Rotons, Stripe Phases, Dimerization: Condensed Matter Physics with Dipolar Molecules

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Rotons in ^{4}He

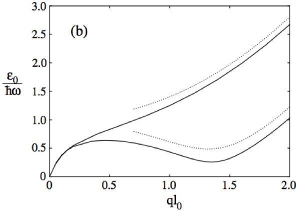
- roton = local minimum (E_r) in the dispersion relation $\epsilon(k)$ at $k = k_r$
- roton = signature of short-range "order" of a dense Bose (or Fermi[1]) liquid
- $k_r \approx \frac{2\pi}{a}$, with a the average nearest neighbor distance
- compare with crystal: phonon dispersion $\epsilon(\frac{2\pi}{a}) = \epsilon(0) = 0$
- note: E_r does not continuously approach 0 at crystallisation of ^{4}He!

Rotons in a dilute system

- layer of dipolar Bose gas created by a 1D trap: infinite in xy, finite in z
- polarization in z
- excitation modes n with parallel momentum k, energy $\epsilon_n(k)$

e.g. Santos et al., PRL **90**, 250403 (2003):

- calculation of $\epsilon_1(k)$ in Gross-Pitaevskii approximation (no pair correlations)
- "rotonization" for $g_d/g > 1/2$ ($g_d = 8\pi d^2/3$)
- different kind of roton (II) than the ^{4}He roton (I)



[1] H. Godfrin et al., Nature 483, 576 (2012)

Can a dipolar Bose solidify?

layer in 1D trap with $\omega_z \to \infty \quad \Longrightarrow \quad$ 2D Bose gas with $1/r^3$ repulsion
express Hamiltonian in dipole units $r_0 = \frac{md^2}{4\pi\epsilon_0\hbar^2}$ and $E_0 = \frac{\hbar^2}{mr_0^2}$:

$$H = -\frac{1}{2}\sum_i \nabla_i^2 + \sum_{i<j}\frac{1}{r_{ij}^3}$$

$\Rightarrow$ only 1 parameter: density n

solidification of 2D dipolar Bose gas? ("self-assembled lattice")

Q Can solidification at some $n = n_{\rm cr}$ be achieved?

A r_0 can be very large (NaCs: $r_0 = 5 \times 10^5$Å; SrO: $r_0 = 0.1$mm!)

QMC simulation at high n $\begin{cases} \text{H. P. Büchler et al., } \textbf{98}\text{, 060404 (2007)} \\ \text{G. Astrakharchik et al., } \textbf{98}\text{, 060405 (2007)} \end{cases}$

for $n_{\rm cr} r_0^2 \approx 290$, solificicication into triangular 2D crystal (NaCs: $n_{\rm cr} \approx 10^7\text{cm}^{-2}$; SrO: $n_{\rm cr} \approx 2 \times 10^6\text{cm}^{-2}$)

Experiments

experimental realizations:

- magnetic dipole moments of atoms:

  ^{52}Cr Lahaye et al, Nature **448**, 672 (2007) [$\mu = 6\mu_B$]
  ^{164}Dy Lev, PRL (2011) [$\mu = 10\mu_B$]
  ^{168}Er Aikawa et al., PRL **108**, 210401 (2012) [$\mu = 7\mu_B$]

- molecular quantum gases:
  permanent electric dipole moments of heteronuclear dimers
  transfer atom pairs to weakly bound state by Feshbach resonance $\longrightarrow$ transfer to rovibrational g.s. by STIRAP laser pulses

  KRb Ni et al., Science **322**, 231 (2008)
  RbCs T. Takekoshi et al., PRA **85**, 032506 (2012)
  OH B. K. Stuhl et al., Nature **492**, 396 (2012) (evap. cooling)
  SrF Steven Hoekstra
  . . .

Overview of Talk

given two dipoles with dipole moment d and orientations $\hat{\mathbf{e}}_i$, $i = 1, 2$, the interaction is

$$\perp \text{ polarized, 2D:} \quad v_{dd}^{\|}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0} \frac{1}{r_{12}^3}$$

$$\text{tilted by } \alpha\text{, 2D:} \quad v_{dd}^{//}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0} \frac{1 - 3(x_{12}/r_{12})^2 \sin^2\alpha}{r_{12}^3}$$

$$\text{polarized, 3D:} \quad v_{dd}^{\|}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0} \frac{1 - 3\cos^2\theta_{12}}{r_{12}^3}$$

$$\textit{un}\text{polarized, xD:} \quad v_{dd}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0} \frac{\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{e}}_2 - 3(\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{r}})(\hat{\mathbf{e}}_2 \cdot \hat{\mathbf{r}})}{r_{12}^3}$$

(units: length $r_0 = \frac{md^2}{4\pi\epsilon_0\hbar^2}$; energy $E_0 = \frac{\hbar^2}{mr_0^2}$; density nr_0^2)

interesting questions in dipolar QGs

effects of strong short-range interactions – pair correlations:

e.g. dipole length $r_0 = 5 \times 10^5$Å for NaCs ($d = 4.6D$)

- rotons I
- stripe phase

effects of long range of interactions – pair correlations:

- correlations between different DBG layers: inter-layer binding

effects of anisotropy of V_{dd}:

"instability well" for head-to-tail orientation
(e.g. homogeneous 3D Bose gas of polarized dipoles is unstable)

- collapse of DBG
- rotons II

effects of molecule rotation in dipolar BEC:

Roman Krems et al.: rotational excitons in optical lattices
Alexey Gorshkov, Kaden Hazzard, Misha Lemeshko: spin Hamiltonians
coupling between rotation and translation,. . .

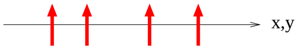
Methodology

methodology:

- quantum many-body method: hypernetted chain Euler-Lagrange for ground state (HNC-EL) and excited states (TDHNC-EL, "dynamic many-body theory")
- QMC: path integral ground state MC (PIGSMC) and diffusion MC (DMC)
- combining QMC for ground state and TDHNC-EL for excitations: previously applied and tested for molecule rotation dynamics in superfluid ^{4}He nanodroplets.
- mean field approach (GP)

polarized, 2D: $\quad v_{dd}^{\parallel}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0}\frac{1}{r_{12}^3}$

Dipoles in 2D



ground state solidification (self-assembled lattice) at density $nr_0^2 = 290$
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Büchler et al., PRL **98**, 060404 (2007)

excitations combining DMC for ground state with **CBF-BW** for excitations (only gas phase)

Calculation of dynamic structure function $S(k,\omega)$

$S(k,\omega)$ ... response to perturbation imparting momentum $\hbar k$ and energy $\hbar\omega$
(cond. mat.: neutron scattering; cold gases: Bragg spectroscopy)
excitations $\Leftrightarrow$ peaks of $S(k,\omega)$ at $\omega =$excitation energy

Many-Body Approach to Excitations

Dynamic many-body approach (Bose)

time-dependent hyper-netted chain Euler-Lagrange method, assuming the many-body ground state Φ_0 is known (e.g. from time-independent HNC-EL or from QMC):

1. t-dependent ansatz:

$$\Psi(R;t) = e^{-iE_0 t} \frac{e^{\delta U(R;t)/2}}{\langle\Psi|\Psi\rangle^{1/2}} \Phi_0(R) \quad \text{with} \quad \delta U(R;t) = \sum_i \delta u_1(\mathbf{r}_i;t) + \sum_{i<j} \delta u_2(\mathbf{r}_i,\mathbf{r}_j;t) + \ldots$$

2. t-dependent generalization of Ritz' principle

$$\delta \int dt \big\langle \Psi(t) \big| H + V_{pert}(t) - i\hbar \frac{\partial}{\partial t} \big| \Psi(t) \big\rangle = 0$$

3. linear response theory:

$$V_{pert}(t) \to V_{pert}(\omega) \to \delta\rho(\omega) = \hat{\chi}(\omega) * V_{pert}(\omega)$$

$\hat{\chi}$ =density-density response operator

- $\delta u_1(\mathbf{r}_i;t)$ only: Bjil-Feynman approximation
- $\delta u_2(\mathbf{r}_i,\mathbf{r}_j;t)$ & some approximations (CBF-BW,. . .):
  accounts for phonon-phonon coupling of Bjil-Feynman modes
  Campbell, Krotscheck PRB **80**, 174501 (2009)
- $\delta u_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k;t)$ triplets (homogeneous system)

Calculation of dynamic structure function $S(k,\omega)$ (homogeneous system):

$$S(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\chi(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\frac{S(k)}{\hbar\omega - \epsilon_F(k) - \Sigma(k,\omega) + i\eta}$$

$S(k)$ ... static structure function ($\leftarrow$ from ground state calculation)

$\epsilon_F(k) = \frac{\hbar^2 k^2}{2mS(k)}$ ... Bjil-Feynman spectrum

$\Sigma(k,\omega)$ ... energy-dependent self energy: coupling between modes, relaxation

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

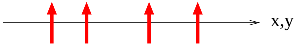
$$V_3(\mathbf{k},\mathbf{p},\mathbf{q}) = \frac{\hbar^2}{2m}\sqrt{\frac{S(p)S(q)}{S(k)}}\left[\mathbf{k}\cdot\mathbf{p}\left(1-\frac{1}{S(p)}\right) + \mathbf{k}\cdot\mathbf{q}\left(1-\frac{1}{S(q)}\right) - k^2 u_3(\mathbf{k},\mathbf{p},\mathbf{q})\right]$$

$$S(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\frac{S(k)}{\hbar\omega - \epsilon_F(k) - \Sigma(k,\omega) + i\eta}$$

Collective excitations:

1. if
$$\hbar\omega - \epsilon_F(k) - \Sigma(k,\omega) = 0$$
has a real solution, $\hbar\omega \in \mathbf{R}$, then $\epsilon(k) = \hbar\omega$ is spectrum of collective excitations with ∞ lifetime ($\mathrm{Im}\Sigma(k,\omega) = 0$)
$\Rightarrow \delta$ peak in $S(k,\omega)$
2. if
$$\hbar\omega - \epsilon_F(k) - \mathrm{Re}\Sigma(k,\omega) = 0$$
has solutions, with a small $\mathrm{Im}\Sigma(k,\omega)$, excitation of energy $\epsilon(k)$ is damped, has finite lifetime
$\Rightarrow$ peak with linewidth $\mathrm{Im}\Sigma(k,\omega)$ in $S(k,\omega)$
3. whereever $\mathrm{Im}\Sigma(k,\omega)$ is large, there are no well-defined excitation modes ("multi-excitation continuum")

Dipoles in 2D



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$S(k,\omega)$ . . . response to perturbation imparting momentum $\hbar k$ and energy $\hbar\omega$
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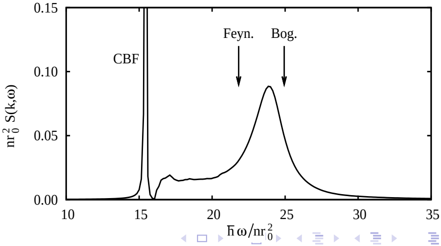
excitations $\Leftrightarrow$ peaks of $S(k,\omega)$ at ω =excitation energy

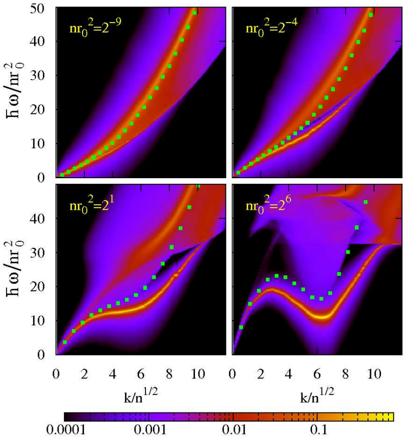
$S(k,\omega)$ for low density $nr_0^2 = 2^{-7}$ ($\frac{k}{\sqrt{n}} = 6.4$):

- broad peak: short life-time
- sharp peak: ∞/long life-time



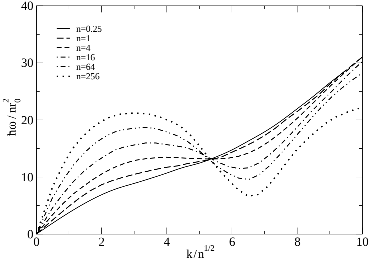
dynamic structure function $S(k,\omega)$:

(artificial broadening by $\eta = 0.15$)



increasing density:

- sharp phonon dispersion splits off from broader peak
- roton I appears at about $nr_0^2 = 4$ due to strong pair correlations



Mazzanti, REZ, Astrakharchik, Boronat, PRL **102**, 110405 (2009)

⟶ **appearance of a maxon-roton dispersion similar to ^{4}He**

⟶ **evolution towards maxon & roton can be studied as density is increased**

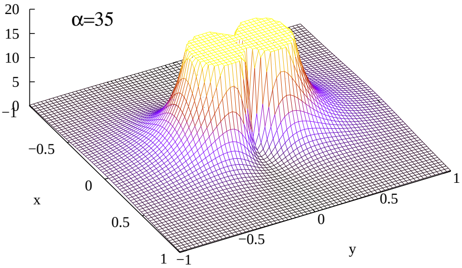
⟶ **now do it for Fermi dipoles**

tilted by α, 2D: $\quad v_{dd}^{//}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0} \frac{1 - 3(x_{12}/r_{12})^2 \sin^2\alpha}{r_{12}^3}$

anisotropy is not probed in 2D with perpendicular polarization axis

$\longrightarrow$ tilt polarization axis along x-axis (i.e. rotate about y-axis) to form homogeneous *anisotropic* 2D quantum gas (similar to "nematic")

$$v_{dd}^{//}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0} \frac{1 - 3(x_{12}/r_{12})^2 \sin^2\alpha}{r_{12}^3} \qquad (\alpha < \alpha_{max} = 0.61548 = 35.26^\circ)$$



strong repulsion in y and weak repulsion in x

HNC-EL for Bose ground state

$$\Phi_0(R) = \prod_i \varphi(\mathbf{r}_i) \prod_{i<j} f(\mathbf{r}_i, \mathbf{r}_j) \cdots = e^{\frac{1}{2}\sum_i u_1(\mathbf{r}_i)} e^{\frac{1}{2}\sum_{i<j} u_2(\mathbf{r}_i, \mathbf{r}_j)} \ldots$$

(Fermi: $\Phi_0^F(R) = e^{\frac{1}{2}\sum_i u_1(\mathbf{r}_i)} e^{\frac{1}{2}\sum_{i<j} u_2(\mathbf{r}_i, \mathbf{r}_j)} \ldots \times \Phi_{sl}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$)

- $u_1(\mathbf{r}_i)$: needed for inhomogeneous systems (u_1 only $\rightarrow$ Hartree)
- $u_2(\mathbf{r}_i, \mathbf{r}_j)$: correlations (Jastrow-Feenberg; used also for QMC)
- $u_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)$: even better

express $E = \langle H \rangle$ as functional of density ρ, pair distribution function g and triplet correlations u_3. Use Ritz' variational principle:

$$\frac{\delta \langle H \rangle}{\delta \rho(\mathbf{r})} = 0 \ , \qquad \frac{\delta \langle H \rangle}{\delta g(\mathbf{r}_1, \mathbf{r}_2)} = 0 \ , \qquad \frac{\delta \langle H \rangle}{\delta u_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)} = 0$$

closure by hyper-netted chain & Ornstein-Zernicke relation (*classical* stat mech!)

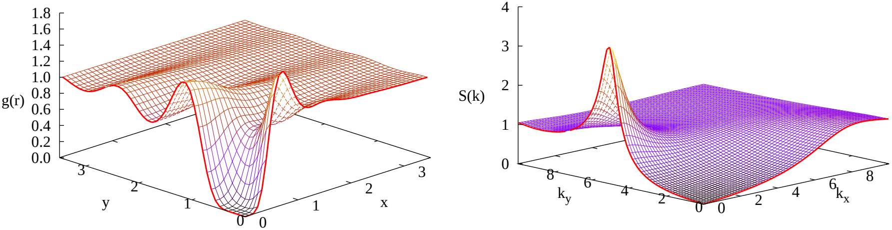
$$g = e^{u_2 + N + B} \quad \& \quad N(1,2) = \int d3\,[g(1,3) - 1 - N(1,3)]\,\rho(3)\,[g(3,2) - 1]$$

- − HNC-EL not exact
- + HNC-EL can be orders of magnitude more efficient than QMC
- + at low densities, u_3 and elementary diagrams B are small ("HNC-EL/0")

anisotropic HNC-EL/0 calculation:

density $nr_0^2 = \underline{256}$, $\alpha = 0.58$: very anisotropic pair structure

pair distribution $g(\mathbf{r})$ static structure factor $S(\mathbf{k})$



- tendency towards long range order in y-direction
- isotropic speed of sound
- Q: excitation spectrum $\epsilon(\mathbf{k})$?
- Q: isotropic solidification at $nr_0^2 = 290$ for $\alpha = 0$
  $\alpha > 0$: anisotropic crystal? or stripe ("smectic") phase?

Note: HNC-EL/0 only qualitative at such high density! $\rightarrow$ QMC

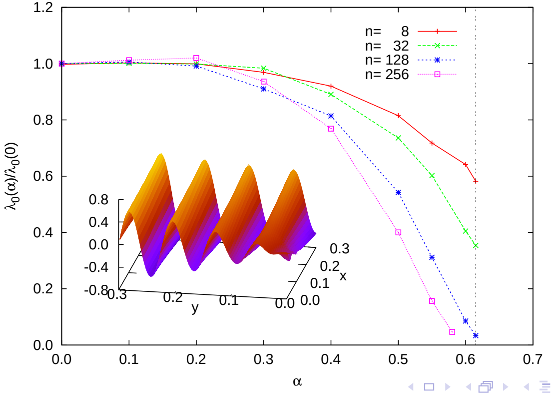
Stability analysis: positivity of eigenvalues λ of

$$\frac{\delta^2 E}{\delta g^{1/2}(\mathbf{r})\,\delta g^{1/2}(\mathbf{r}')}\,, \quad \mathbf{r} \equiv (x, y)$$

$$\Leftrightarrow \left[-\frac{\hbar^2}{m}\nabla^2 + V_{dd}(\mathbf{r}) + w_I(\mathbf{r})\right] f(\mathbf{r}) - \rho g^{1/2}(\mathbf{r}) \int d^2r\ W(\mathbf{r}-\mathbf{r}')g^{1/2}(\mathbf{r}')f(\mathbf{r}') = \lambda f(\mathbf{r})$$

where $\tilde{w}_I(\mathbf{k}) = -\frac{\hbar^2 k^2}{4m}(1-1/S(\mathbf{k}))^2(2S(\mathbf{k})+1)$ and $\tilde{W}(\mathbf{k}) = \frac{\hbar^2 k^2}{m}(1-1/S^3(\mathbf{k}))$.

solve for lowest eigenvalue/vector by imaginary time propagation:



Path integral ground state Monte Carlo (PIGSMC)

N-body Schrödinger equation in imag. time = diffusion equation:

$$-\frac{\partial}{\partial t}\Psi(t) = H\Psi(t) \quad \Rightarrow \quad \Psi(t) = \sum_n \Psi_n e^{-\omega_n t} \to\sim \Psi_0$$

idea:

1. start at $t = 0$ with "trial" wave function Ψ_T
2. propagate in imag. time towards ground state with $G(\beta) = e^{-\beta H}$

$$\Psi_0(R) \propto \lim_{\beta\to\infty} \int dR'\, G(R,R',\beta)\Psi_T(R')$$

3. factorize $G(\beta)$ into small time steps: $G(\beta) = G(\epsilon)^M$, with $\epsilon = \frac{\beta}{M}$
4. use short time approximation for $G(\epsilon)$

implementation:

- probability distribution to be sampled ($R = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$):

$$P(R_0,\ldots,R_{2M}) = \Psi_T(R_0)\; G(R_0,R_1;\epsilon)\ldots G(R_{2M-1},R_{2M};\epsilon)\; \Psi_T(R_{2M}),$$

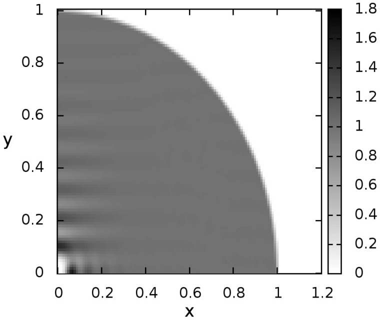
- ground state expectation value $\langle\Psi_0|A|\Psi_0\rangle$ evaluated at central t-step: $A(R_M)$.
- MC: Metropolis sampling of $d \times N \times 2M$ integrations

→ Path integral ground state Monte Carlo (PIGSMC) results:

Pair distribution function $g(x, y)$:

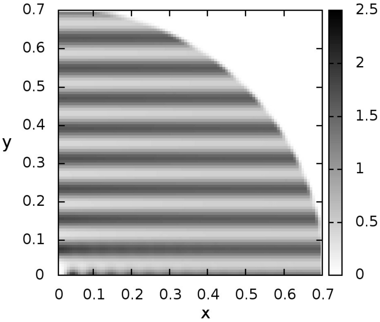
density $nr_0^2 = 128$, $\alpha = 0.58$:
no long range order:

GAS PHASE



density $nr_0^2 = 256$, $\alpha = 0.61$:
long range order in y-direction:

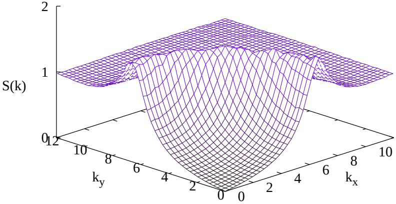
STRIPE PHASE



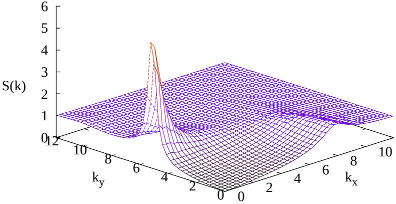
A. Macia et al, PRL **109**, 235307(2012)

static structure factor $S(\mathbf{k})$ (gas phase):

density $nr_0^2 = 128$, $\alpha = 0.0$:



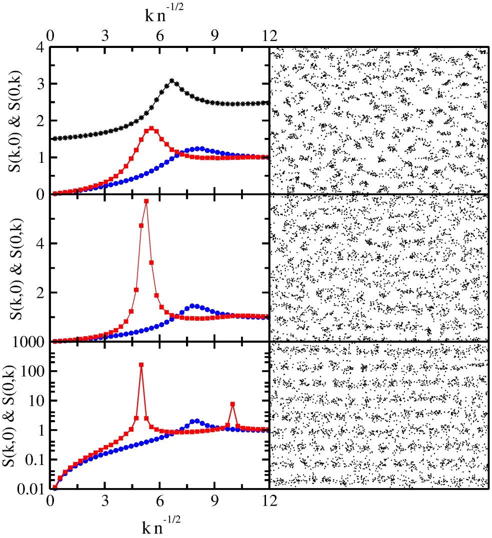
density $nr_0^2 = 128$, $\alpha = 0.58$:



Tilted Dipoles in 2D

$S(\mathbf{k})$ and simulation snapshorts:

1. $nr_0^2 = 64, \alpha = 0.58$
2. $nr_0^2 = 128, \alpha = 0.58$:
   very large peak of $S(\mathbf{k})$ in
   y-direction, but still liquid:
   peak height independent of N
3. $nr_0^2 = 256, \alpha = 0.61$: $S(\mathbf{k})$
   has a Bragg peak in
   y-direction
   peak height almost linear in
   N



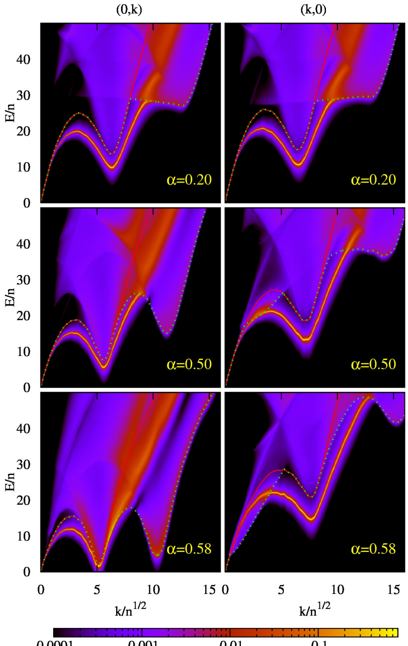
Tilted Dipoles in 2D

dynamic structure function $S(\mathbf{k}, E)$ for $nr_0^2 = 128$: **gas phase**

1. $\alpha = 0.20$:
   - almost isotropic dispersion relation
   - "Pitaevskii" plateau at twice the roton energy

2. $\alpha = 0.50$:
   - roton energy in y-direction decreases, roton momentum decreases

3. $\alpha = 0.58$:
   - roton energy in y almost reaches zero
   - $\Rightarrow$ continuous transition to stripe phase
   - *second* roton with much smaller spectral weight at twice the wave number
   - $\leftrightarrow$ compare with phonon dispersion of crystal: $\epsilon(\frac{2\pi n}{a}) = 0$



$$\text{polarized, 3D:} \quad v_{dd}^{\parallel}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0}\frac{1 - 3\cos^2\theta_{12}}{r_{12}^3}$$

Quasi-2D: Layer of Dipolar Bose Gas

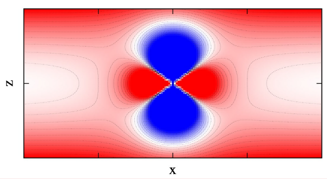
experiment

pancake-shaped harmonic traps: $\omega_z \gg \omega_{x,y}$
layer: $\omega_z > 0$, $\omega_{x,y} \to 0 \Rightarrow$ translational invariance

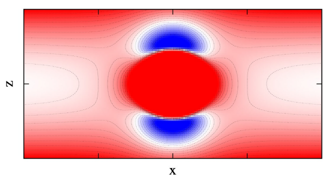
dipoles in 1D harmonic trap

pure dipole system unstable via tunneling towards head-to-tail configurations
$\Rightarrow$ stabilize with repulsion $(\sigma/r)^{12}$

$\sigma = 0$:



$\sigma \neq 0$:



using again units length $r_0 = \frac{md^2}{\hbar^2}$ and energy $\epsilon_0 = \frac{\hbar^2}{mr_0^2}$, the system is characterized by

- repulsion σ — unstable for $\sigma \to 0$
- trap frequency Ω — unstable for $\Omega \to 0$
- area density $n = \int dz\, \rho(z)$ — unstable for $n \to \infty$

ground state calculation: HNC-EL; excitations: CBF-BW

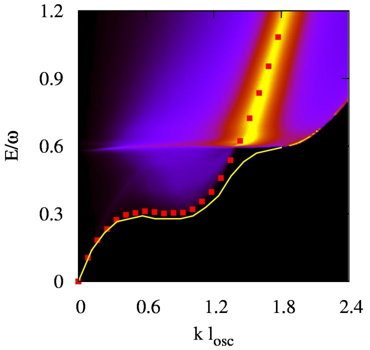
Roton II in dilute gas

in ^{4}He: roton excitation due to strong correlations
Q: roton excitation in dilute gas?
A: Santos et al., PRL 90, 250403 (2003): yes! (based on mean field approximation)

CBF-BW results:

- "rotonization" due to attractive part of v_{dd}
- strong damping at $2 \times E_{roton}$: "Pitaevskii plateau"
- system unstable towards $\sigma \downarrow$, $n \uparrow$, $\Omega \downarrow$
- HNC-EL calculation unstable before roton energy E_{roton} (presumably) vanishes
- above: repulsion & high density $\rightarrow$ roton I
  here: attraction & any density $\rightarrow$ roton II
- instability for similar parameters as for binding of 2-body problem $\Rightarrow$ dimerization

$S(k, E)$ for $nr_0^2 = 2$, $\Omega^2 = 10$, $\sigma = 0.3$:



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

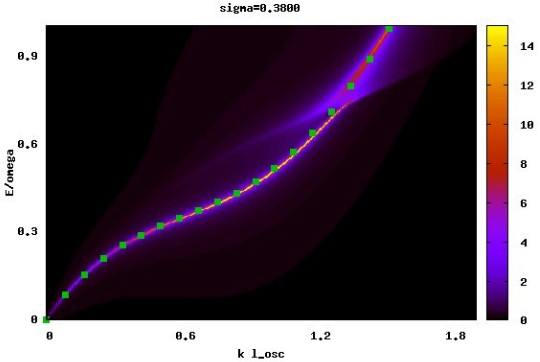
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$
with decreasing σ:

$\sigma = 0.3800$



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

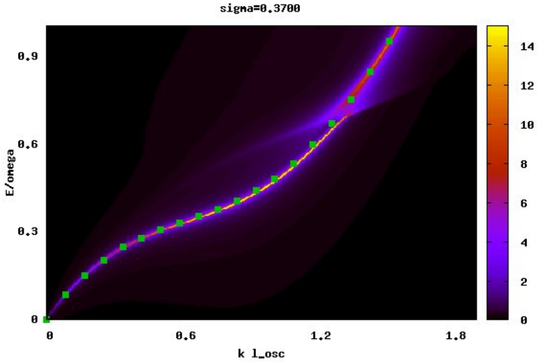
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$
with decreasing σ:

$\sigma = 0.3700$



Er_2 (magnetic dipoles):

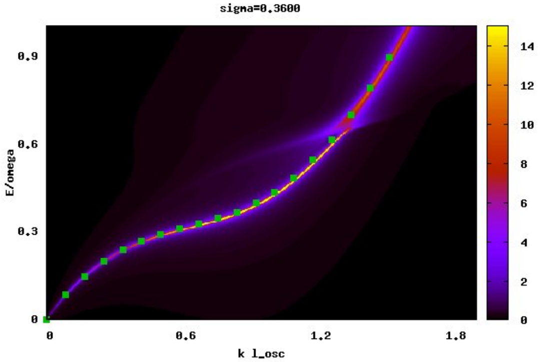
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850$Å
- $\Omega = 10$kHz
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$ with decreasing σ:

$\sigma = 0.3600$



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

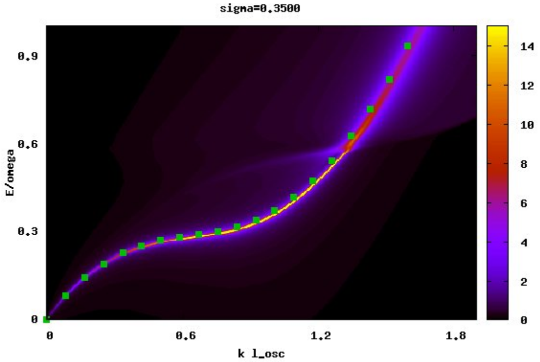
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$
with decreasing σ:

$\sigma = 0.3500$



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

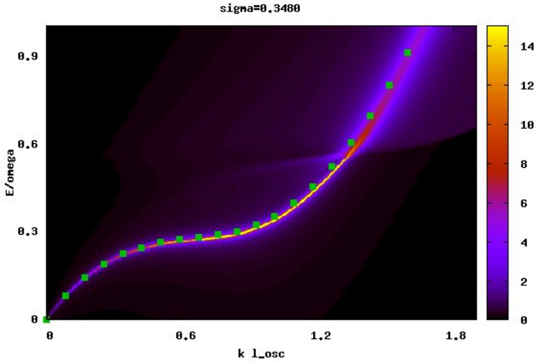
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$
with decreasing σ:

$\sigma = 0.3480$



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

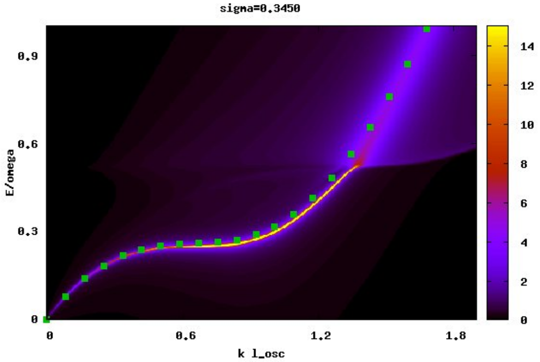
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$ with decreasing σ:

$\sigma = 0.3450$



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

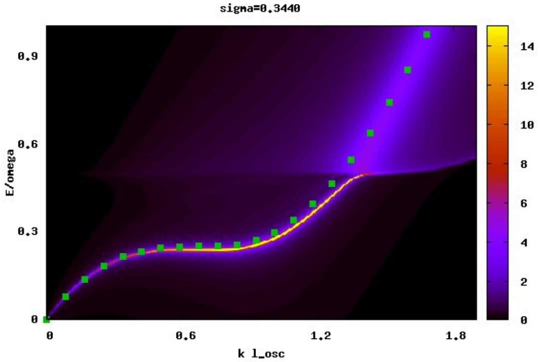
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$ with decreasing σ:

$\sigma = 0.3440$



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

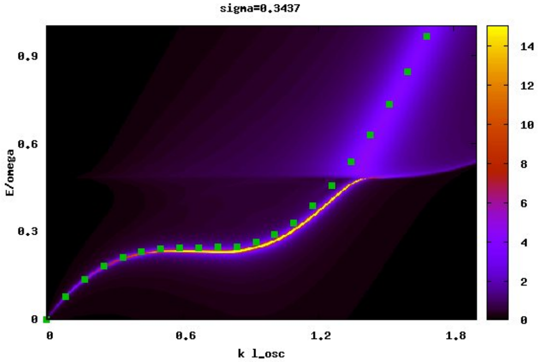
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$
with decreasing σ:

$\sigma = 0.3437$



Er_2 (magnetic dipoles):

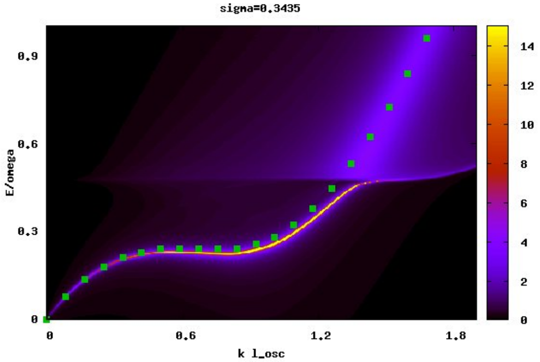
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k, \omega)$ with decreasing σ:

$\sigma = 0.3435$



Roton in dilute system: Er_2

Er_2 (magnetic dipoles):

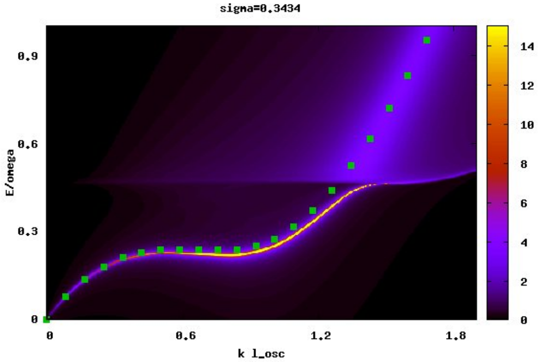
- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850\text{Å}$
- $\Omega = 10\text{kHz}$
- $nr_0^2 = 0.3$

evolution of $S(k,\omega)$
with decreasing σ:

$\sigma = 0.3434$

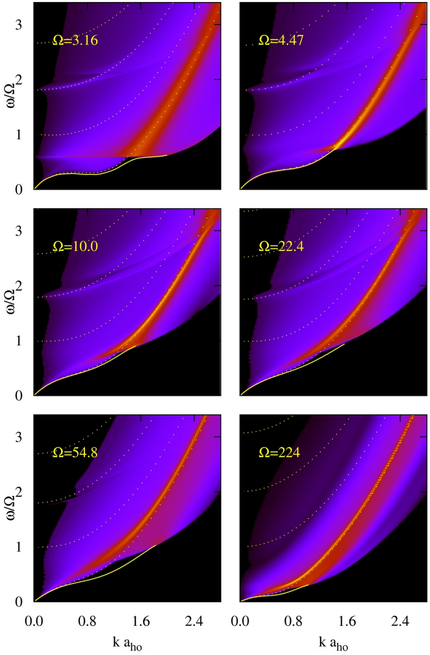


Q: can we switch between roton I and roton II?

$S(k,\omega)$ for density $nr_0^2 = 2$, repulsion $\sigma = 0.3$ and trap frequency Ω increasing from $\Omega = 3.16$ (top left) to $\Omega = 224$ (bottom right):

- weak trapping: roton I, caused by perpendicular correlations due to attractive part of dipole-dipole interaction
$$k_{roton} \approx a_{ho}^{-1}$$
- strong trapping: roton II, caused by parallel correlations due to repulsive part of dipole-dipole interaction
$$k_{roton} \approx 6n^{1/2}$$

D. Hufnagl et al., PRL 107, 065303 (2011)

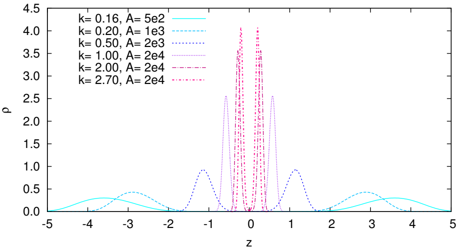


Bilayer dipolar Bose Gas

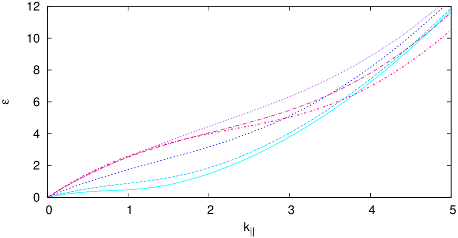
dipole interaction is long-ranged $\rightarrow$ coupling between layers

double-well potential: $U_{ext}(\vec{r}_i) = A\{\cos(Kz_i - \pi) + \lambda\cos(2Kz_i - 2\pi)\}$

- density profile $\rho(z)$ $(nr_0^2 = \int dz\rho(z) = 1)$



- dispersion relatiom of lowest mode in Bjil-Feynman approximation

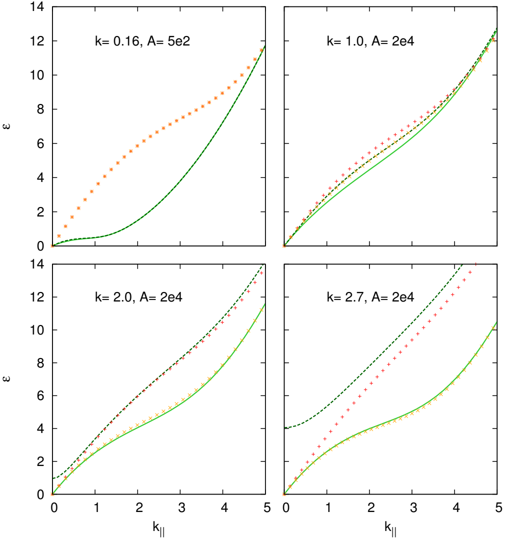


first two excitation spectra:

- **top left:**
  - layers far apart
    ⇒ negligible coupling
  - almost degenerate collective excitations
  - weak trap
    ⇒ intra-layer dimerization instability, same as for single layer

- **bottom right:**
  - layers close together ⇒
    inter-layer dimerization instability
  - splitting of collective excitations
  - strong trap
    ⇒ each layer almost 2D

Bjil-Feynman spectra for bilayers
(symbols: corresponding 2D limit)



inter- and intra-layer pair distribution function:

- inter-layer:

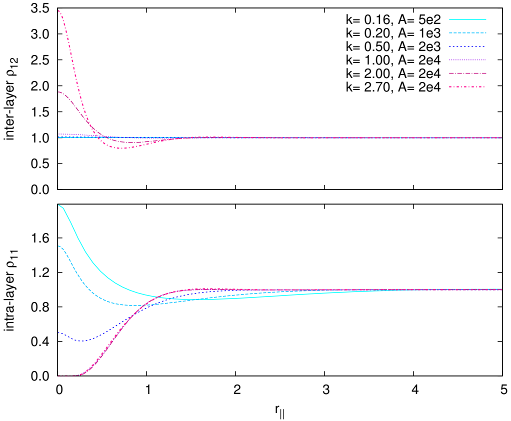
$$\rho_{12}(r_{\parallel}) = \int_{-\infty}^{0}\int_{0}^{\infty} dzdz' \; \rho_2(r_{\parallel}, z, z')$$

$\Rightarrow$ intra-layer dimerization
$\Rightarrow$ collapse

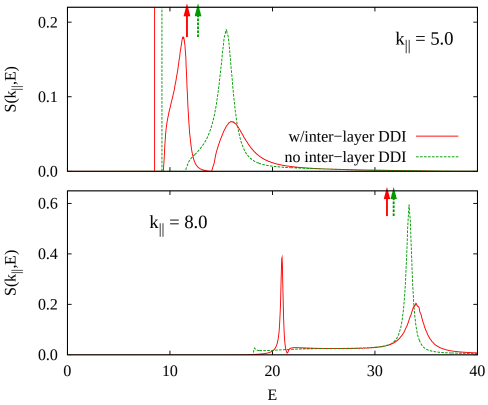
- intra-layer:

$$\rho_{11}(r_{\parallel}) = \int_{0}^{\infty}\int_{0}^{\infty} dzdz' \; \rho_2(r_{\parallel}, z, z')$$

$\Rightarrow$ inter-layer dimerization



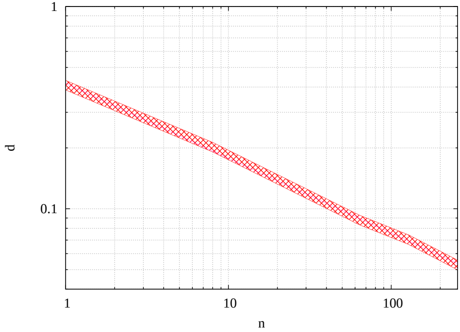
dynamic structure function $S(k_{\|}, \omega)$**:** close narrow layers



Bilayer dipolar Bose Gas

Q: how to stabilize against inter-layer "instability"/dimerization?
A: increase distance or *increase density*

critical distance d as function of density nr_0^2 for two 2D layers:



note: $n \to 0$ (2 particles on different 2D planes) leads to bound state regardless of d!

what next? bi/multilayers of *tilted* dipoles *un*polarized, 3D: $$v_{dd}(\mathbf{r}_{12}) = \frac{d^2}{4\pi\epsilon_0} \frac{\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{e}}_2 - 3(\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{r}})(\hat{\mathbf{e}}_2 \cdot \hat{\mathbf{r}})}{r_{12}^3}$$

Rotating Dipoles

mean field approach (GP):

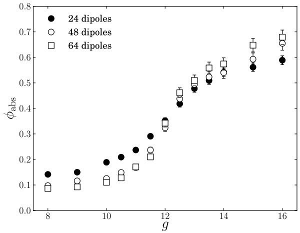
- unpolarized molecules: splitting of first rotational excitation ($j = 1$): $\Delta E = \frac{\rho d^2}{3\epsilon_0}$

  e.g. $n = 10^{14}\text{cm}^{-3}$ and $d = 5D$: $\Delta E \approx 1.6\text{MHz}$
- polarized molecules: fixed-orientation approximation with $d = \langle d \rangle$ generally good, but corrections for very small polarization $d = \langle d \rangle$

Phys. Chem. Chem. Phys. **13**, 18835 (2011)

PIGSMC simulations:

MC sampling of rotations
e.g. 1D dipole lattice:
ordering as $g = \frac{d^2}{Ba^3}$ increases:



B. Abolins et al., JLTP **165**, 249 (2011)

HNC-EL calculations:

preliminary results: at high density, system collapses via self-polarization

what next:

- self-assembled crystalline phases: stable?
- 3-body physics of rotating dipoles?
- ions in dipolar gases

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