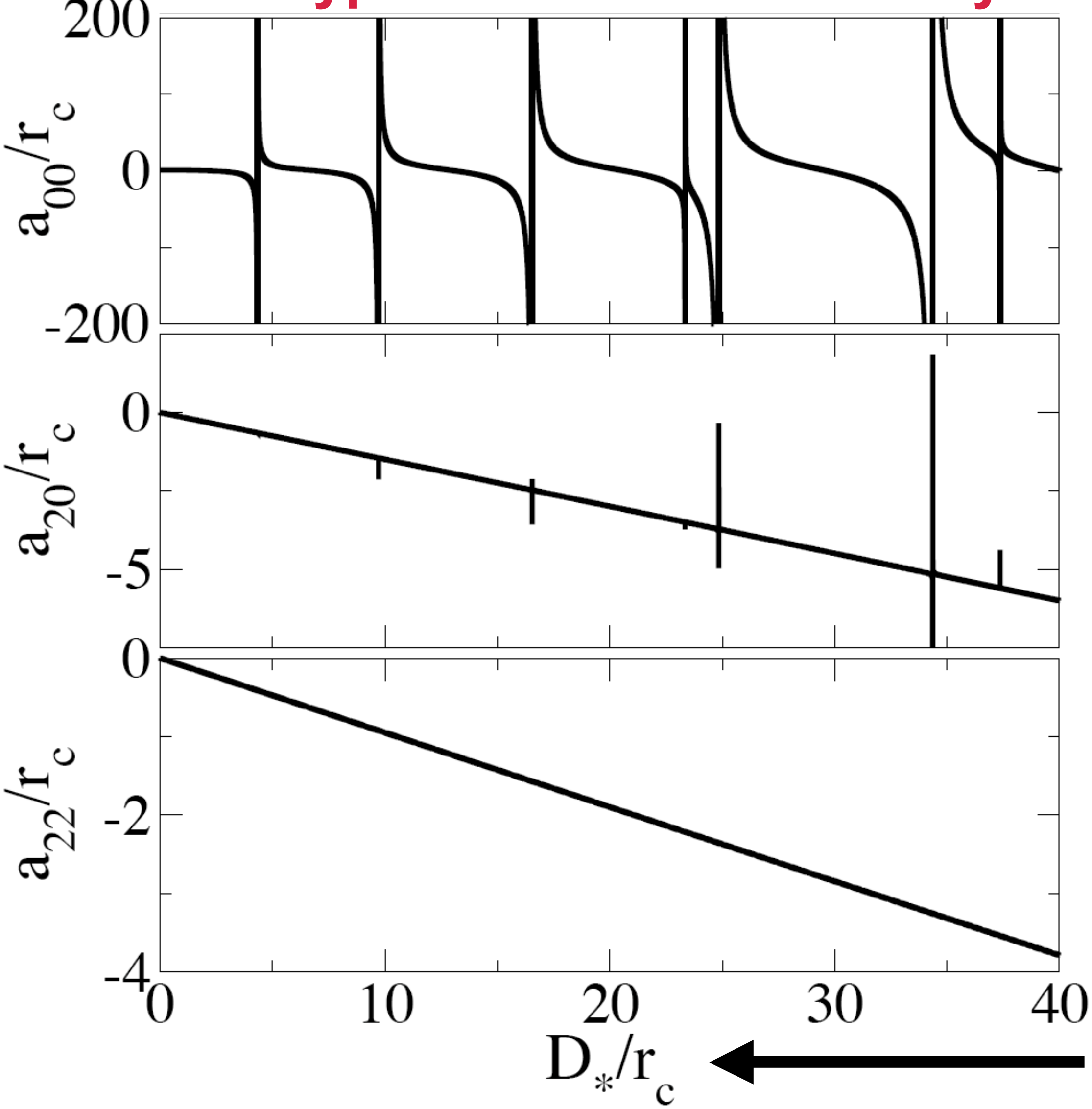
No s-wave bound states

One s-wave bound state

Two s-wave bound states

Scattering Lengths for Two Aligned Identical Bosonic Point Dipoles

Two types of resonances. Why?



Scattering length $a_{ll'}$ for each partial wave:

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

$a_{ll'}$ constant as $E \to 0$.

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

$a_{ll'} \propto D_*$ for l,l' > 0 (except near resonance).

[dipole length $D_* = \mu d^2/\hbar^2$. SR cutoff r_c=b]

Tuning SR or LR physics.

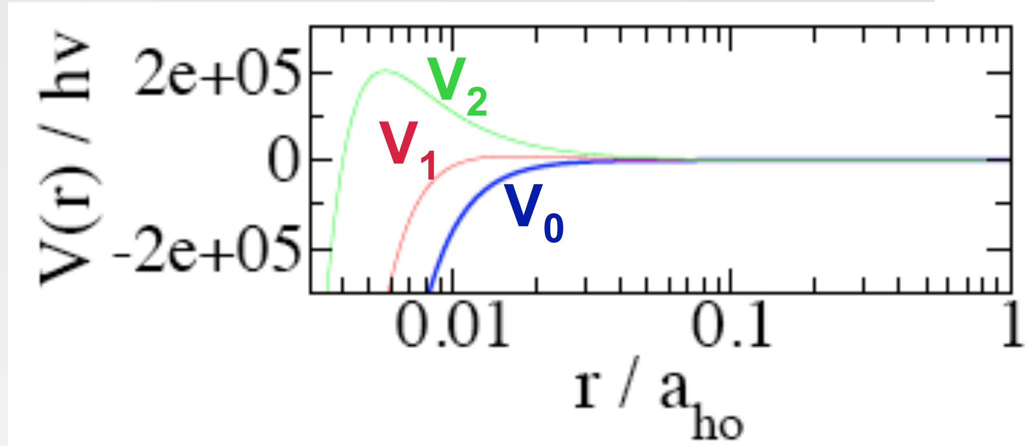
Rationalizing the Results of Coupled Channel Calculation

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

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

Understanding Resonances: Adiabatic Potential Curves and WKB Phase

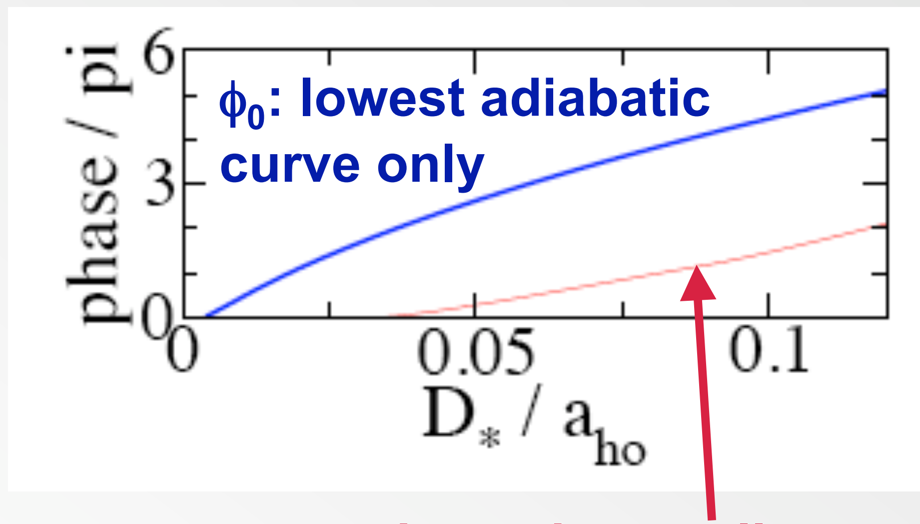
- **Diagonalizing Hamiltonian in angular momentum basis for fixed r determines adiabatic potential curves.**



- **Neglecting coupling/adiabatic correction, WKB phases ϕ_i give good prediction for resonance positions.**

  Look for ϕ_i/π = integer, where

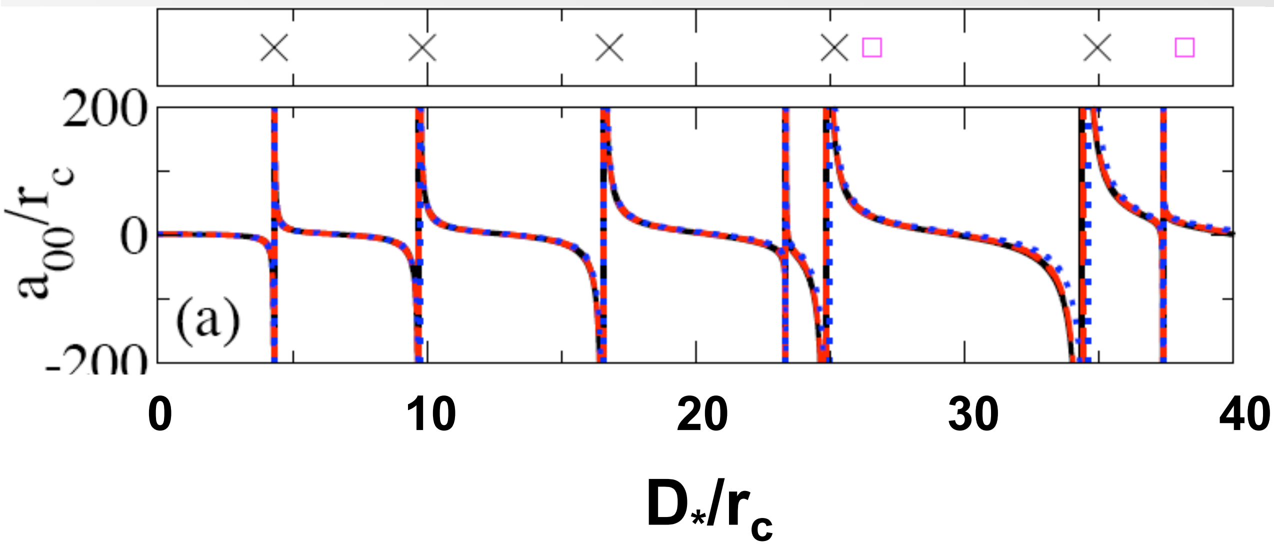
  $\phi_i = \int_{cl.\ allowed} [2\mu V_i(r)/\hbar^2]^{1/2}\, dr$.



$\Sigma_i\ \phi_i$: phase due to all other adiabatic curves

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

WKB Prediction of Resonance Positions for Two Identical Bosons



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

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

Kanjilal and Blume, PRA 78, 040703(R) (2008); see also Deb and You, PRA 64, 022717 (2001).

Finite-Range Pseudo-Potential For Two Interacting Dipoles

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

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

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

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

- **This pseudo-potential works because its scattering amplitudes, calculated in the first Born approximation, agree with the full scattering amplitudes of the model potential.**

Mean-Field Gross-Pitaevskii Description of Dipolar Bose Gas

$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \Big[-\frac{\hbar^2}{2M}\nabla^2 + \frac{M\omega_\rho^2}{2}(\rho^2+\lambda^2 z^2) + (N-1)\Big[\frac{4\pi\hbar^2 a}{M}|\psi(\mathbf{r},t)|^2 + \int d\mathbf{r}' V_d(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}',t)|^2\Big]\Big]\psi(\mathbf{r},t)$$

Mean-field interaction:

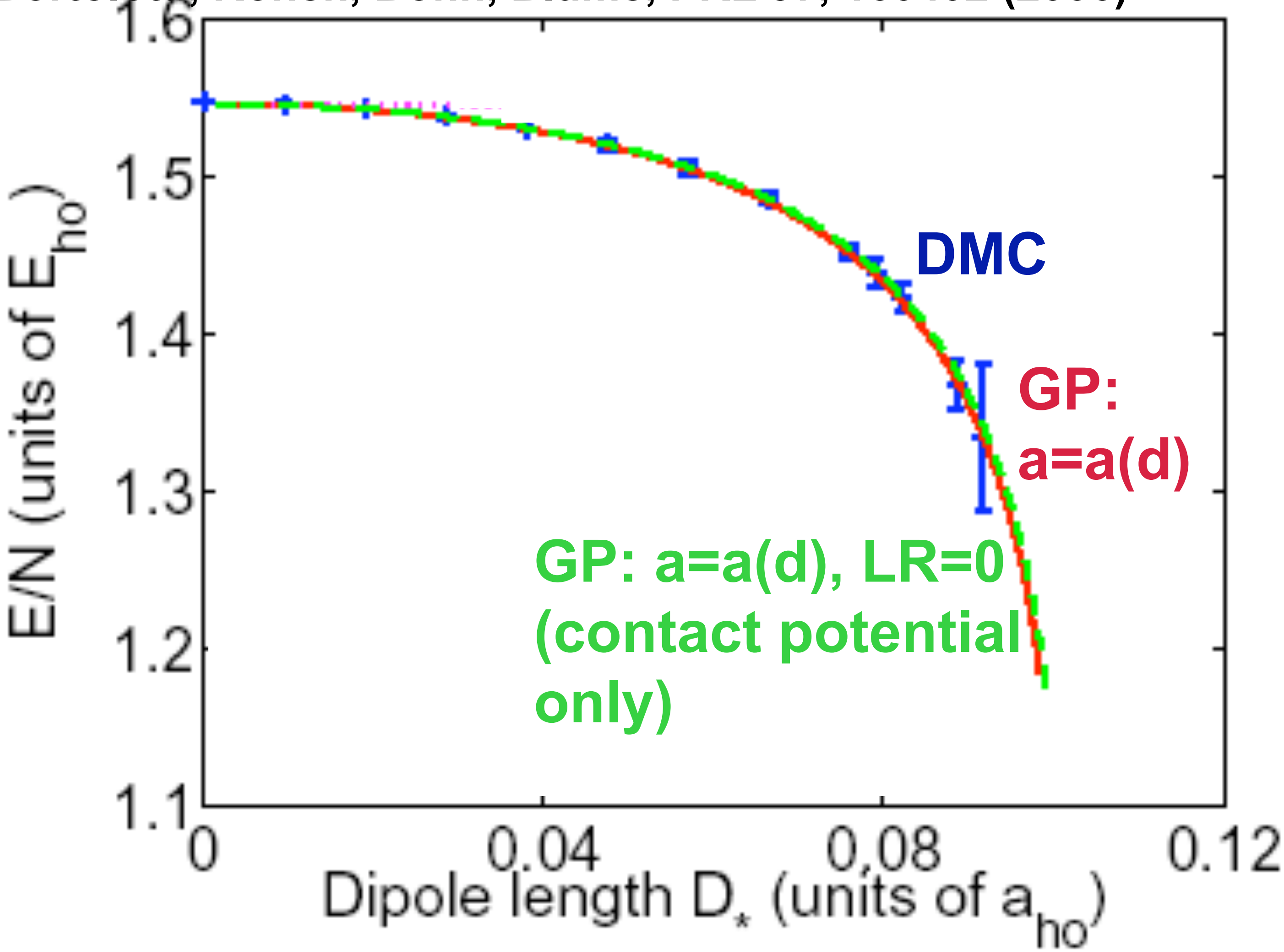
contact s-wave (SR) + dipole-dipole (LR)

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

Compare with results from many-body Schroedinger equation that uses model potential (hardwall + V_{dd}) as input.

Spherical Confinement (N=10, $b=0.0137a_{ho}$): GP versus Many-Body DMC Energies

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



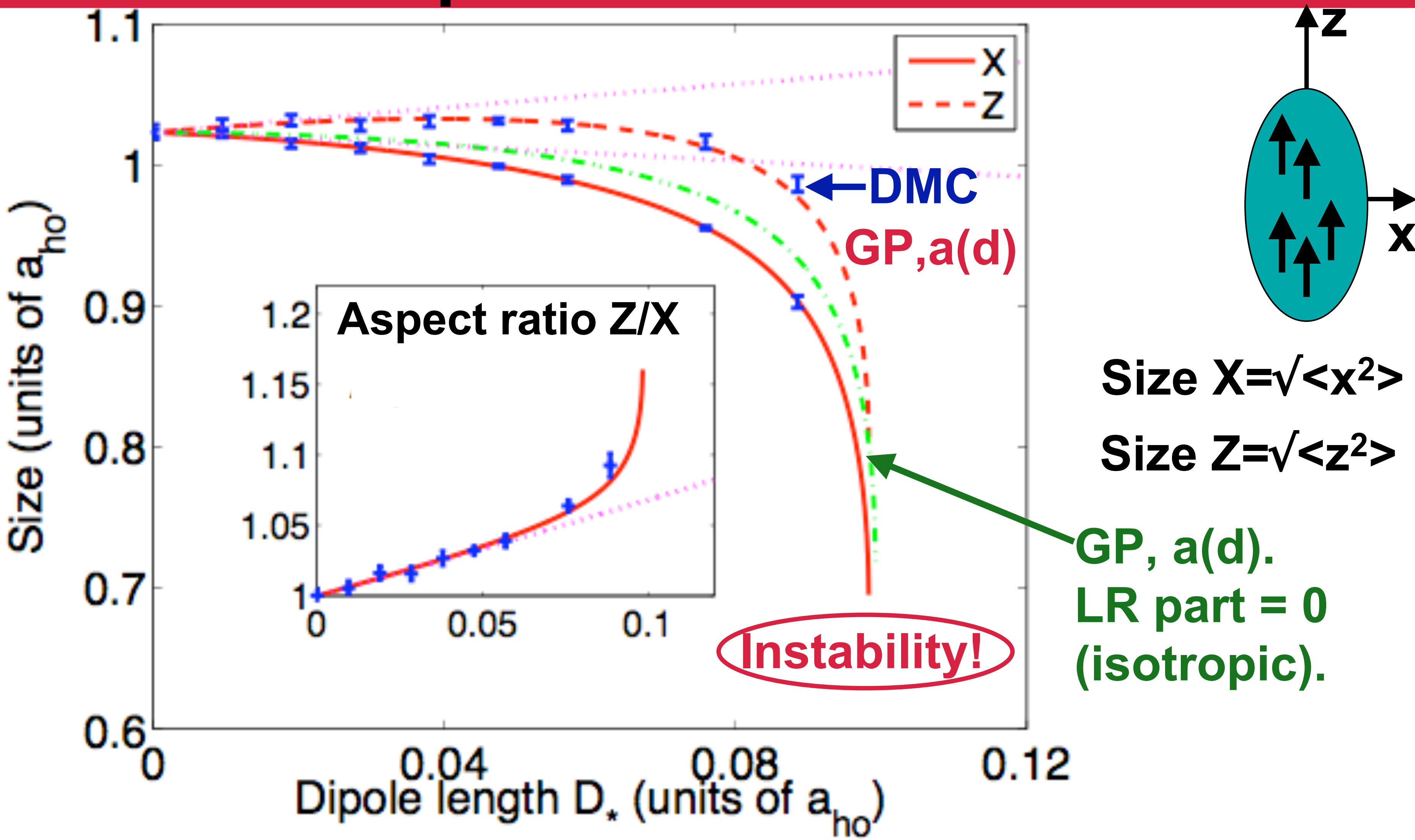
increasing E-field / dipole moment

Excellent agreement between GP and DMC many-body energies!

Validation of mean-field treatment!

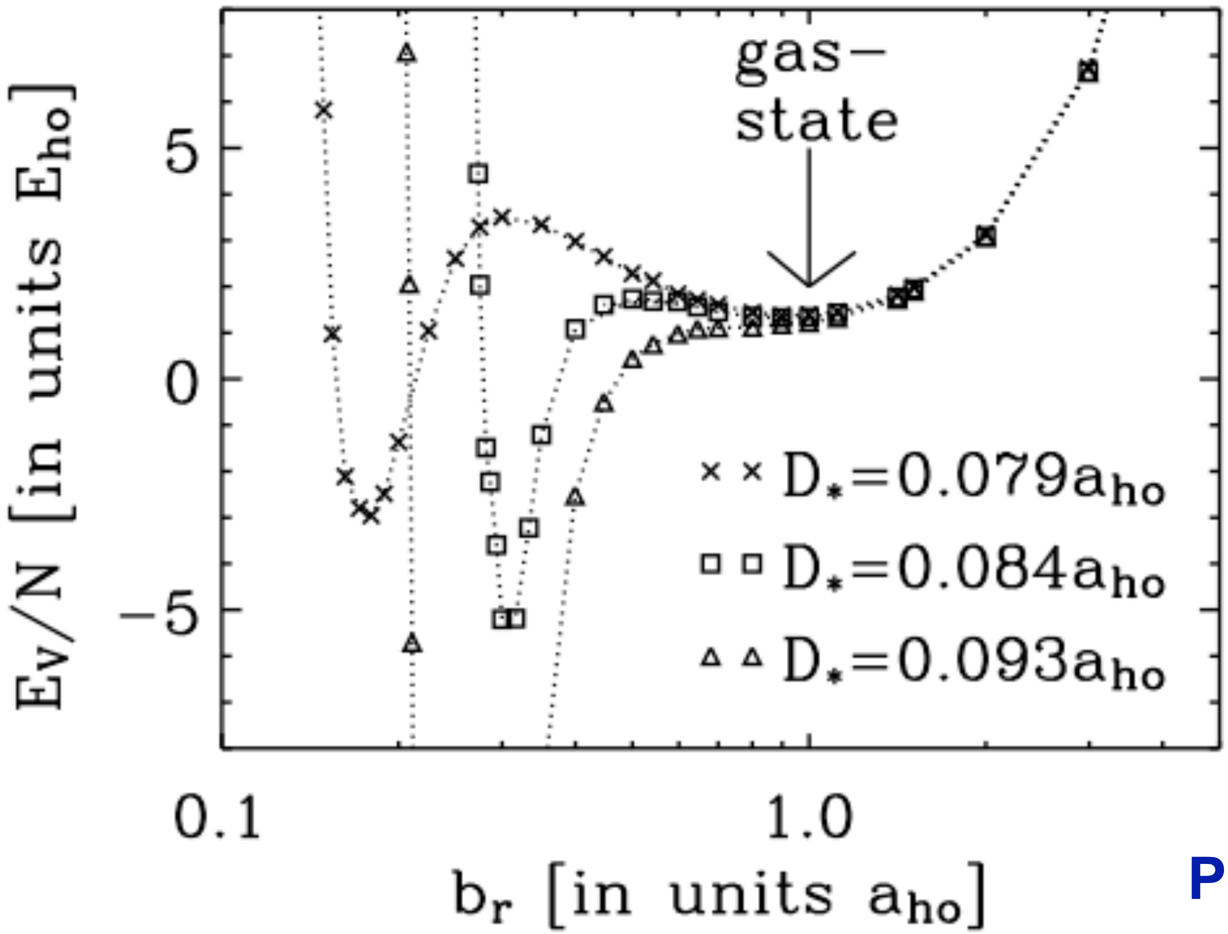
s-wave induced instability.

Spherical Confinement (N=10, b=0.0137a_{ho}): Size and Aspect Ratio



Structural properties depend on dipole moment!

Many-Body Variational Calculation: Nature of the Mechanical Instability



$N=20$, $b=0.0137a_{ho}$.

Variational wave function:

$$\Psi = \prod \Phi(r_i) \prod \varphi(\vec{r}_{jk})$$

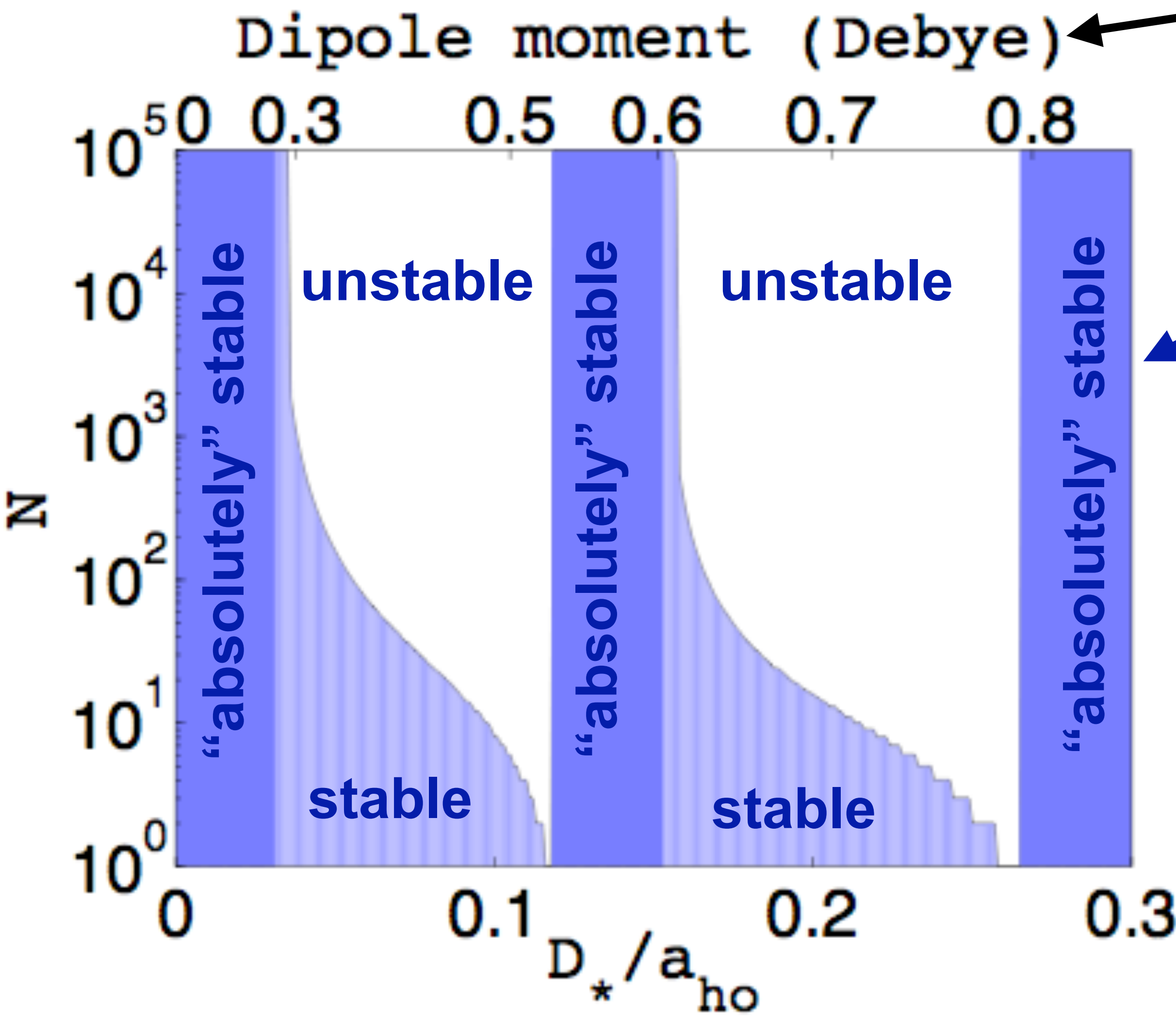
one-body term: $\exp[-(r^2/2b_r^2)]$
Parameter b_r: size.

two-body term

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

Field-Induced S-wave Collapse Within GP Formalism: Stability Diagram

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



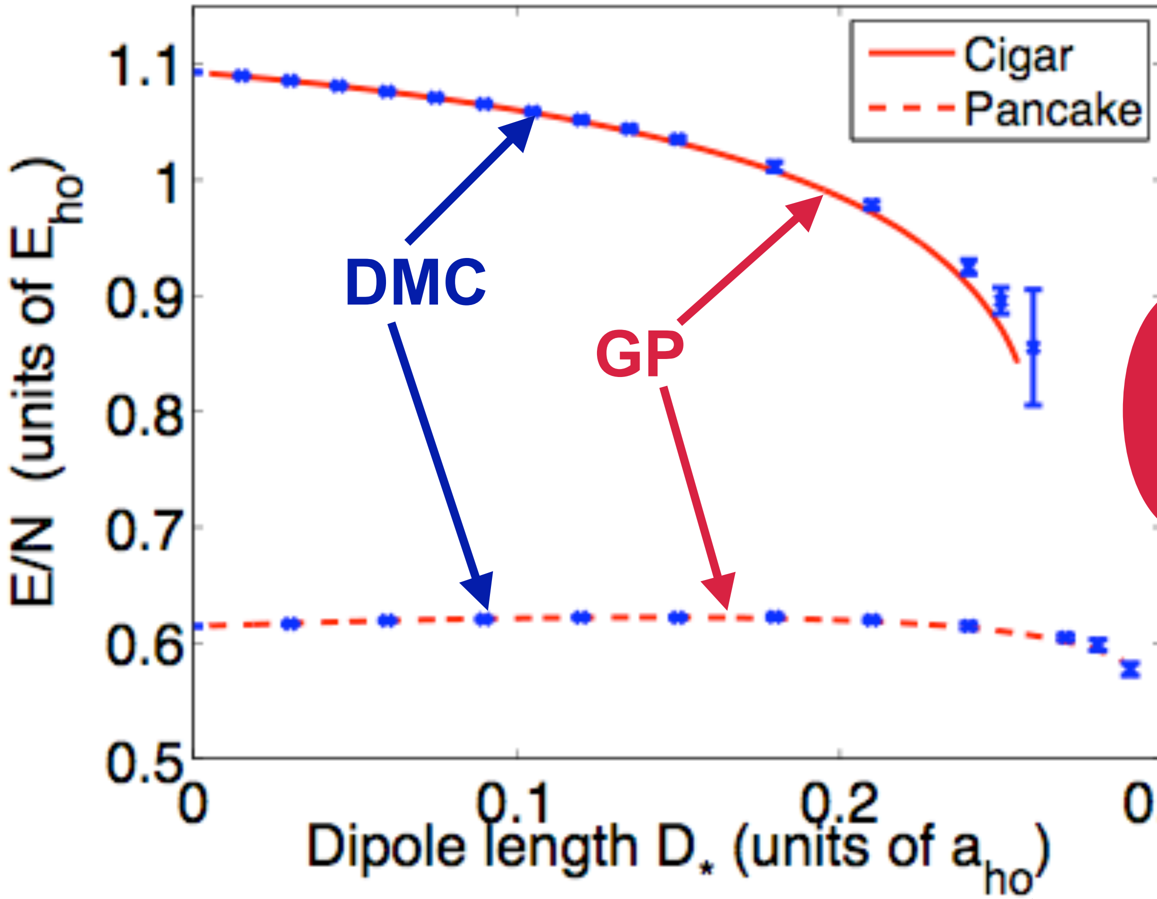
Using OH mass and ν=1kHz.

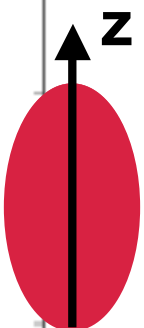
Would be stable even w/o trap, a(d) > $D_*/12\pi$

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

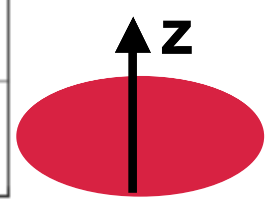
Experiment for fixed N: Sequence of stable and unstable regions.

N=10: Tuning Interactions By Changing Confining Potential





E/N increases with increasing D_*.



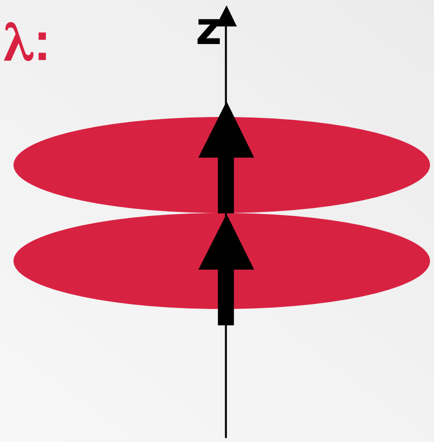
E/N first increases with increasing D_*, and then decreases.

defined by largest frequency

Non-interacting gas:
Spherical: (0.5+0.5+0.5)hν =1.5hν
Cigar: (0.5+0.5+0.05)hν_ρ =1.05hν_ρ
Pancake: (0.05+0.05+0.5)hν_z =0.6hν_z

Double-Well Potential Along z-Direction

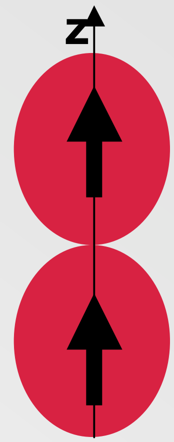
- **Large λ:**



z: high energy coordinate

- **Two "sheets" of dipoles:**
  - **Interaction within each sheet predominantly repulsive.**
  - **Interaction between sheets predominantly attractive.**
  - **Interplay?**
- **Building up a lattice of pancake-shaped dipolar gases.**

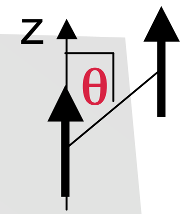
- **Small λ:**



z: low energy coordinate

- **Analogy between two weakly-coupled superconductors and two-weakly-coupled BECs (barrier ~ weak link).**
- **Josephson oscillation and macroscopic quantum self-trapping have been observed for s-wave interactions (Oberthaler group).**
- **Can they be observed for dipolar Bose gas?**

Mean-Field Gross-Pitaevskii Description of Dipolar Bose Gas

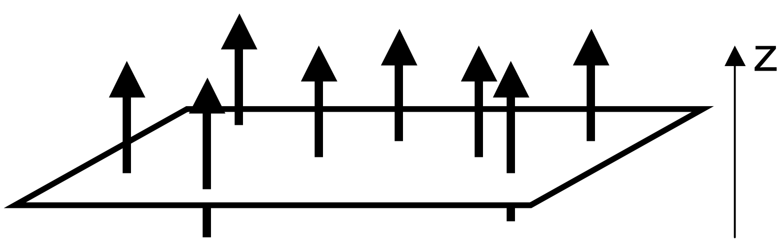


$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2M}\nabla^2 + \frac{M\omega_\rho^2}{2}(\rho^2+\lambda^2 z^2) + A\exp(-0.5z^2/b^2) + (N-1)\left[\frac{4\pi\hbar^2 a}{M}|\psi(\mathbf{r},t)|^2 + \int d\mathbf{r}' V_d(\mathbf{r}-\mathbf{r}')|\psi(\mathbf{r}',t)|^2\right]\right]\psi(\mathbf{r},t)$$

Mean-field interaction:

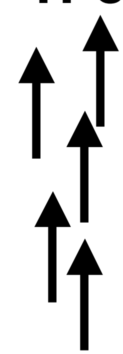
contact s-wave (SR) + dipole-dipole (LR) $V_d=d^2(1-3\cos^2\theta)/r^3$

A=0, λ > 1: pancake-shape trap



Effectively (more) repulsive

A=0, λ < 1: cigar-shape trap



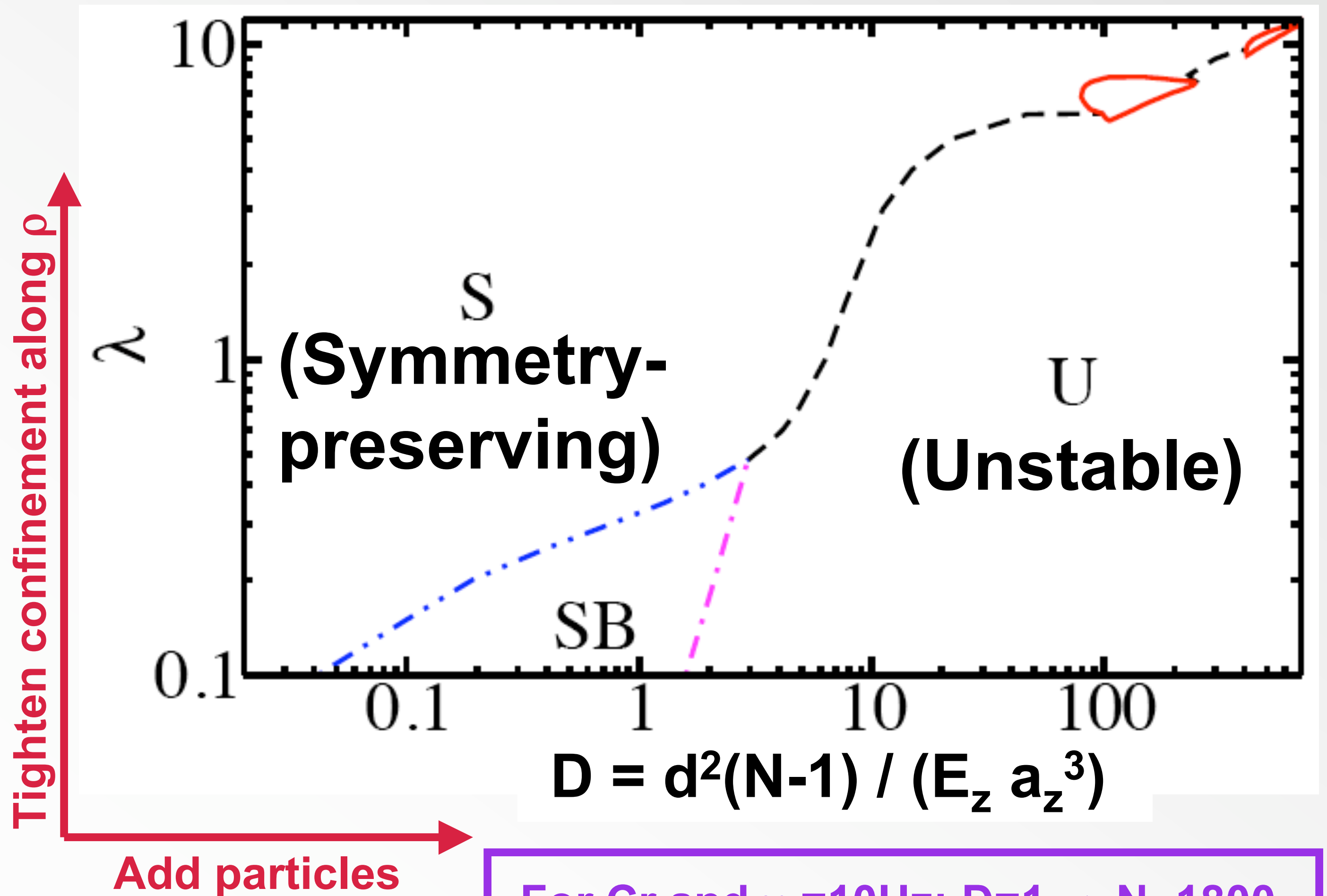
Effectively (more) attractive

---

5 parameters: (N-1)a, λ, (N-1)d², A, b. Here: Fix (N-1)a, b, A; vary λ, (N-1)d².

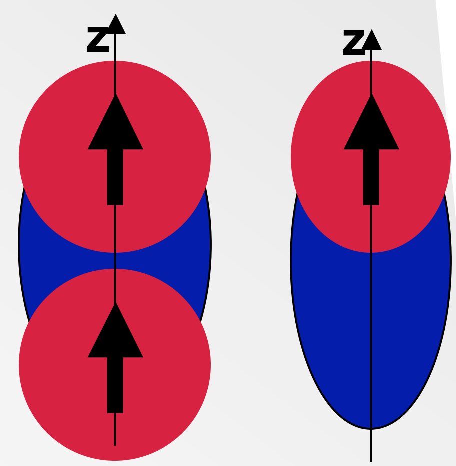
MF-GP Treatment of Pure Dipolar BEC in Double-Well Trap

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

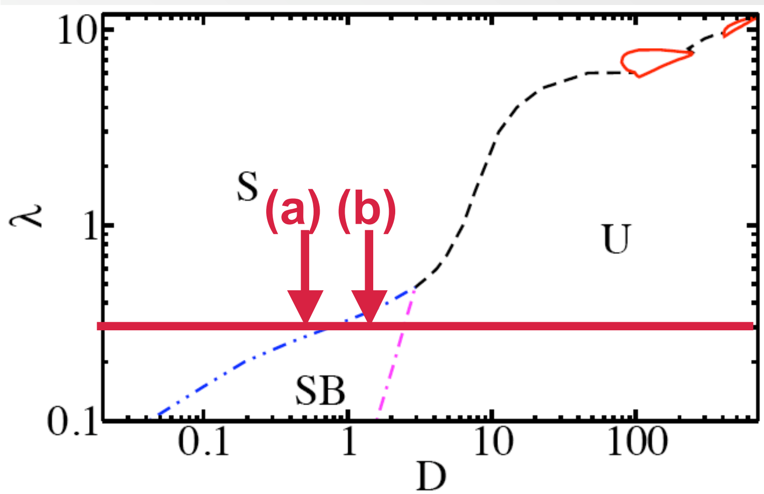


For Cr and ν_z=10Hz: D=1 → N~1800

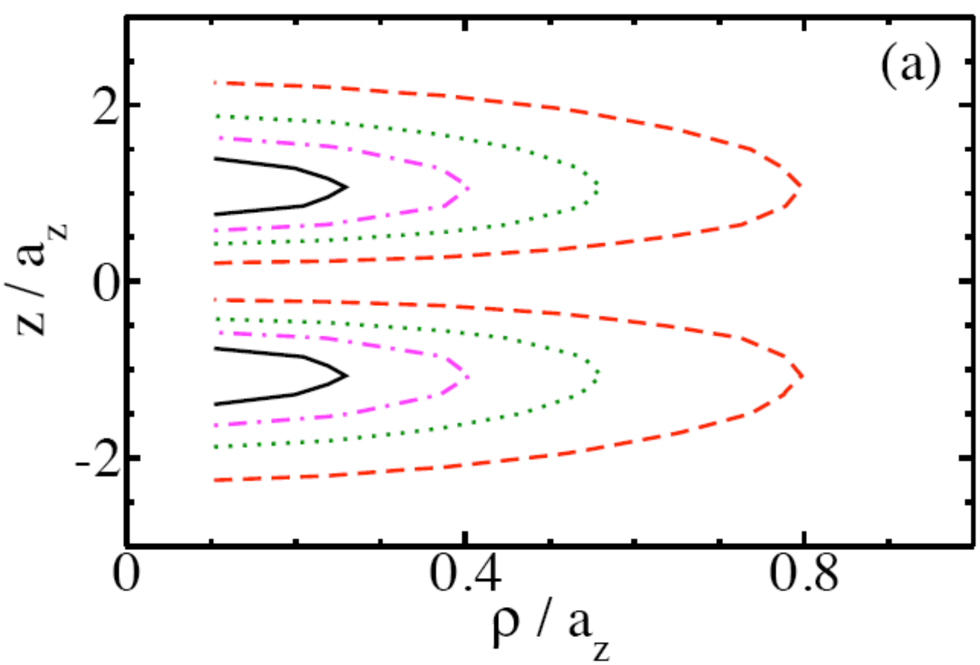
Transition from symmetry-preserving (S) to symmetry-breaking (SB) is driven by mean-field interaction.

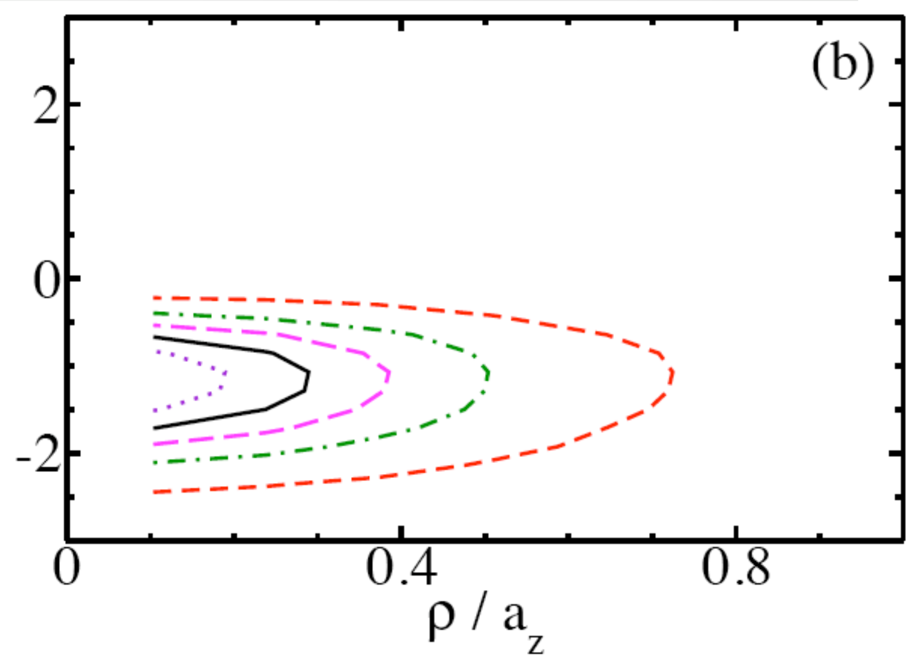


Ground State GP Densities for Aspect Ratio λ=0.3



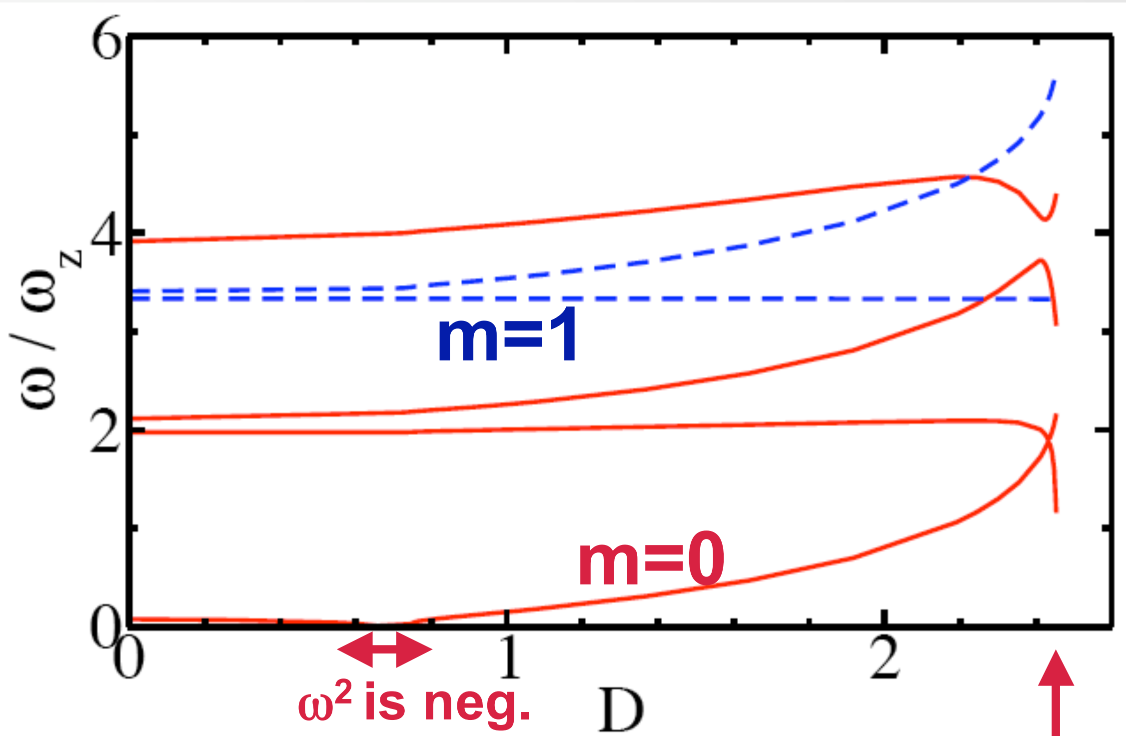
Asad-uz-Zaman and Blume, PRA 80, 053622 (2009).
For a related study, see
Xiong, Gong, Pu, Bao, Li, Phys. Rev. A (2009) [this study tunes dipole-dipole interactions by changing axis along which dipoles are aligned]





Excitation Frequencies for Aspect Ratio λ=0.3

Bogoliubov de Gennes excitation spectrum:



ω^2 is neg. (unstable mode)

Three distinct regimes as function of D:
i) Josephson oscillation.
ii) Self-trapping regime.
iii) Collapse.

Collapse is "triggered" by m=0 mode.

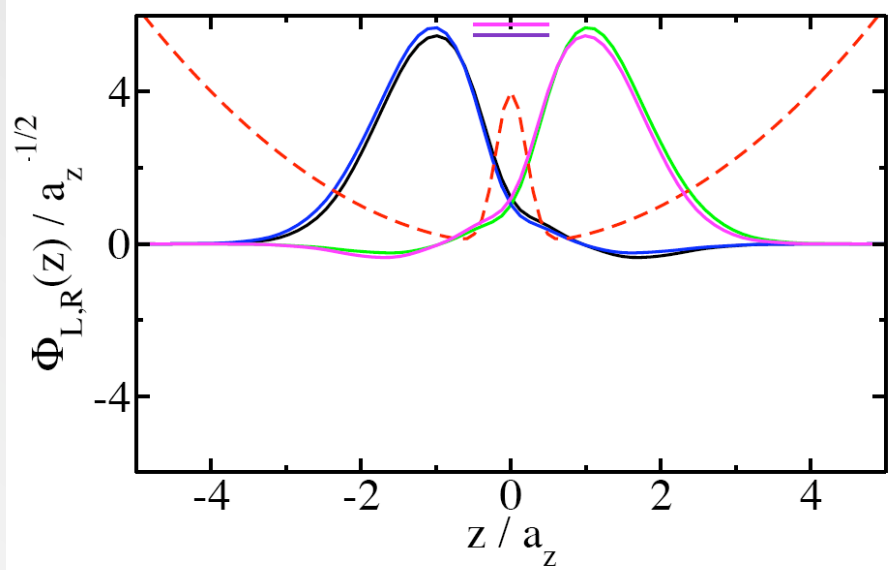
Lowest m=0 eigenmode:
Population transfer between L and R well
(BdG frequency is nearly identical to Josephson oscillation frequency obtained by time evolving initial state with small population imbalance)

Two-Mode Variational Description

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

$\Phi_{L,R}(\rho,z) \propto \Phi_+(\rho,z) \pm \Phi_-(\rho,z)$
(Φ_+ and Φ_- are stationary GP solutions)

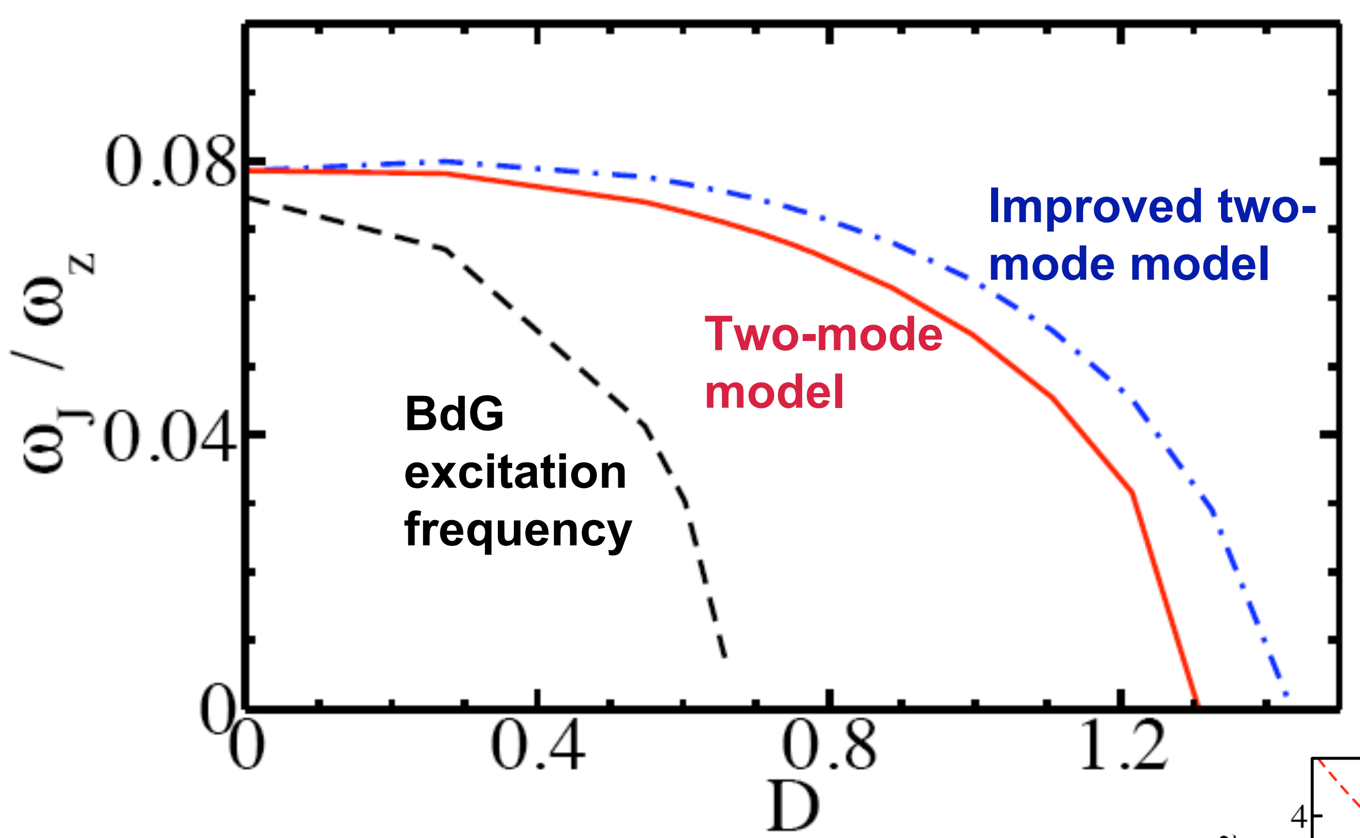
$\psi_{L,R}(t) = \sqrt{N_{L,R}(t)} \exp[i\theta_{L,R}(t)]$



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

See, e.g., Smerzi et al., PRL 79, 4950 (1997).

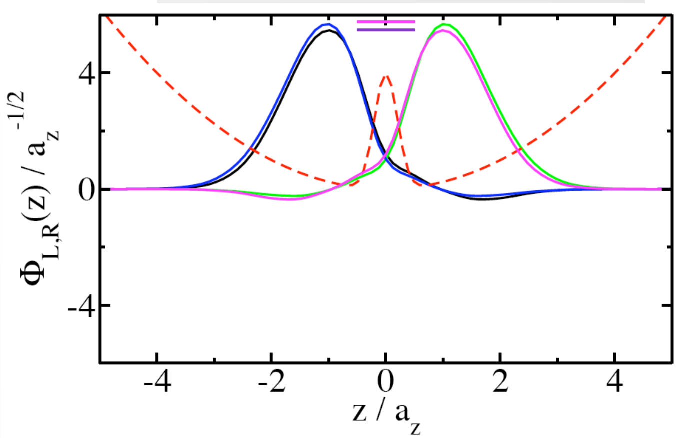
Bogoliubov de Gennes versus Two-Mode Model Prediction (λ=0.3)



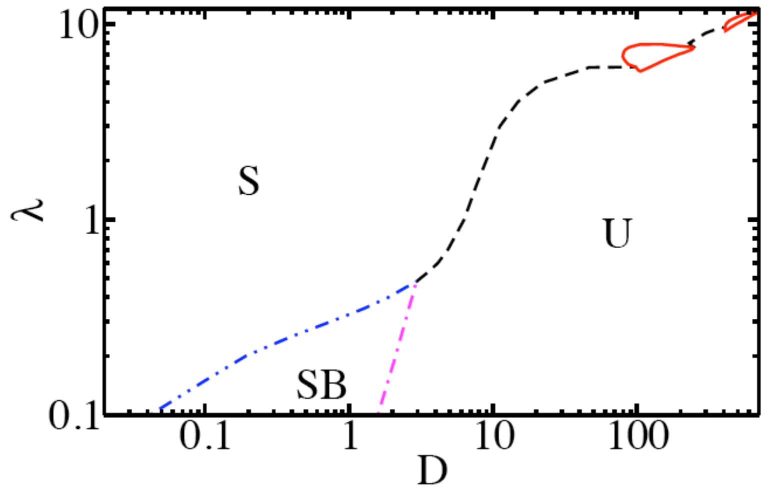
Improved two-mode model [Ananikian and Bergeman, PRA 73, 013604 (2006)] does not lead to improvement.

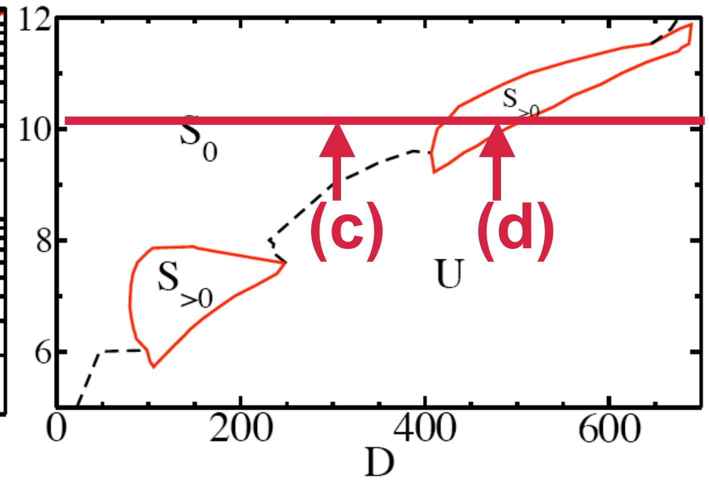
Two-mode model provides qualitative but not quantitative description.

Overlap between amplitudes in left and right well appreciable.

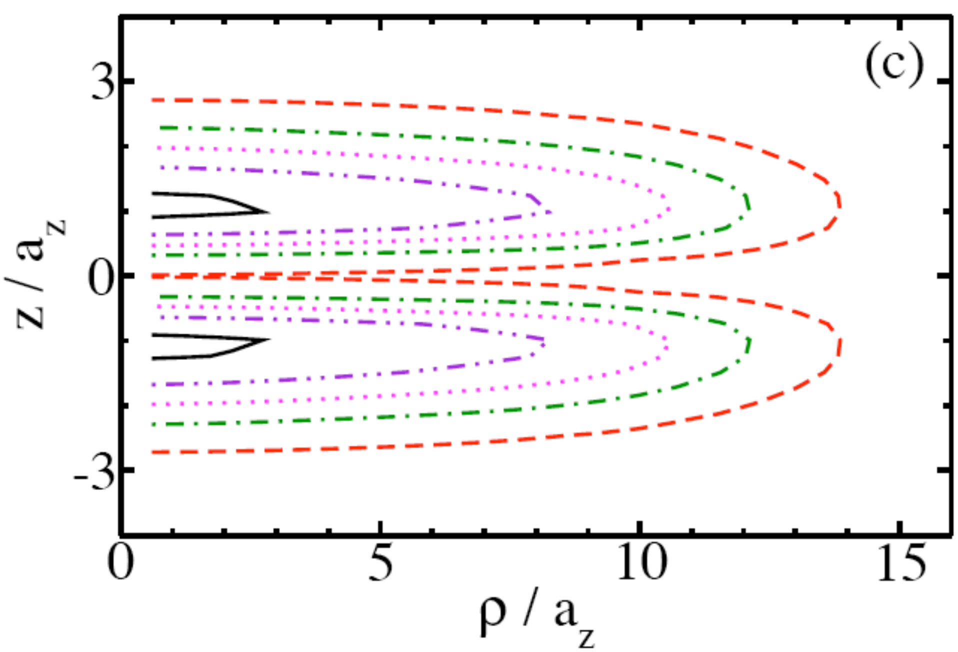


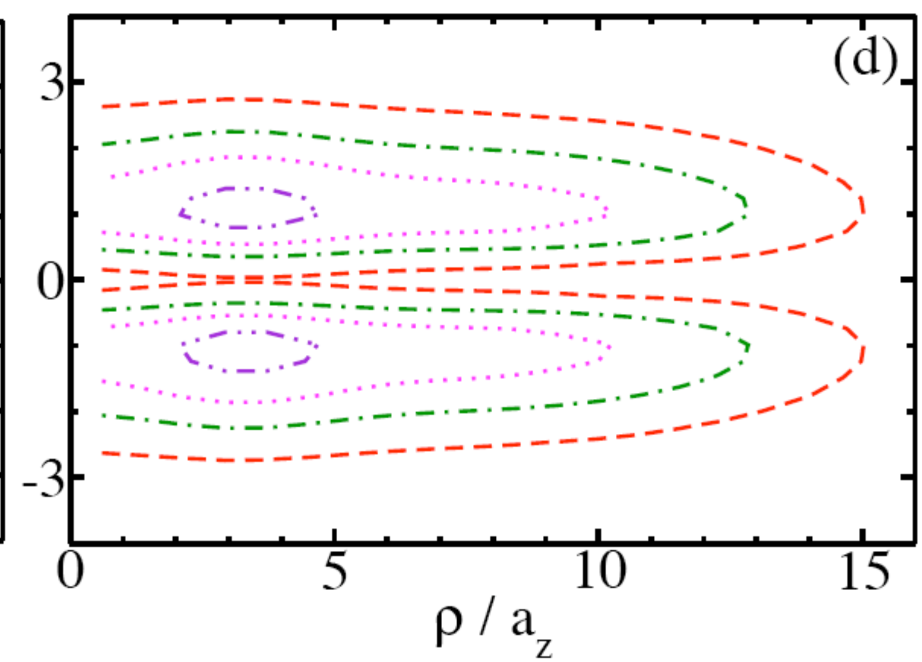
Ground State Densities for Large Aspect Ratio: λ=10



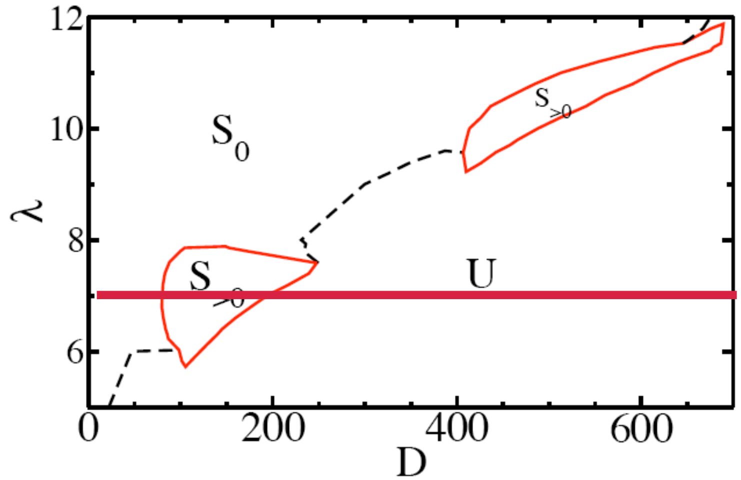


For A=0, “red blood cell” was predicted by Ronen et al., PRL 98, 030406(2007):

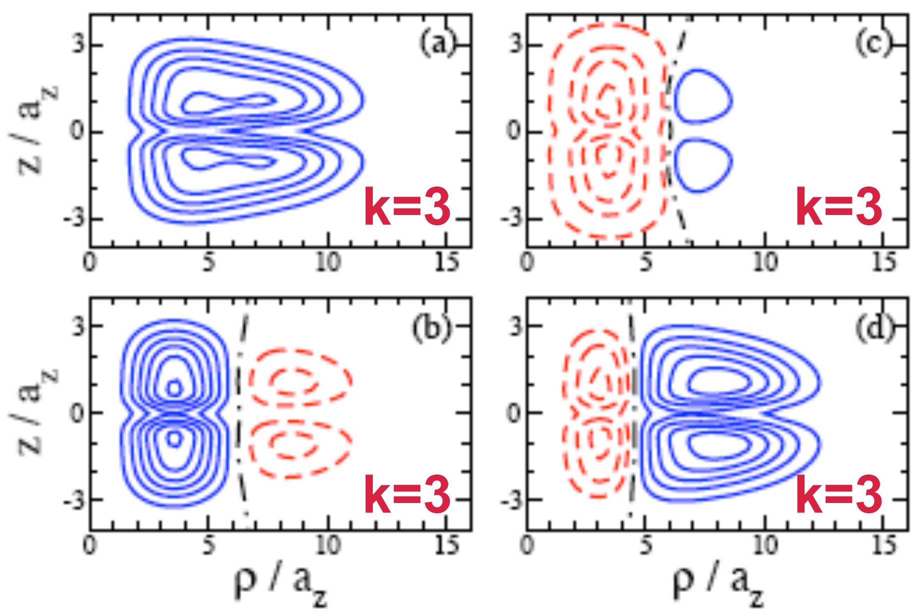


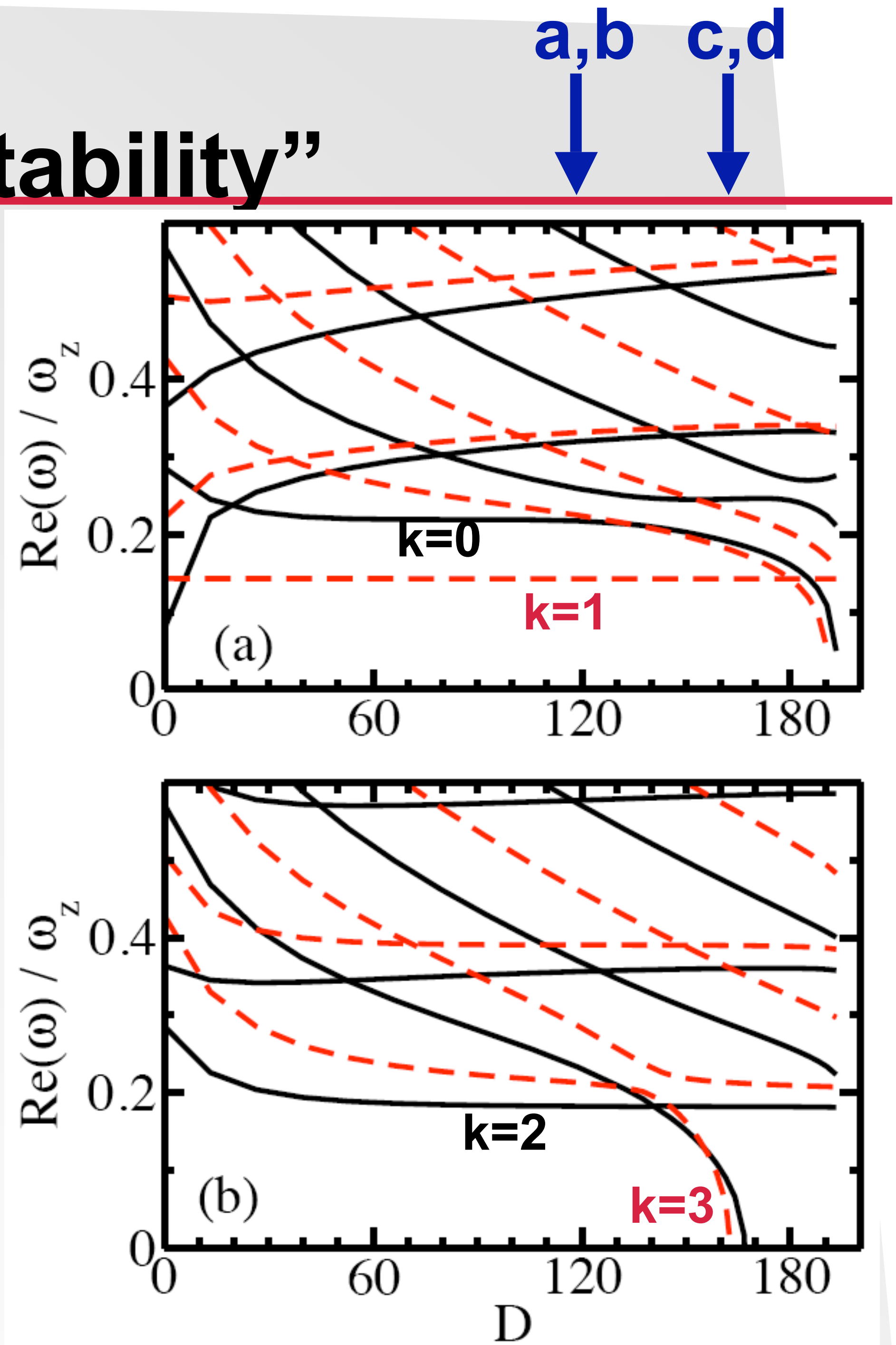


"Angular Roton Instability"



BdG eigenmodes (density osc.):





Summary

- Aligned dipolar Cr Bose gases with long-range and anisotropic interactions have been condensed.
- Huge progress toward condensing cold molecular sample with large electric dipole moment.

- Two-dipole system shows interesting scattering properties that need to be accounted for in comparisons between mean-field and many-body calculations.

- Effective interactions of aligned dipolar Bose gas can be tuned through variation of external confining potential.

- Rich stability and phase diagram as functions of dipole strength and aspect ratio.

- There's a lot more to do to fully uncover the physics of dipolar systems!