Low-dimensional dipolar gases

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One dimensional bosonic dipolar gas

First quantization Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \mathcal{C} \sum_{i<j} \frac{\vec{d}_i \cdot \vec{d}_j - 3 d_i^x d_j^x}{|x_i - x_j|^3},$$

$\vec{d}_i$: vector dipole moment (electric or magnetic).

Fully polarized case $\Rightarrow \vec{d}_i = d\hat{e}_z$

$\Rightarrow$ Repulsive interactions

$$r_0 = \frac{2\mathcal{C} d^2}{\hbar^2}$$

Repulsive bosons in one dimension

- phonons with linear spectrum
- Stringari-Pitaevskii $\Rightarrow$ neither superfluid nor crystal
- Quasi long range order $\rightarrow$ fluctuating "supersolid"

Captured by the Luttinger liquid concept

Luttinger liquid theory I

Luther-Peschel (1975); Haldane (1980).

Effective Hamiltonian

$$H = \hbar \int \frac{dx}{2\pi} \left[uK(\pi\Pi)^2 + \frac{u}{K}(\partial_x \phi)^2 \right]$$

$$[\phi(x), \Pi(x')] = i\delta(x - x')$$

$\theta = \pi \int^x dx' \Pi(x') =$ Superfluid phase

$\partial_x \phi =$ density (dual variable)

Linearized quantum hydrodynamics

Luttinger Liquid Theory II

Representation of operators

$$\psi_B(x) = e^{i\theta}\left[\sum_{m=0} B_m \cos(2m\phi - 2m\pi\rho_0 x)\right]$$

$$\rho_B(x) = \rho_0 - \frac{\partial_x \phi}{\pi} + \sum_{m=1}^{\infty} A_m \cos(2m\phi(x) - 2m\pi\rho_0 x)$$

Luttinger Liquid Theory III

Correlation functions

$$\langle e^{in\theta(x)} e^{-in\theta(x')} \rangle = \left(\frac{\alpha}{|x-x'|}\right)^{\frac{n^2}{2K}}$$

$$\langle e^{i2m\phi(x)} e^{-i2m\phi(x')} \rangle = \left(\frac{\alpha}{|x-x'|}\right)^{2m^2 K}$$

- $K \searrow$ as repulsion $\nearrow$.
- $K = \infty \rightarrow$ Free Bose gas
- $K = 1 \rightarrow$ Free Fermi / Tonks-Girardeau gas.

Finding the parameters u, K

Galilean invariance

$$uK = \frac{\hbar \pi \rho_0}{m},$$

Compressibility

$$\frac{\hbar \pi u}{K} = \frac{\partial^2 e}{\partial \rho_0^2}$$

Low density dipolar Bose gas

Two-body problem in the center of mass frame:

$$\frac{\hbar^2}{m}\left(-\frac{d^2}{dx^2}+\frac{r_0}{2x^3}\right)\psi = E\psi$$

WKB approximation

$$\psi(x) = \exp[-C(r_0/|x|)^{1/2}]$$

$\rightarrow$ Wavefunction vanishes $\Leftrightarrow$ Tonks Girardeau limit (K=1)
$e(\rho_0) \sim \rho_0^3$

Dipolar gas at high density

classical limit

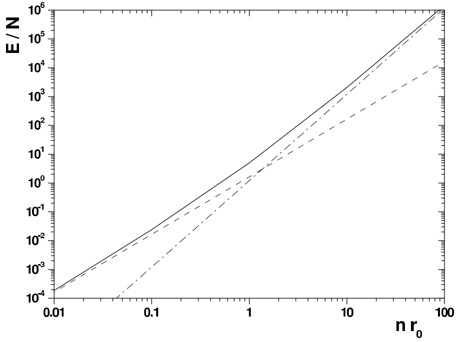
Potential energy dominates → Crystal with lattice spacing $1/\rho_0 = a$.
Potential energy per unit length $= \frac{d^2}{4\pi\epsilon_0}\zeta(3)\rho_0^4$ (dominates kinetic energy $\propto \rho_0^3$).

This crystal is melt by the quantum fluctuations.

$$K \sim \frac{1}{\sqrt{6\zeta(3) r_0 \rho_0}}$$

⇒ Crossover from Tonks-Girardeau at low density to quasi-solid ("super-Tonks") at high density.

Energy vs Density by DMC calculation



From A.S.Arkhipov, G.E.Astrakharchik, A.V.Belikov and Yu. E. Lozovik JETP Lett. **82**, 39 (2005).

Ground State Energy from Monte Carlo Methods

$$E_{VMC} = \frac{\langle \Phi_{Trial} | H | \Phi_{Trial} \rangle}{\langle \Phi_{Trial} | \Phi_{Trial} \rangle} = \frac{1}{M} \sum_{i=1}^{M} E_L(\{R_i\})$$

$E_L(\{R\}) = \frac{H\Phi_{Trial}(R)}{\Phi_{Trial}(R)}$ is the local energy

R_i configuration is sampled from $|\Phi_{Trial}|^2$

Project out the ground state wave-function

$$\Psi(R_1, R_2 \dots R_N; \beta) = e^{-\beta H} \Phi_{Trial}(R_1, R_2 \dots R_N)$$

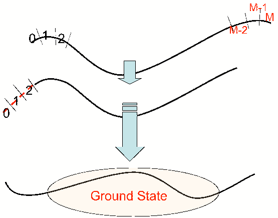
$$E = \lim_{\beta \to \infty} \frac{\langle \Phi_{Trial} | H | \Psi \rangle}{\langle \Phi_{Trial} | \Psi \rangle} = \lim_{\beta \to \infty} \frac{\int dR P(\{R\}; \beta) E_L}{\int dR P(\{R\}; \beta)}$$

$P(\{R\}) = \Phi_{Trial} \Psi(R_1, R_2 \dots R_N; \beta)$ is the *mixed* probability distribution to be sampled

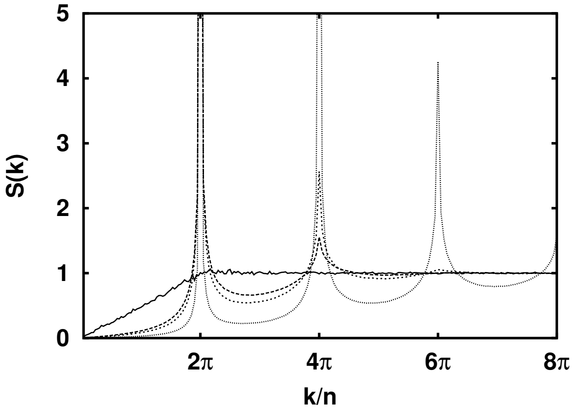
Reptation Quantum Monte Carlo (RQMC)

$$P(R_1, R_2 \ldots R_M) = \Phi_{Trial}(R_0)\Pi_{i=1}^{M-1} G(R_i, R_{i+1}; \epsilon)\Phi_{Trial}(R_M)$$

- use Trotter decomposition $\Rightarrow \beta = \epsilon M$, $\epsilon \rightarrow 0$
- choose a suitable Green function $G(R_i, R_{i+1}; \epsilon)$
- use Metropolis : reptation algorithm



RQMC simulation: static structure factor



From R. Citro, EO, S. De Palo and M. L. Chiofalo Phys. Rev. A **75**, 051602(R) (2007).

Structure factor

$$S(q) = \int_0^L dx e^{iqx} \left[\langle \rho(x)\rho(0)\rangle - \langle \rho_0^2 \rangle\right]$$

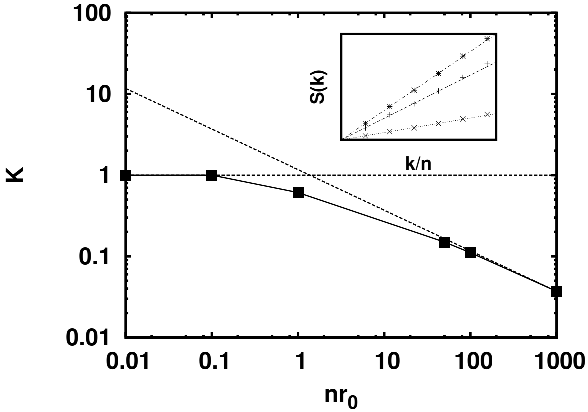
$$S(q) = \frac{K|q|}{2\pi} (q \ll \pi\rho_0)$$

$$S(q) \sim L^{1-2m^2K} \frac{\Gamma(1-2m^2K)\Gamma(m^2K + kL/(2\pi))}{\Gamma(1-m^2K+kL/(2\pi))} \sin(\pi m^2 K)$$

$q = k + 2m\pi\rho_0, 2m^2K < 1.$

$\Rightarrow$ Development of quasi-Bragg peaks as $K \to 0$.

RQMC simulations: Luttinger exponent



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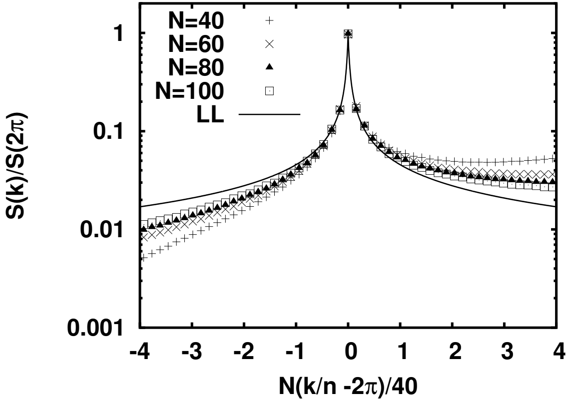
RQMC simulation vs. Luttinger liquid



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Experimental systems ?

- magnetic dipoles: ^{52}Cr atoms ($6\mu_B$) Stuhler et al. Phys. Rev. Lett. **95**, 150406 (2005).
- electric dipoles: polar molecules (SrO) Büchler et al. Phys. Rev. Lett., **98**, 060404 (2007).

Condition for one dimensional regime: $\rho_0 \ell_\perp \ll 1$ where $\ell_\perp = (r_0/(4a_\perp))^{1/5} a_\perp$.

- Magnetic dipoles (Chromium) $\ell_\perp = 31$ nm, $r_0 = 4.8$ nm $\Rightarrow \rho_0 r_0 \lesssim 0.1$
- Electric dipoles (SrO) $\ell_\perp = 0.2\ \mu$m, $r_0 = 240\ \mu$m $\Rightarrow \rho_0 r_0 \lesssim 10^3$

Longitudinal trapping

LDA + Luttinger liquid approach

$$e[\rho(x)] + \frac{1}{2} m\omega_0^2 x^2 = \frac{1}{2} m\omega_0^2 R^2$$

$$H = \int dx \left[u(x)K(x)(\pi\Pi)^2 + \frac{u(x)}{K(x)}(\partial_x\phi)^2 \right]$$

$$u(x)K(x) = \frac{\pi\rho(x)}{m}; \frac{u(x)}{K(x)} = \frac{1}{\pi}\frac{\partial^2 e}{\partial\rho^2}(\rho(x))$$

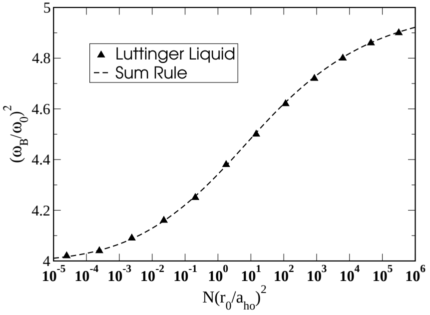
Boundary conditions: $j(\pm R) = 0 \Rightarrow \phi(\pm R) = 0.$

Modes of the trapped dipolar gas

$$u(x)K(x)\partial_x\left(\frac{u(x)}{K(x)}\partial_x\phi_n\right) = -\omega_n^2\phi_n$$

When $e(\rho) \propto \rho^{\gamma+1}$ exact solution
Petrov, Gangardt Shlyapnikov J. Phys. IV **116** p. (2004)
$\omega_n^2 = \omega_0^2(n+1)(1+n\gamma/2)$
$n=1$: Breathing mode $\omega_B = \omega_0(2+\gamma)^{1/2}$
Low density $\gamma = 3 \Rightarrow \omega_B = 2\omega_0$
High density $\gamma = 4 \Rightarrow \omega_B = \sqrt{5}\omega_B$

Evolution of the breathing mode



R. Citro, S. De Palo, E. Orignac, P. Pedri, M.-L. Chiofalo New J. Phys. **10**, 045011 (2008).

Dynamical structure factor

Feynman approximation:

$$\omega(q) \geq \frac{q^2}{2mS(q)} = \omega_{SMA}(q)$$

peaks in the static structure factor suggest
$\omega_{SMA}(q = 2\pi n\rho_0) \to 0$
Is there a roton mode ?

Dynamical structure factor

In Matsubara time,

$$\rho(q,\tau) = e^{\tau H}\rho(q)e^{-\tau H}$$
$$F(q,\tau) = \langle T_\tau \rho(q,\tau)\rho(-q,0)\rangle$$
$$F(q,\tau\to\infty) \sim e^{-\tau\omega(q)}$$

Existence of a roton mode can be established by studying the exponential decay of $F(q,\tau)$.

From bosonization

$$F(q = \frac{2\pi n}{L}, \tau) = L 2^{2K+1-n} \frac{e^{-\frac{2\pi u}{L}(K+n)\tau}}{\left(1 + e^{-\frac{2\pi u \tau}{L}}\right)^{K+n}} \frac{\Gamma(n+K)}{\Gamma(K)\Gamma(n+1)} \times {}_2F_1\left(K+n, K; n+1; e^{-\frac{2\pi u \tau}{L}}\right)$$

$$\omega(q) = \frac{2\pi u K}{L} + u|q|$$

$\Rightarrow$ apparent roton mode, but disappears as $L \to \infty$.

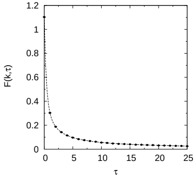
Imaginary-time correlation functions by RQMC

Observables can be easily evaluated on ground state distribution in the middle of the path.

Density fluctation operator $\rho_k = \sum_i e^{-ikr_i}$

$$F(k,\tau) = \langle \rho_k(\tau)\rho^*_{-k}(0)\rangle / N$$

$$S(k) = F(k,0) = \int_0^\infty S(k,\omega)\frac{d\omega}{2\pi}$$



Dynamical structure factor from RQMC

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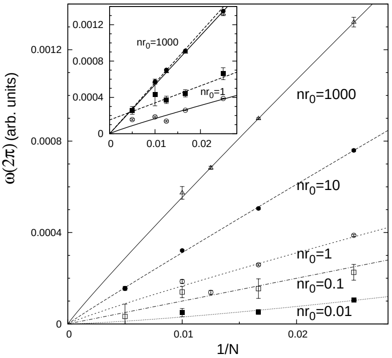

S. De Palo, E. Orignac, R. Citro, M. L. Chiofalo arXiv:0801.1200

Conclusions

- Luttinger liquid description of the dipolar bose gas
- Accounts for static and dynamic correlations
- no long-range order, tendency to crystallization at large density
- absence of a roton mode
- prediction of increase of breathing mode frequency with density

Open problems

- Effect of the cutoff on interaction provided by transverse trapping.
- Effect of population of higher transverse modes.
- Case where the dipolar gas is not fully polarized (spin-charge separation).

References

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- P. Pedri, S. De Palo, EO, R. Citro, M. L. Chiofalo Phys. Rev. A **77**, 015601 (2008).
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- S. De Palo, EO, R. Citro, M.L. Chiofalo arXiv:0801.1200