Dipolar quantum gases

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Outline

Introduction

Dipolar quantum gases: 2D
- perpendicular polarization
- tilted polarization

Dipolar quantum gases: Slabs

Dipolar quantum gases: weakly/unpolarized dipoles

Introduction to dipolar QGs

experiments:

- permanent magnetic dipole moments of atoms (Cr):
  Pfau group (Lahaye et al, Nature **448**, 672 (2007))
- 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; JILA, NIST: Ni et al., Science **322**, 231 (2008),...)
- Diatomic molecules in optical lattices (Danzl et al., Nature Physics **6**, 265 (2010): Cs_2)

dipole-dipole interaction:

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

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

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

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

our interest:

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

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 group here (quasi-6th order,...) and by REZ and Chin on high order propagators ("any-order")

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

ground state: HNC-EL

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

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

- $u_1(\mathbf{r}_i)$ 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...

excitations: TDHNC-EL

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

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

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

- $\delta u_1(\mathbf{r}_i;t)$ 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

Perpendicular dipoles in 2D

→ recent work with Ferran, Gregory, and Jordi:
excitation spectrum by combining DMC with CBF-BW
(PRL **102**, 110405 (2009))

increase density:

- roton energy not going to 0 in vicinity of solidification
- phonon-roton splits off from Bogoliubov mode

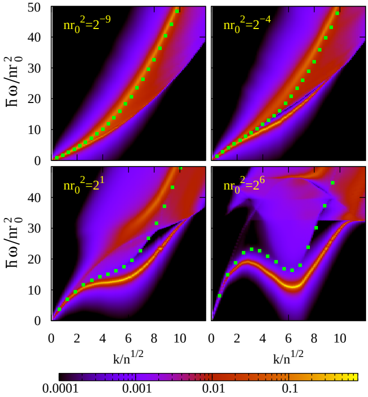
Bogoliubov-deGennes (linearzed GP)

Bijl-Feynman approximation $\frac{\hbar^2 k^2}{2mS(k)}$

CBF-BW approximation

w/triplets δu_3

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

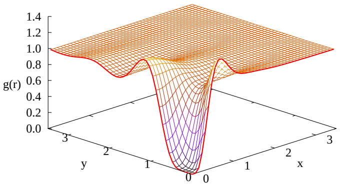


Tilted dipoles in 2D with HNC/0-EL

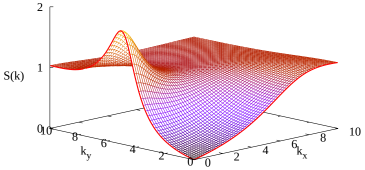
anisotropy is not probed in 2D with perpendicular polarization axis
$\longrightarrow$ tilt polarization axis to form homogeneous *anisotropic* 2D quantum gas (i.e. nematic quantum gas)
HNC/0-EL ground state calculation (no elementaries, no triplets):

- test system to study well-defined instability (at angle $\alpha_{cr} = 35.26°$?)
- 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: <u>an</u>isotropic speed of sound

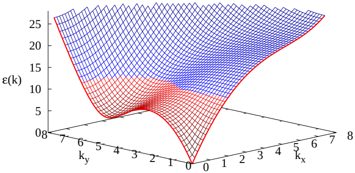
$g(\mathbf{r})$



$S(\mathbf{k})$



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

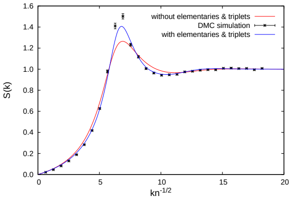


all plots for $\rho = 64$, $\alpha = \alpha_{cr}$

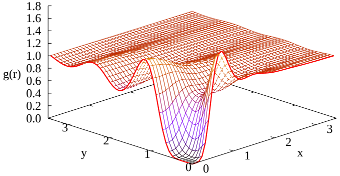
Tilted dipoles in 2D with HNC/0-EL

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

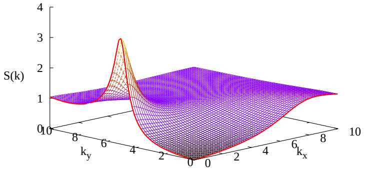
HNC-EL/0 not reliable anymore: $\rho = 128$



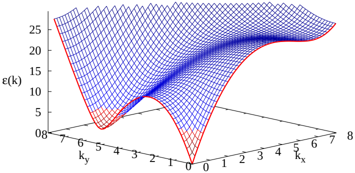
$g(\mathbf{r})$



$S(\mathbf{k})$



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



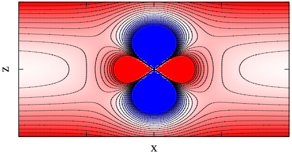
roton energy $\to 0$? $\longrightarrow$ QMC + CBF-BW (or better)!

quasi-2D: Slabs of dipolar quantum gases

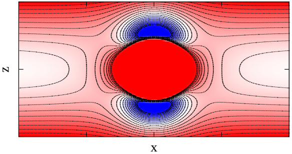
relax infinitely strong confinement in z-direction
$\Rightarrow$ system unstable via tunneling towards head-to-tail configurations
$\Rightarrow$ stabilize with repulsive interaction

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

$\sigma = 0$:



$\sigma \neq 0$:



studied in mean field approximation (GP + linearized GP) by Santos et al., PRL **90** 250403 (2003): rotonization, followed by instability

completely different roton than roton in dense, strongly interacting systems like LHe!

Roton in dilute system

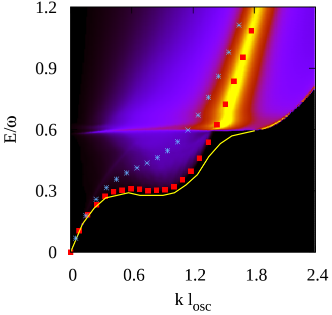
Bijl-Feynman approximation

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

beyond Bijl-Feynman approximation

- dynamic structure function $S(k, E)$ with CBF-BW approximation of TDHNC-EL (no triplet correlations; convolution approximation)
- roton energy almost unchanged
- strong damping at $2 \times E_{roton}$

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

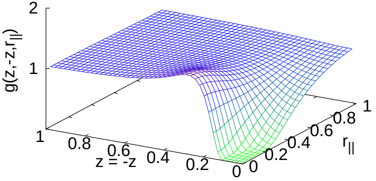


system (meta)stable up to $E_{roton} = 0$, but HNC-EL collapses to lower-energy phase before that happens...

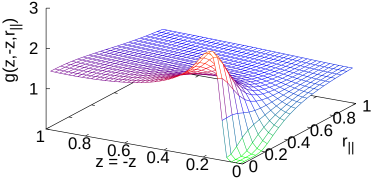
Pair distribution function: dimerization?

pair distribution function $g(z, z', r_{\parallel})$... probability to find particle at (x, y, z) and (another) particle at (x', y', z') ($r_{\parallel} = \sqrt{(x - x')^2 + (y - y')^2}$), divided by $\rho(z_i)$

$\sigma = 0.4$:



$\sigma = 0.3$:



- $z' = -z$
- correlation hole at $(0, 0, 0)$ due to repulsion $(\sigma/r)^{12}$
- strong peak at $\mathbf{r}_{\parallel} = 0$ – expected for dimer (2 bound dipoles)
- dimerization? $\longrightarrow$ check other side of phase transition with QMC
- E_{roton} small: system stable or just metastable $\longrightarrow$ energetics with QMC

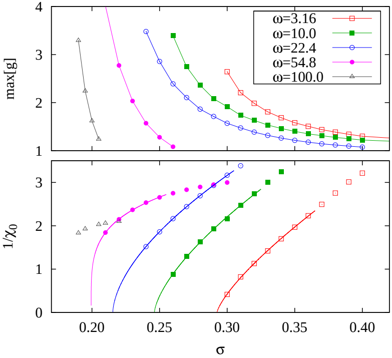
(D. Hufnagl, E. Krotscheck, REZ, JLTP **158**, 85 (2010))

Stability analysis: static response function

tracking E_{roton} not practical in HNC-EL...

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

- $\longrightarrow$ 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 $a(\sigma-\sigma_0)^b$)

Outlook on unpolarized / partially polarized DBG

molecular DBG has inner degree of freedom: molecule rotation, $\hat{\mathbf{e}}_i$

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

Weak interactions

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

  coupling rotational degrees of freedom of molecules by dipole-dipole interaction: 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 $n = 10^{14}\text{cm}^{-3}$

Strong interactions

- HNC-EL w/rotations
- PIGSMC w/rotations

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unpolarized molecular BG
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