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Quantum Polar Liquids

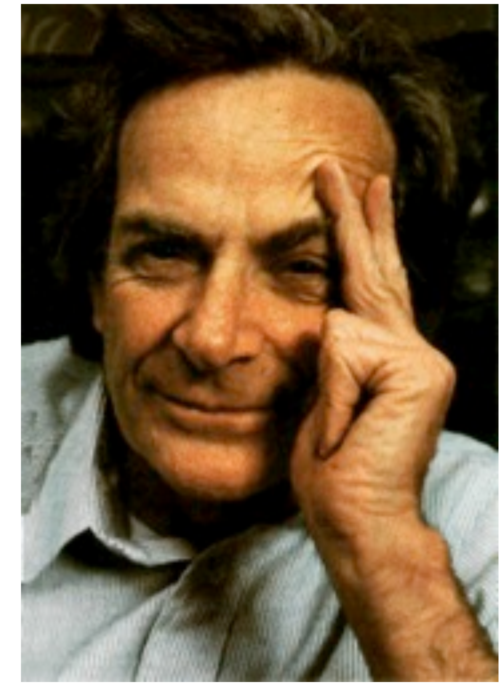
Saeed Abedinpour Harzand

Institute for Advanced Studies in Basic Sciences
Gava Zang, Zanjan, Iran

Collaborators:
Reza Asgari (Tehran), Marco Polini (Pisa) and Bilal Tanatar (Ankara)

Simulating physics with computers (1981):

Simulate a (quantum) system using another more controllable one



April 2012

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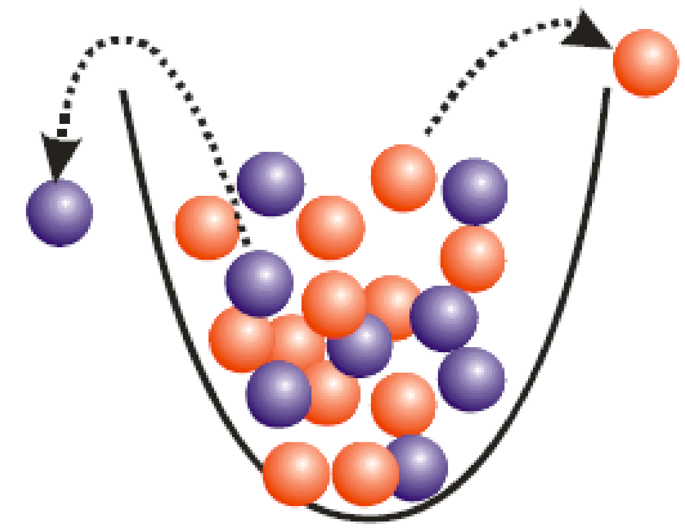
Outline

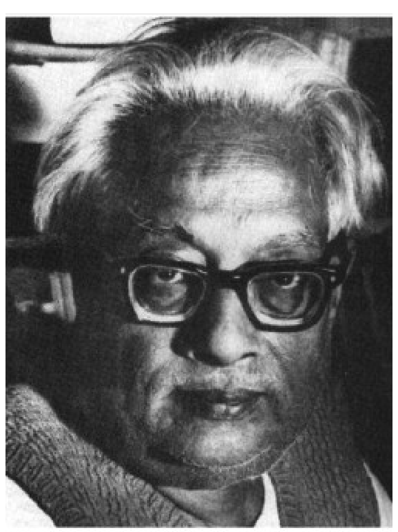
- Why ultra-cold gases?
- Why polar molecules?
- How to deal with *homogenous* many-body systems?
- Results for 2D polar liquids
- Summary and future directions

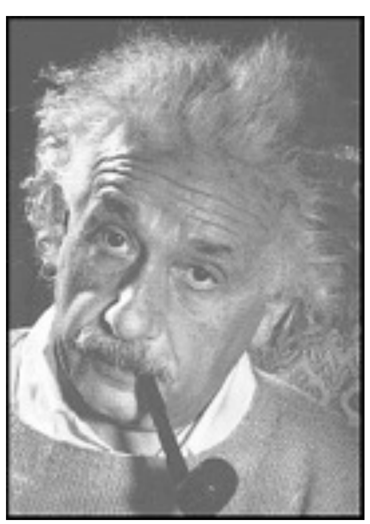
Why ultra-cold gases?

Bose-Einstein Condensation (BEC) in bosonic systems

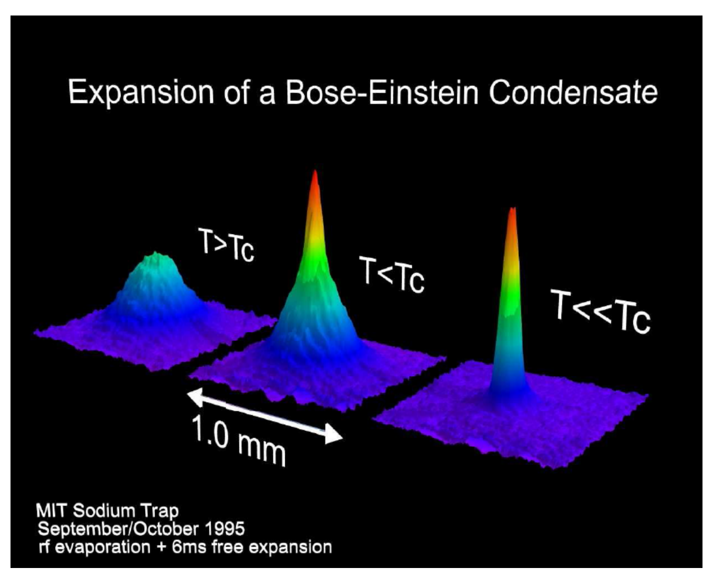


predicted: 1925



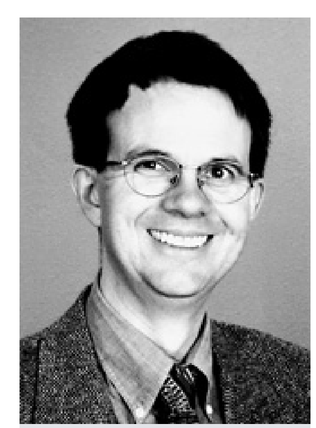


observed: 1995

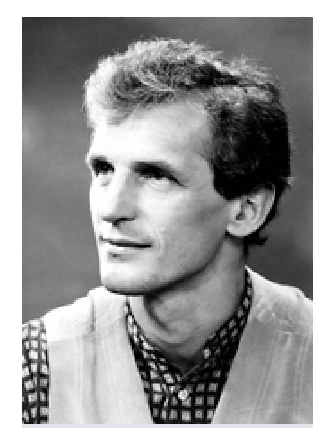


The Nobel Prize in Physics 2001

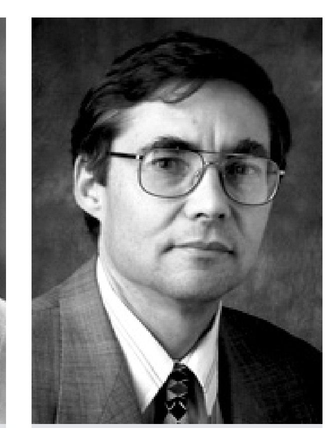
"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"



Eric A. Cornell



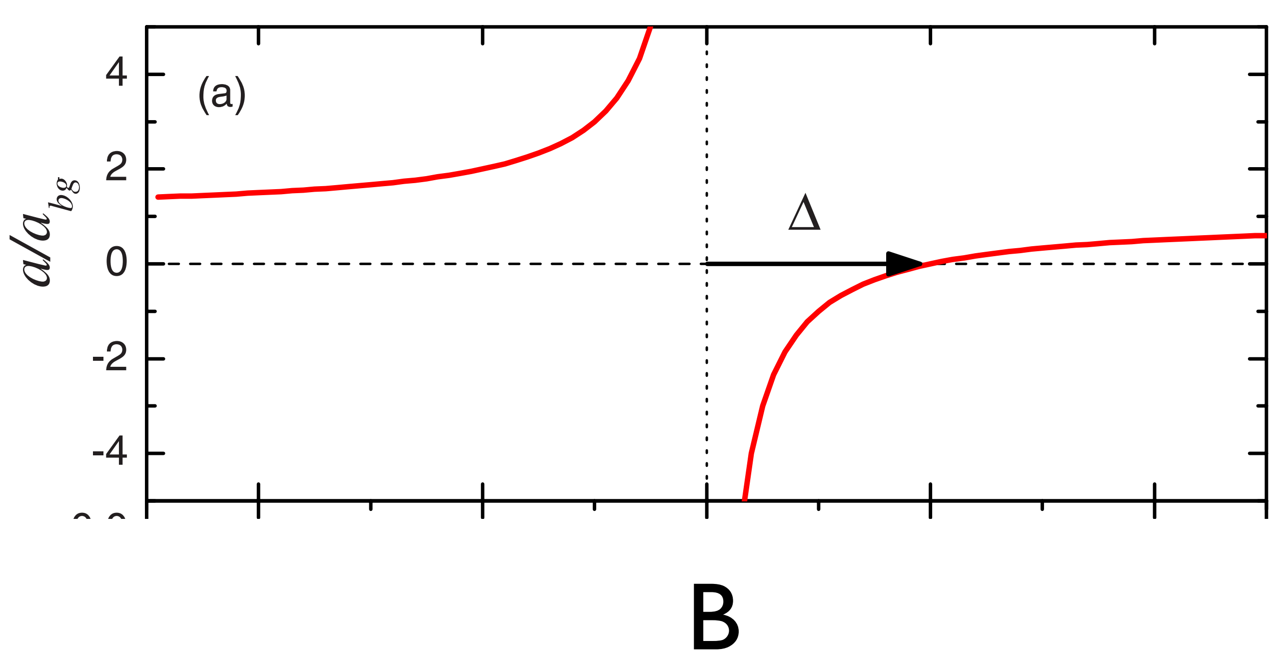
Wolfgang Ketterle

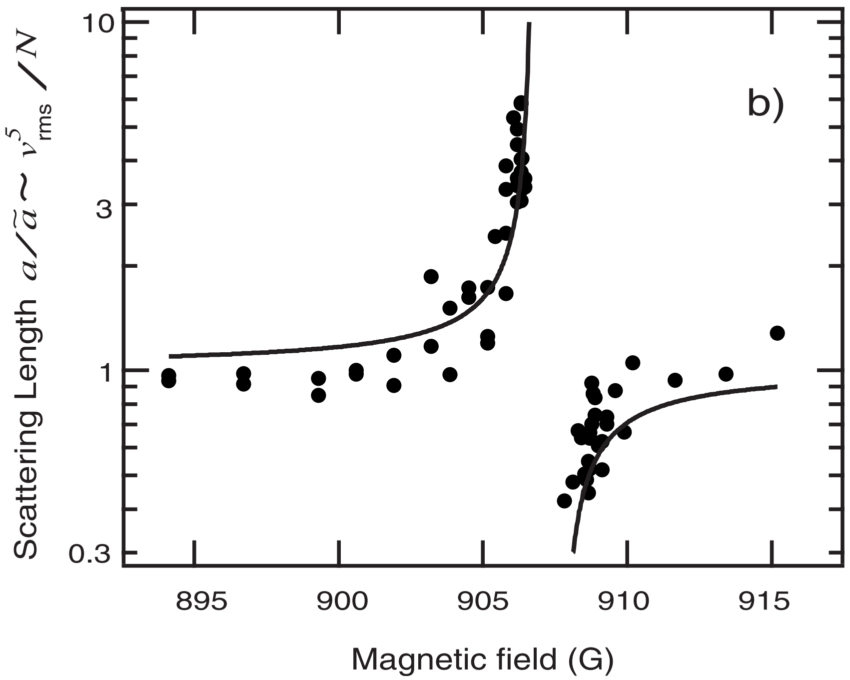


Carl E. Wieman

In atomic gases interactions are *"short-range"* and totally *"tunable"*

Feshbach resonance: $a(B) = a_{\rm bg}(1 - \frac{\Delta_B}{B - B_{res}})$



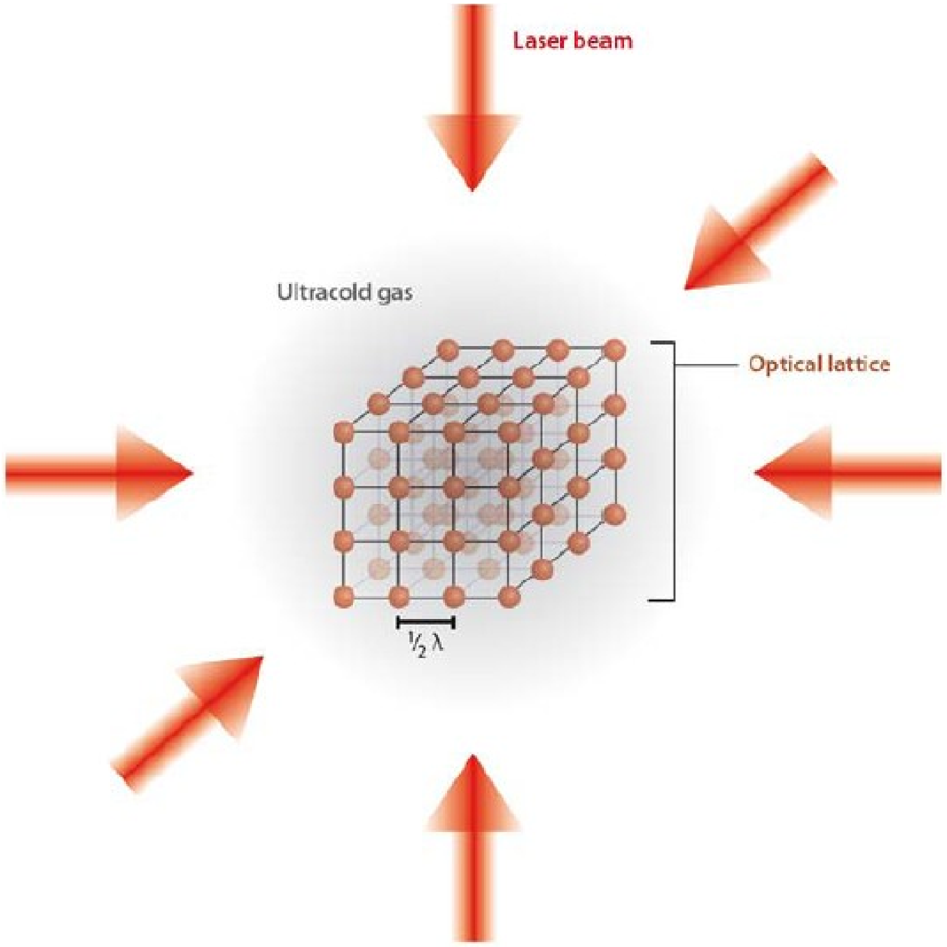


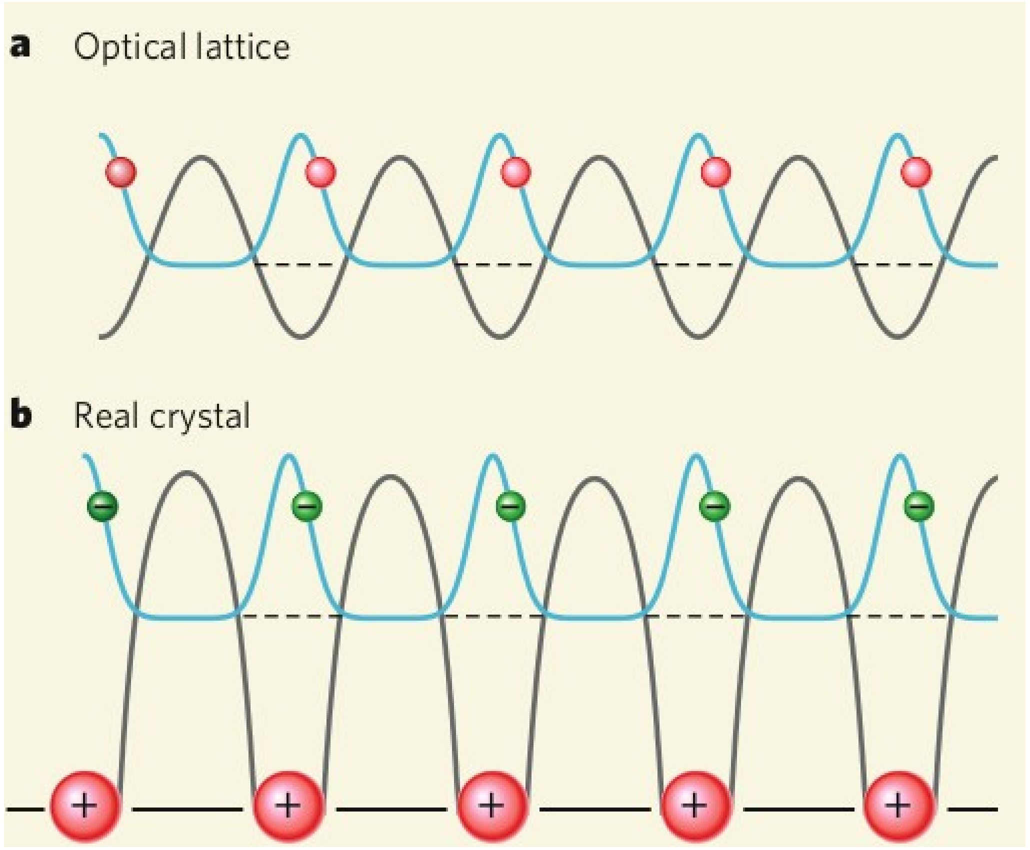
Reviews of Modern Physics **82**, 1225 (2010)

- non-interacting particles at $B = B_{\rm res} + \Delta_{\rm B}$
- BCS of weakly attractive fermions
- BEC of strongly attractive fermions
- Universal regime at $B_{\rm res}$

Optical lattices:

Artificial crystals with different geometries and dimensionalities





Nature **453**, 736 (2008)

Short-range (on-site) interactions: Hubbard model

Synthetic gauge fields in cold atoms

Many interesting phenomena in condensed matter physics occur when electrons are placed in an electric or magnetic field, or possess strong spin-orbit coupling. But neutral atoms, neither possess gauge coupling to electromagnetic fields nor have spin-orbit coupling.

Spielman's group (NIST):

- Uniform gauge field: *Phys. Rev. Lett. 102, 130401 (2009)*
- Magnetic field: *Nature 462, 628 (2009)*
- Electric field: *Nature Physics, 7, 531, (2011)*
- Spin-orbit coupling: *Nature, 471, 83 (2011)*

Bosons with spin-orbit couplings!

Topological cold-atomic insulators!

For a short review see: Hui Zhai, Int. J. Mod. Phys. B (2012)

Why polar molecules?

Even a short-range contact interaction between atoms leads to a very rich physics. A long-range richer interaction would be very interesting to investigate.

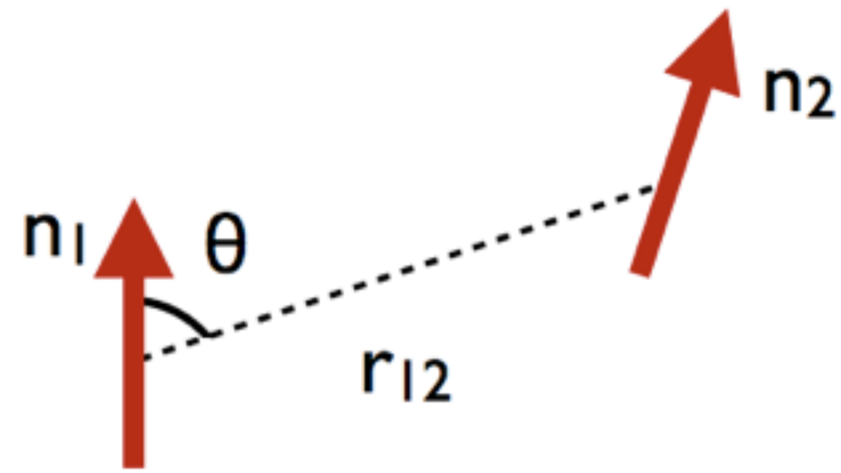
Dipole-dipole interaction between particles with permanent electric or magnetic dipole moments leads to a novel degenerate quantum gas already in the weak coupling.

Experimental realization:

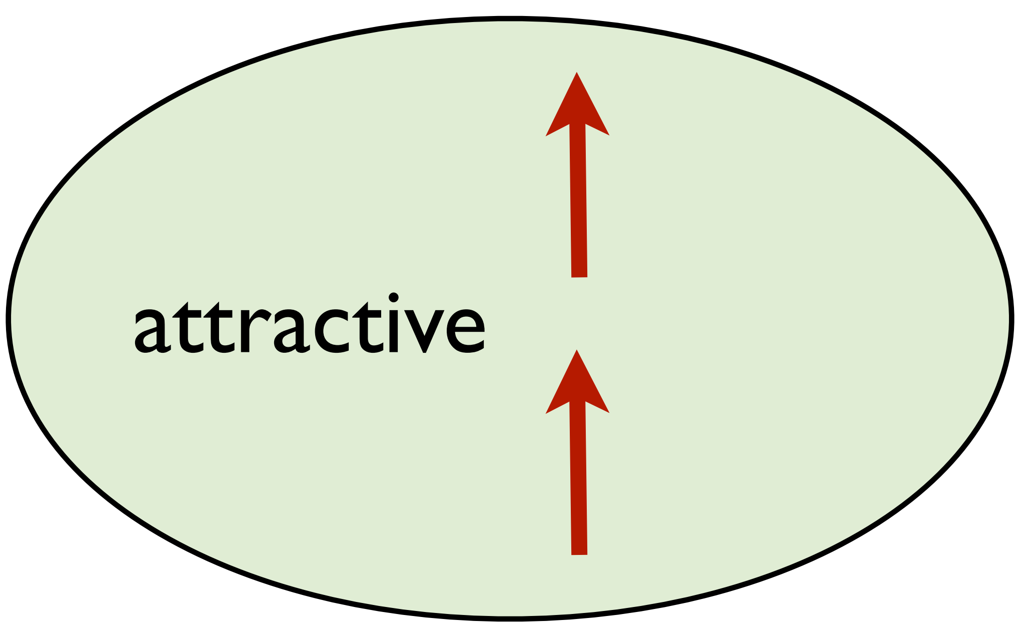
Polar molecules: Rb; K, LiCs
Magnetic dipoles: ^{52}Cr

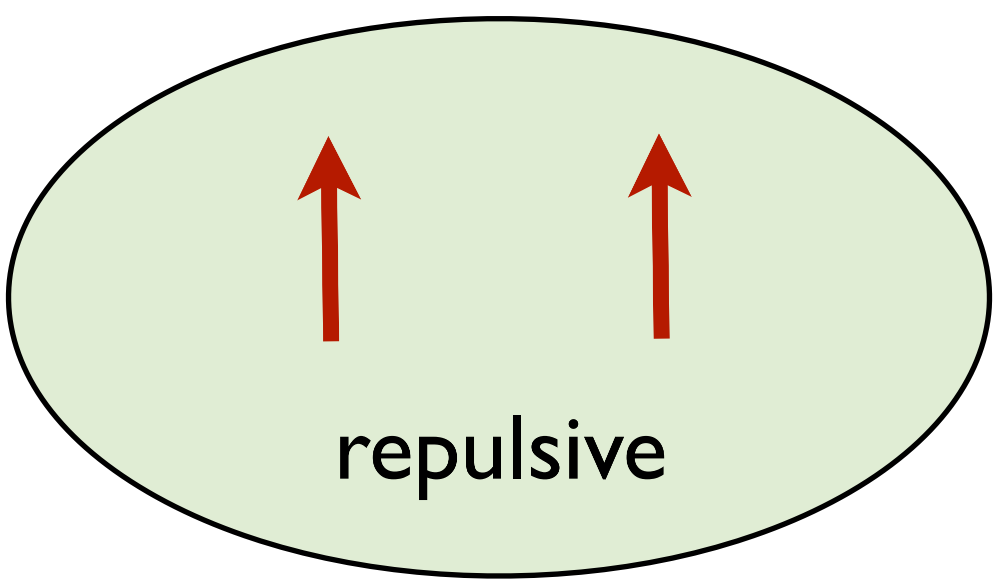
Why polar molecules? (cont.)

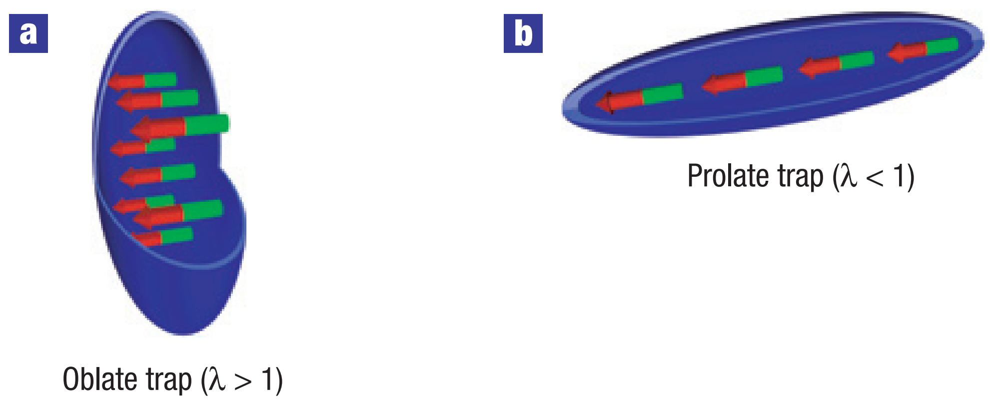
$$v_{\rm dd}(\mathbf{r}_{12}) = \frac{C_{\rm dd}}{4\pi}\,\frac{(\mathbf{n}_1\cdot\mathbf{n}_2)r_{12}^2 - 3(\mathbf{n}_1\cdot\mathbf{r}_{12})(\mathbf{n}_2\cdot\mathbf{r}_{12})}{r_{12}^5}$$

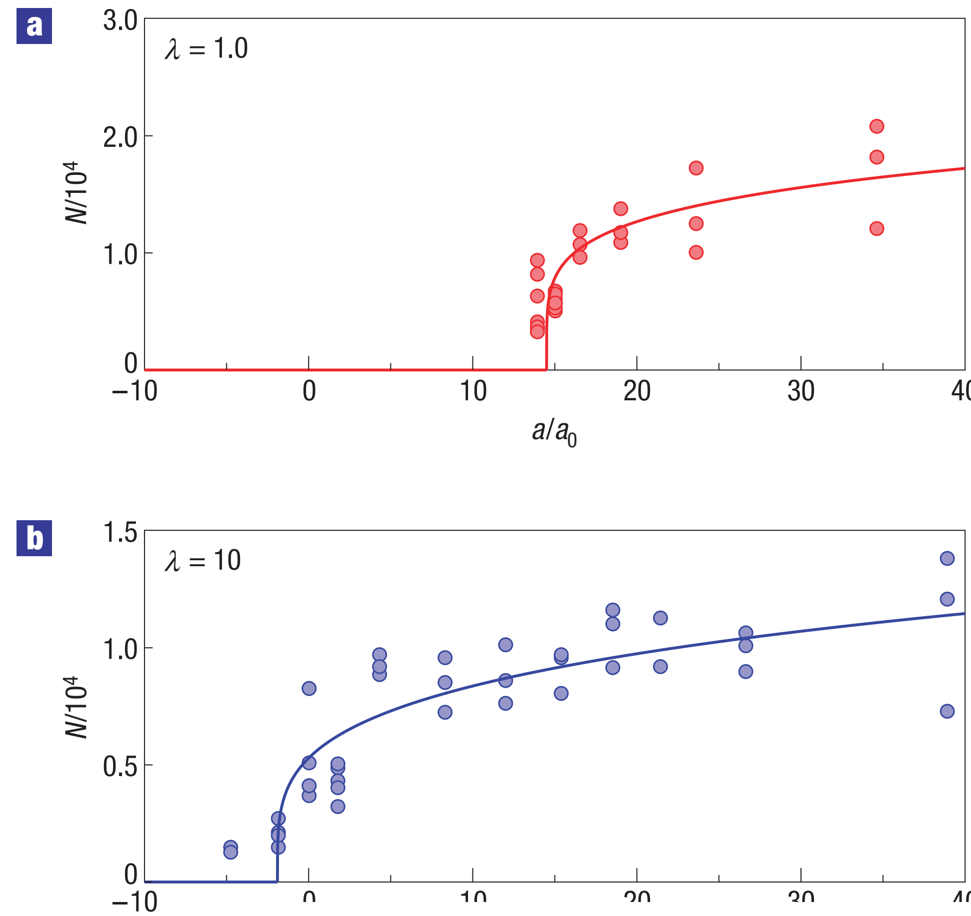


Long-range & anisotropic



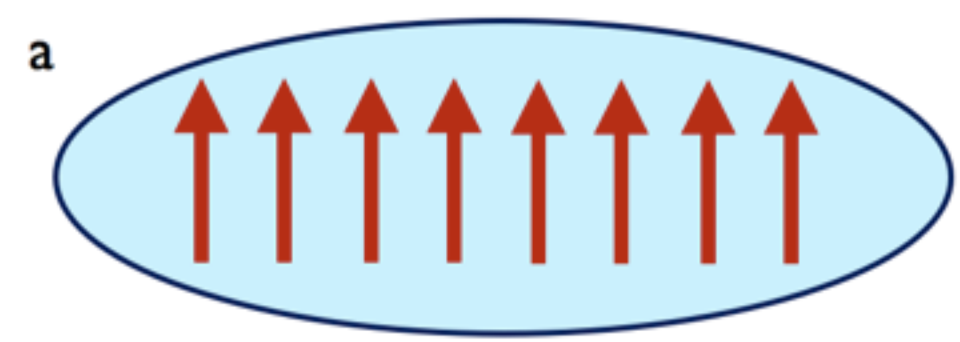






T. Koch *et al.*, Nature Physics (2008)

$$v_{\mathrm{dd}}(\mathbf{r}_{12}) = \frac{C_{\mathrm{dd}}}{4\pi}\,\frac{1}{r_{12}^3}$$



Isotropic but still long-range

Now we have to deal with too many *interacting* particles

$$\left[\sum_{i=1}^{N}\frac{p_i^2}{2m}+\sum_{i<j}^{N}V(r_{ij})\right]\Psi\left(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N\right)=E\ \Psi\left(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N\right)$$

$\Psi\left(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N\right)$:e.g. HF, RPA, QMC, BA

The *homogenous* limit is especially interesting as it can provide input for e.g. DFT calculations of *inhomogenous* systems

Cheat list:

Density:

$$\rho(\mathbf{r}) = \int \mathrm{d}\mathbf{r}_2 ... \mathrm{d}\mathbf{r}_N \;\; \Psi^* \left(\mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N\right) \Psi \left(\mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N\right)$$

One-body density-matrix:

$$\rho(\mathbf{r}, \mathbf{r}') = \int \mathrm{d}\mathbf{r}_2 ... \mathrm{d}\mathbf{r}_N \;\; \Psi^* \left(\mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N\right) \Psi \left(\mathbf{r}', \mathbf{r}_2, ..., \mathbf{r}_N\right)$$

$$\rho(\mathbf{r}, \mathbf{r}) = \rho(\mathbf{r})$$

Pair- distribution function:

$$g(r - r') = \frac{(N-1)}{\rho^2} \int \mathrm{d}\mathbf{r}_3 ... \mathrm{d}\mathbf{r}_N \;\; \Psi^* \left(\mathbf{r}, \mathbf{r}', \mathbf{r}_3, ..., \mathbf{r}_N\right) \Psi \left(\mathbf{r}, \mathbf{r}', \mathbf{r}_3, ..., \mathbf{r}_N\right)$$

Static structure factor:

$$S(q) - 1 = \mathrm{FT}[g(r) - 1]$$

HNC (Bosons)

Self-consistent solution

$$\left[-\frac{\hbar^2}{m}\nabla^2 + V_{\rm eff}(r)\right]\sqrt{g(r)} = 0$$

Formally exact and describes a zero-energy two-body scattering problem in the many-body fluid

$$V_{\rm eff}(r) = v(r) + W_{\rm B}(r)$$

$$W_{\rm B}(k) = W_{\rm B}^0(k) + \alpha(\gamma) W_{\rm B}^3(k)$$

Scaling parameter

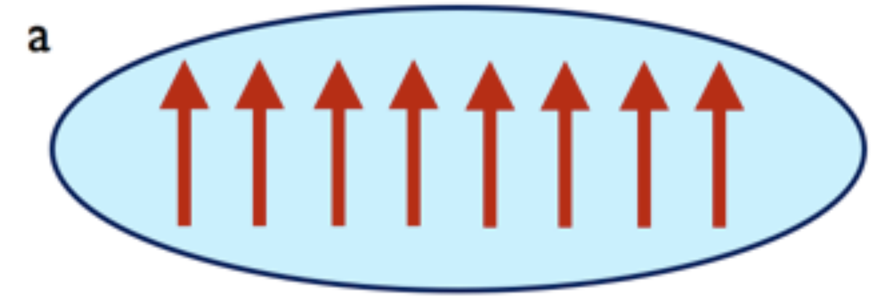
Triplet correlations

FHNC (Fermions)

$$V_{\rm eff}(r) = v(r) + W_{\rm B}(r) + W_{\rm F}(r)$$

Numerical Results: 2D polar Bose liquid

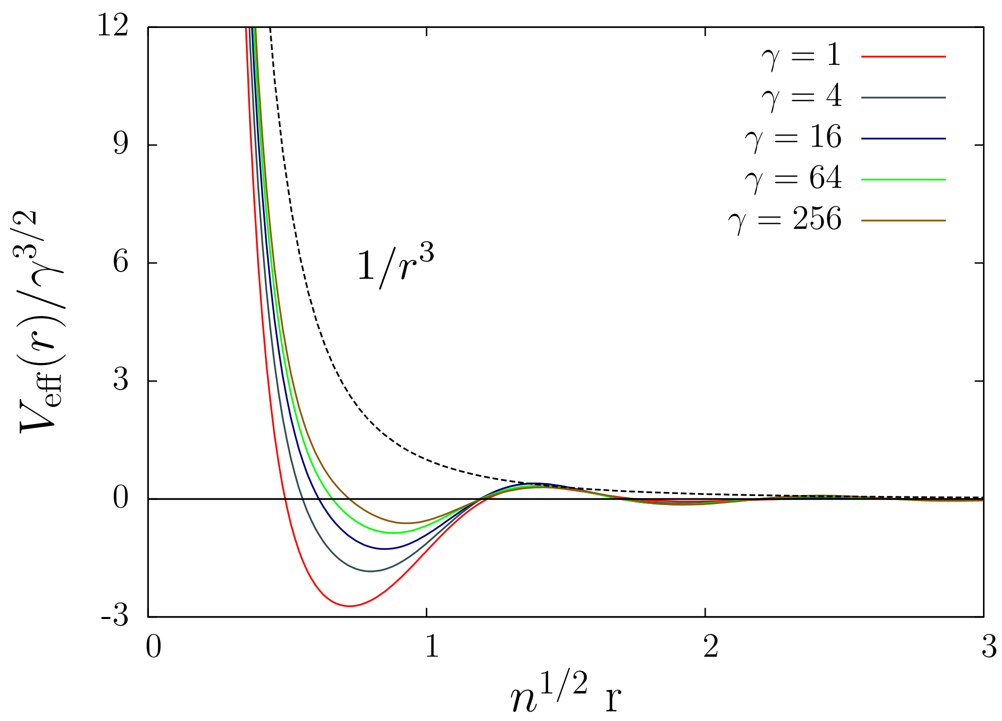
$$\left[-\frac{\hbar^2}{m}\nabla^2 + V_{\rm eff}(r)\right]\sqrt{g(r)} = 0$$



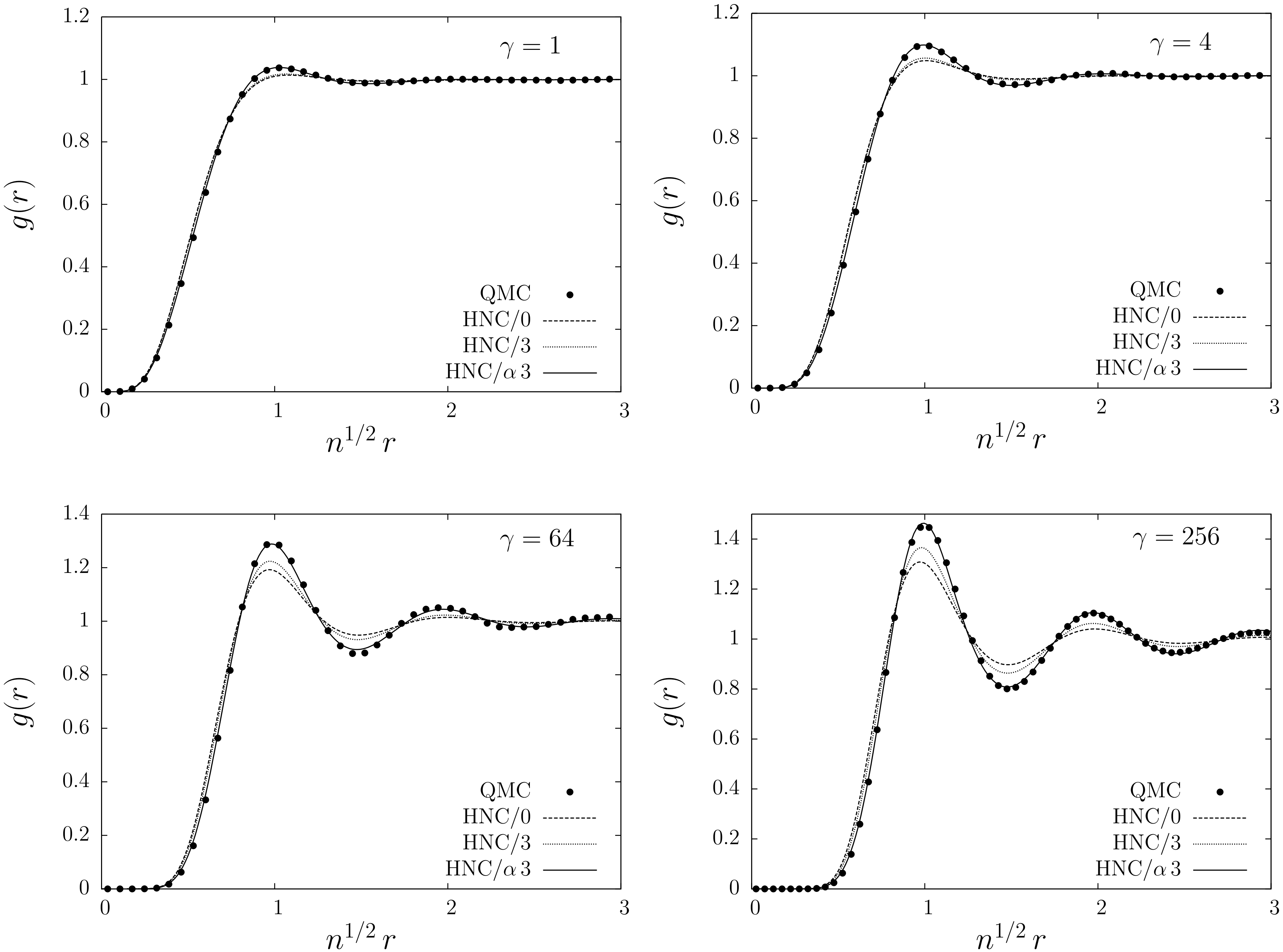
$$V_{\rm eff}(r) = \frac{C_{\rm dd}}{4\pi}\frac{1}{r^3} + W_{\rm B}(r)$$

$$\gamma = n r_0^2$$

$$r_0 = \frac{mC_{\rm dd}}{4\pi\hbar^2}$$



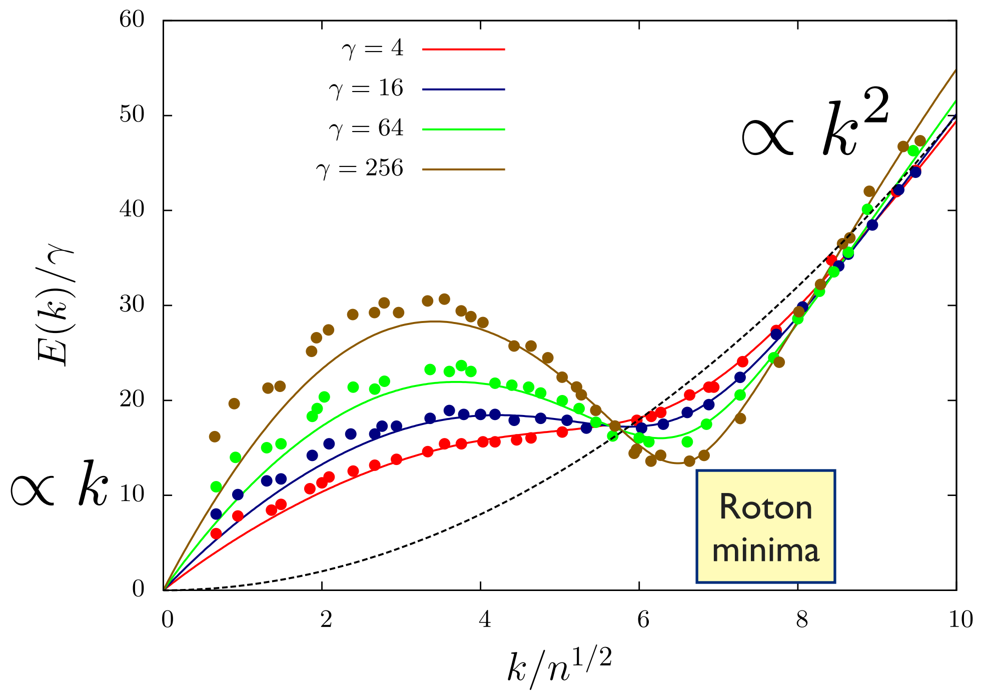
Pair distribution function



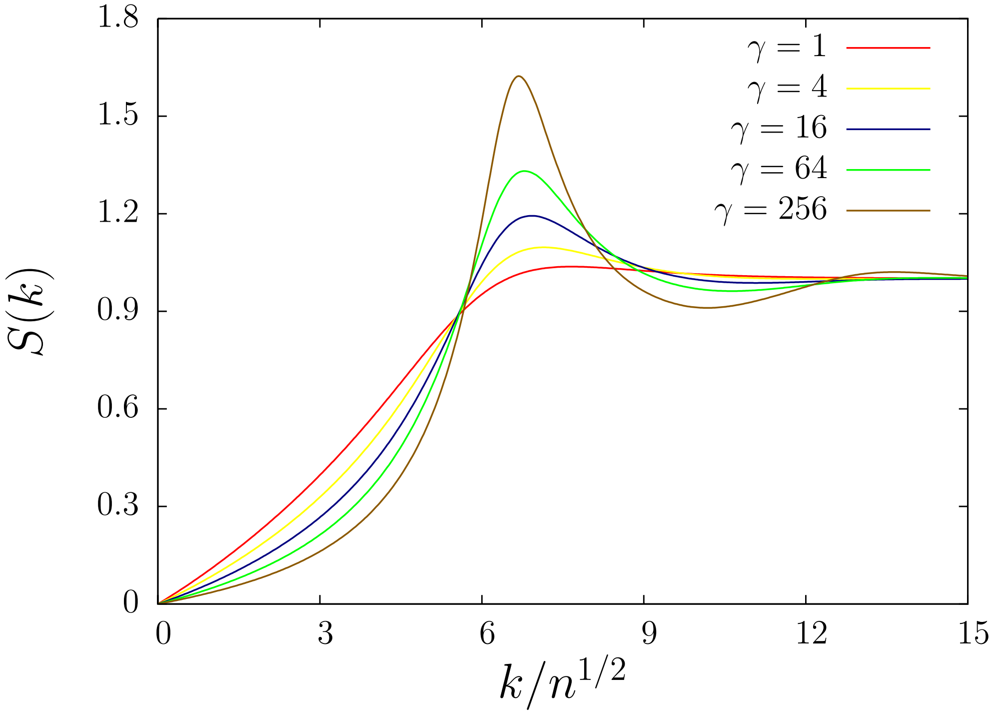
QMC data: courtesy of Gregory Astrakharchik

Excitation spectrum

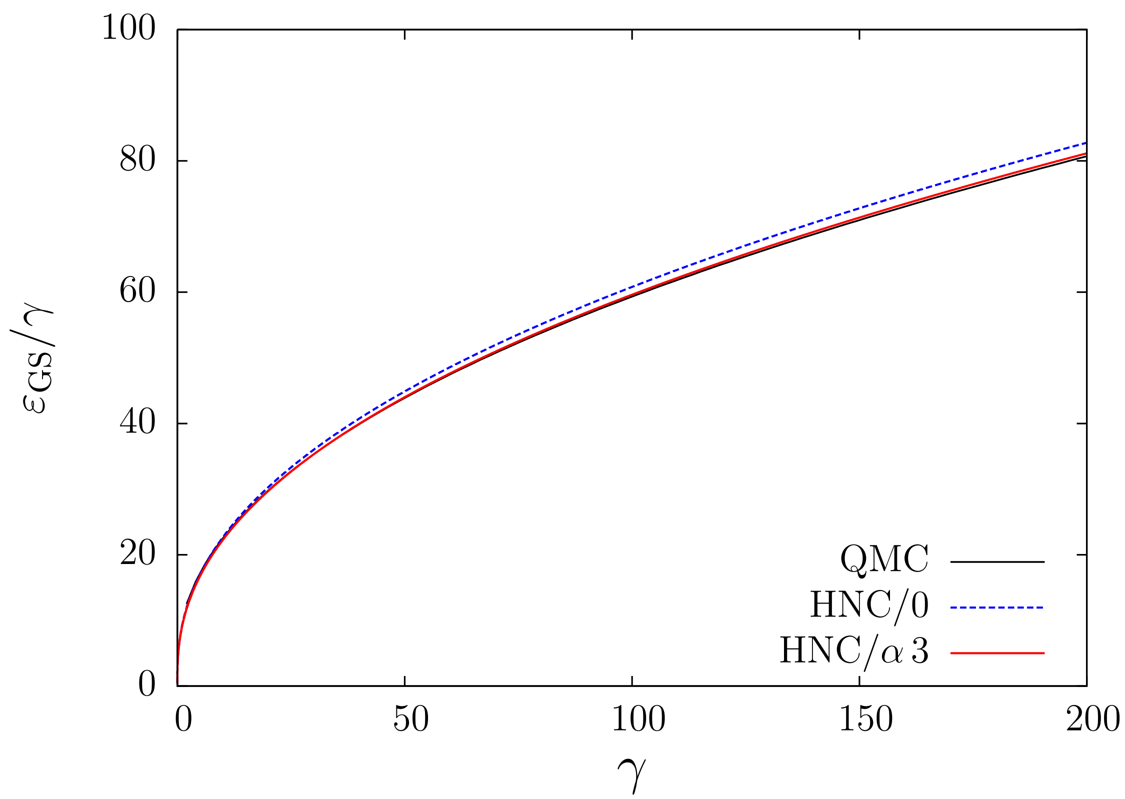
$$E(k) = \frac{\hbar^2 k^2/(2m)}{S(k)}$$



Structure factor

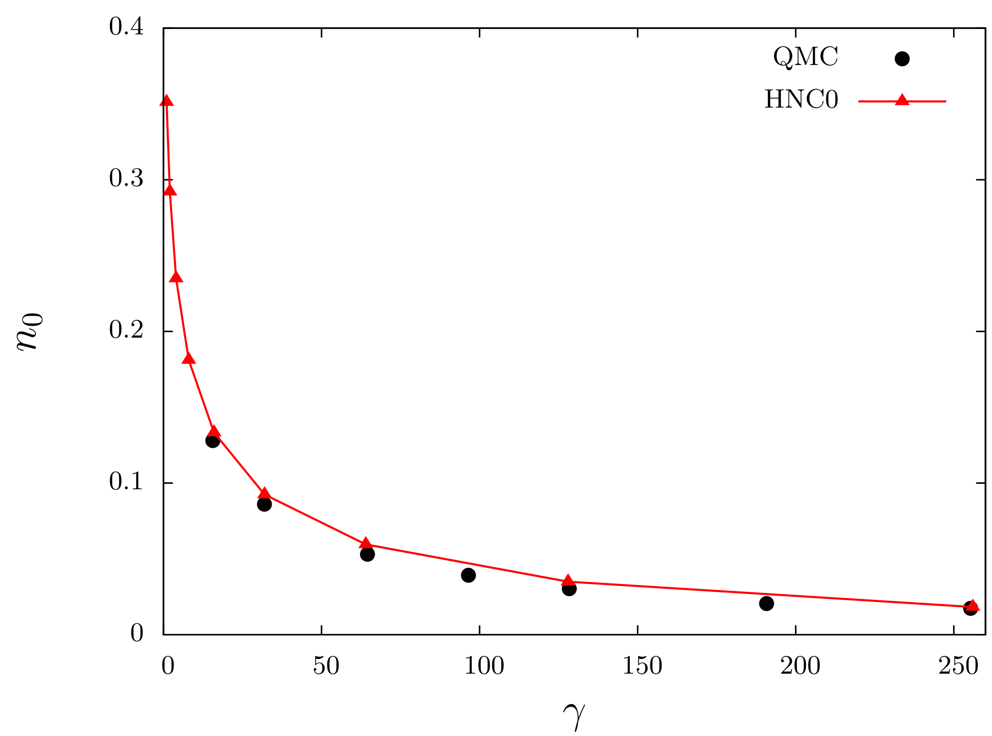


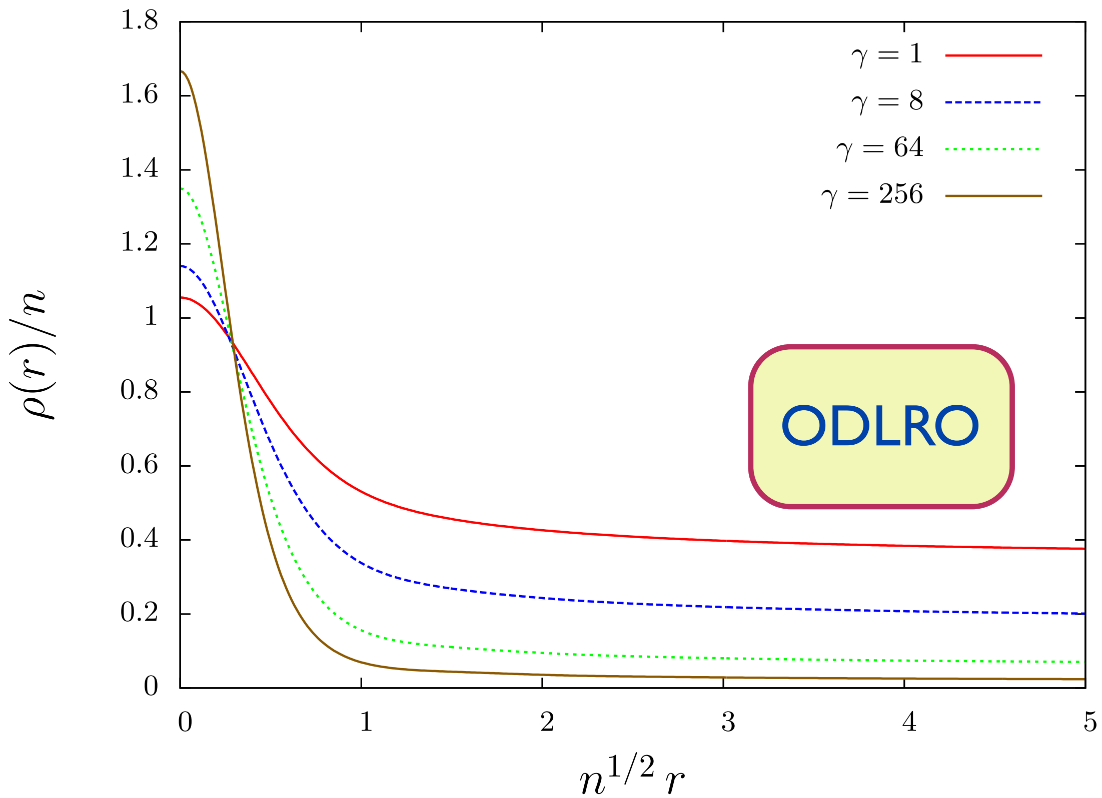
Ground-state energy



One-body density matrix and condensation fraction

Condensation fraction

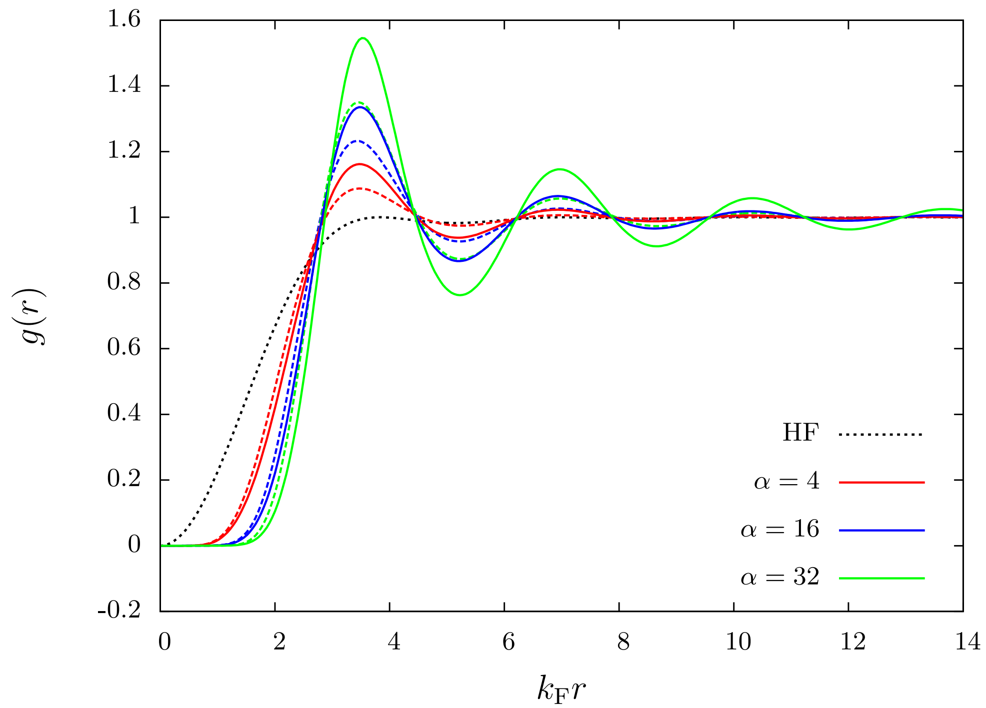


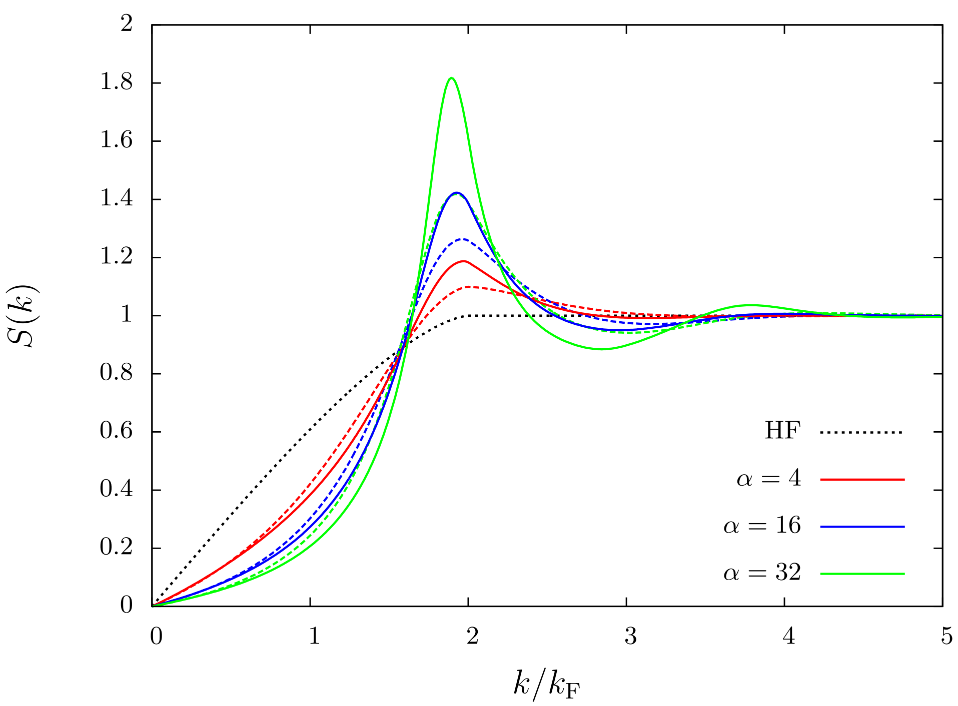


1BDM

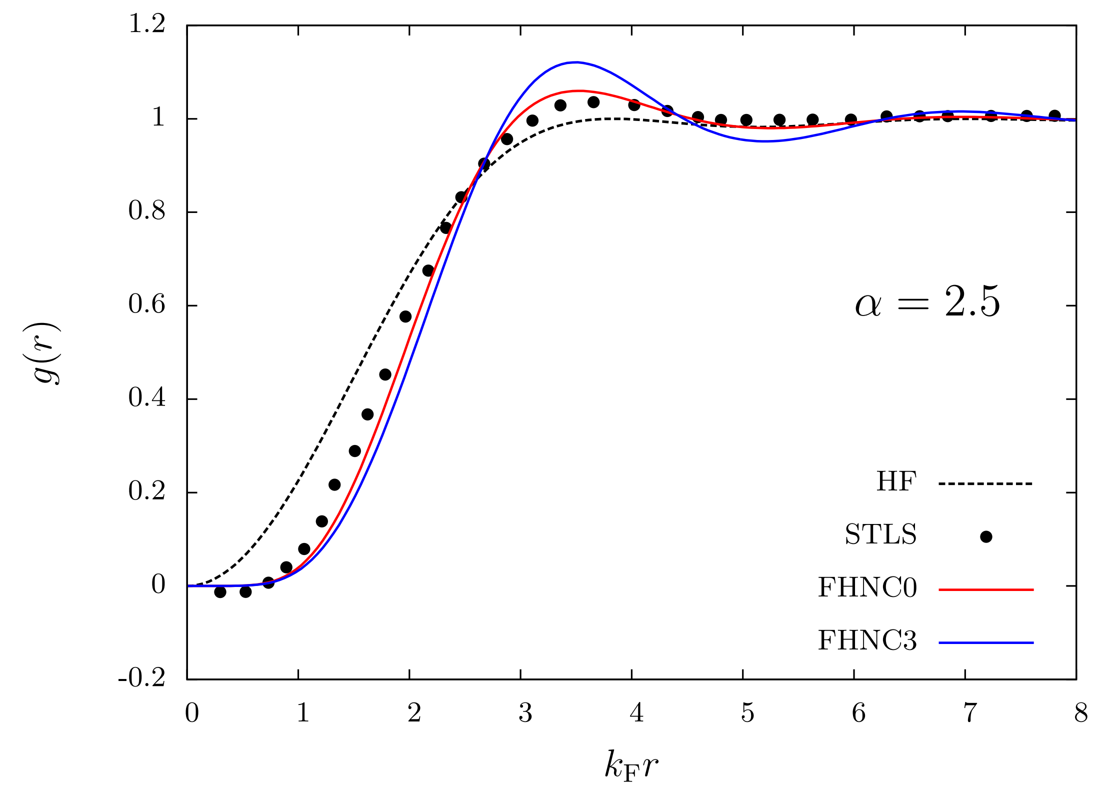
Numerical Results: 2D polar Fermi liquid

(still no exact results in the market)



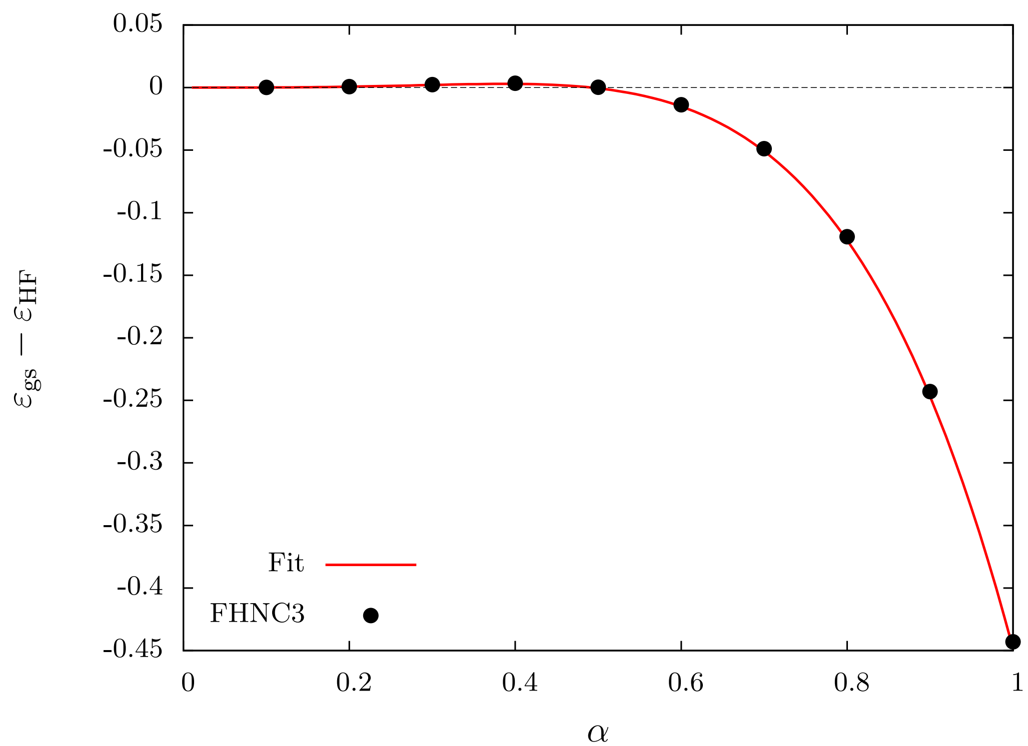


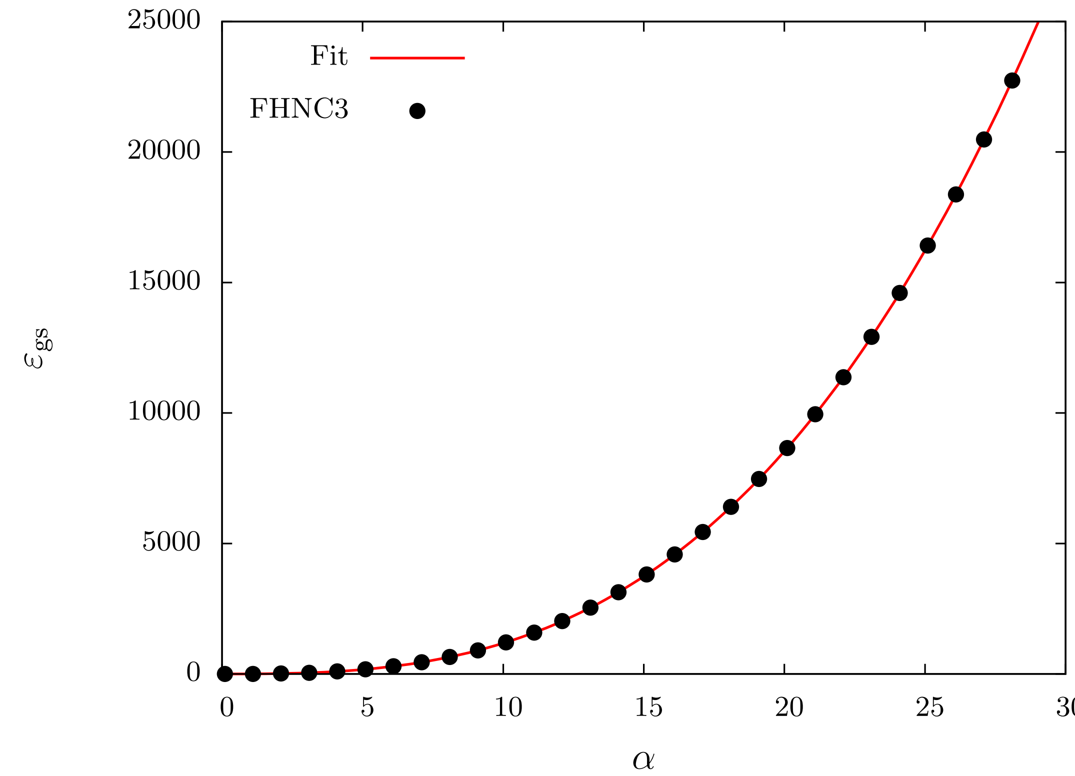
$$\alpha = \sqrt{\pi\gamma}$$



STLS: Parish & Marchetti, PRL (2012)

Ground-state energy





$$\varepsilon_{\rm GS}(\alpha \to 0) = \alpha^2 + \frac{256}{45\pi}\alpha^3 + \alpha^4 \ln(\alpha) + \mathcal{O}(\alpha^4)$$

Lu & Shlyapnikov, PRA (2012)

Summary

- Ground-state properties of a 2D system of polar bosons studied within HNC approximation.
- An excellent agreement with QMC results obtained wherever the liquid phase is stable.
- Ground-state properties of a 2D system of polar fermions studied within FHNC approximation.
- Results were in agreement with available weak-coupling results in the weak-coupling regime.

Where to go from here?

- Dynamical properties and elementary/collective excitations!
- Polar systems with anisotropic interaction!
- Confined in-homogenous systems!
- Effects of finite temperature!
- Fermi-Bose mixture!
- Higher/Lower dimensions!
- Multilayer polar systems!
- Polar interaction + synthetic gauge fields!

Thanks for your attention!