Condensed Matter Theory of Dipolar Quantum Gases

ILL, Grenoble, Aug. 2010

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August 7, 2010

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Outline

Dipolar QGs: Experiments

experiments:

- magnetic dipole moments of atoms:
  Cr: Lahaye et al, Nature **448**, 672 (2007)
  Er, Er_2: Ferlaino, Innsbruck
- permanent electric dipole moments of heteronuclear dimers (RbK, etc): transfer atom pairs to weakly bound state by Feshbach resonance $\longrightarrow$ transfer to rovibrational g.s. by STIRAP laser pulses (Innsbruck: Danzl et al., Science **321**, 1062 (2008); JILA, NIST: Ni et al., Science **322**, 231 (2008), RbK)
- Diatomic molecules in optical lattices
  (Danzl et al., Nature Physics **6**, 265 (2010): Cs_2)

our interest in dipolar QGs:

- effects of strong interactions – pair correlations
- effects of anisotropy of V_{dd}
- effects of rotational degrees of freedom of molecular BEC

Dipole-Dipole Interaction

abstract approach of the condensed matter physicist:

> *given two dipoles with dipole moments d and resp. orientation $\hat{\mathbf{e}}_i$, $i = 1, 2$, the interaction is*

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

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

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

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

units: length $r_0 = \frac{md^2}{\hbar^2}$; energy $\epsilon_0 = \frac{\hbar^2}{mr_0^2}$; density $\rho = nr_0^2$

Methodology

methodology:

- quantum many-body method: hypernetted chain Euler-Lagrange for ground state (HNC-EL) and excited state (TDHNC-EL)
  recent progress by Campbell and Krotscheck on the TDHNC-EL front
- QMC: path integral ground state MC (PIGSMC) for ground state and path integral MC (PIMC) for $T > 0$
  recent progress in Barcelona group (quasi-6th order,...) and by REZ and Chin on high order propagators ("any-order")
- combining QMC for ground state and TDHNC-EL for excitations:
  previously applied and tested for molecule rotation dynamics in superfluid ^{4}He nanodroplets (HENDI spectrosopy), e.g.:
  HCCH rotation spectrum in ^{4}He (REZ, Kwon, Whaley, PRL **93** 250401 (2004))
- combining QMC and HNC-EL for ground state:
  Φ_0 from HNC-EL $\longrightarrow$ Φ_T for DMC or PIGSMC
  very recent progress for tilted dipoles

(time-dependent) hyper-netted chain Euler-Lagrange

ground state: HNC-EL

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

$$\frac{\delta\langle H\rangle}{\delta u_1(\mathbf{r})} = 0\ , \qquad \frac{\delta\langle H\rangle}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)} = 0\ , \qquad \frac{\delta\langle H\rangle}{\delta u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)} = 0$$

. . . coupled nonlinear integro-differential equations

- $u_1(\mathbf{r}_i)$ only (& effective δ-potential): Hartree (GP)
- $u_2(\mathbf{r}_i, \mathbf{r}_j)$: minimal requirement for repulsive interaction
- $u_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)$: even better. . .

− HNC-EL not exact

\+ HNC-EL can be orders of magnitude more efficient than QMC

HNC-EL validated by numerous applications to ^{4}He:

- accuracy of E_0, $g(r)$, $\rho(\mathbf{r})$ close to QMC
- caveat: for high accuracy, HNC-EL require one phenomenological factor (scaling of elementary diagrams), kept fixed
- for weaker interactions, elementary diagrams negligible

(time-dependent) hyper-netted chain Euler-Lagrange

excitations: TDHNC-EL

$$\Psi(R;t) = e^{-iE_0 t} \frac{e^{\delta U(R;t)/2}}{\langle\Psi|\Psi\rangle^{1/2}} \Phi_0(R)$$

$$\text{with} \quad \delta U(R;t) = \sum_i \delta u_1(\mathbf{r}_i;t) + \sum_{i<j} \delta u_2(\mathbf{r}_i,\mathbf{r}_j;t) + \dots$$

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

- $\delta u_1(\mathbf{r}_i;t)$ only: Bjil-Feynman approximation (Bogoliubov-deGennes/linearized GP)
- $\delta u_2(\mathbf{r}_i,\mathbf{r}_j;t)$ & some approximations: CBF-BW
- $\delta u_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k;t)$ triplets & less approximation: Krotscheck & Campbell

– TDHNC-EL not exact

\+ TDHNC-EL can be orders done at all, when QMC unfeasible

application to phonon-roton spectrum in ^{4}He at ρ_{eq}:

- Feynman roton about $\times 2$ too high
- CBF-BW roton about 30% too high
- even closer with δu_3

excitations: hierarchy of approximations

Bogoliubov-deGennes	*linearization of Gross-Pitaevskii (GP) equation: 1-body fluctuations based on mean field ground state*
Bijl-Feynman approximation	*1-body fluctuations based on real ground state (or approx. w/pair correlations);* $\frac{\hbar^2 k^2}{2mS(k)}$ *in bulk*
CBF-BW approximation	*2-body fluctuations based on real ground state (or approx. w/high correlations)*
w/triplets δu_3	*3-body fluctuations based on real ground state (or approx. w/high correlations)*

Perpendicular dipoles in 2D

ground state solidification (self-assembled lattice) at density $\rho = 290$ (Astrakharchik PRL **98**, 060405 (2007))

excitations combining DMC for g.s with CBF-BW for excitations (Mazzanti, REZ, Astrakharchik, Boronat, PRL **102**, 110405 (2009))

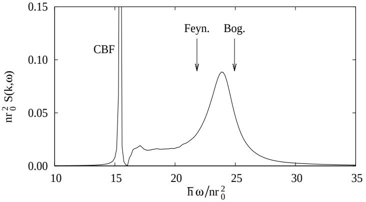
Calculation of dynamic structure function $S(k,\omega)$

$S(k,\omega)$ ... response to perturbation imparting momentum $\hbar k$ and energy $\hbar\omega$ to system (neutron scattering; Bragg spectroscopy)

determined in CBF-BW approximation

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

- broad peak (excitation with short life-time) near Bogoliubov prediction
- similar for Feynman prediction
- sharp peak (excitation with ∞ life-time) at lower energy, small spectral weight at such low density

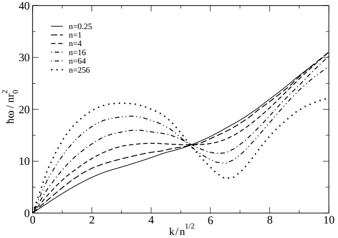


Perpendicular dipoles in 2D

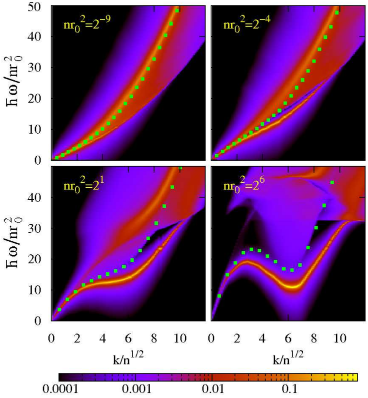
for ^{4}He, dispersion relation is well studied: phonon-roton dispersion

increasing density:

- sharp phonon dispersion splits off from broader peak
- roton appears at about $\rho = 4$ due to strong pair correlations
- roton energy not going to 0 in vicinity of solidification



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

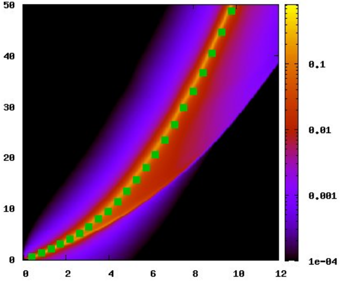


(artificial broadening by $\eta = 0.15$)

Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

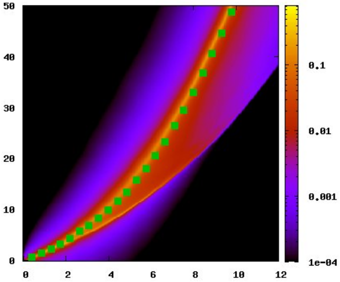
$nr_0^2 = 2^{-12}$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

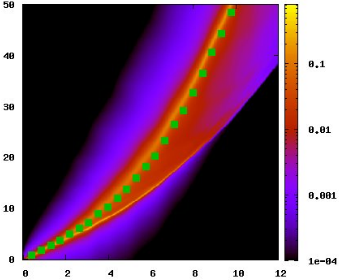
$nr_0^2 = 2^{-10}$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

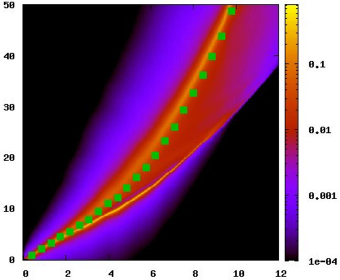
$nr_0^2 = 2^{-8}$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

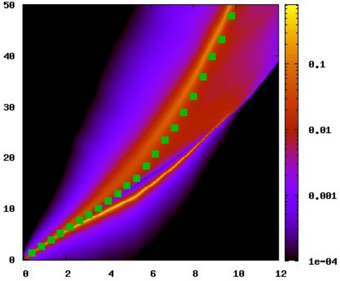
$nr_0^2 = 2^{-6}$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

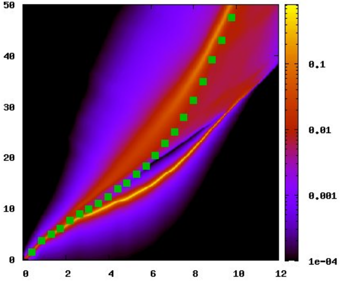
$nr_0^2 = 2^{-4}$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

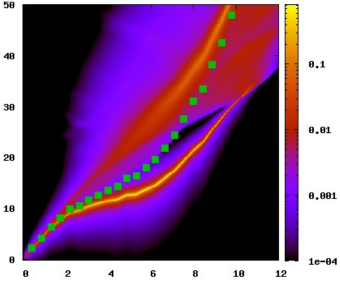
$nr_0^2 = 2^{-2}$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

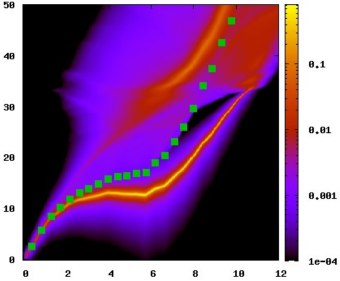
$nr_0^2 = 2^0$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

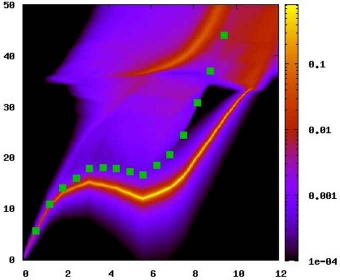
$nr_0^2 = 2^2$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

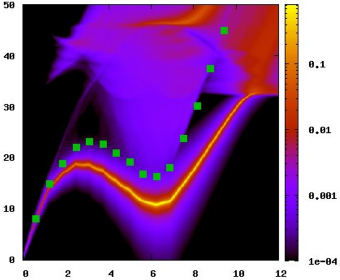
$nr_0^2 = 2^4$



Perpendicular dipoles in 2D

evolution from Bogoliubov to phonon-roton:

$nr_0^2 = 2^6$

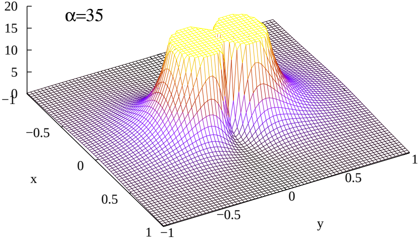


Tilted dipoles in 2D with HNC/0-EL

anisotropy is not probed in 2D with perpendicular polarization axis

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

$$v_{dd}^{/\!/}(\mathbf{r}_{12}) = d^2 \frac{1 - 3(x_{12}/r_{12})^2 \sin^2\alpha}{r_{12}^3}$$

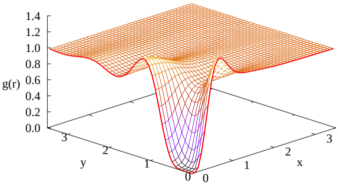


HNC/0-EL ground state calculation (no elementaries, no triplets):

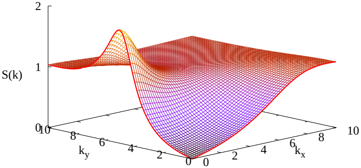
Tilted dipoles in 2D with HNC/0-EL

intermediate density $\rho = 64$, $\alpha = \alpha_{cr}$

$g(\mathbf{r})$

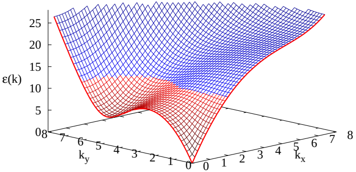


$S(\mathbf{k})$



- test system to study well-defined instability (at angle $\alpha_{cr} = 35.26^\circ$?)
- coupling of excitations: rotons in strongly correlated direction, but not in weakly correlated direction
- anisotropic solidification?
  gas state: isotropic speed of sound $\leftrightarrow$
  solid state: anisotropic speed of sound

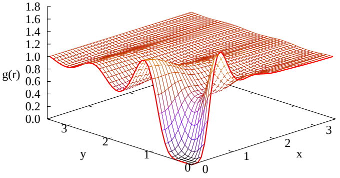
$\epsilon^F(\mathbf{k})$



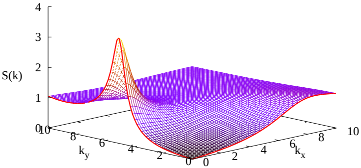
Tilted dipoles in 2D with HNC/0-EL

increase density towards solidification: $\rho = 256$, $\alpha = 33.23^\circ$

$g(\mathbf{r})$



$S(\mathbf{k})$



- test system to study well-defined instability (at angle $\alpha_{cr} = 35.26^\circ$?)
- coupling of excitations: rotons in strongly correlated direction, but not in weakly correlated direction
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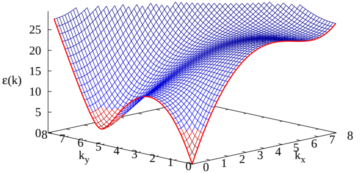
  gas state: isotropic speed of sound ↔
  solid state: anisotropic speed of sound

$\epsilon^F(\mathbf{k})$



HNC/0 approximation not good enough at high density...

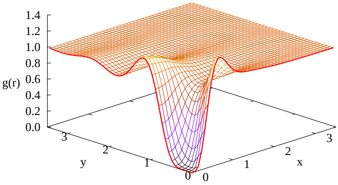
Tilted comparison HNC/0-EL and DMC

tabulate $u_2(x,y)$ $(\Phi_0(R) = \exp[\frac{1}{2}\sum_{i<j} u_2(\mathbf{r}_i,\mathbf{r}_j)])$

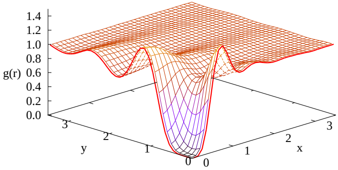
$\longrightarrow$ use Ψ_0 as trial wave function for DMC:

intermediate density $\rho = 64$, $\alpha = \alpha_{cr}$

$g(\mathbf{r})$ from **HNC/0**:



$g(\mathbf{r})$ from **DMC** (mixed estimator):



roton energy $\rightarrow 0$? $\longrightarrow$ CBF-BW (or better)!

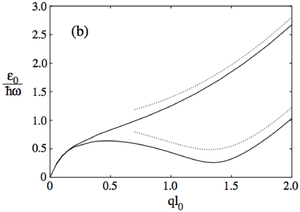
quasi-2D: Slabs of dipolar quantum gases

relax infinitely strong confinement in z-direction: slab = infinite pancake

mean field approach

linearized GP results by Santos, Shlyapnikov, Lewenstein, PRL **90**, 250403 (2003):

excitation spectrum $\epsilon_0(k = k_{||})$:



- dipole + contact interaction $g\delta(\mathbf{r} - \mathbf{r}')$
- top: $g/g_d > 1/2$ ($g_d = 8\pi d^2/3$)
- bottom: $g/g_d < 1/2$ – "rotonization"
- dynamical instability upon further decreasing g/g_d

mean field: no information about microscopic correlations

Note: this is a *different* roton than roton in a dense system, like above.

(both types of rotons possible in a single spectrum?)

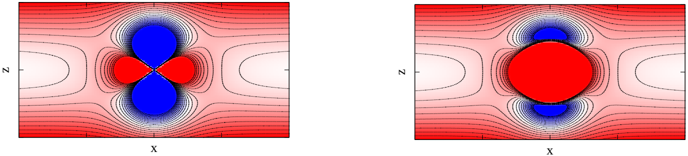
quasi-2D: Slabs of dipolar quantum gases

many-body problem

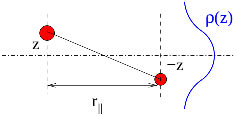
pure dipole system unstable via tunneling towards head-to-tail configurations
⇒ stabilize with repulsive interaction (D. Hufnagl, E. Krotscheck, REZ, JLTP **158**, 85 (2010))

$$H = \sum_i \left[-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{m\omega^2}{2} z_i^2 \right] + \sum_{i<j} \left[v_{\rm dd}(\mathbf{r}_{ij}) + \frac{\sigma^{12}}{r_{ij}^{12}} \right]$$

$\sigma = 0$: $\sigma \neq 0$:



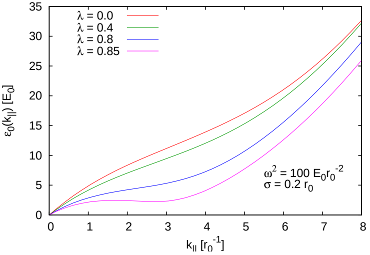
pair distribution function $g(z, z', r_{\|})$:
probability to find particle at (x, y, z) and (another) particle at (x', y', z')
$(r_{\|} = \sqrt{(x-x')^2 + (y-y')^2})$, divided by $\rho(z_i)$
$g \longrightarrow 1$ for large separation



Quasi-2D dipolar quantum gases

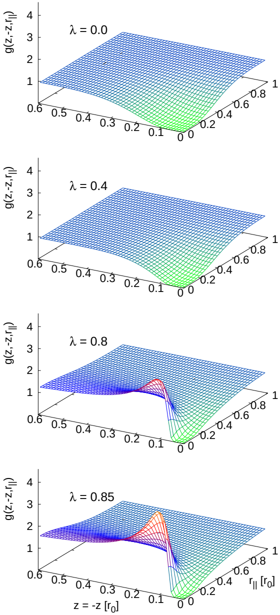
Results with $\sigma = 0.2$, $\rho = 2$, $\omega^2 = 100$:

- parameter λ for anisotropy:
  $v_{dd}^{\|}(\mathbf{r}_{12}) = (1 - 3\lambda \cos^2\theta_{12})/r_{12}^3$
- increase $\lambda \longrightarrow$ peak in $g(z, -z, r_\|)$ at $r_\|$
- rotonization $\leftrightarrow$ dimerization?
  dispersion of lowest mode $\omega(k_\|)$ in Feynman approximation:



- critical λ similar for bound state of free dimer

set $\lambda = 1$ and vary physical parameters ρ, σ, ω...



Roton in dilute system

Bogoliubov-deGennes approximation

- comparison non-trivial: scattering length a
- a from repulsive core σ?
- a from *full* interaction V in vacuum (Bortolotti et al., PRL **97**, 160402 (2006))?
- a from *full* interaction V in harmonic *trap*!

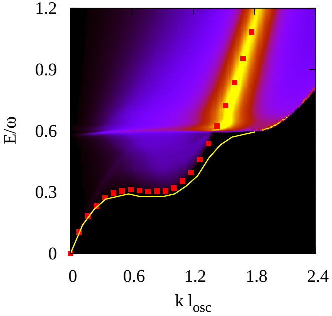
Bijl-Feynman approximation

- like in mean field: "rotonization"
- system unstable towards $\sigma-$, $n+$, $\omega-$
- But: HNC-EL g.s. calculation does not reach point of instability where roton energy E_{roton} (presumably) vanishes
- in ^{4}He: Feynman roton too high by factor of 2

CBF-BW approximation

- dynamic structure function $S(k, E)$ with CBF-BW approximation of TDHNC-EL (convolution approximation)
- roton energy little changed
- strong damping at $2 \times E_{roton}$, but $S(k, \omega)$ looks simpler

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

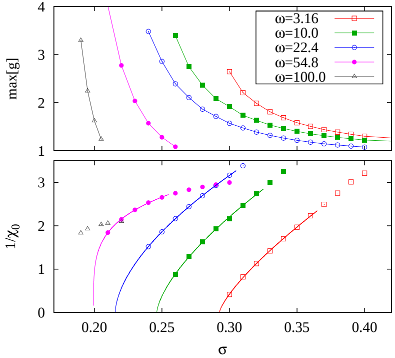


Stability analysis: static response function

static response function $\chi(z, z', r_\parallel)$ ... density response to a (weak) perturbation $\sum_i U_{\rm pert}(\mathbf{r}_i)$:

$$\delta\rho(\mathbf{r}) = \int d^3r' \; \chi(z, z', |\mathbf{r}_\parallel - \mathbf{r}'_\parallel|) \; U_{\rm pert}(\mathbf{r}')$$

- $\longrightarrow$ F.T. w/resp to $r_\parallel$: $\chi(z, z', k)$
- $\longrightarrow$ diagonalize w/resp to z, z': $\chi_n(k)$
- $\longrightarrow$ maximal response: $\chi_0 \equiv \max[\chi_n(k)]$



(extrapolation by fitting $a(\sigma - \sigma_0)^b$)

Roton in dilute system: Er_2

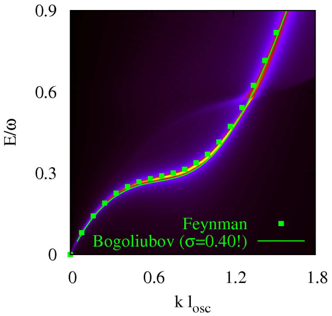
experiment with Er_2 by F. Ferlaino (magnetic dipoles):

- $\mu = 14\mu_B$

choice of other parameters:

- $r_0 = 850$Å
- $\omega = 10$kHz
- $\rho (= nr_0^2) = 0.3$

$S(k, E)$ for $\rho = 0.3$, $\omega^2 = 0.145$, $\sigma = 0.35$:



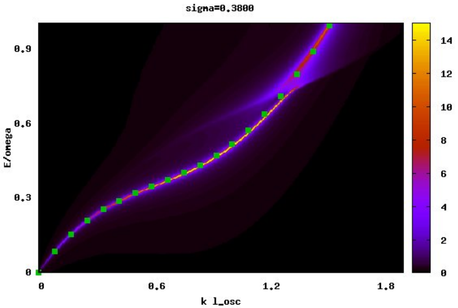
in summary:

- analysis of χ: system (meta)stable up to and beyond rotonization
- but: HNC-EL typically collapses to lower-energy phase close to rotonization

Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

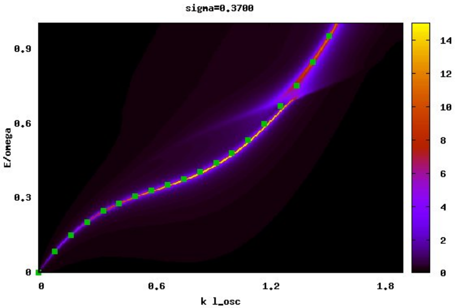
$\sigma = 0.3800$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

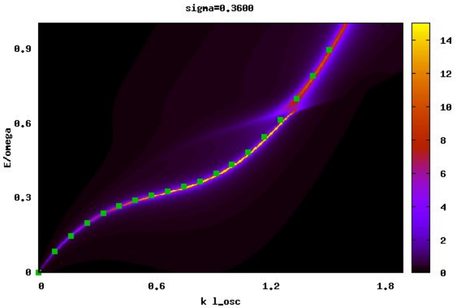
$\sigma = 0.3700$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

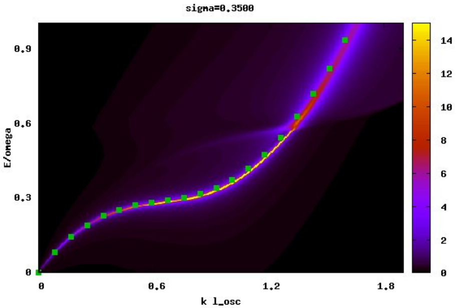
$\sigma = 0.3600$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

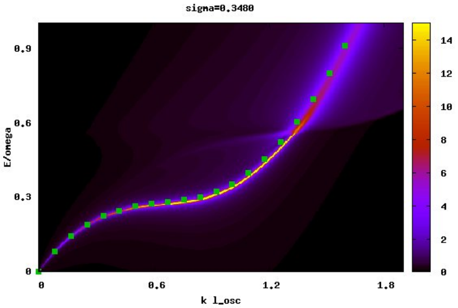
$\sigma = 0.3500$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

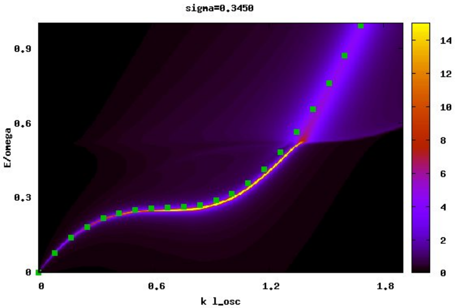
$\sigma = 0.3480$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

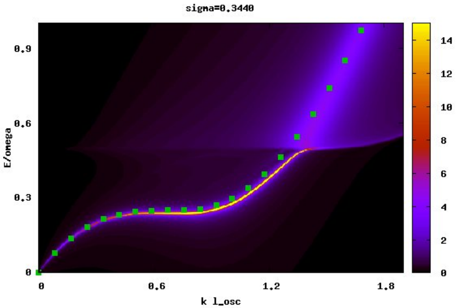
$\sigma = 0.3450$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

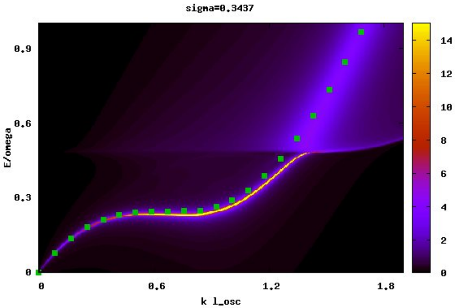
$\sigma = 0.3440$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

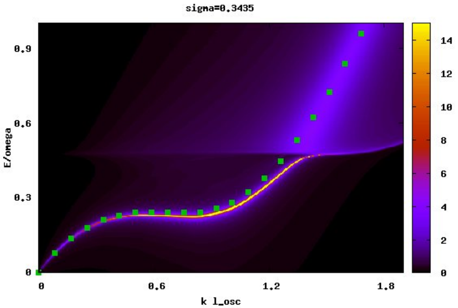
$\sigma = 0.3437$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

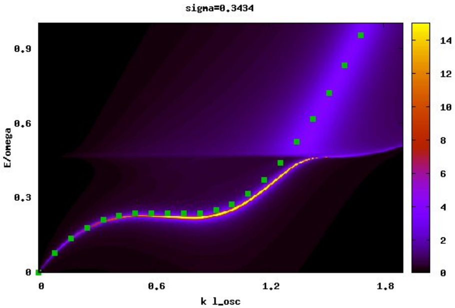
$\sigma = 0.3435$



Roton in dilute system: Er_2

evolution from Bogoliubov to phonon-roton:

$\sigma = 0.3434$



Outlook on unpolarized / partially polarized DBG

molecular DBG has inner degree of freedom: molecule rotation, $\hat{\mathbf{e}}_i$
even in ideal gas, rotation affects BEC (T_c decreases with B, increases with external field)

$\longrightarrow$ w/dipolar interaction: $$v_{dd}(\mathbf{r}_{12}) = d^2 \, \frac{\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{e}}_2 - 3(\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{r}})(\hat{\mathbf{e}}_2 \cdot \hat{\mathbf{r}})}{r_{12}^3}$$

Weak interactions

mean field estimate: linearized GP equation for excitations $\Psi_0(\mathbf{r}, \Omega)$

- coupling rotational degrees of freedom of molecules by dipole-dipole interaction in homogeneous system: splitting of $j = 1$ state by $\Delta \approx \frac{1}{3\epsilon_0} n d^2$

  $\Delta = O(10^{-3}\text{cm}^{-1})$ for $d = 5$Debye and $n = 10^{14}\text{cm}^{-3}$
- apply electric field $\Rightarrow$ finite polarization $\langle \mathbf{d} \rangle$:
  similar to fully polarized, if $\mathbf{d} = \langle \mathbf{d} \rangle$

Strong interactions

role of rotational zero point motion in self-assembled dipole lattice?

- many-body theory approach: HNC-EL w/rotations
- Monte Carlo approach: path integral ground state (PIGSMC) w/rotations

Summary

2D dipolar gas

- evolution towards phonon-roton spectrum with increasing density
- tilted w/resp to confinement plane – nematic quantum gas: long-range order in "hard" direction

quasi-2D dipolar gas

- quasi-2D (pancake): appearance of roton even with weak interactions
- stability of quasi-2D: probably only metastable
- dimerization? $\longrightarrow$ QMC

unpolarized/partially polarized dipolar gas

- splitting of rotational $J = 1$ line

Acknowledgements

collaborators:

2D DBG

Adrian Macia, Ferran Mazzanti, Gregory Astrakharchik, Jordi Boronat

quasi-2D DBG

Diana Hufnagl (HNC-EL), Rainer Kaltseis (mean field), Vesa Apaja (CBF-BW), Eckhard Krotscheck (HNC-EL); Dorte Blume (calculation of a)

unpolarized molecular BG

Brendan Abolins, K. Birgitta Whaley: PIGSMC

€€€:

Austrian Science Foundation FWF #21264

Acciones Integradas ES-19/2009

Path Integral Ground State — diffusion to ground state

Imaginary Time Propagation

exact ground state wave function $\Phi_0(R)$, $R \equiv (\mathbf{r}_1, \ldots, \mathbf{r}_N)$, can be obtained from trial wave function $\Psi_T(R)$ as

$$\Phi_0(R) \sim \lim_{\beta/2\to\infty} \langle Re^{-\frac{\beta}{2}H} \rangle \Psi_T = \lim_{\beta/2\to\infty} \int G(R, R', \beta/2)\Psi_T(R')dR'$$

with the imaginary-time propagator or Greens function

$$G(R, R', \beta/2) = \langle R| e^{-(\beta/2)H} |R'\rangle.$$

Split β into shorter imag. time steps, $\frac{\beta}{2} = M\tau$.

$$G(R, R', \beta/2) = \int G(R, R_1, \tau)G(R_1, R_2, \tau) \cdots G(R_{M-1}, R', \tau)\, dR_1 \cdots dR_{M-1}$$

good trial wave function $\Psi_T \Rightarrow$ short imaginary time β

Split imaginary time into steps ($\rightarrow$ "beads"):

$$\left\langle \hat{O} \right\rangle \propto \lim_{\beta\to\infty} \int dY\, P'(Y, \beta)\hat{O}(R_M, \tilde{R}_M) = \lim_{N_{mov}\to\infty} \frac{1}{N_{mov}} \sum_{i=1}^{N_{mov}} \hat{O}(R_M^i, \tilde{R}_M^i)$$

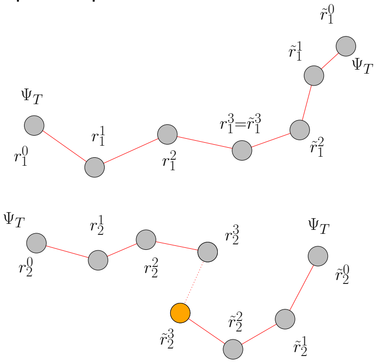
with

$$P'(Y, \beta) = \frac{1}{\text{Norm}} \Psi_T(R_0) \times \prod_{j=0}^{M-1} G(R_j, R_{j+1}, \tau) \times \prod_{j=0}^{M-1} G(\tilde{R}_j, \tilde{R}_{j+1}, \tau) \times \Psi_T(\tilde{R}_0)$$

(expectation value is not normalized correctly if $R_M \neq \tilde{R}_M$, such as for OBDM)

PIGSMC sketch – classical isomorphism

imaginary time paths for 2 particles and 7 time slices ("beads").
path of particle 2 is cut in the center.



- each bead has weight $e^{-\alpha\tau V}$
- red lines: kinetic energy $e^{-(\mathbf{r}_i^\tau - \mathbf{r}_i^{\tau+1})^2/4D\tau}$
- end beads: trial wave function Ψ_T
- center bead: true ground state Ψ_0, unbiased by Ψ_T
- cut path in middle for off-diagonal properties such as OBDM
  caution: normalization
- Metropolis random walk using bisection method

$G(R, R', \tau)\ldots$ **quasi-6th** order PIGSMC, error$[E_0]$=O(τ^6)
S. A. Chin and C. R. Chen, JCP'02
$G(R, R', \tau)\ldots$ **any** order PIGSMC, error$[E_0]$=O(τ^n)
REZ, Mayrhofer, S. A. Chin, JCP (2010)