Monte Carlo simulations of the Unitary Bose gas

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[*S. Piatecki & W. Krauth, Efimov-driven phase transitions of the unitary Bose gas, Nature Communications* ***5*** *(2014)*, *3503]*

Ultracold atoms

Cooling techniques allow to bring atomic gases to **ultracold temperatures** (down to 10-100 nK).

Clean and tunable systems, where **quantum effects** are dominant.

1990s: **Bose-Einstein condensation** of Rb-87 atoms.

Simplest model: **ideal gas of bosonic atoms**.
Length scales:

- thermal wave length: $\lambda \sim 1/\sqrt{T}$
- mean interparticle distance: $(\mathrm{vol}/N)^{1/3}$

When $\lambda \sim (\mathrm{vol}/N)^{1/3}$, **phase transition** between **normal gas** and **BEC** (macroscopic ground-state occupation)

Unitary Bose gas

Add interactions (e.g. van der Waals) → one more length scale (**scattering length** *a*).

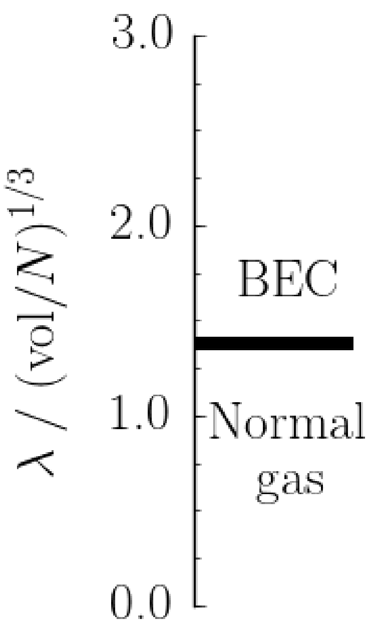
Feshbach resonances: tuning scattering length to very large values (“infinite”, i.e. much larger than any other length scale).
→ **unitary regime**.

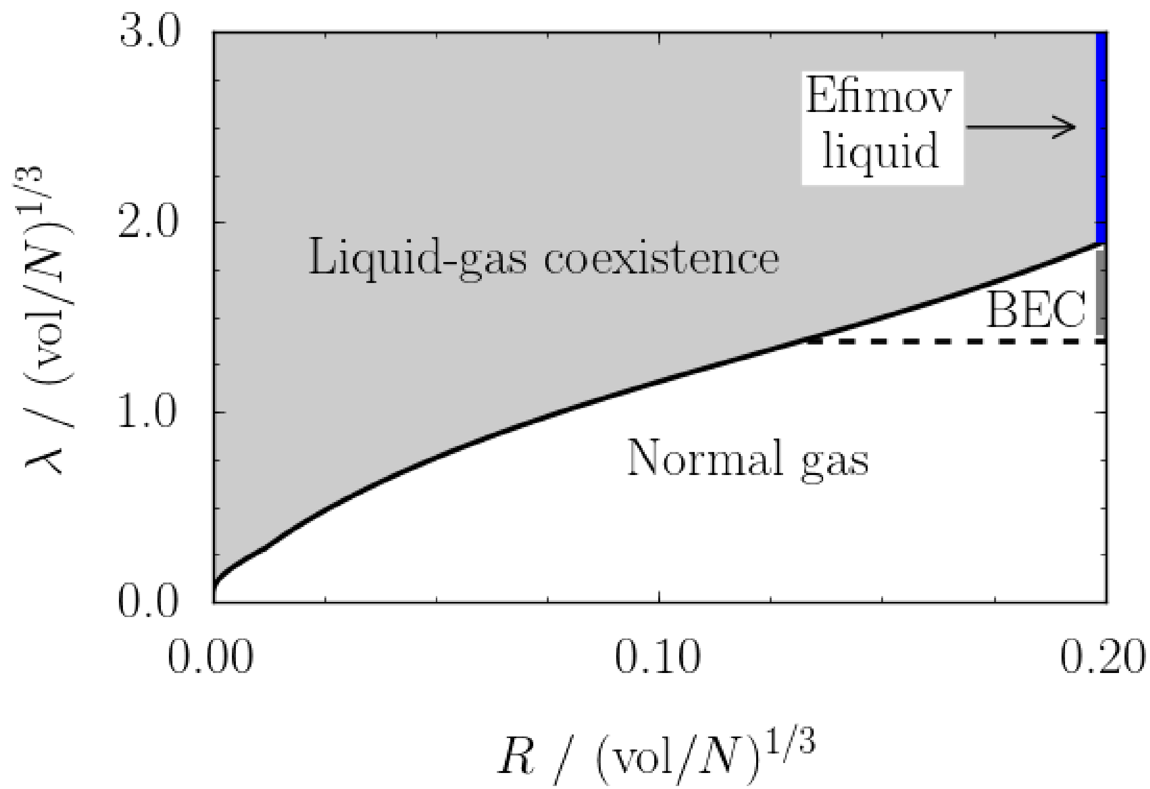
Universal behavior (independent on interaction details), with the appearance of an **additional three-body length-scale** (*R*)

First observation of the **Efimov effect** (three-body quantum effect, predicted in nuclear physics in the 1970s).

Experiments with bosons: **stability problem** (3-body losses).
Simulations: no such problem (**only thermodynamics**).

Unitary Bose gas (continued)





Results from simulations with **harmonic trap** (Piatecki&Krauth, 2014)
Inhomogeneous system → quantitative study of transitions is hard.

Homogeneous periodic box → appropriate system to study phase transitions (correlation functions, superfluid behavior, Bose-Einstein condensate fraction, finite-size scaling, ...)

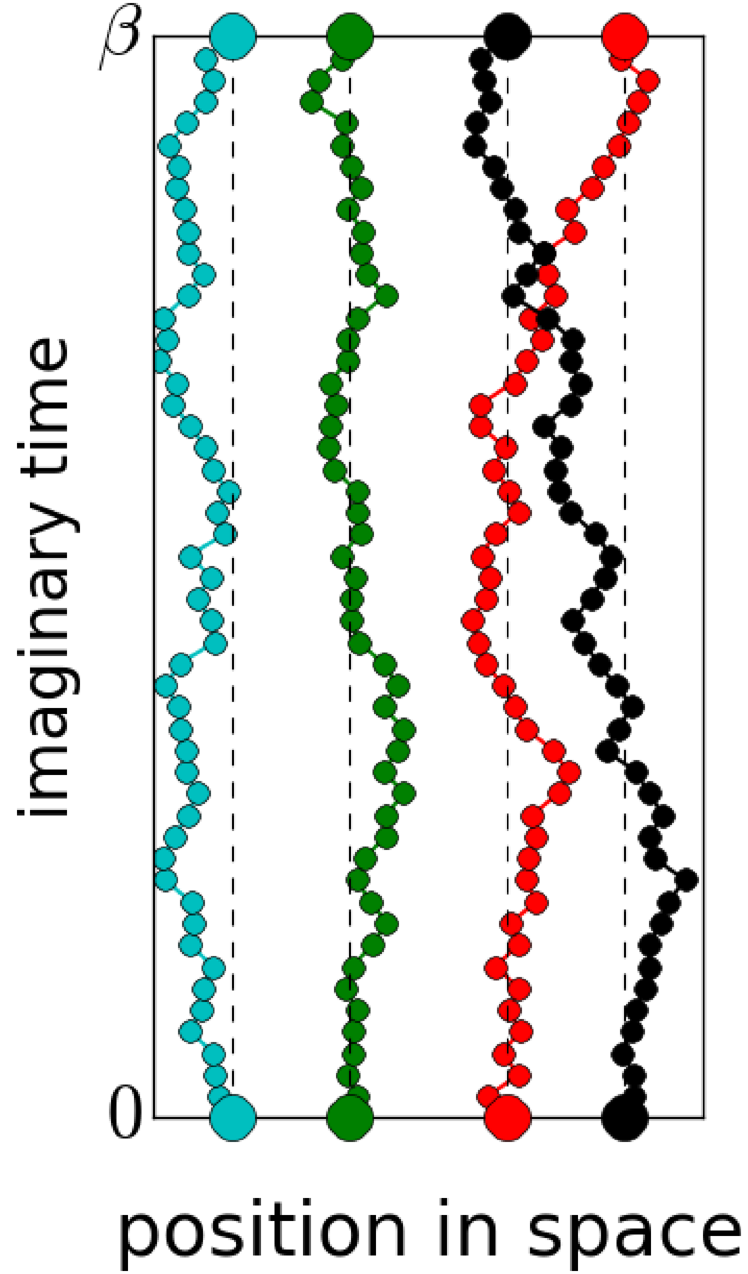
Path-integral Monte Carlo simulations

Physical model → probability distribution **P(X)** for a configuration **X**.

Direct-sampling Monte Carlo (a dream): draw independent samples from **P(X)**, and use it to compute average values (i.e. thermodynamics).

Path-integral representation for quantum particles (unbiased for bosons): **X** is 20000-dimensional, and **P(X)** is complicated
→ **Markov-chain sampling**

Design and improve algorithms to **sample P(X) efficiently**, i.e. many independent samples in few steps.
[see Manon Michel's talk at 14h]



On-going work on mesoPSL

Running programs in **python2+numpy**.

Using custom version of libraries on mesopsl1 (thanks to support.mesopsl*)*.

Intrinsic **naive parallelizations**:
- many independent points of the phase diagram
- many identical simulations (to improve statistics)

Possibility of smarter parallelization (different portions of the imaginary-time axis).

Interest in exploring parallel python libraries (*multiprocessing* built-in library or others), in progress.