Microscopic Description of Anisotropic Quantum Bose Dipoles in 2D

A. Macia, F. Mazzanti, J. Boronat

in collaboration with R.E. Zillich, D. Hufnagl and G.E. Astrakharchik

Departament de Física i Enginyeria Nuclear
Universitat Politècnica de Catalunya

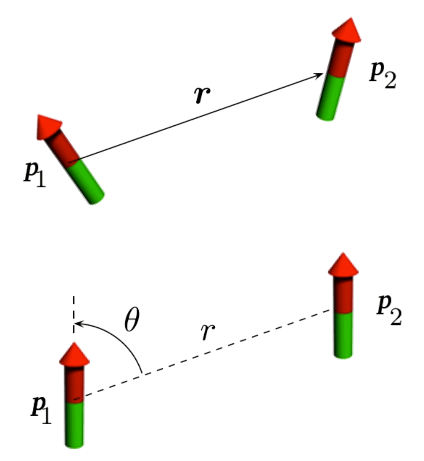
Outline

- The dipolar interaction
- Low density regime and universal properties
  - Building a trial wave function
- High density regime and the effect of the anisotropy
  - Density Response Function
  - The phase diagram

The Dipolar Interaction

The general form of the interacting potential between two dipoles p_1 and p_2 is

$$V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi}\left[\frac{\hat{p}_1\cdot\hat{p}_2 - 3(\hat{p}_1\cdot\hat{r})(\hat{p}_1\cdot\hat{r})}{r^3}\right]$$



There are 2 types of dipolar interactions:

Magnetic dipoles: Typical example: ^{52}Cr

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

Electric dipoles: Essentially polar molecules

$$C_{dd} = d^2/\epsilon_0$$

Species	Dipole moment	a_{dd}	$\varepsilon_{\mathrm{dd}}$
^{87}Rb	$1.0\,\mu_B$	$0.7\,a_0$	0.007
^{52}Cr	$6.0\,\mu_B$	$16\,a_0$	0.16
KRb	0.6 D	$2.0\times10^3 a_0$	20
ND_3	1.5 D	$3.6\times10^3\,a_0$	36
HCN	3.0 D	$2.4\times10^4\,a_0$	240

T. Lahaye *et al.* Rep.Prog.Phys. **72,** 126401 (2009)

$$a_{dd} = \frac{mC_{dd}}{12\pi\hbar^2}$$: dipolar length

What really matters is the ratio of dipolar to contact lengths:

$$\epsilon_{dd} = \frac{a_{dd}}{a}$$

The Dipolar Interaction

The general form of the interacting potential between two dipoles p_1 and p_2 is

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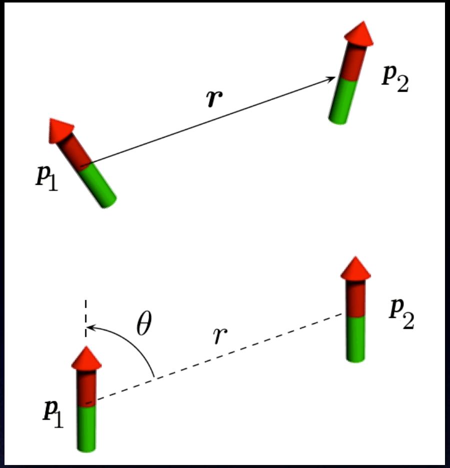
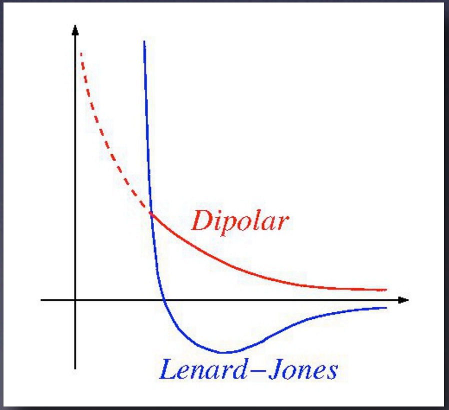


Interaction Features:

- Long ranged compared to common interactions in Condensed Matter which typically have Van der Waals tails

Dipolar : $V_{dd}(r \to \infty) \approx \dfrac{1}{r^3}$ Van der Waals : $V(r \to \infty) \approx \dfrac{1}{r^6}$

- Diverges at the origin as $1/r^3$ at $r=0$
  Not realistic as in real systems the complete interaction has an additional standard Lenard-Jones-like potential with an infinitely repulsive Hard Core near the origin

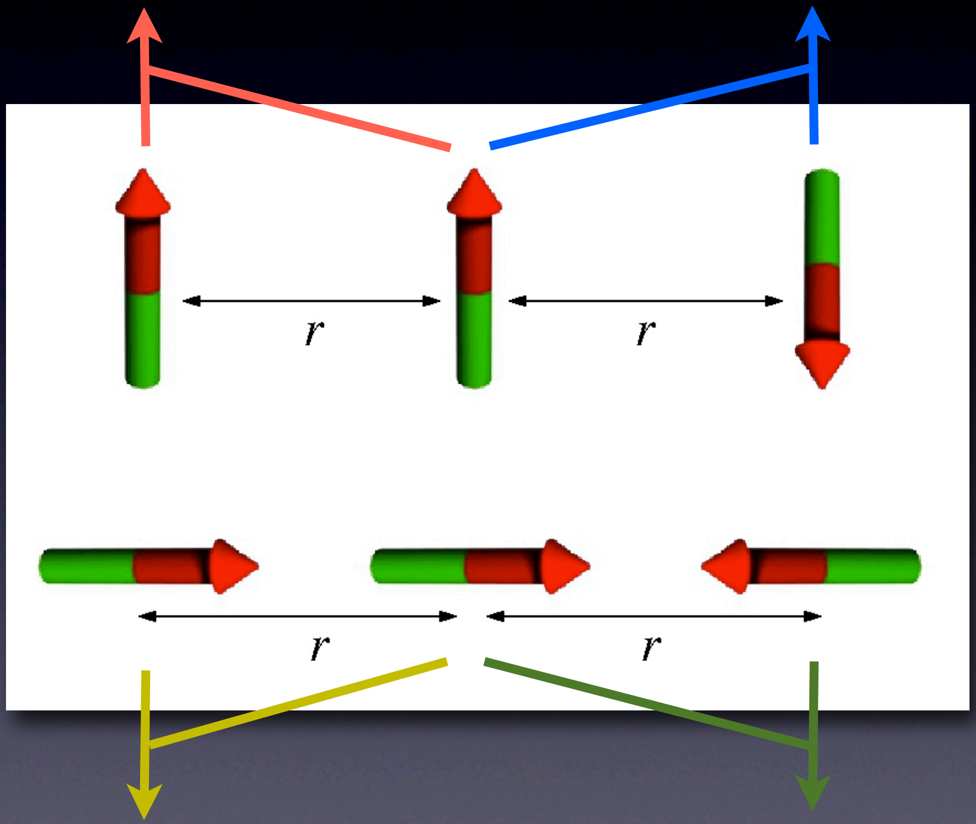


- It is anisotropic

SIMPLE CASES

Repulsion $\frac{1}{r^3}$

$-\frac{1}{r^3}$ Attraction



Twice as
attractive $-\frac{2}{r^3}$

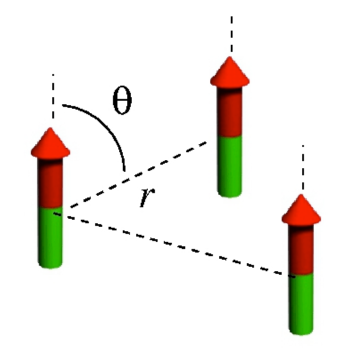
$\frac{2}{r^3}$ Twice as
repulsive

- It is anisotropic and depends on the dimensionality of the space

Assuming a fully polarized system

In 3D

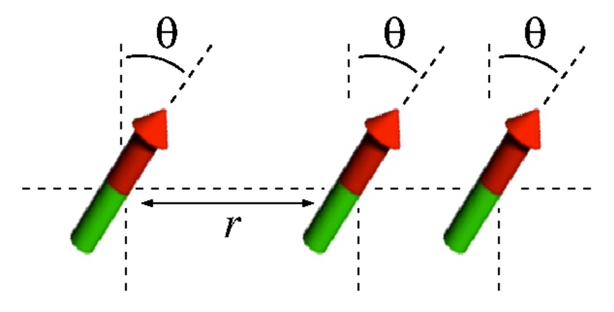
$$V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi}\left[\frac{1-3\cos^2\theta}{r^3}\right]$$



Different pairs have different angles θ and the interaction varies with the angle and the distance.

Critical angle θ_c=54°7

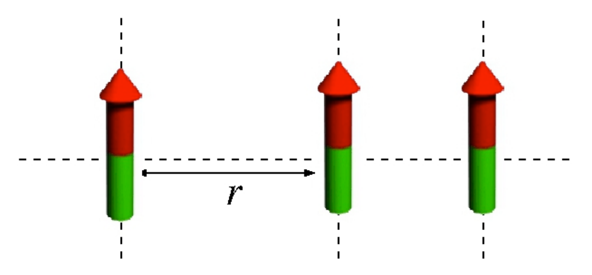
In 1D



$$V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi}\left[\frac{1-3\sin^2\theta}{r^3}\right]$$

Very similar expression to the 3D case. But a very important difference!

For fixed polarization angle θ, $1\text{-}3\cos^2\theta$ is a constant. This acts as a renormalization of C_{dd} and the system behaves as if all dipoles were polarized perpendicularly to the line. Critical angle θ_c=35°3



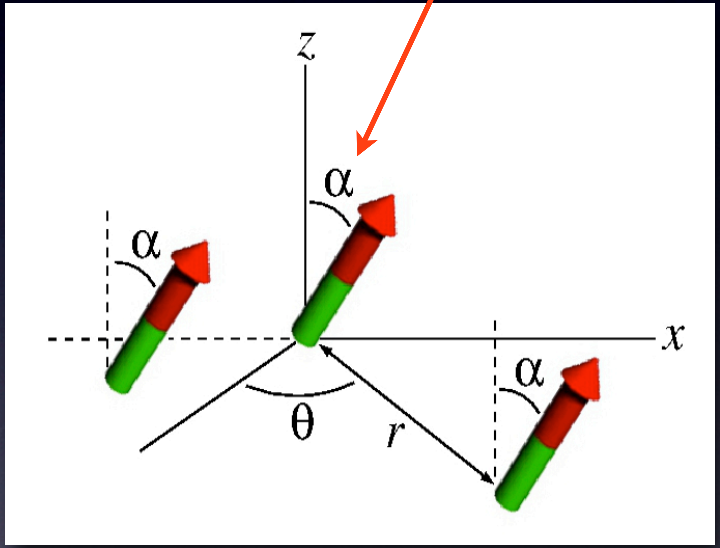
In 2D

$$V_{dd}(\vec{r}) = \frac{C_{dd}}{4\pi}\left[\frac{1-3\lambda^2 cos^2\theta}{r^3}\right]$$

Looks similar to the 3D case but it is in fact different

{r, θ} are IN PLANE spherical coordinates

$\lambda = \sin\alpha$ α : Polarization angle



Now for a polarized system, λ becomes a constant.

We can then use λ as an expansion parameter to see how the anisotropy enters in the wave function of the system

The interaction $V_{dd}(r)$ depends on λ and the system properties change when λ varies. The special case λ=0 is the simplest to analyze and we take it as the reference case to start with.

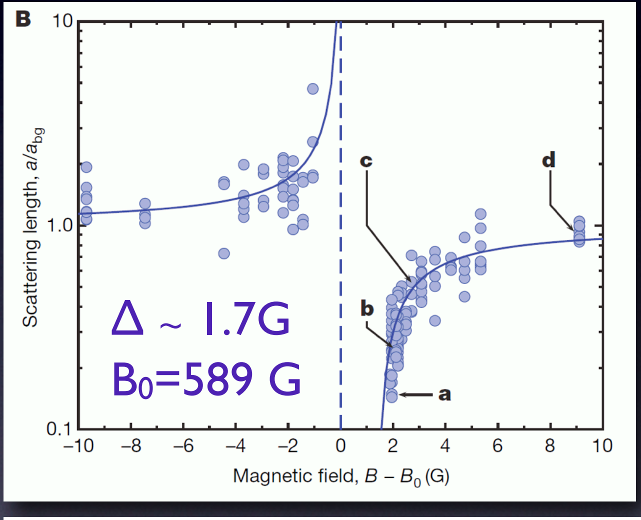
The Dipolar Interaction

The dipolar coupling is much higher in the electric case

$$\frac{\mu_o\mu^2}{d^2/\epsilon_0} \sim \frac{1}{4}\alpha^2 \sim 10^{-5}$$

α : fine structure constant

It is clearly possible to see dipolar effects! ^{52}Cr close to a Feshbach resonance



Δ ~ 1.7G

B_0=589 G

$$a = a_{bg}\left(1 - \frac{\Delta}{B - B_0}\right)$$

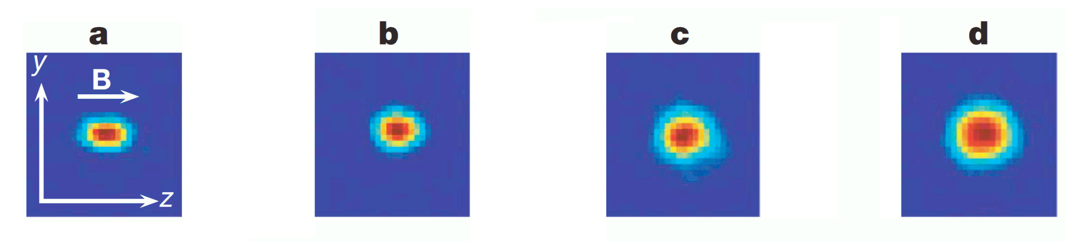
a_{bg} : background scattering length

B_0 : resonance magnetic field

Δ : resonance width

$a \rightarrow 0$ when $B \rightarrow B_0 + \Delta$

DIpolar effects are then enhanced

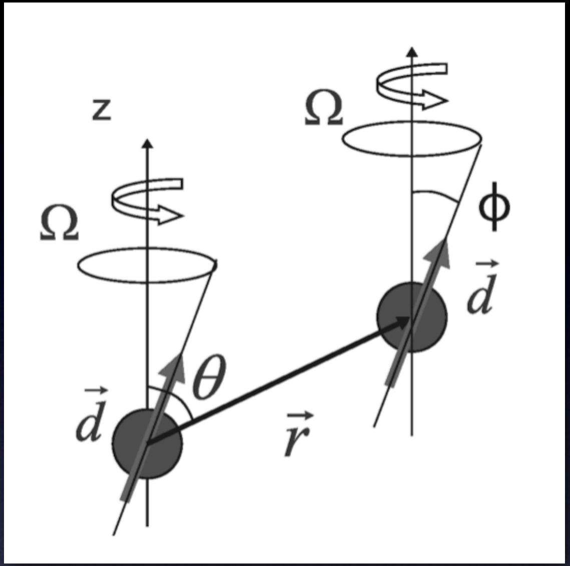


$B\text{-}B_0$=2G $B\text{-}B_0$=2.2G $B\text{-}B_0$=2.7G $B\text{-}B_0$=9G

T. Lahaye *et al.*
Nature, **448,** 672 (2007)

Tuning the Interaction in magnetic systems

Magnetic dipoles: external fields allow tuning the strength and sign of the dipolar interaction



A static field in the z direction together with a fast rotating field in the XY plane induce a dipolar moment

$$\mathbf{d}(t) = p\Big[\hat{\mathbf{e}}_z \cos\phi + \big[\hat{\mathbf{e}}_x \cos(\Omega t) + \hat{\mathbf{e}}_y \sin(\Omega t)\big] \sin\phi\Big]$$

with ϕ determined by the ratio of the amplitudes of the static and rotating fields

When Ω is large enough, particles feel an average interaction

$$\langle V_d(r)\rangle = \frac{p^2}{r^3}\left(1 - 3\cos^2\theta\right)\boxed{a(\phi)} \longrightarrow a(\phi) = \frac{3\cos^2\phi - 1}{2} \in \left[-\frac{1}{2}, 1\right]$$

This technique allows reversal of the sign in the dipole-dipole interaction as well as its cancellation at the critical angle

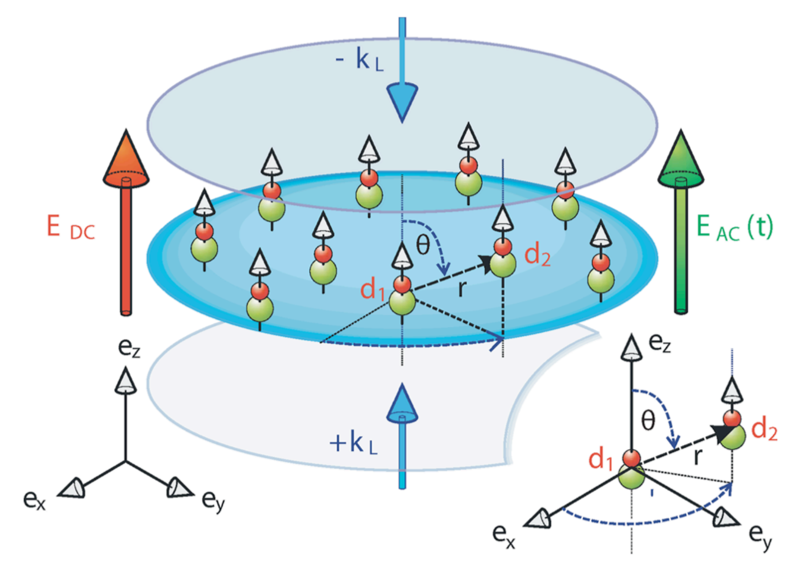
$$\cos^2\phi_c = 1/3 \longrightarrow 54^\circ 7$$

Tuning the Interaction in electric systems

Electric dipoles: mostly talking about polar molecules.

Electric fields mix internal rotational states of the molecule and that induces a n electric moment that varies with the field. These can be very large!

$$H = \sum_{i=1}^{N}\left[\frac{\mathbf{p}_1^2}{2m} + V_{\rm trap}(\mathbf{r}_i) + H_{\rm int}^{(i)} - \mathbf{d}_i\cdot\mathbf{E}\right] + \sum_{i<j} V_{dd}(\mathbf{r}_i - \mathbf{r}_j)$$



External fields mix internal rotational states that increase $\mathbf{d}_i$
and that in turn enhances $V_{dd}(\mathbf{r})$

The effective potential creates an attractive component at short distances that induces collapse in head-to-tail configurations

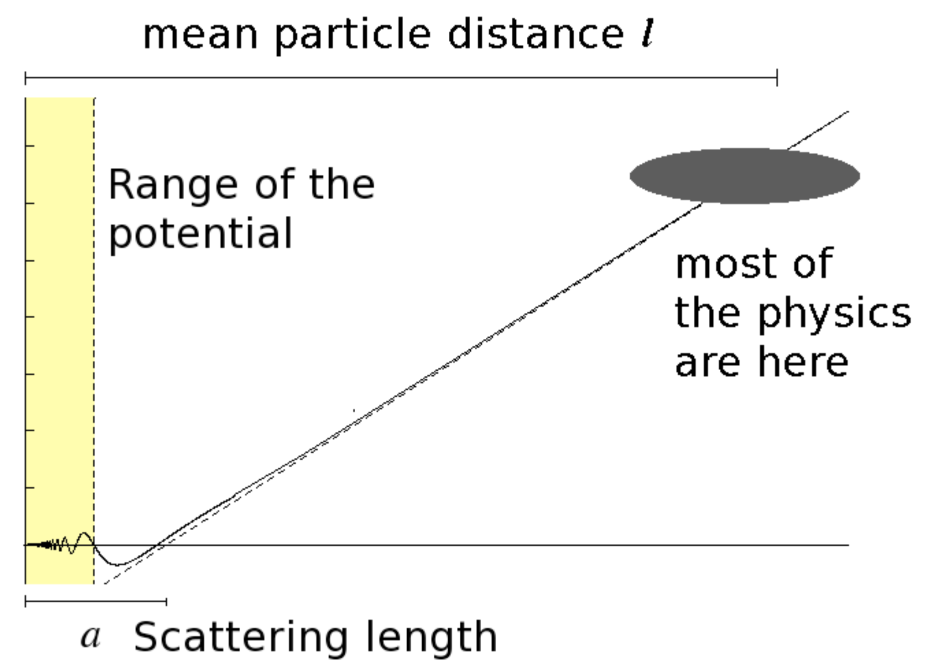
↓

Solution: tightly trap along the Z direction

Weakly Interacting Systems and Universal Regime

Dilute systems are dominated by two-body correlations

System in gaseous phase



Mean interparticle distance

$d = \rho^{-1/3}$ large

Low-Energy two-body processes

$$E = \frac{\hbar^2 k^2}{2m} \quad \longrightarrow \quad \tan\delta_l(k) \sim k^{2l+1}$$

only s-wave scattering (l=0)

$$\cot\delta_l = -\frac{1}{ka} + \frac{1}{2} k r_0 + \cdots$$

a = scattering length

only the s-wave scattering length is relevant when $ka \rightarrow 0$

Universal Regime at T=0: $x = \rho a^3 \rightarrow 0 \quad ka \rightarrow 0$

...but what about dipoles, with a (nearly, in 2D) long-range interactions ?

Diffusion Monte Carlo

Schrödinger Eq. in imaginary time for the *mixed* distribution $f(R;\tau) = \psi_T(R)\Psi(R;\tau)$

with: ψ_T = variational wave function used for Importance Sampling

$$-\frac{\partial f(R;\tau)}{\partial \tau} = \underbrace{-\frac{\hbar^2}{2m}\nabla^2 f(R;\tau)}_{\text{A}_1\text{: isotropic diffusion}} + \underbrace{\frac{\hbar^2}{2m}\vec{\nabla}\left(\vec{F} f(R;\tau)\right)}_{\text{A}_2\text{: Drift term}} + \underbrace{\left[E_L(R) - f(R;\tau)\right] f(R,\tau)}_{\text{A}_3\text{: Branching term}}$$

$$-\frac{\partial}{\partial \tau} f(R;\tau) = \left[A_1 + A_2 + A_3\right] f(R;\tau)$$

Formal solution: $f(R;\tau+\Delta\tau) = \int dR' \boxed{G(R,R';\tau)} f(R';\tau)$ Green's function

→ $G(R,R';\tau) = \langle R|\, e^{-H\Delta\tau}\, |R'\rangle$ = 2nd. order Chin approx. splits the propagator as products of simpler Green's function we know

Repeated iteration of this scheme finally yields $f(R;\tau \to \infty) \to \psi_T(R)\Psi_0(R)$

→ We NEED a GOOD trial wave function for this scheme to work well

The 2-body problem

The Hamiltonian for the relative motion of two dipoles becomes

$$H = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2\mu r^2} + \frac{C_{dd}}{4\pi}\left[\frac{1-3\lambda^2\cos^2\theta}{r^3}\right]$$

written in terms of the angular momentum operator

Symmetry $\theta \to -\theta$

$$\hat{L}^2 = -\hbar^2\frac{\partial^2}{\partial\theta^2}$$

and its orthogonal basis $\xi_m(\theta) = \cos(m\,\theta)$

The eigenstates of H can be expanded in that basis $\Psi_0(\vec{r}) = \sum_{m=0}^{\infty}\varphi_m(r)\,\cos(m\,\theta)$

However: $\left[\hat{H},\hat{L}^2\right] \neq 0$

Parity symmetry considerations
under $\vec{r} \to -\vec{r}$ rule out modes

Even modes: BOSONS
Odd modes: FERMIONS

BOSONS: $\hat{P}\Psi_0 = +\Psi_0$

$$\Psi_0(\vec{r}) = \sum_{m=0}^{\infty}\varphi_m(r)\,\cos(m\,\theta)$$

only EVEN modes

$m = 0, 2, 4, \ldots$

Solution of the Zero Energy Two-Body problem

Expand the wave function in partial waves

$$\Psi_0 = \sum_{m=0}^{\infty} \psi_m(r)\, \cos(m\,\theta)$$

Each separate mode satisfies the equation

$$m = 0, 2, 4, \ldots$$

$$-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \psi_m}{\partial r}\right) + \frac{m^2}{r^2}\psi_m + \frac{1}{r^3}\psi_m = 0$$

→ Change variables

$$x = \frac{2}{\sqrt{r}}$$

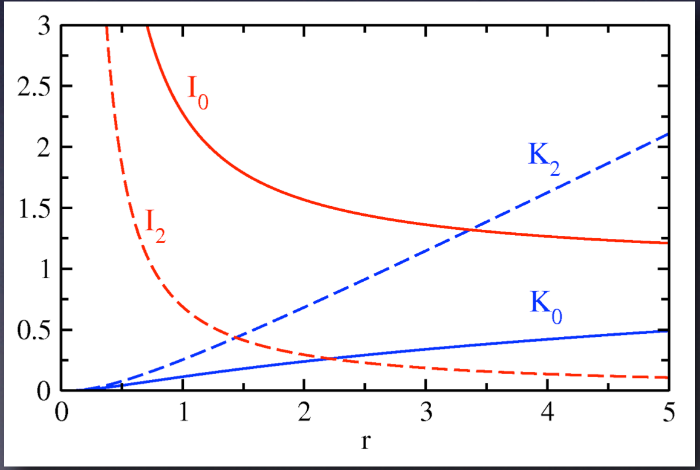
Finally rearrange terms to find the following Modified Bessel's Equation with general solution

$$x^2\psi_m'' + x\psi_m' - \left[(2m)^2 + x^2\right]\psi_m = 0$$

$$\psi_m(r) = A_m K_{2m}\left(\frac{2}{\sqrt{r}}\right) + \cancel{B_m I_{2m}\left(\frac{2}{\sqrt{r}}\right)}$$

1/r^3 diverges at r=0 and the contribution to the potential energy would diverge → Boundary condition

$$\psi_m(r=0) = 0$$



General Anisotropic case (λ≠0)

Separate explicitly the anisotropic part of the interacton

$$-\nabla^2\Psi + \left[\frac{1-3\lambda^2\cos^2\theta}{r^3}\right]\Psi = 0 \quad \longrightarrow \quad -\nabla^2\Psi + \frac{1}{r^3}\Psi = \frac{3\lambda^2\cos^2\theta}{r^3}\Psi$$

and solve $\Psi(\vec{r}) = \Psi_h(\vec{r}) + \Psi_p(\mathbf{r})$

Particular solution

Homogeneous: (λ=0) solution

The homogeneous problem is isotropic and so we know $\Psi_h(\vec{r}) = K_0\left(\frac{2}{\sqrt{r}}\right)$

The particular solution can be built from the exact Green's function, and the complete solution of the problem becomes

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + 3\lambda^2 \int d\vec{s}_1\, G(\vec{r},\vec{s}_1)\frac{\cos^2\theta_1}{s_1'^3}\Psi(\vec{s}_1)$$

and solve by iteration to get the different orders in λ^2

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + 3\lambda^2 \int d\vec{s}_1\, G(\vec{r},\vec{s}_1)\frac{\cos^2\theta_1}{s_1'^3}\Psi_h(\vec{s}_1) + \\ + (3\lambda^2)^2 \int d\vec{s}_1 \int d\vec{s}_2\, G(\vec{r},\vec{s}_1)\,G(\vec{s}_1,\vec{s}_2)\frac{\cos^2\theta_1}{s_1'^3}\frac{\cos^2\theta_2}{s_2'^3}\Psi_h(\vec{s}_2) + \cdots$$

General Anisotropic case (λ≠0)

The Green’s function is the solution of the problem

$$\Big[-\nabla^2+V_{dd}(\vec{r})\Big]G(\vec{r},\vec{s})=-\delta(\vec{r}-\vec{s})$$

and we expand
it in partial waves

$$G(\vec{r},\vec{r})=\frac{1}{2\pi}\,g_0(r,r')+\frac{1}{\pi}\sum_{m=1}^{\infty}g_m(r,r')\cos\left[m(\theta-\theta')\right]$$

where $g_m(r,r')$ is the Green’s function of each separate mode, which reads

$$g_m(r,s)=\begin{cases}2\,K_{2m}\left(\frac{2}{\sqrt{r}}\right)\,I_{2m}\left(\frac{2}{\sqrt{s}}\right) & \text{if } r<s\\ 2\,I_{2m}\left(\frac{2}{\sqrt{r}}\right)\,I_{2m}\left(\frac{2}{\sqrt{s}}\right) & \text{if } r>s\end{cases}$$

Upon substitution on the expression of the solution one can see how the different modes couple with increasing orders in λ

$$\Psi(\vec{r})=\Psi_h(\vec{r})+3\lambda^2\int d\vec{r}'\,\frac{\cos^2\theta'}{r'^3}\left[\frac{1}{2\pi}g_0(r,r')+\frac{1}{\pi}\sum_{m=1}^{\infty}g_m(r,r')\cos\left[m\left(\theta-\theta'\right)\right]\right]\Psi(\vec{r}')$$

General Anisotropic case ($\lambda \neq 0$)

How does the coupling between different modes appears?

We can see this looking at the lowest order in λ^2

Order λ^0 : only m=0 (isotropic)

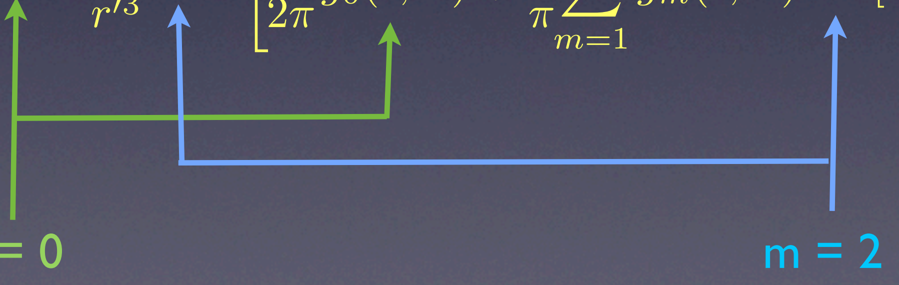
$$\Psi(\vec{r}) = \Psi_h(\vec{r}) = K_0\left(\frac{2}{\sqrt{r}}\right)$$

Order λ^2 : the coupling induces the coupling to the m=2 mode

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + 3\lambda^2 \int d\vec{r}' \, \frac{\cos^2\theta'}{r'^3}\left[\frac{1}{2\pi} g_0(r,r') + \frac{1}{\pi}\sum_{m=1}^{\infty} g_m(r,r')\cos\left[m\left(\theta-\theta'\right)\right]\right]\Psi_h(\vec{r}')$$

developing

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + \frac{3\lambda^2}{2}\int d\vec{r}' \, \frac{1+\cos(2\theta')}{r'^3}\left[\frac{1}{2\pi} g_0(r,r') + \frac{1}{\pi}\sum_{m=1}^{\infty} g_m(r,r')\cos\left[m\left(\theta-\theta'\right)\right]\right]\Psi_h(\vec{r}')$$



General Anisotropic case (λ≠0)

In this way to order λ^2 the wave function couples the m=0 mode to m=0 and m=2

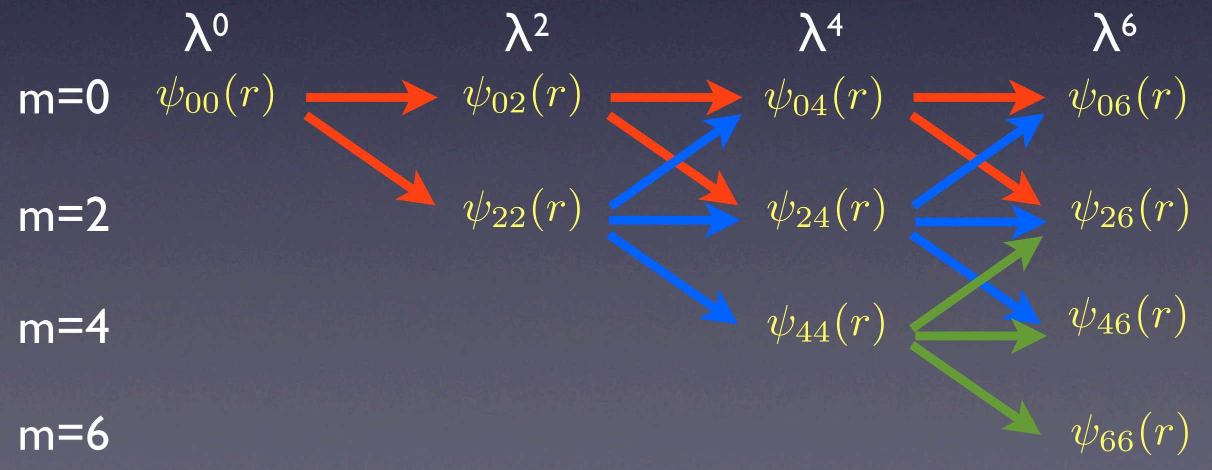
$$\Psi(\vec{r}) = \psi_{00}(r) + \lambda^2 \Big[\psi_{o2}(r) + \psi_{22}(r)\Big] \cos(2\theta)$$

Plug it back into the general equation and obtain the contribution to order λ^4

$$\Psi(\vec{r}) = \Psi_h(\vec{r}) + \frac{3\lambda^2}{2}\int d\vec{r}\,' \frac{1+\cos(2\theta')}{r'^3}\left[\frac{1}{2\pi} g_0(r,r') + \frac{1}{\pi}\sum_{m=1}^{\infty} g_m(r,r')\cos\left[m\left(\theta-\theta'\right)\right]\right]\Psi(\vec{r}\,')$$

two cosine terms couple state m to states m

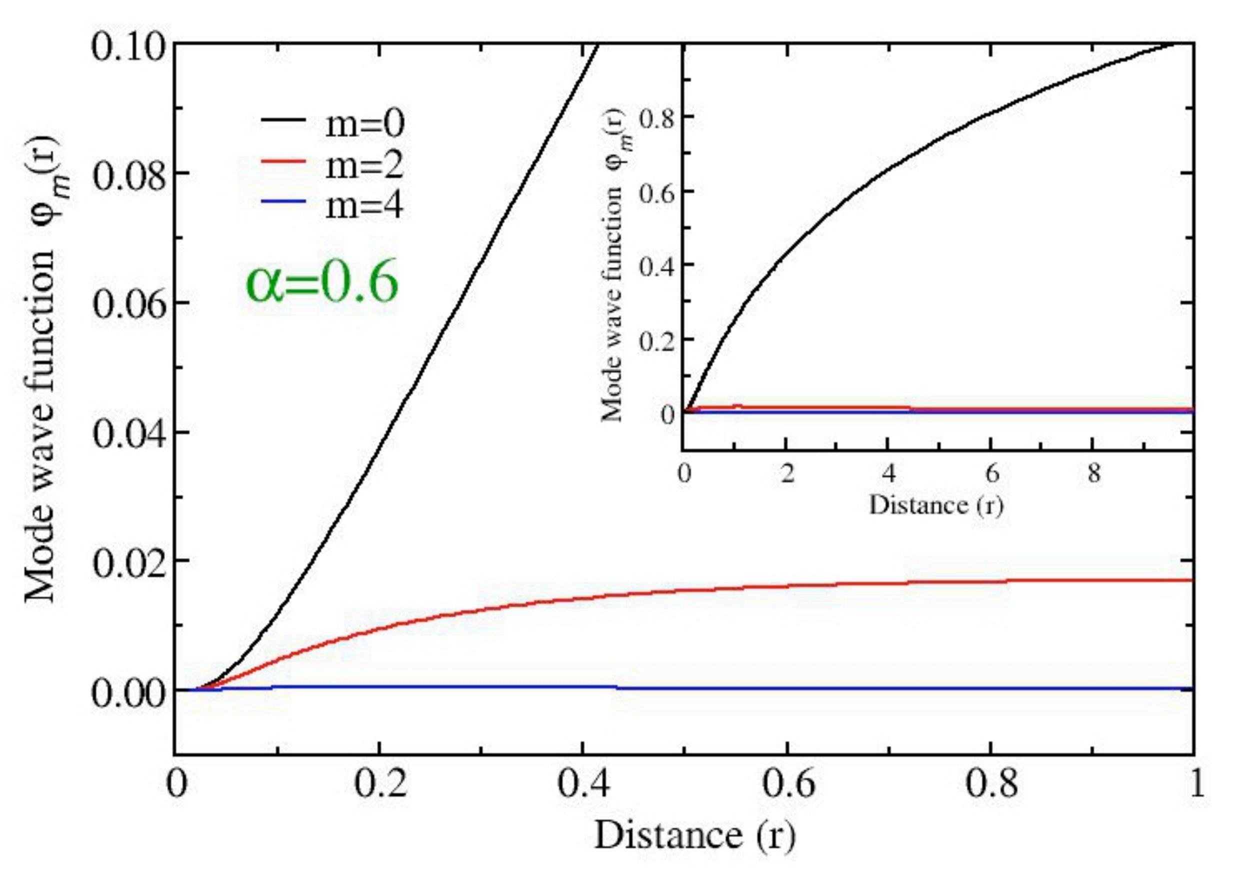
three cosine terms couple state m to states m ± 2



	λ^0	λ^2	λ^4	λ^6
m=0	$\psi_{00}(r)$	$\psi_{02}(r)$	$\psi_{04}(r)$	$\psi_{06}(r)$
m=2		$\psi_{22}(r)$	$\psi_{24}(r)$	$\psi_{26}(r)$
m=4			$\psi_{44}(r)$	$\psi_{46}(r)$
m=6				$\psi_{66}(r)$

coupling scheme

Contribution of the different modes



The anisotropy is there, but the coupling to modes m≥4 is very weak

Scattering length

The exact Schrödinger equation for the m=0 mode $\psi_0(r)$ reads

$$-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi_0(r)}{\partial r}\right)+\frac{1}{r^3}\psi_0(r)=\frac{3\lambda^2}{2r^3}\left[\psi_0(r)+\psi_2(r)\right]$$

At large distance $r \gg 1$ we know $\psi_0(r) \gg \psi_2(r)$ and therefore the previous equation is well approximated by

$$-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi_0(r)}{\partial r}\right)+\frac{1}{r^3}\left(1-\frac{3\lambda^2}{2}\right)\psi_0(r)=0$$

Change variables $x=r/(1-3\lambda^2/2)$ to find

$$-\frac{1}{x}\frac{\partial}{\partial x}\left(x\frac{\partial\psi_0(x)}{\partial x}\right)+\frac{1}{x^3}\psi_0(x)=0$$

$\longleftarrow$ same as λ=0 !

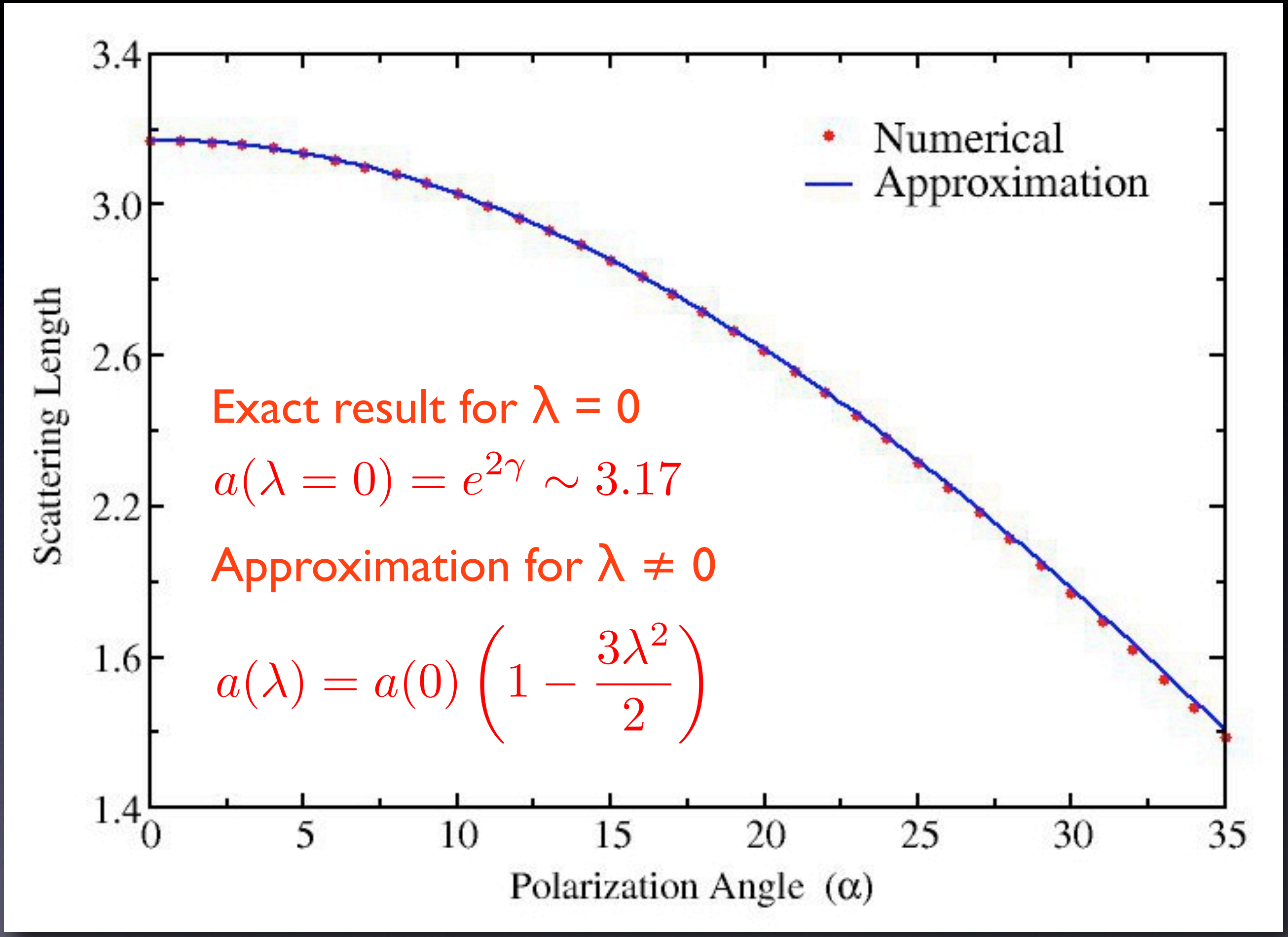
so the solution at large distances reads

$$\varphi_0(r)\approx K_0\left(2\sqrt{\frac{1-3\lambda^2/2}{r}}\right)\approx\frac{1}{2}\ln\left(\frac{r}{a_\lambda}\right)$$

Scattering length

$$a_\lambda=e^{2\gamma}\left(1-\frac{3\lambda^2}{2}\right)$$

Scattering length as a function of the polarization angle $\lambda = \sin(\alpha)$



Exact result for λ = 0

$$a(\lambda = 0) = e^{2\gamma} \sim 3.17$$

Approximation for λ ≠ 0

$$a(\lambda) = a(0)\left(1 - \frac{3\lambda^2}{2}\right)$$

The Many-Body problem

Many-Body Hamiltonian
$$H = -\frac{1}{2}\sum_{j=1}^{N}\nabla_j^2 + \sum_{i<j}\frac{1-3\lambda^2\cos^2\theta_{ij}}{r_{ij}^3}$$

Isotropic interactions at low densities follow a universal curve describing the energy per particle as a function of the gas parameter $x = na^2$

$$\left(\frac{2ma^2}{\hbar^2}\right)\left(\frac{E}{N}\right) = \frac{4\pi x}{|\ln(x)|}\left[1+\mathcal{O}(\ln(x))\right]$$

In isotropic systems and for a given interaction, a=cte. and the density fixes the value of the gas parameter x.

In the anisotropic dipolar case considered, a given value of x can be obtained from different densities and polarization angles since $a = a(\lambda)$

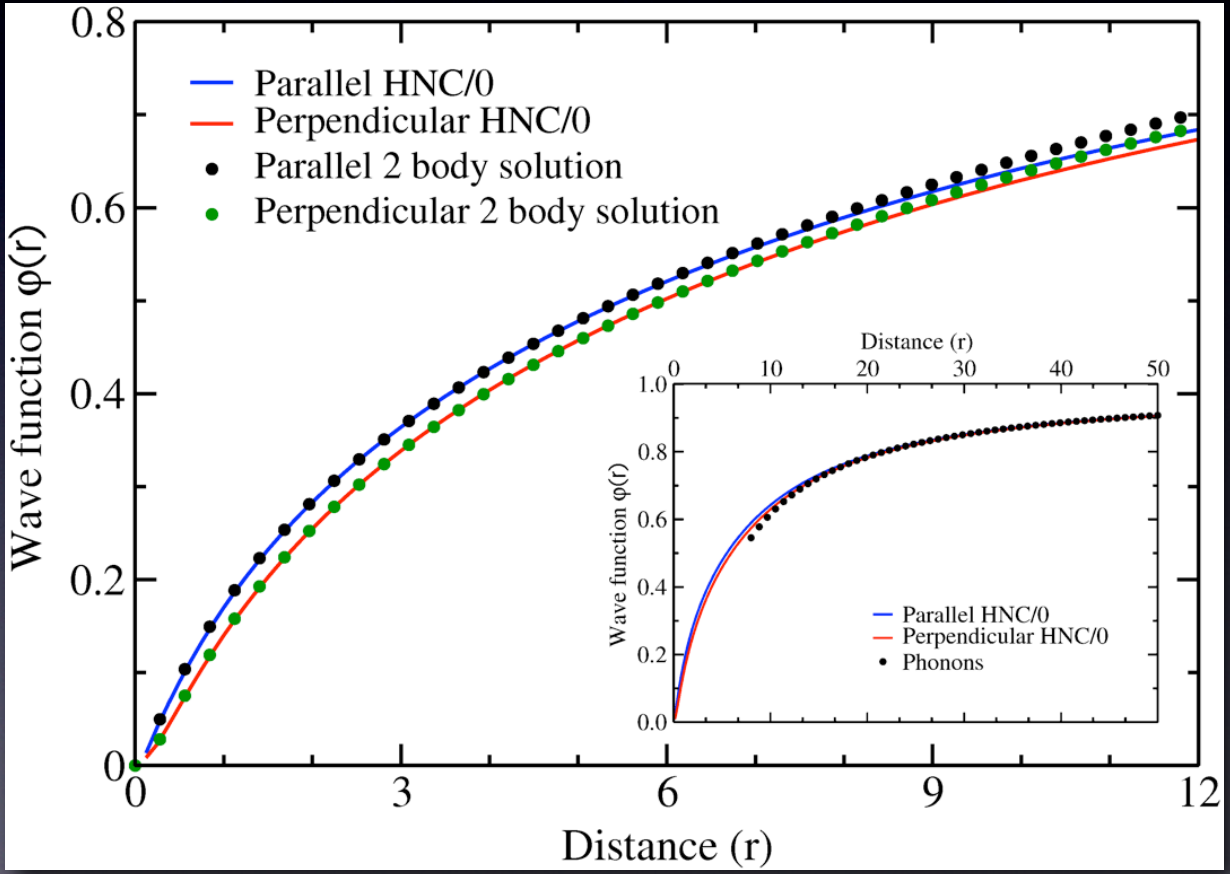
$$a_\lambda = e^{2\gamma}\left(1-\frac{3\lambda^2}{2}\right)$$

Keeping x fixed and varying λ means varying the density accordingly

Many-Body energies can be obtained by means of variational methods (HNC, VMC) or *exact* ones (DMC)

The Many-Body problem

Two-Body wave function compared with optimal HNC/0 Jastrow factor



Optimal HNC

$$\Psi = \prod_{i<j} f(\vec{r}_{ij})$$

$$\frac{\delta E}{\delta f} = 0$$

Phonons in 2D

$$f(r) = e^{u_2(r)}$$

$$u_2(r) = -\frac{c}{r}$$

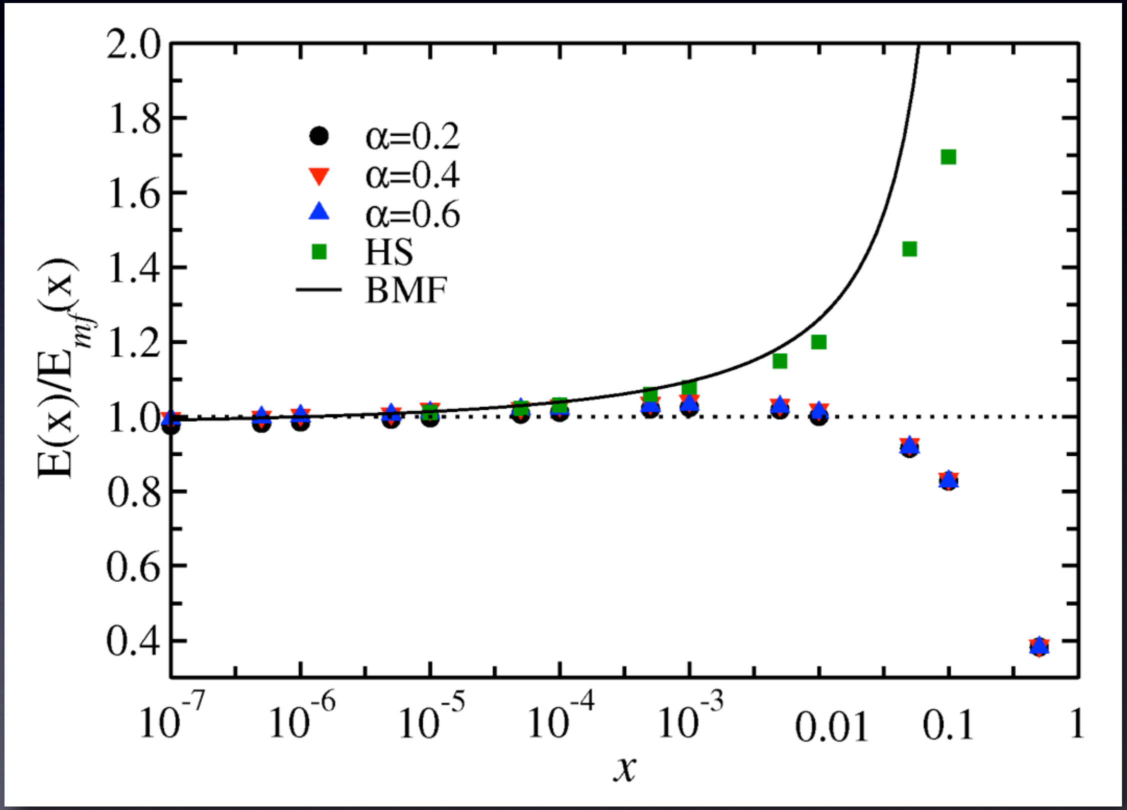
$$\alpha = 0.6$$

$$x = 0.01$$

The Many-Body problem

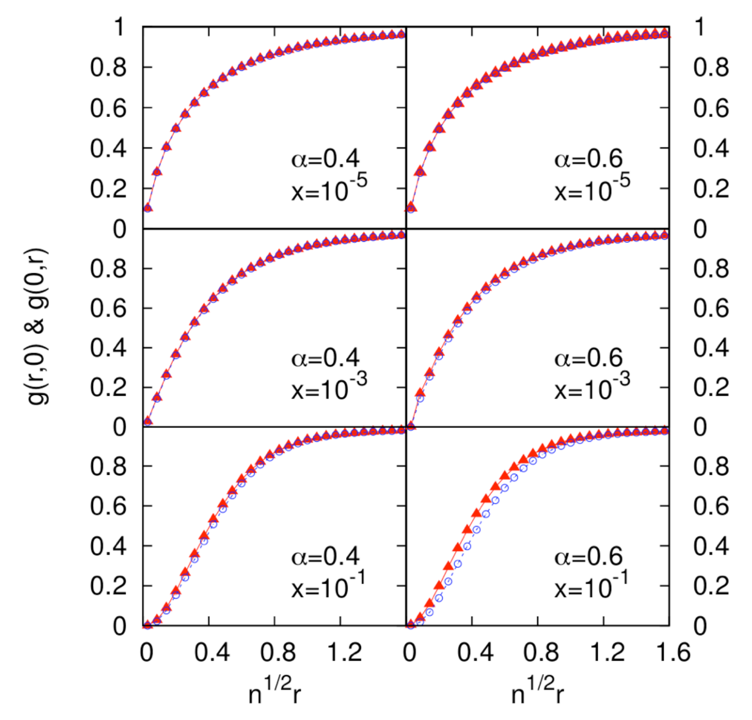
Universal Energy per particle.
Scaled energies

$$\tilde{E} = \left(\frac{2ma^2}{\hbar^2}\right)\left(\frac{E}{N}\right)$$

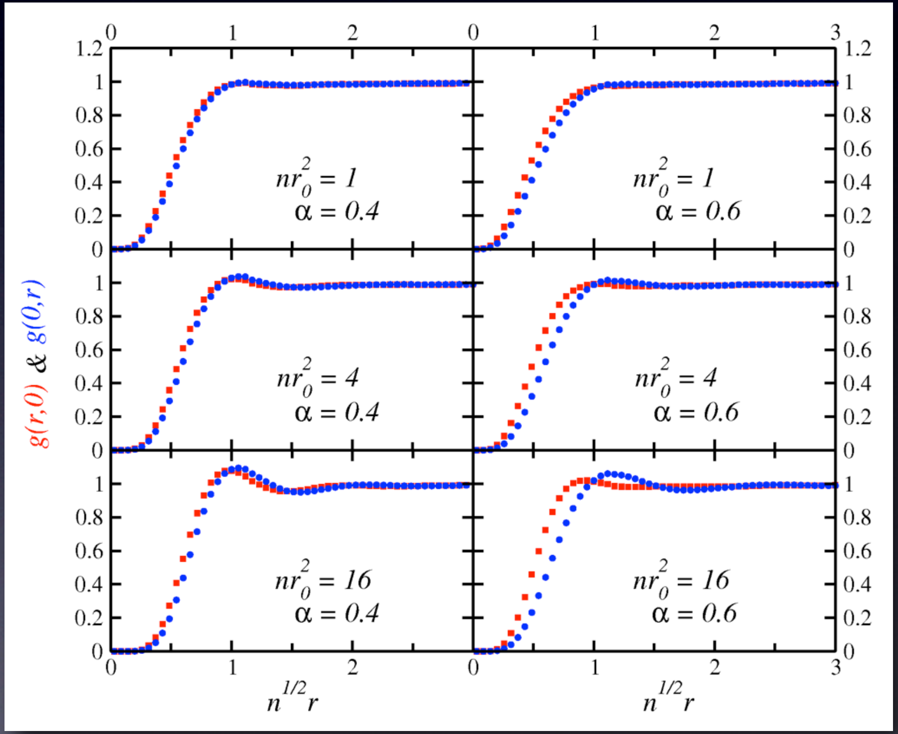


BMF : G. E, Astrakharchik *et al.* Phys. Rev. **A** 79, 051602 (2009)
HS : F. Mazzanti *et al.* Phys. Rev. **A** 71, 033615 (2005)

Pair Distribution Function

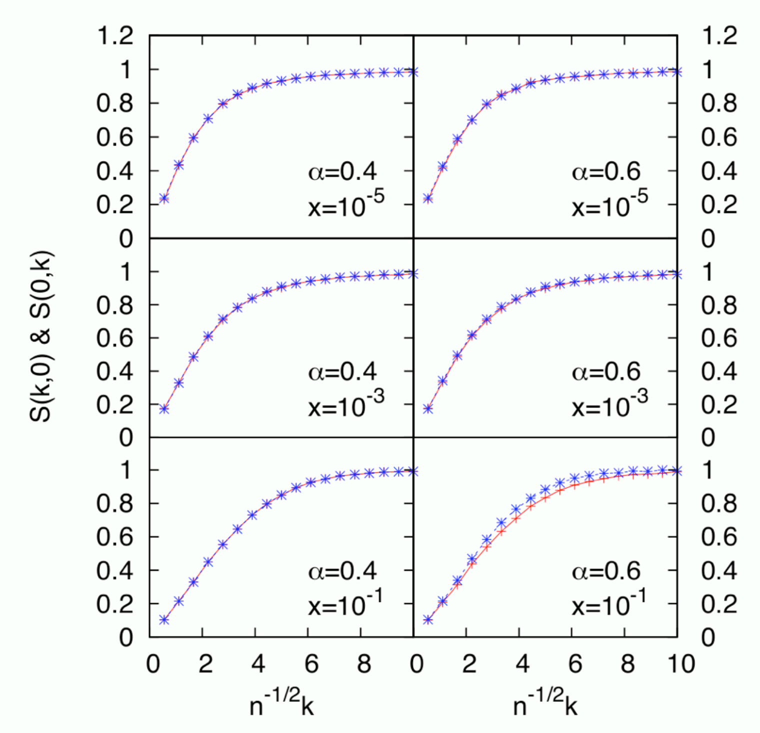


Low densities
Universal regime



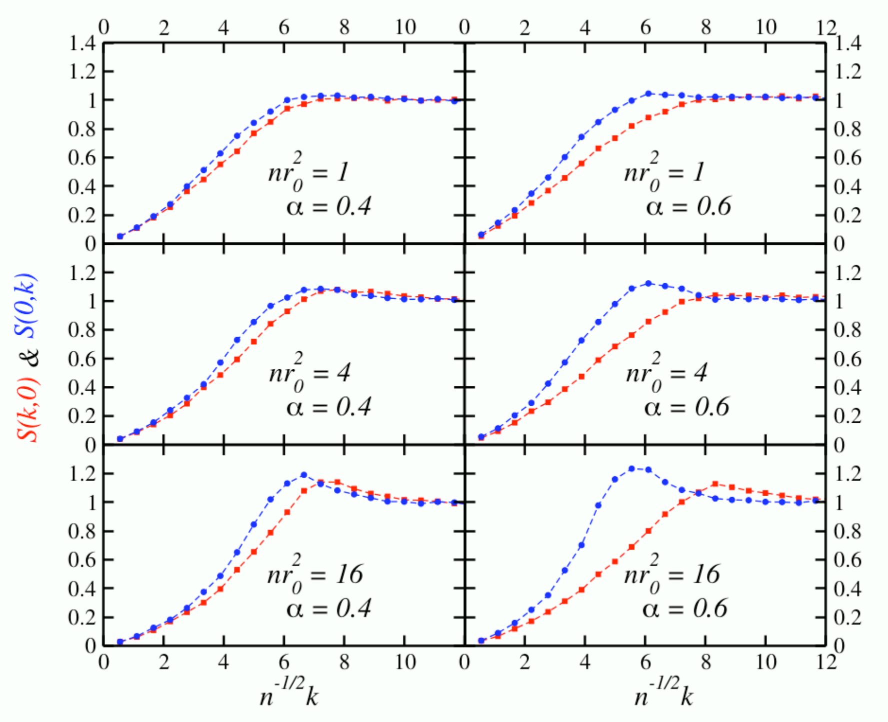
Intermediate densities

Static Structure Factor



Low densities

Universal regime



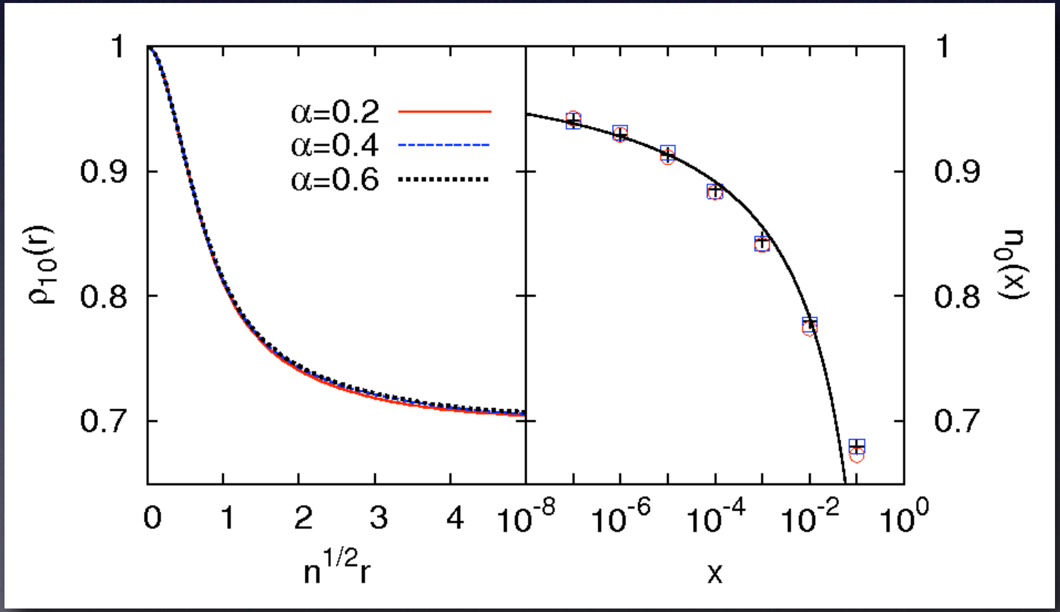
Intermediate densities

Condensate Fraction

The condensate fraction is obtained from the asymptotic behavior of the m=0 mode of the Off-Diagonal One-Body Density Matrix

$$\rho_1(\mathbf{r}_1, \mathbf{r}_1') = N \frac{\int d\mathbf{r}_2 \cdots \mathbf{r}_N \Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \Psi_0(\mathbf{r}_1', \mathbf{r}_2, \ldots, \mathbf{r}_N)}{\int d\mathbf{r}_1 d\mathbf{r}_2 \cdots \mathbf{r}_N \Psi_0^2(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)}$$

$$x = 0.05$$



Momentum Distribution

$$\rho_1(\mathbf{r}_{11'}) = FT[n(\mathbf{k})]$$

$$n_0 = \lim_{r_{11'} \to \infty} \frac{1}{\rho} \rho_1(r_{11'})$$

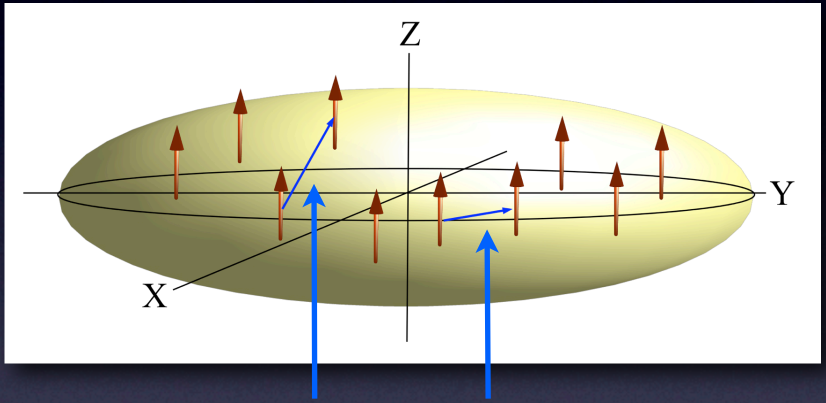
Bogoliubov
(universal)
prediction

$$n_0(x) = 1 - \frac{1}{|\ln x|}$$

Density Response and System Instabilities

Pancake geometry: harmonic confinement along the Z direction

L. Santos, G.V. Shlyapnikov and M. Lewenstein,
Phys. Rev. Lett. 90, 250403 (2003)



unstable configuration

stable configuration

In the Gross-Pitaevskii framework the authors described a roton-instability associated with the quantity

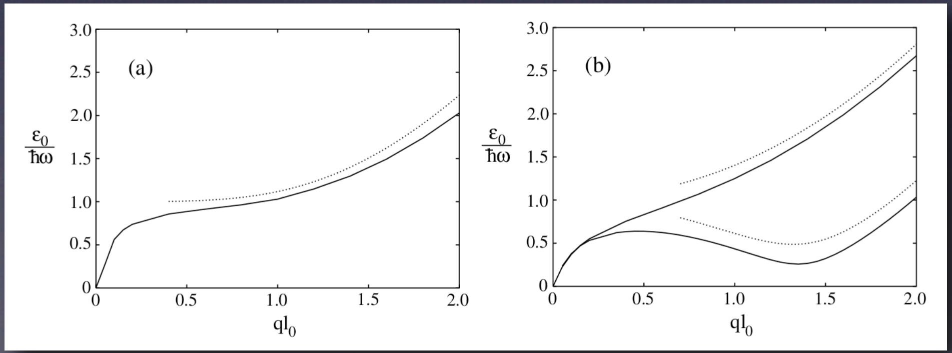
$$\beta = g/g_d$$

coupling constant of the short-range interaction

$8\pi p^2/3$

effective dipolar coupling constant

Below a critical value β_c depending on the density and trap confinement leads to the roton collapse



Density Response Function in CBF Approximation

$S(q,\omega)$ is the Imaginary part of the Density-Density response induced by a time-dependent perturbation

$$S(q,\omega) = -\frac{1}{\pi}\mathrm{Im}\Big[\chi(k,\omega)\Big] \equiv -\frac{1}{\pi}\mathrm{Im}\left[\frac{\delta\rho_1(k,\omega)}{\rho_0 U_{ext}(k,\omega)}\right]$$

with a time-dependent variational wave function

$$\Psi = \frac{1}{\sqrt{\mathcal{N}(t)}} e^{\delta U(t)} e^{-iE_0 t/\hbar}\Psi_0$$

and time-dependent correlations

$$\delta U(t) = \sum_j \delta u(\mathbf{r}_j;t) + \sum_{i<j}\delta u_2(\mathbf{r}_i,\mathbf{r}_j;t) + \cdots$$

minimize the action

$$\delta S = \delta \int_0^t dt\, \langle\Psi|\; H - i\frac{\partial}{\partial t}\;|\Psi\rangle$$

Lowest order: setting $\delta u_n = 0\ \forall n > 1$ leads to the Feynman approximation

$$S(k,\omega) = S(k)\delta(\omega - \epsilon_F(k)) \quad , \quad \epsilon_F(k) = \frac{\hbar^2 k^2}{2m}$$

Density Response Function in CBF Approximation

Keeping δu_2 improves over Feynmann. Use continuity equations for the one- and two-particle densities and currents to isolate δu_1 and δu_2 in terms of one- and two-body density fluctuations.

Disregarding triplet correlations one arrives at

$$\chi(k,\omega) = \frac{S(k)}{\hbar\omega - \epsilon_F(k) - \Sigma(k,\omega)} - \frac{S(k)}{\hbar\omega + \epsilon_F(k) - \Sigma^*(k,\omega)}$$

with the Self-Energy

$$\Sigma(k,\omega) = \frac{1}{2}\int \frac{d\mathbf{p}\,d\mathbf{q}}{(2\pi)^3\rho}\,\delta(\mathbf{k}+\mathbf{p}+\mathbf{q})\frac{|\,V_3(\mathbf{k};\mathbf{p},\mathbf{q})\,|^2}{\hbar\omega - \epsilon_f(p) - \epsilon_F(q)}$$

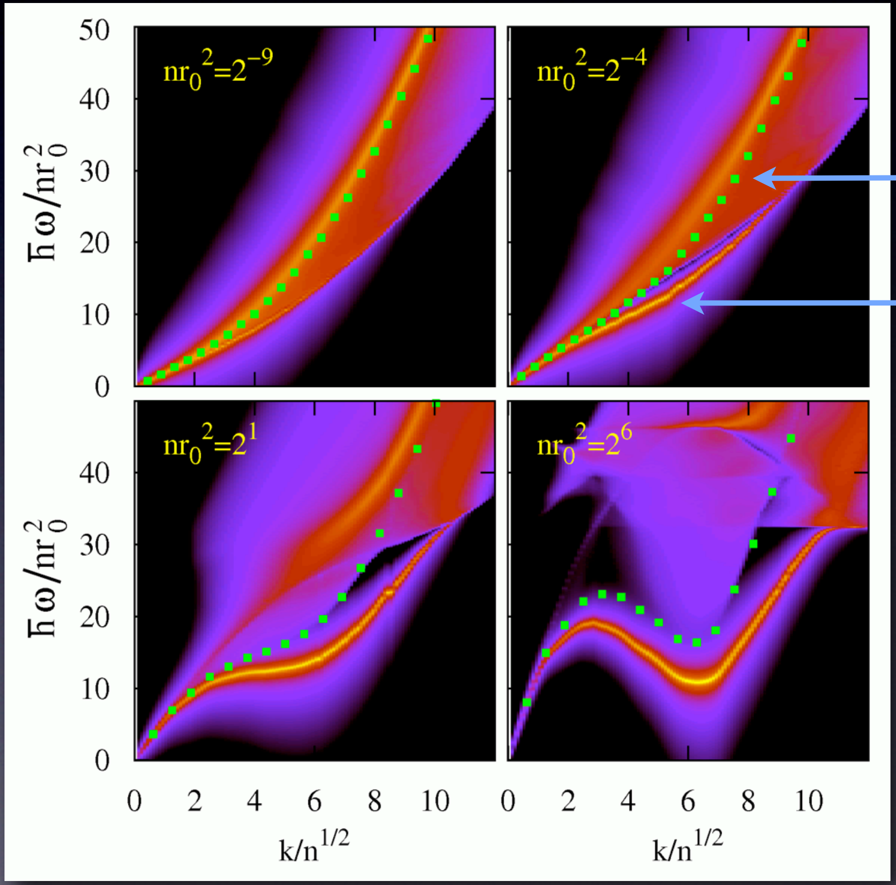
and the two-phonon coupling vertex

$$V_3(\mathbf{k};\mathbf{p},\mathbf{q}) = \frac{\hbar^2}{2m}\sqrt{\frac{S(p)S(q)}{S(k)}}\left[\mathbf{k}\cdot\mathbf{p}X(p) + \mathbf{k}\cdot\mathbf{q}X(q) - k^2 u_3(\mathbf{k};\mathbf{p},\mathbf{q})\right]$$

in terms of S(k) ONLY through $X(q) = 1 - \dfrac{1}{S(q)}$

Density Response Function in CBF Approximation

2D dipoles polarized perpendicular to the plane (λ=0)



Feynman spectrum
(upper bound to the exact one)

CBF prediction

At this level no
instability is seen

F.Mazzanti, R.E.Zillich, G.E.Astrakharchik and J.Boronat
Phys.Rev.Lett. **102**, 110405 (2009)

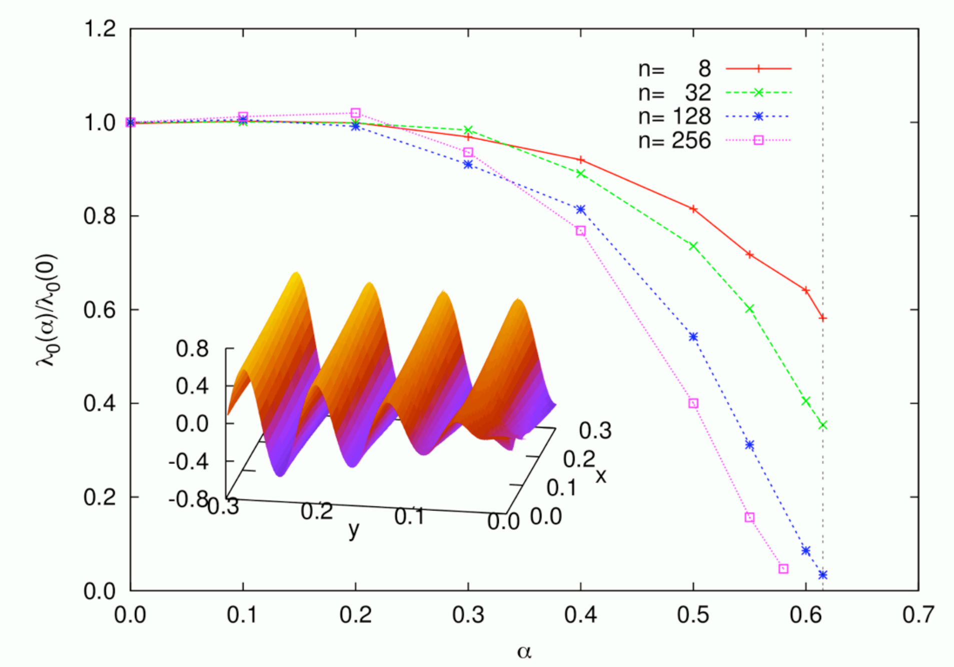
System Instabilities in the phase diagram

Can we determine transition lines in the phase diagram ?

In Optimized HNC theory one can tell when solutions can no longer be found

Castillejo *et al.* showed that when the lowest eigenvalue of the Hessian is non-positive, the system becomes unstable against infinitesimal fluctuations in $g(r)$

$$K(\mathbf{r},\mathbf{r}') = \frac{\partial^2 E[g]}{\delta\sqrt{g(\mathbf{r})}\delta\sqrt{g(\mathbf{r}')}}$$



...still this is an approximate result as HNC solutions become less accurate at larger densities

Variational Path Integral (VPI)

also called Path Integral Ground State (PIGS)

Start from the Time Evolution Operator in imaginary time

$$G = e^{iHt} = \left\{ it \to \tau \right\} \longrightarrow e^{-\tau H}$$

Devise a Variational Wave function $|\Phi\rangle$ not orthogonal to the true ground state, (may not be completely trivial). The closest to the exact ground state, the better.

The iterated action of G on $|\Phi\rangle$ becomes

$$G^n |\Phi\rangle = \left[e^{-H\tau} \right]^n \left[a_0 |\Psi_0\rangle + a_1 |\Psi_1\rangle + \cdots \right]$$

$$= a_0 e^{-\tau E_0^n} |\Psi_0\rangle + a_1 e^{-\tau E_1^n} |\Psi_1\rangle + \cdots \longrightarrow a_0 e^{-\tau E_0^n} |\Psi_0\rangle$$

... and thus all excited states contributions are killed, yielding a wave function proportional to the actual ground state.

⟶ a key ingredient is a good representation of G that ensures fast convergence

Variational Path Integral (VPI)

S. Chin derived a One-Parameter family of propagator representations that are exact up to fourth order in time. Our choice is:

$$e^{\epsilon H} = e^{\epsilon V/6} e^{\epsilon T/2} e^{2\epsilon \tilde{V}/3} e^{\epsilon T/2} e^{\epsilon V/6}$$

Basic propagator structure

special case of the general ACB propagator with $t_0=0$

S.Chin, J.Chem.Phys.117, 1409 (2002)

The iteration of the propagator leads to the single-particle chains of the simulation

Bose symmetry is taken into account by the symmetry of the variational model $|\Phi\rangle$

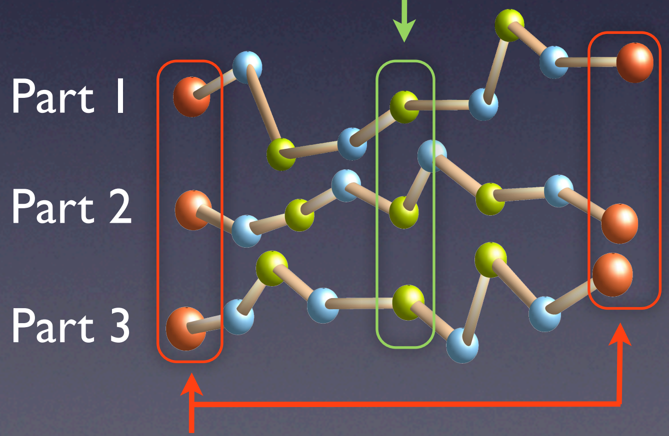
The tilde potential

$$\tilde{V} = V + \frac{\hbar^2}{m}\epsilon^2 \frac{u_0}{v_2}\left(\sum_j \nabla_j V\right)^2$$

brings a characteristically new contribution not present in other, simpler approximations like the primitive.

Central bead

exact ground state at both sides



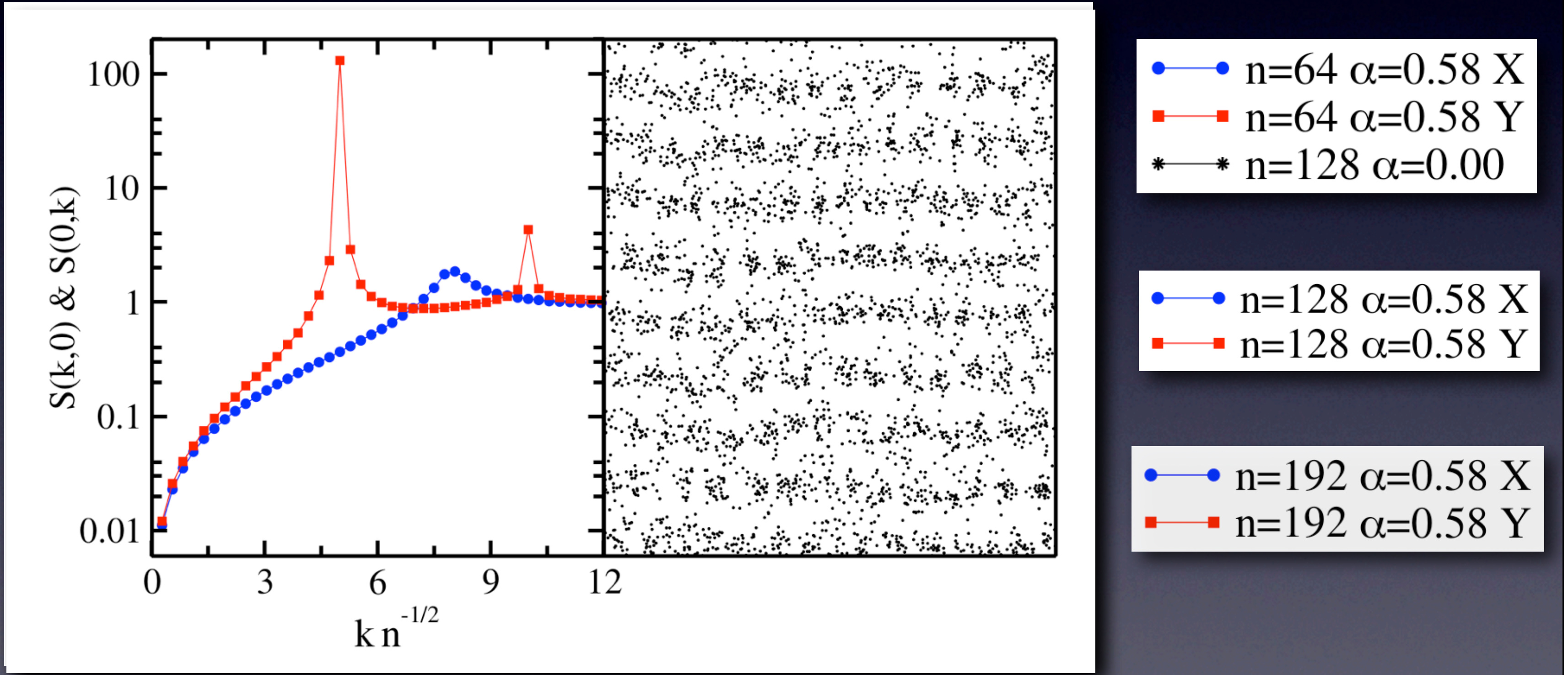
Variational Model Wave Function $|\Phi\rangle$

Static Structure Factor and Stripe Phase Formation

When do the stripes form?

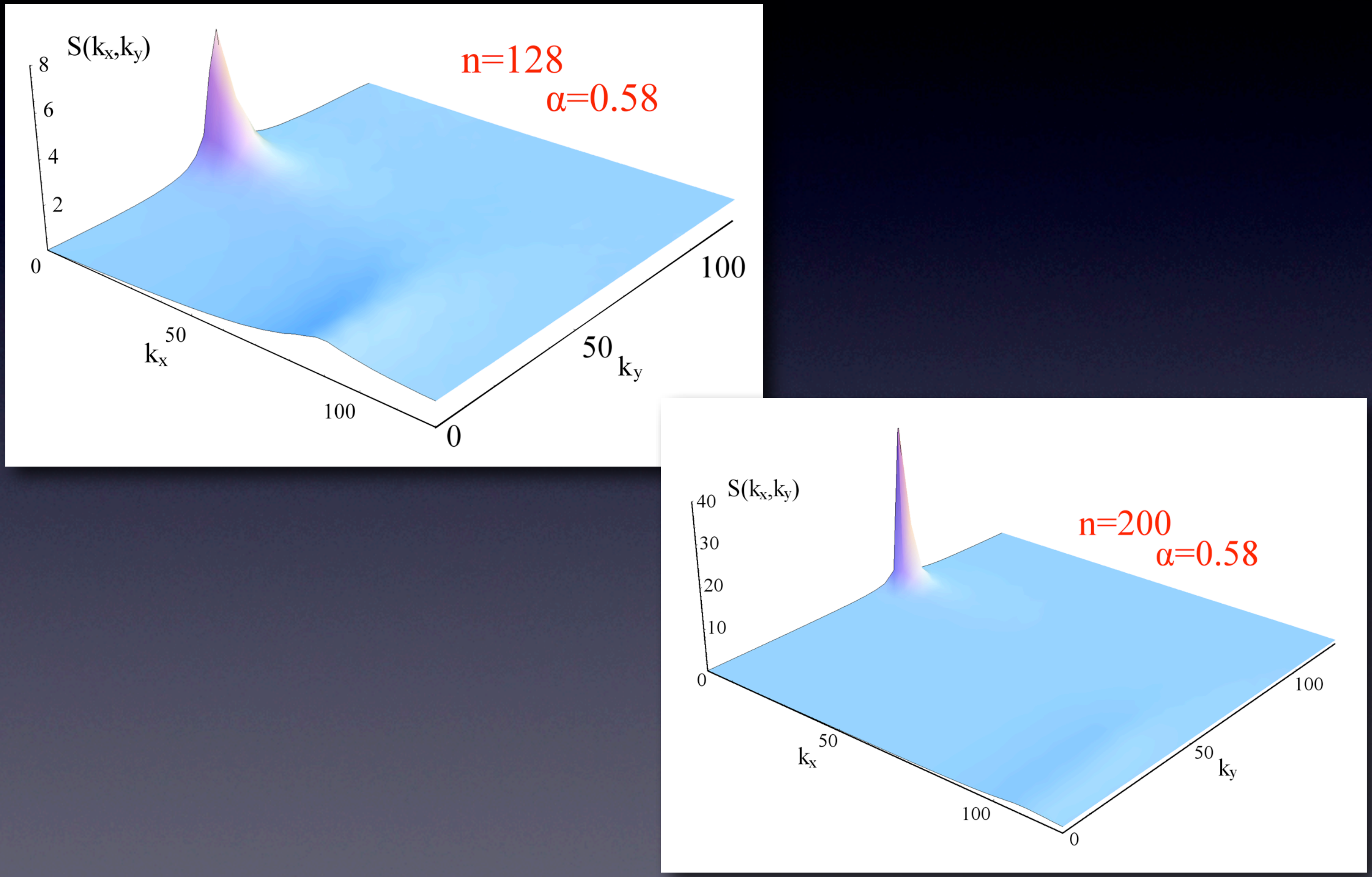
Structure Factor
in X and Y directions

Particles snapshot



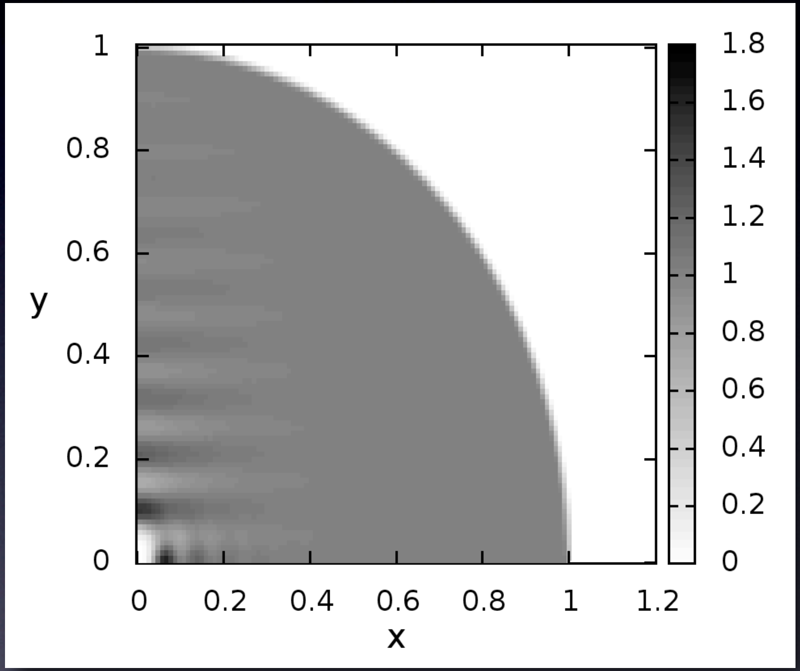
... at large densities & close to the critical angle

Static Structure Factor and Stripe Phase Formation

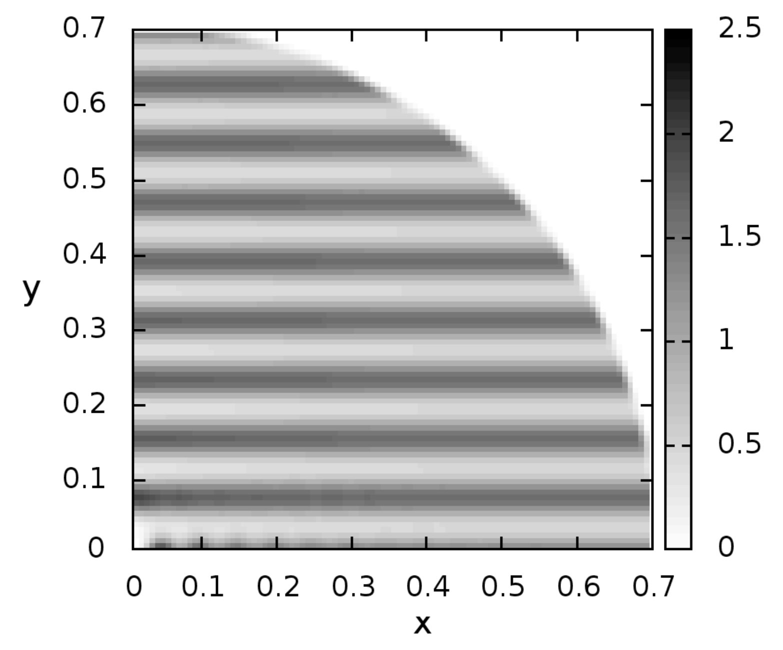


Pair Distribution Function and the Stripe Phase

Stripes can be clearly seen in the Pair Distribution function g(r)

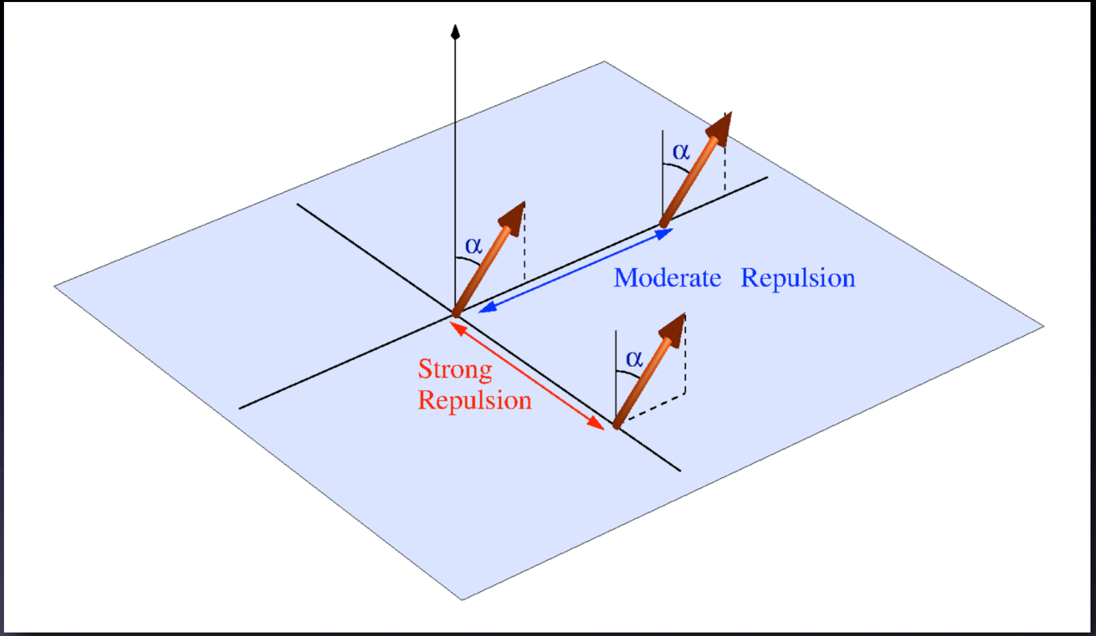


$n = 128 \ , \ \ \alpha = 0.58$



$n = 256 \ , \ \ \alpha = 0.61$

Static Structure Factor and Stripe Phase Formation in continuous systems



Strong repulsion induces order

Moderate repulsion let's the system behave as a fluid

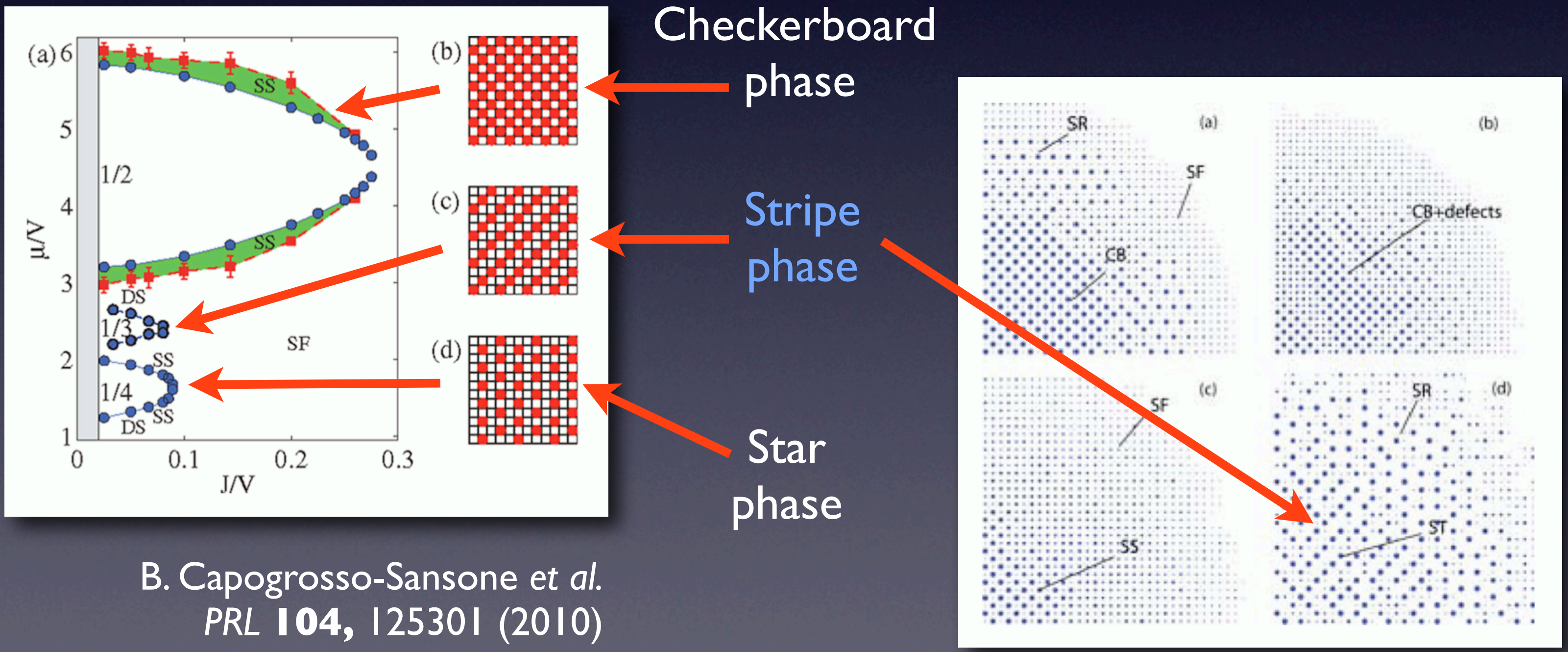
A new Stripe Phase develops when the density increases for a large enough polarization angle α because:

- side-by-side dipoles interact through $\frac{1}{r^3}$ forces
- head-to-tail dipoles interact through $\frac{1-3\lambda^2}{r^3}$ forces

Many different phases in Optical Lattices

Extended Bose-Hubbard models predict a rich phase diagram in 2D dipolar systems on the lattice

$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + V \sum_{i<j} \frac{n_i n_j}{r_{ij}^3} - \mu \sum_i n_i$$



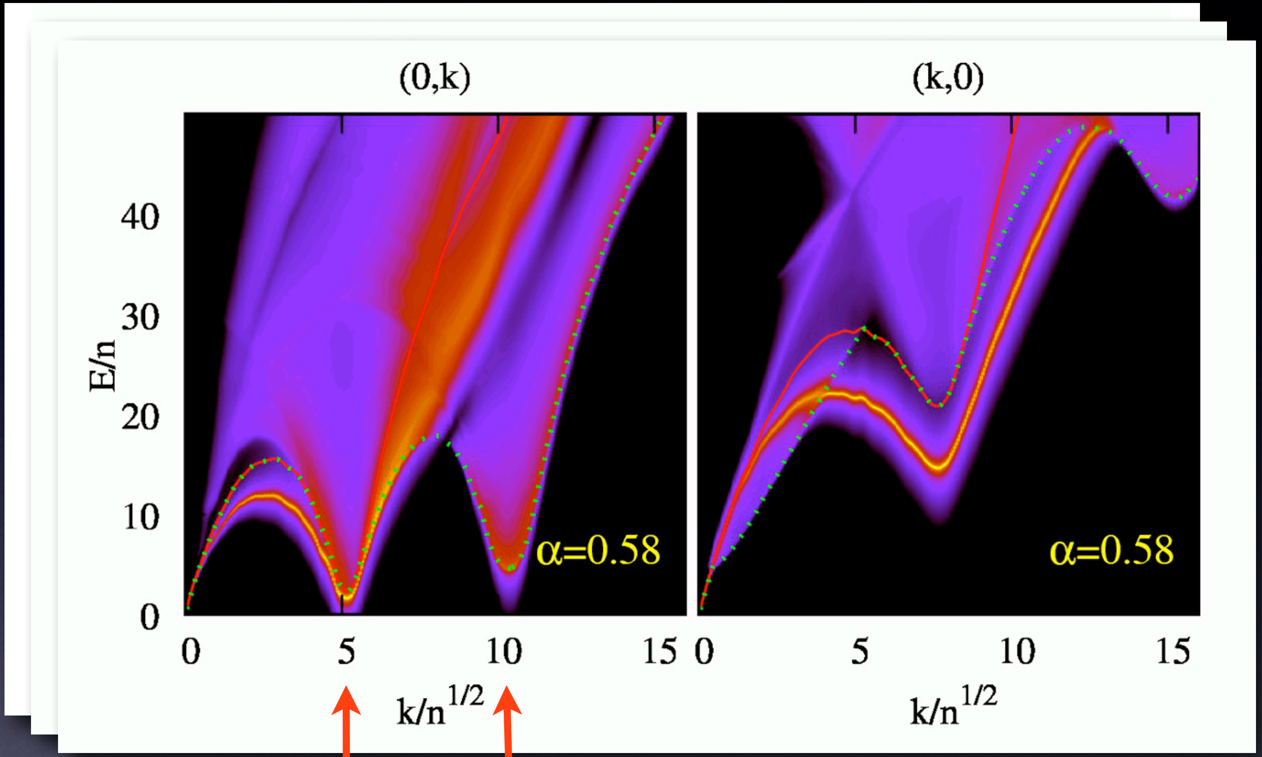
Checkerboard
phase

Stripe
phase

Star
phase

B. Capogrosso-Sansone *et al.*
PRL **104,** 125301 (2010)

The Stripe Phase and the Dynamic Response



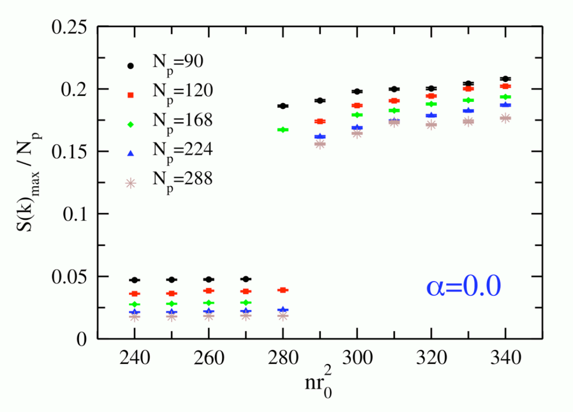
$n = 128$

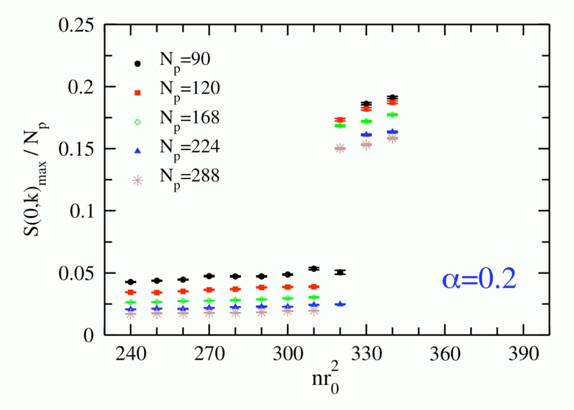
... the roton minimum in the Y direction drops to zero

...and a strongly marked second roton seems to develop

Maximum of S(k_x,k_y)

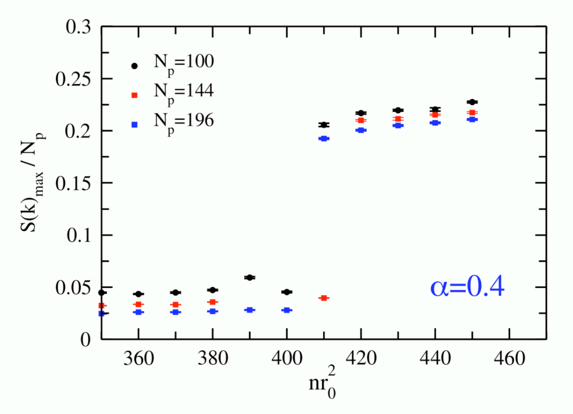
Evolution with the density and tilting angle

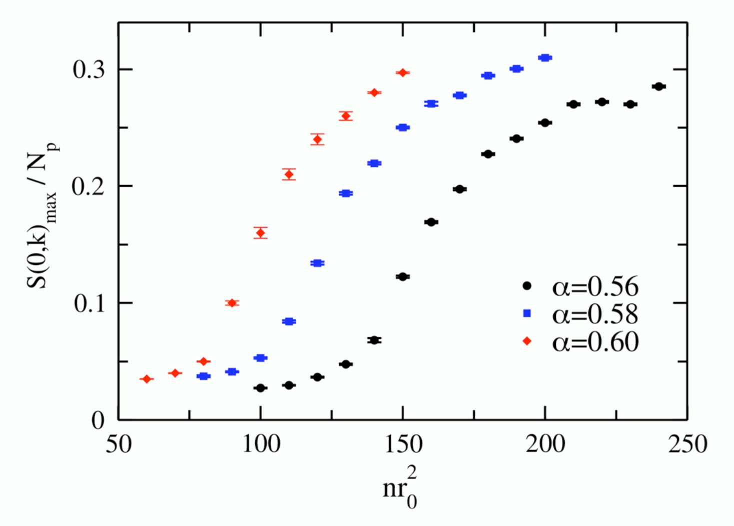




Gas-Solid
transition

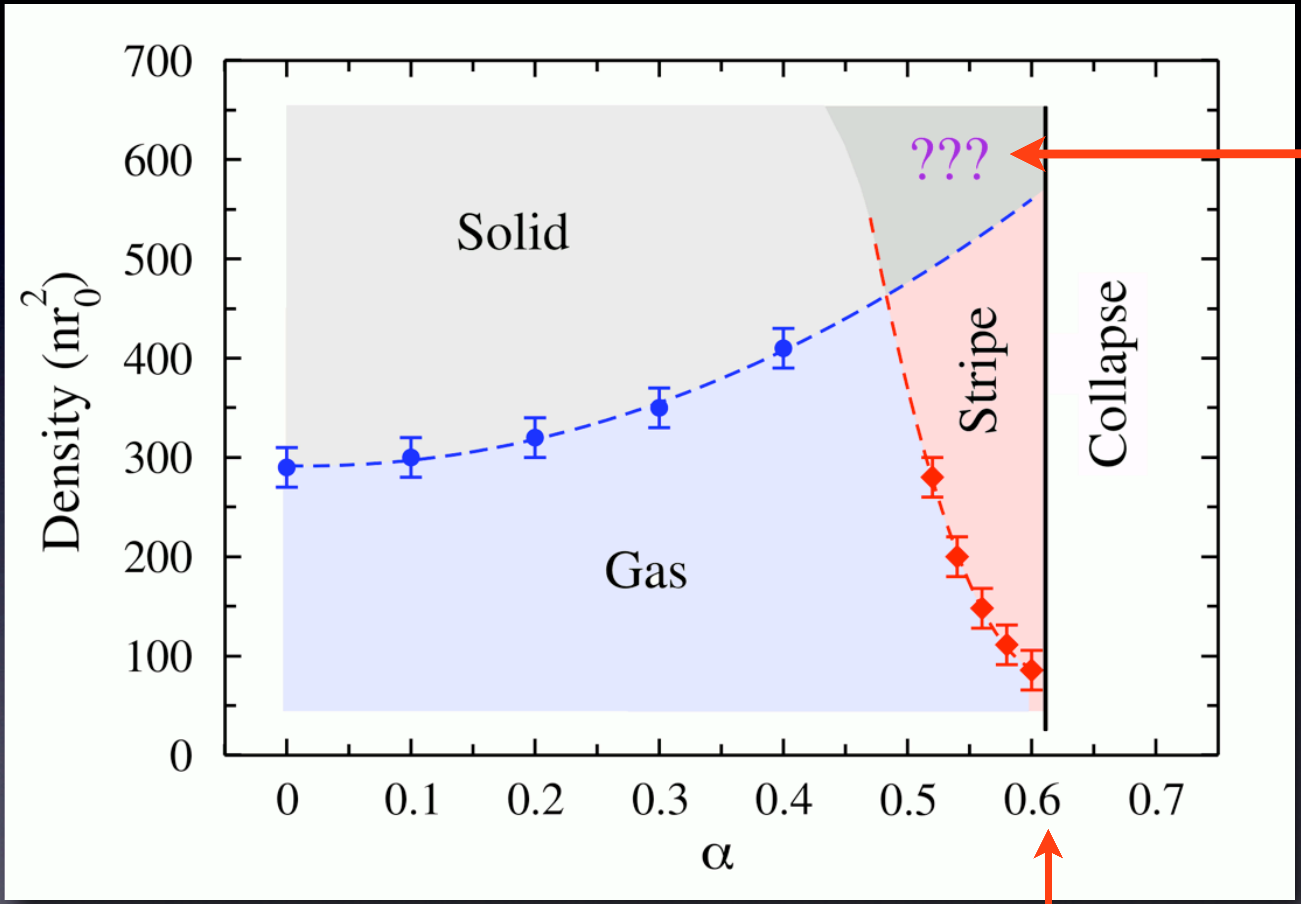
Use $\frac{S(0,k)}{N_p}$
as the
order parameter





Gas-Stripe
transition

A hint at the Phase Diagram



What do we have in this region?

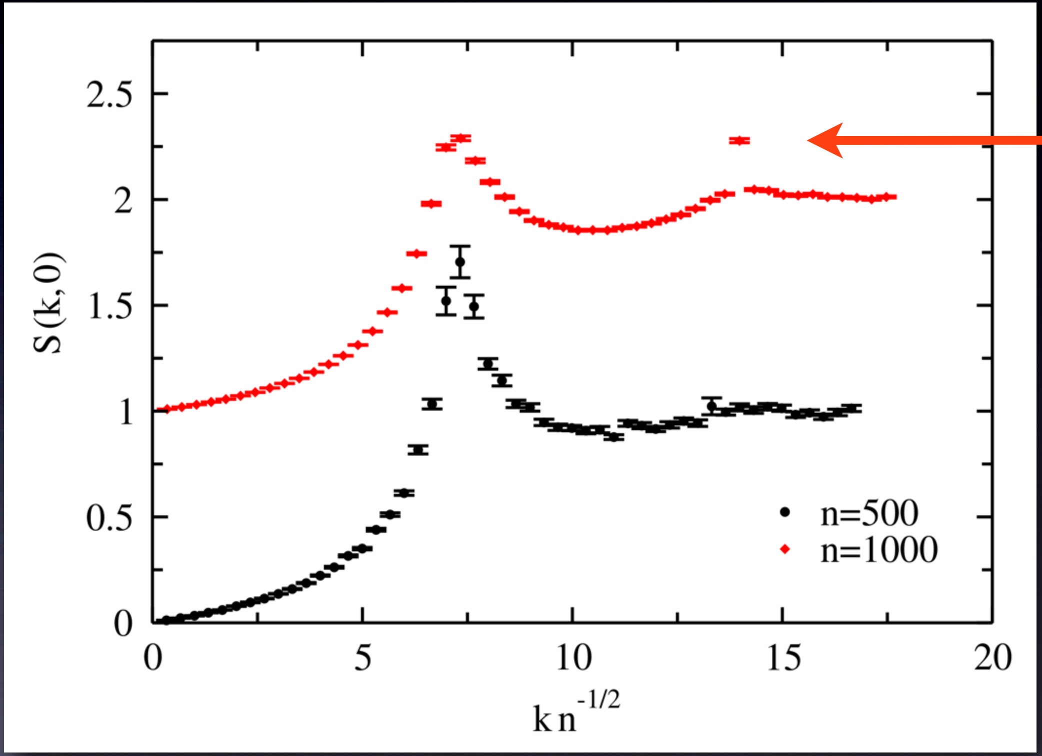
(At this point) we can't decide where does the stripe phase ends and where the solid forms...

Critical Angle

...work in progress

Stripe-Solid transition (?)

Static Structure factor along the X direction



A new peak reveals crystaline order, or is it a quirk of the simulation induced by finite size effects ?

work in progress !!!

Thank you very much :)