Thermodynamics of the unitary Bose gas from first principles

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Abstract

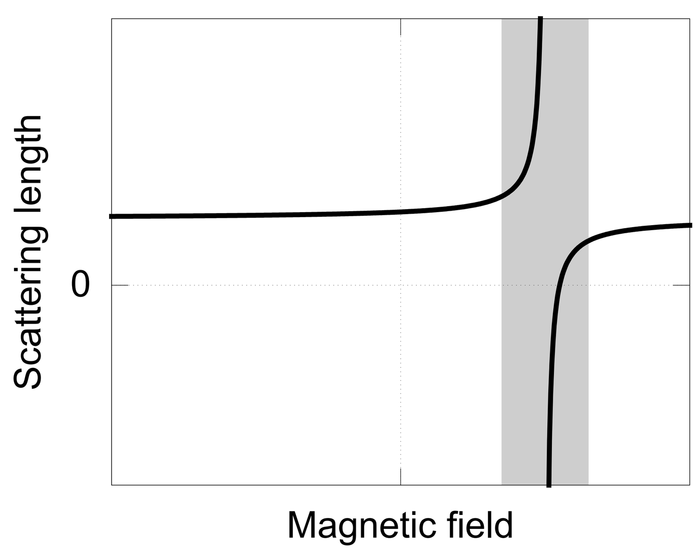
We consider N bosonic atoms with short-range interactions in the unitary limit (that is, with infinite scattering length). The few-body case ($N \gtrsim 3$) is governed by universal Efimov physics, and its signatures were experimentally observed with ultracold gases. We address the many-body problem at thermal equilibrium through the path-integral quantum Monte Carlo technique. The phase diagram includes a normal-gas phase at high temperature and two low-temperature phases: The Efimov liquid and the Bose-Einstein condensate. We determine the critical temperature for Bose-Einstein condensation (found to be 10% smaller than for non-interacting bosons) and compute the momentum distribution, which shows the characteristic power-law decay at large momentum.

T. Comparin and W. Krauth, Momentum Distribution in the Unitary Bose Gas from First Principles, *Phys. Rev. Lett.* **117**, 225301 (2016).

Physical system: Unitary Bose gas

Ultracold atomic gases

- Scattering length a: Single parameter to encode low-energy interactions (at low density and temperature).
- Feshbach resonances to tune a via external magnetic field.



Efimov effect and unitary Bose gas

- Efimov effect (nuclear physics): Scale-invariant three-body bound states, at large a.
- Large $a \rightarrow$ Universality (additional three-body length scale needed when Efimov effect is present).
- First Efimov-effect signature in ultracold caesium (Innsbruck, 2006).
- Three-body recombination losses pose a challenge for realizing the degenerate unitary Bose gas.

Model

- Pair interactions: Zero-range limit with $|a| = \infty$.
- Three-body hard-core repulsion for any triplet (i, j, k):

$$V_3(R_{ijk}) = \begin{cases} \infty & \text{if } R_{ijk} < R_0 \\ 0 & \text{if } R_{ijk} > R_0 \end{cases},$$

with $R_{ijk}^2 = (r_{ij}^2 + r_{jk}^2 + r_{ki}^2)/3$.

Method: Path-integral quantum Monte Carlo

Path-integral representation

- Quantum particles represented as polymers (size $\lambda \sim 1/\sqrt{T}$), indistinguishability enforced via permutations.
- $\lambda \ll$ typical interparticle distance $\rightarrow$ normal gas,
  $\lambda \gg$ typical interparticle distance $\rightarrow$ quantum gas, long permutation cycles, superfluid phase (bosons).

Monte Carlo sampling

- Probability distribution for configuration $X = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$:

$$P(X) = \langle \mathbf{x}_1, \dots, \mathbf{x}_N | \exp(-\beta H) | \mathbf{x}_1, \dots, \mathbf{x}_N \rangle$$

- A Markov-chain Monte Carlo algorithm is used to produce a sequence of configurations distributed according to $P(X)$.

Short-ranged, strong interactions

- Singularities in the probability distribution:

$$P(X) \propto \frac{1}{r_{ij}^2}, \qquad \text{for } r_{ij} \equiv |\mathbf{x}_i - \mathbf{x}_j| \rightarrow 0.$$

- Physical reason: $\lim_{r\rightarrow 0} [r^2 g_2(r)] \propto c_2$, with the contact density c_2 being the central quantity in Tan's universal relations.
- Singularities slow down Monte Carlo sampling.
  Our solution: Adding to the algorithm the exact sampling of the two-body density matrix (optimal solution for $N = 2$).

Phase diagram and observables

Phase diagram

- High temperature: Normal gas.
  Low temperature: Phase coexistence of gas and Efimov liquid (small R_0), or homogeneous superfluid (large R_0).
- Critical temperature T_c for superfluidity approximately 90% of T_c for the ideal Bose gas, to be compared with ^{4}He (70%) and weakly-interacting Bose gas ($> 100\%$).
- Is the liquid droplet a signature of the cluster bound states already predicted for $N \lesssim 15$?

Contact density and momentum distribution

- The contact density c_2 controls the large-k asymptotics of the momentum distribution: $n(\mathbf{k}) \simeq (c_2 V)/k^4$.
- Starting from large temperature, c_2 increases (in agreement with virial expansion) and then has a non-monotonous behavior. At low temperature, $c_2\rho^{-4/3} \approx 10$.
- Approximate ground-state theories: $c_2\rho^{-4/3} = 8 - 12$.
- $c_2\rho^{-4/3} \simeq 22$ from the fit of experimental data with universal theory [Smith *et al.*, Phys. Rev. Lett., 2014]. Why the discrepancy?