Monte Carlo simulations of the unitary Bose gas

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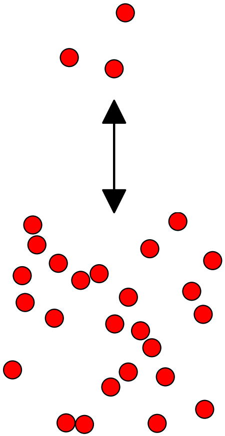
S. Piatecki & W. Krauth, Efimov-driven phase transitions of the unitary Bose gas, *Nature Communications* **5**, 3503 (2014)

S. Piatecki, The Bose gas at large scattering lengths, PhD thesis (ENS Paris, 2014)

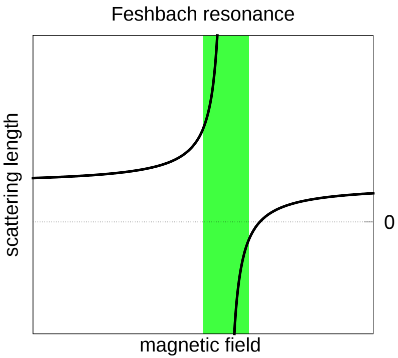
1. Unitary bosons
   - Efimov effect (three bosons)
   - Trimers in ultracold atoms

2. Path integral Monte Carlo study
   - Three bosons
   - Many-body phase diagram in a trap
   - Homogeneous system (in progress)



Scattering length

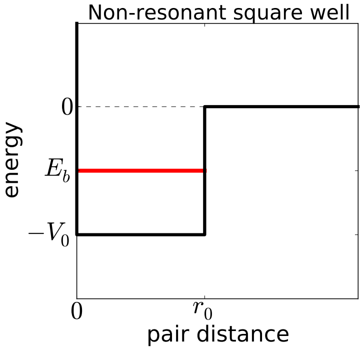
Scattering at low energy (temperature) $\Rightarrow$ scattering length a
Quantum hard spheres of radius $\sigma \Rightarrow a = 2\sigma$
Attractive square well potential $\Rightarrow$ a can be both positive or negative
Feshbach resonance: tuning a to large values

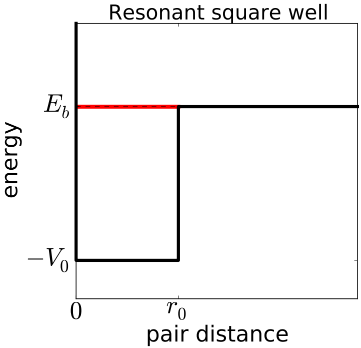


Efimov effect 1/2

Unitary limit: $|a| \to \infty$ (larger than every other length scale)
a.k.a. **resonant interaction**: pair binding is at its threshold ($E_b \to 0$)
Binding energy of the dimer (if present) is universal for $a \gg r_0$:

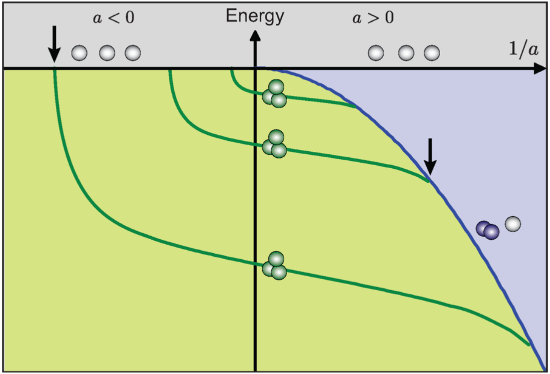
$$E_b = -\frac{\hbar}{ma^2}$$





Efimov effect 2/2

Three identical bosons at unitarity ⇒ **Efimov effect**: infinite number of **trimers** (three-body bound states) even without dimers.



[Ferlaino & Grimm, 2010]

Geometric scaling of trimers (asymptotically universal for $a \to \infty$)

$$\mathrm{size}_{n+1} = \lambda \times \mathrm{size}_n$$

$$\mathrm{energy}_{n+1} = \frac{\mathrm{energy}_n}{\lambda^2}$$

$(\lambda \simeq 22.7)$

Trimers in ultracold atoms

Strongly interacting fermions: many experiments, BEC-BCS crossover.
Strongly interacting bosons: **three-body losses**.

On the good side..
losses provide the indirect observation of the existence of trimers and geometrical scaling:
- identical bosons: first/second resonances (Kraemer 2006, Huang 2014)
- mixtures: up to three resonances (e.g. Tung 2014, with Li-Cs)

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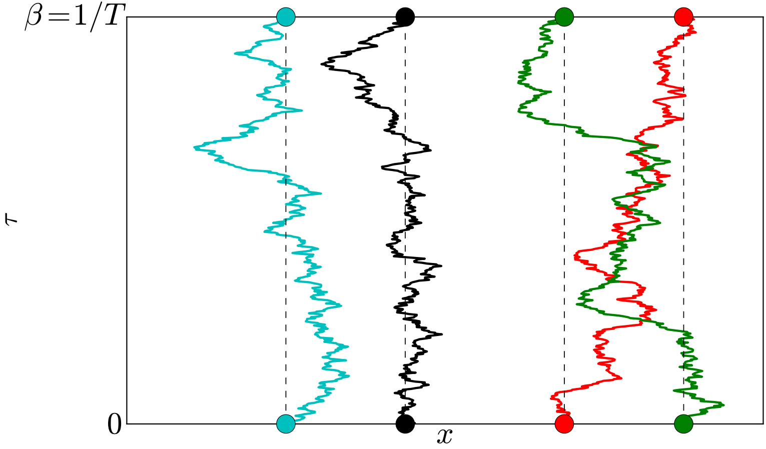
On the not-so-good side..
they lead to a **stability problem**, is it feasible to study unitary bosons?
Experiments at JILA: three-body losses are slow enough, at least to measure the momentum distribution (Makotyn 2014).

Path integral Monte Carlo for the unitary Bose gas

Path integral Monte Carlo

Quantum-classical mapping: one atom $\leftrightarrow$ one path along $\tau \in [0, \beta]$,



Many-body model

Model:

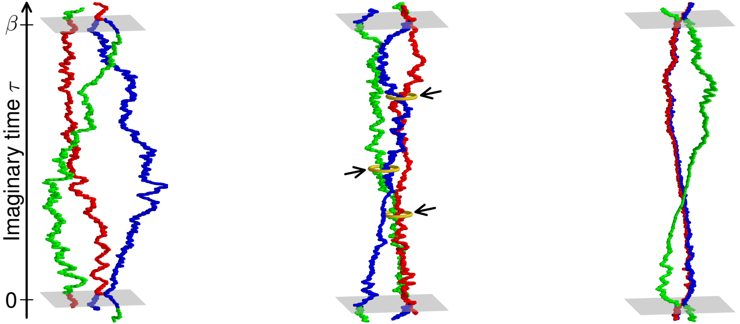
- N bosons at inverse temperature $\beta = 1/T$;
- only thermodynamics, no observation of single states;
- ground state properties for $T \to 0$;
- resonant two-body interaction (solved exactly, in the zero-range limit);
- three-body cut-off on the hyperradius R:

$$R^2 \equiv \frac{r_{12}^2 + r_{23}^2 + r_{31}^2}{3} \geq R_0^2$$

Checks:

- at high T: 3rd order expansion of the virial equation of state,
- three particles at low T: universal trimer.

Trimer in path integral



Non-bound particles
$R_0/a \sim -1$

Unitarity
$R_0/a = 0$

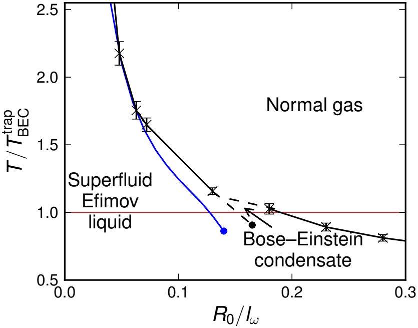
Bound pair + particle
$R_0/a \sim 1$

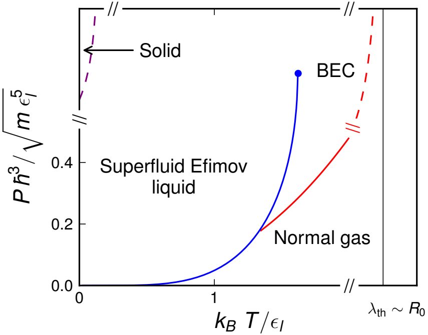
[Piatecki & Krauth, 2014]

(same effect predicted for three DNA strands: Maji, NJP 2010)

Many-body phase diagram

Simulations of trapped system ⇒ numerical phase diagram
Simple theoretical model for the liquid-gas transition (incompressible liquid + virial normal gas) matches with MC.





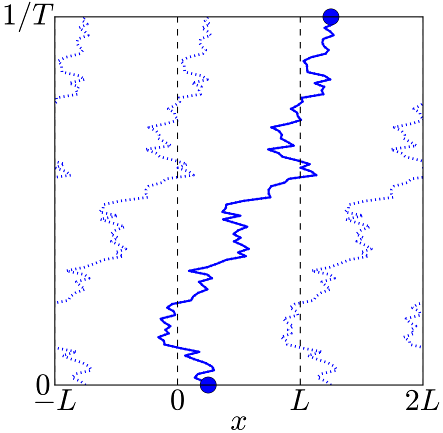
[Piatecki & Krauth, 2014]

Homogeneous system (in progress)

Work in progress: homogeneous periodic box, possible **winding** around the box.

Why making it harder?

- measure superfluid fraction,
- measure momentum distribution,
- precise study of transitions, finite-size scaling, ...



References

- Trimers and universal scaling:
  Ferlaino & Grimm, Physics **3**, 9 (2010);
  Kramer *et al.*, Nature **440** 315 (2006);
  Huang *et al.*, PRL **112**, 190401 (2014);
  Tung *et al.*, arXiv:1402.5943 (2014);
- Unitary Bose gas:
  Makotyin *et al.*, Nat. Phys. **10**, 116 (2014);
- Numerical simulations and clusters:
  von Stetcher, J. Phys. B **43**, 101002 (2010);
  Piatecki & Krauth, *Nat. Communications* **5**, 3503 (2014);
- DNA:
  Maji *et al.*, New J. of Phys. **12**, 083057 (2010);
  Pal *et al.*, PRL **110**, 028105 (2013).