Thermodynamics of the unitary Bose gas from first principles

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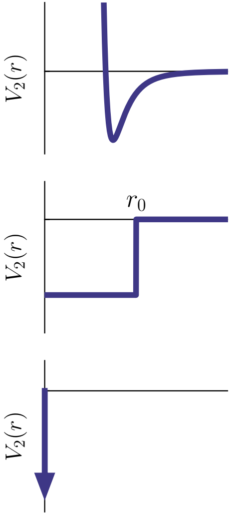
1. Interactions in ultracold gases

2. Efimov effect for $N = 3$ bosons

3. Unitary Bose gas ($N \gg 1$)

Interactions in ultracold gases



Range of interatomic potential (r_0) is small:

$$r_0 \ll \rho^{-1/3} \qquad \text{(low density)}$$

$$r_0 \ll \lambda_{\text{th}} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}} \qquad \text{(low temperature)}$$

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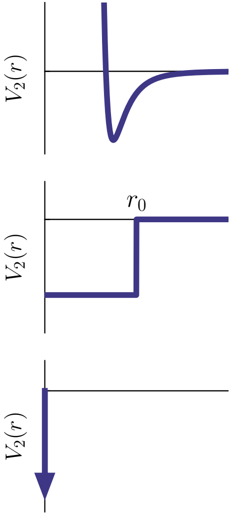

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- Low-energy scattering properties encoded in s-wave scattering length a.
- Theory: Use a model potential for $V_2(r)$, with given a.
- Zero-range pseudopotential ($r_0 \to 0$) removes any detail other than a.

Interactions in ultracold gases – strength

- First experiments with ultracold Bose gases $\rightarrow$ weak interactions:

$$\rho a^3 \ll 1$$

  Successfully treated by Gross-Pitaevskii theory (for small T and a).
- Beyond mean-field corrections (Lee-Huang-Yang, 1957):

$$\frac{E}{V} = \frac{4\pi\hbar^2 a}{m}\frac{\rho}{2}\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + \dots\right)$$

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- Unitary limit:

$$|a| \to \infty$$

- Experimentally accessible (Feshbach resonances).
- Easily realized with theoretical model potentials.

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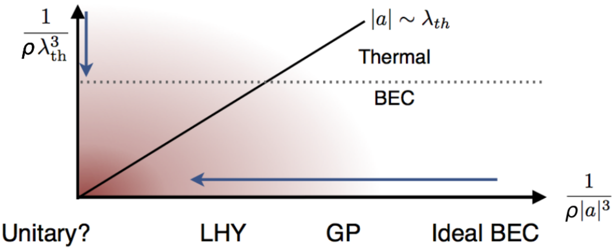

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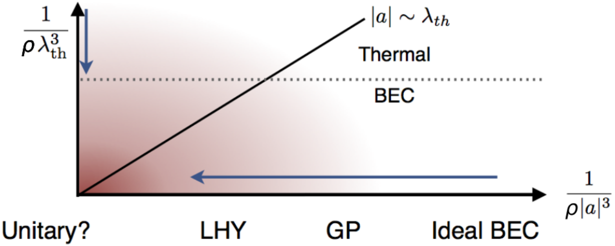

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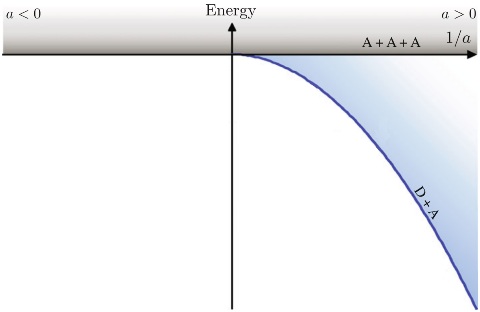
Dynamical instability

- Three-body inelastic recombinations lead to atom losses.
- Loss rate scales as a^4 (at $T = 0$) or as $\frac{1}{T^2}$ (at $|a| = \infty$).

Efimov trimers

Three spinless bosons, with $r_0 \ll |a|$.
For $a > 0$, shallow dimer bound state:

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



[Ferlaino *et al.*, FBS, 2011]

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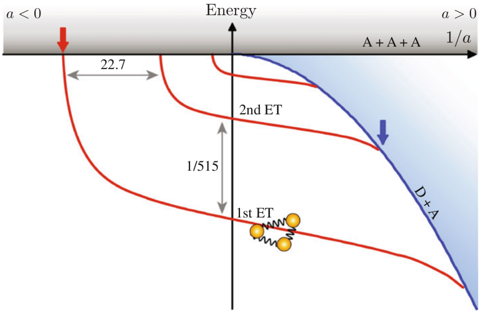


[Ferlaino *et al.*, FBS, 2011]

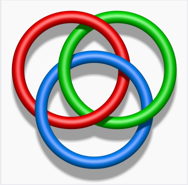
Efimov trimers

Three-body bound states [Efimov, 1970]:

- Geometric sequence:

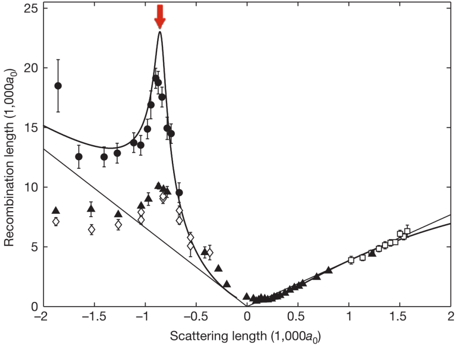
$$\begin{cases} E_{n+1} \simeq E_n/515 \\ \mathrm{size}_{n+1} \simeq 22.7 \times \mathrm{size}_n \end{cases}$$

- Universal (for large n).
- Borromean, for $a \leq 0$:



Efimov trimers - experiments

- Predicted for nucleons, first observed with ultracold atoms (2006).
- Appearance of first Efimov trimer → enhanced three-body losses.



[Kraemer *et al.*, Nature, 2006]

Efimov trimers - theory

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- A solution is to add a three-body repulsion $V_3(R)$:

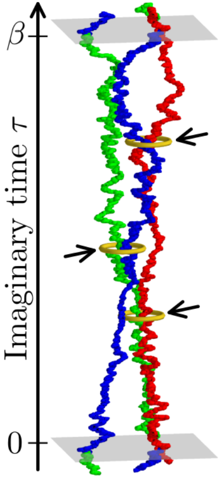
$$H = \sum_{i=1}^{3} \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} V_2(r_{ij}) + V_3(R) \qquad \left[R \equiv \sqrt{\frac{r_{12}^2 + r_{23}^2 + r_{31}^2}{3}} \right]$$

- Hard-core repulsion: $V_3(R) = \infty$ for $R < R_0$, zero otherwise [von Stecher, JPB, 2010]:

To verify

Does the three-body-cutoff model reproduce universal trimers?

Efimov trimers - theory



[Piatecki&Krauth, NC, 2014]

- Path-integral formalism at $T > 0$: Partition function = weighted sum over imaginary-time paths.

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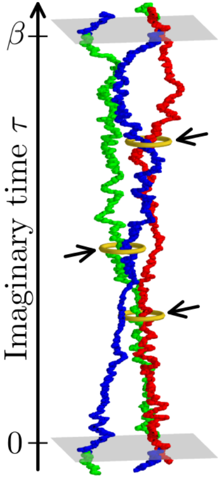

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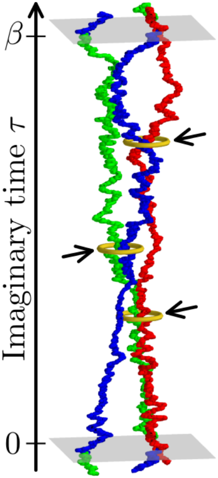
- Path-integral formalism at $T > 0$: Partition function = weighted sum over imaginary-time paths.
- Positive weights $\rightarrow$ interpret as probability.
- Monte Carlo method: Sample path-integral configurations according to weights, to compute average observables.
- Controlled approximations in constructing the many-body density matrix.
- Efimov trimer: Alternate pinning of particle pairs.

Efimov trimers - theory



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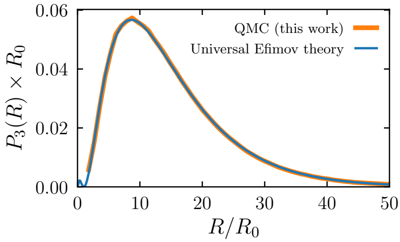

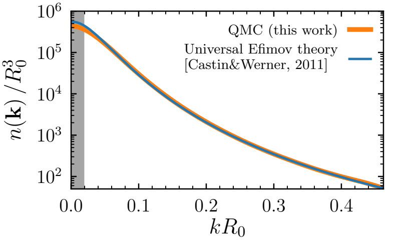

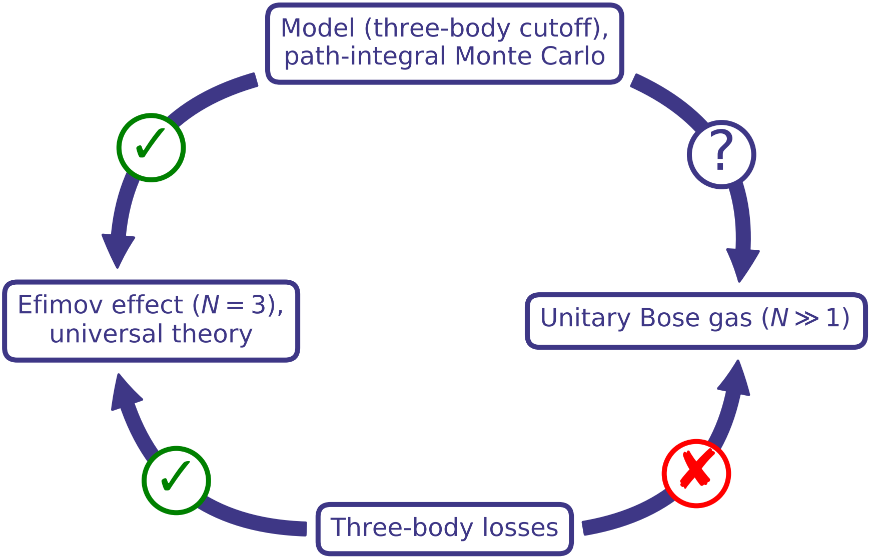
Model (three-body cutoff),
path-integral Monte Carlo
Efimov effect ($N = 3$),
universal theory
Unitary Bose gas ($N \gg 1$)
Three-body losses
✓
✓
?
✗

Unitary bosons – phase diagram

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} V_2(r_{ij}) + \sum_{i<j<k} V_3(R_{ijk})$$

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- Homogeneous system:
  1. Clean measure of correlation functions.
  2. Homogeneous box available in experiments.
- Trapped system: [Piatecki&Krauth, NC, 2014].
- NVT ensemble, three length scales: $\lambda_{\mathrm{th}}, \rho^{-1/3}, R_0$.
- R_0 is linked to l_{vdW}.

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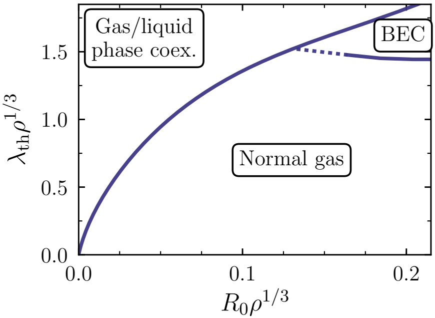
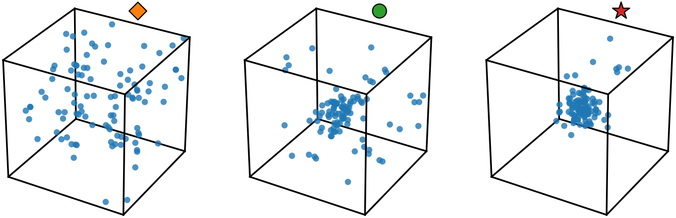
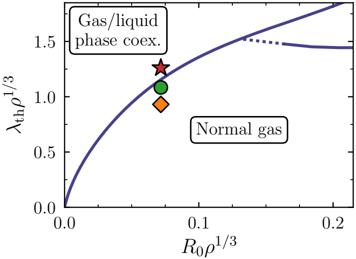


Unitary bosons – Efimov liquid





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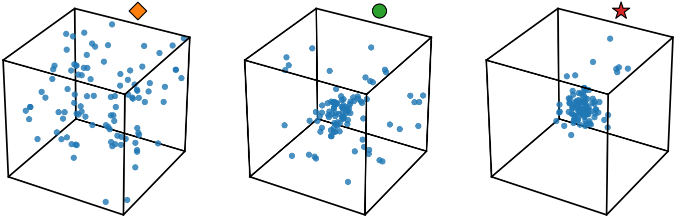

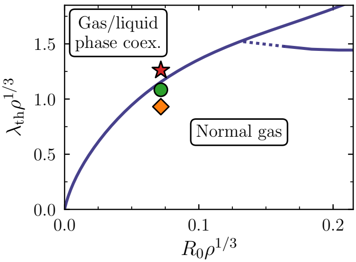

- NVT: Gas/liquid phase separation.
- Instability line predicted through approximate gas/liquid models, supported by quantum Monte Carlo.
- Density: $\rho_{\rm liq} \simeq (3.6R_0)^{-3} \gg \rho_{\rm gas}$.

Unitary bosons – Efimov liquid

Universal N-body bound state?

- Efimov effect does not exist for $N \geq 4$ (no new length scale).
- Universal tetramers associated with trimers [theo/exp: von Stecher *et al.*, Ferlaino *et al.*, 2009].
- Universal bound state of N unitary bosons? Open question, with predictions for up to $N \approx 15$ atoms.
- Is the Efimov liquid the finite-T, large-N limit of these states?

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Experimentally observable?

- Approximate model: Incompressible liquid + normal gas
  $\rightarrow$ Coexistence free energy.
- Free-energy barrier: Droplets are stable when bigger than ≈ 5 atoms.
- In current experiments, dynamical instability (three-body losses) may hide thermodynamic instability (nucleation of liquid).

Unitary bosons – observables for homogeneous system

- One-body reduced density matrix: $g^{(1)}(\mathbf{r}) \leftrightarrow n(\mathbf{k})$.
- Pair-correlation function: $g^{(2)}(\mathbf{r})$.

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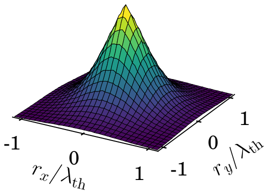
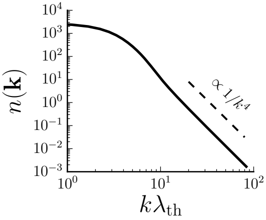
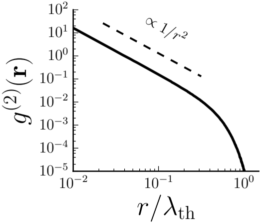
Short-range features

- Two-body contact C_2
- $n(\mathbf{k}) \overset{k\to\infty}{\simeq} \frac{C_2}{k^4}$
- $g^{(2)}(\mathbf{r}) \overset{r\to 0}{\simeq} \frac{C_2/V}{(4\pi r)^2}$







Unitary bosons – Bose-Einstein condensation

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Other (homogeneous) systems:

- Weak repulsive interactions: $T_c \overset{a\to 0}{\simeq} \left(1 + 1.32 \times a\rho^{1/3}\right) T_c^0$
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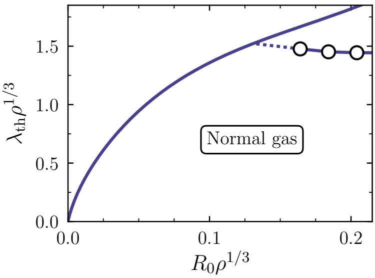
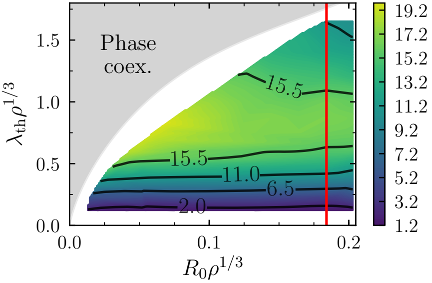
Unitary gas:

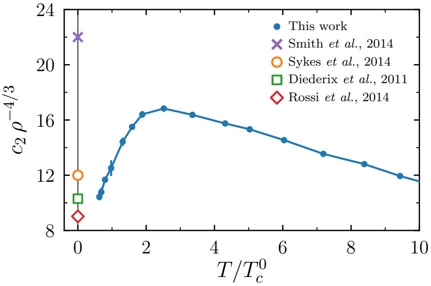
- Quantum Monte Carlo results for superfluid fraction ($N \leq 256$).
- Finite-size-scaling analysis.
- $\mathbf{T_c/T_c^0 \simeq 0.87 - 0.91}$.
- Depletion of the condensate fraction N_0/N.



Unitary bosons – two-body contact

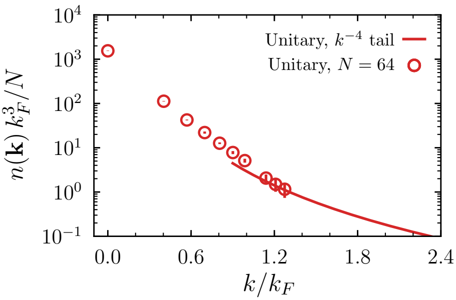
Contact density $c_2 \equiv C_2/V$.

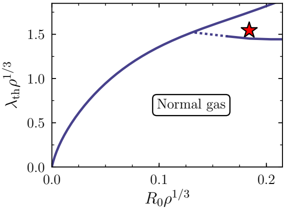




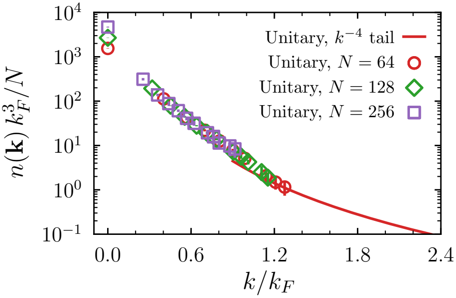
- At large T, well described by virial expansion: $c_2 \propto T^{-2}$.
- Weak dependence on three-body cutoff R_0.
- $c_2(T)$ is non-monotonic. At low-T, similar to $T = 0$ predictions.
- No signature of BEC transition.

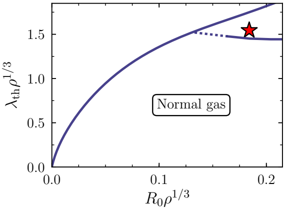
Unitary bosons – momentum distribution





- Units: $k_F = (6\pi^2\rho)^{1/3}$.
- Direct measure of $n(\mathbf{k})$ merges with C_2/k^4 (contact parameter from $g^{(2)}(\mathbf{r})$).





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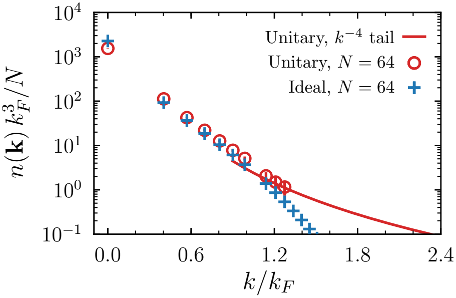

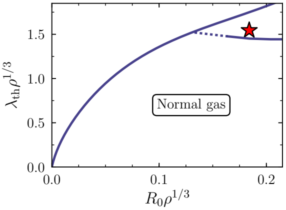

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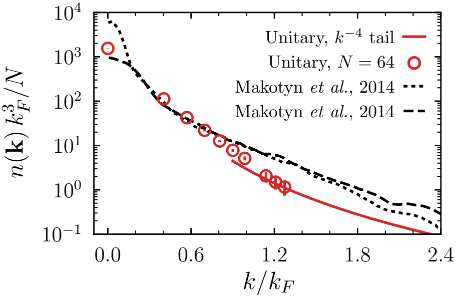
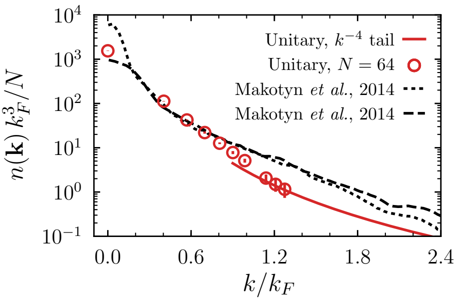
- Depletion of $n(\mathbf{k} = \mathbf{0})$.
- Reweighting of middle-k.



Experiment:

- Trapped BEC at $T < 10$ nK, fast ramp to unitarity.
- Lifetime: ≈ 600 μs.
- Large-k equilibration: 100 μs.
- T after the ramp? Local equilibration?

Unitary bosons – momentum distribution



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Comparison:

- Discrepancy at large k, approximately $\times 2$.
- Trap average would increase theoretical C_2.
- Is experimental T larger?

Conclusion

- Ultracold atoms to study strongly interacting systems.
  Microscopic model + quantum Monte Carlo for equilibrium theory.
- For $N = 3$, model captures universal Efimov physics.
- Unitary Bose gas: Homogeneous *vs* phase-separated.
- Efimov liquid: Possibly universal, currently hard to observe ($\leftarrow$ losses).
- BEC transition: 10% decrease of T_c.
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T. Comparin & W. Krauth,
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Phys. Rev. Lett., in press (arXiv:1604.08870).