Universal Short Range Correlations in Bosonic Helium Clusters

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arXiv:1901.11247

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Illustration: Goethe UniversitÃt Frankfurt

Universality

- Consider particles interacting through 2-body potential with range R.
- Classically, the particles 'feel' each other only within the potential range.
- But, in the case of resonant interaction, the wave function has much larger extent.
- At low energies, the 2-body physics is govern by the scattering length, a.

$$\lim_{k\to 0} k \cot \delta(k) = -\frac{1}{a} + \frac{1}{2} r_0 k^2$$

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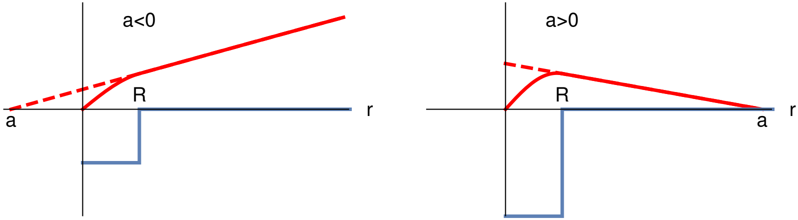

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Universality

- Naturally, $a \approx r_0 \approx R$.
  Universal systems are fine-tuned to get $a \gg r_0, R$.
- Corrections to universal theory are of order of r_0/a and R/a.
- For $a > 0$, we have universal dimer with energy $E = -\hbar^2/ma^2$.
- Nucleus: $a_s \approx -23.4$ fm, $a_t \approx 5.42$ fm, $R = \hbar/m_\pi c \approx 1.4$ fm.
  Deuteron binding energy, 2.22 MeV, is close to $\hbar^2/ma_t{}^2 \approx 1.4$ MeV.
- ^{4}He atoms: $a \approx 95$ Å$\gg r_{vdW} \approx 5.4$ Å.
- Ultracold atoms near a Feshbach resonance,

$$a(B) = a_{bg}\left(1 + \frac{\Delta}{B - B_0}\right)$$

S. Inouye *et al.*, Nature 392, **151** (1998)

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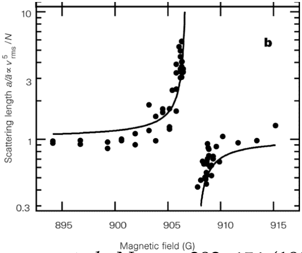

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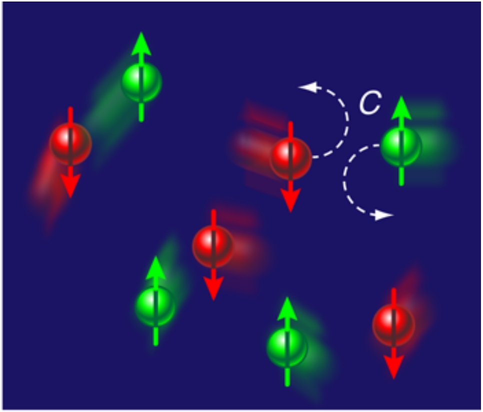
The Contact

The contact C measures the number of pairs of particles with small separations, $C = \int d\boldsymbol{R}\mathcal{C}(\boldsymbol{R})$



S. Tan, Ann. Phys. (N.Y.) **323**, 2952 (2008); **323**, 2971 (2008); **323**, 2987 (2008).

The Contact - Tan's Relations

Tan relations connects the contact C with:

1. **Tail of momentum distribution** $|a|^{-1} \ll k \ll r_0^{-1}$

$$\boxed{n_\sigma(\mathbf{k}) \longrightarrow \frac{C}{k^4}}$$

2. **The energy relation**

$$E = T + U + V$$

The kinetic energy diverges

$$T = \sum_\sigma \int \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} n_\sigma(\mathbf{k})$$

but the sum $T + U$ is regular

$$\boxed{T + U = \sum_\sigma \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \left(n_\sigma(\mathbf{k}) - \frac{C}{k^4} \right) + \frac{\hbar^2}{4\pi m a} C}$$

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3. **Density-Density correlator at short distances**

$$\left\langle n1\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right)n2\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right)\right\rangle \longrightarrow \frac{1}{16\pi^2}\left(\frac{1}{r^2}-\frac{2}{ar}\right)\mathcal{C}(\boldsymbol{R})$$

4. **Adiabatic relation**

$$\left(\frac{dE}{da^{-1}}\right)_S = -\frac{\hbar^2}{4\pi m}C$$

5. **Virial theorem** For a system in a harmonic trapping potential,

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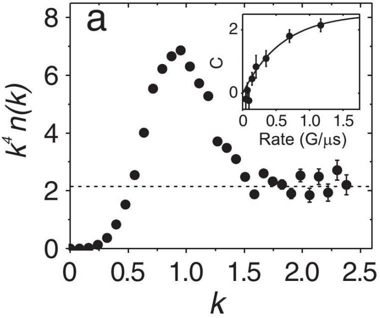
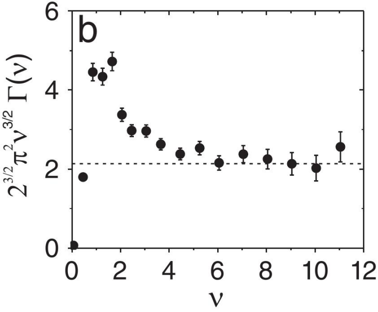
The Contact - Experimental Results

Momentum Distribution



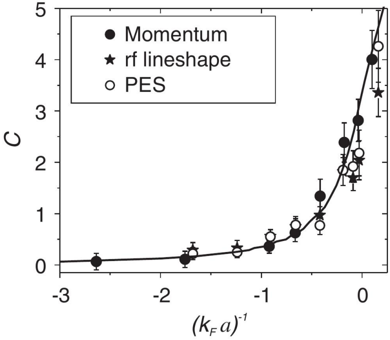
RF line shape



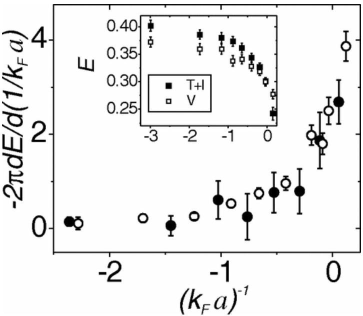
Ultra cold gas of fermionic ^{40}K

J. T. Stewart et al. PRL **104**, 235301 (2010)

The Contact - Experimental Results (II)



Adiabatic relation



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Strong and Weak Universality

- *Wave function factorization:* when two particles approach each other,

$$\Psi \xrightarrow[r_{ij}\to 0]{} \phi_2(\boldsymbol{r}_{ij}) A_{ij}(\boldsymbol{R}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j})$$

$$C \propto \textstyle\sum_{ij} \langle A_{ij}|A_{ij}\rangle; \qquad \langle A_{ij}|A_{ij}\rangle = \int \prod_{k\neq i,j} d\boldsymbol{r}_k\, d\boldsymbol{R}_{ij} \left| A_{ij}\left(\boldsymbol{R}_{ij}, \{\boldsymbol{r}_k\}_{k\neq i,j}\right)\right|^2$$

- In the zero-range limit, *strong* universality holds,

$$\phi_2(r) \propto \frac{1}{r} - \frac{1}{a}$$

- For finite-range potential, *weak* universality holds, $\phi_2(r)$ is not sensitive to the system size or state.

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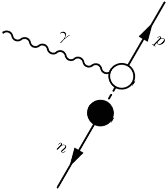
Photoabsorption of Nuclei

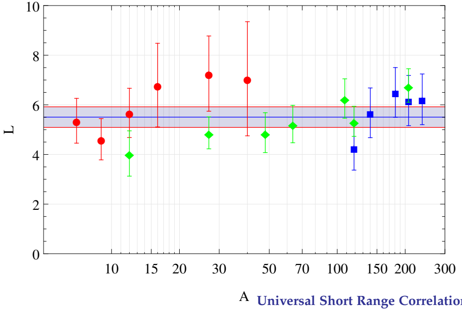
quasi-deuteron model: $\sigma_A(\omega) = L\frac{NZ}{A}\sigma_d(\omega)$

Levinger, Phys. Rev. **84**, 43 (1951)

$$\sigma_A(\omega) = \frac{a_t}{4\pi}\bar{C}_{pn}\sigma_d(\omega)$$

Weiss, **BB**, and Barnea, PRL **114**, 012501 (2015);
PRC **92**, 054311 (2015); Eur. Phys. J. A **52** 92 (2016); ...





Weak Universality

- The 2-body contact in the N-body system

$$C_2^{(N)} = \binom{N}{2} \langle A_2^{(N)} | A_2^{(N)} \rangle$$

- The pair density function at short distances

$$\rho_2^{(N)}(r) = \langle \Psi | \hat{\rho}_2^{(N)}(r) | \Psi \rangle \xrightarrow[r \to 0]{} C_2^{(N)} \rho_2(r)$$

where $\hat{\rho}_2^{(N)}(r) = \frac{1}{r^2} \sum_{i<j} \delta(r_{ij} - r)$, $\rho_2(r) = \int d\Omega_2 |\phi_2(\boldsymbol{r})|^2$.

Weak Universality

- The 1-body momentum distribution

$$n^{(N)}(\boldsymbol{k}) \xrightarrow[k\to\infty]{} 2C_2^{(N)}|\tilde{\phi}_2(\boldsymbol{k})|^2$$

- The static structure factor

$$S(Q) \xrightarrow[Q\to\infty]{} 1 + \frac{2C_2^{(N)}}{N}\frac{4\pi}{Q}\int drr\sin(Qr)\rho_2(r)\ ,$$

  where Q is the momentum transfer.

- The potential energy

$$\langle V_2^{(N)}\rangle = C_2^{(N)}\langle V_2^{(2)}\rangle$$

Werner and Castin, Phys. Rev. A **86**, 013626 (2012).

Coalescence of more particles

- In a bosonic system, coalescence of more particles should provide further factorizations of the wavefunction,

$$\Psi \xrightarrow[r_{ijk}\to 0]{} \phi_3(\boldsymbol{x}_{ijk}, \boldsymbol{y}_{ijk}) A_3^{(N)}(\boldsymbol{R}_{ijk}, \{\boldsymbol{r}_l\}_{l\neq i,j,k})$$

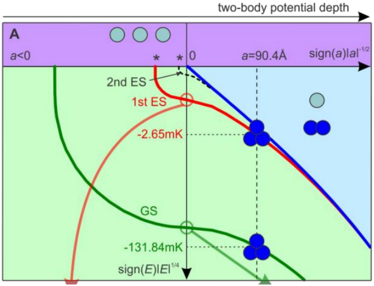
Braaten, Kang, and Platter, PRL **106**, 153005 (2011)

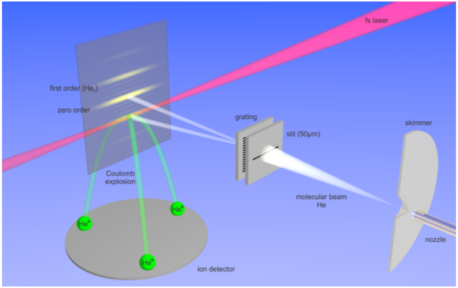
Similar factorization holds for $n > 3$, giving for the n-body density function

$$\rho_n^{(N)}(r) \xrightarrow[r\to 0]{} C_n^{(N)} \rho_n(r)$$

Universality in ^{4}He Atoms

- For $a \longrightarrow \infty$, an infinite tower of Efimov trimers exists.
- For ^{4}He Atoms, a is finite, and therefore only two trimers survive.
- Recently the excited trimer was observed experimentally.

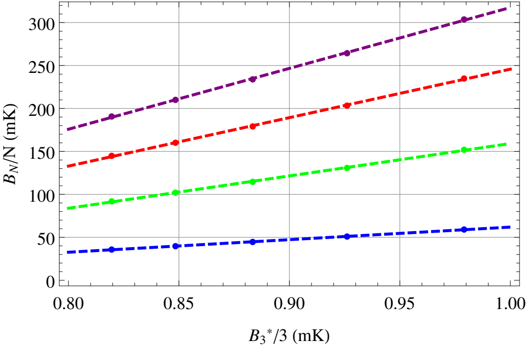




Theory: Hiyama and Kamimura, Phys Rev A. **85**, 062505 (2012);
Experiment: Kunitski *et al.*, Science **348** 551 (2015).

Clusters of He atoms in Effective Field Theory

- Tjon line: correlation between triton and alpha binding energies.
  Tjon, Phys. Lett. B **56**, 217 (1975)
- Therefore, there is no need for four-body parameter at leading order.
  Platter, Hammer, Meissner, Phys. Lett. B **607**, 254 (2005)
- Same is true for 5- and 6-body clusters, also attached to an Efinov trimer.



BB, Eliyahu and van Kolck, PRA **94**, 052502 (2016)

- But four-body parameter is needed at NLO! cf. Johannes Kirscher talk
  BB, Kirscher, Konnig, Valderrama, Barnea, and van Kolck, PRL **122**, 143001 (2019)

Computational methods: VMC + DMC

- We solve the N-body Schrödinger equation with LM2M2 pair-potential
  Aziz and Slaman, J. Chem. Phys. **94**, 8047 (1991).
- Variational Monte Carlo (VMC)

$$E_{var} = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

  with $\Psi_T = \prod_{i<j} f(r_{ij})$, where

$$f(r) = \exp\left[-(p_5/r)^5 - (p_2/r)^2 - p_1 r \right] / r^{p_0}.$$

- Diffusion Monte Carlo (DMC):

$$\frac{\partial \Psi(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N, \tau)}{\partial \tau} = (T + V - E_R)\, \Psi(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N, \tau)$$

  is treated as a diffusion-reaction process for walkers, distributed according to Ψ. Ψ converges to Ψ_0 and E_R to E_0.
- Ψ_T, optimized with VMC, is used to guide the walkers.

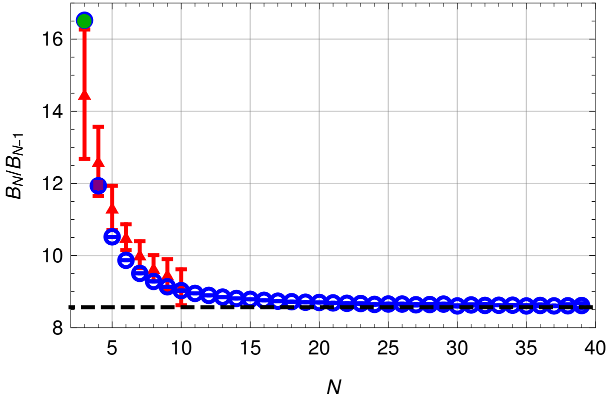
Benchmark: energies of small He clusters

Ground-state energies (in mK); The dimer energy is 1.30348 mK [2].

N	Ref [1]	Ref [2]	Ref [3]	Ref [4]	This work
3	126.39	126.40	125.5(6)	124(2)	125.9(2)
4	557.7	558.98	557(1)	558(3)	557.4(4)
5			1296(1)	1310(5)	1300(2)
6			2309(3)	2308(5)	2315(2)
7			3565(4)	3552(6)	3571(2)
8			5020(4)	5030(8)	5041(2)
9			6677(6)	6679(9)	6697(2)
10			8495(7)	8532(10)	8519(3)

[1] Lazauskas and Carbonell, Phys. Rev. A **73**, 062717 (2006).
[2] Hiyama and Kamimura, Phys. Rev. A **85**, 022502 (2012).
[3] Blume and Greene, J. Chem. Phys. **112**, 8053 (2000).
[4] Guardiola, Kornilov, Navarro, and Toennies, J. Chem. Phys. **124**, 084307 (2006).

$2D$ Bosons Droplets



$B_3/B_2 = 16.522688(1)$ Hammer and Son, Phys. Rev. Lett. **93**, 250408 (2004).

$B_4/B_2 = 197.3(1)$ Platter, Hammer, and Meissner, Few-Body Syst. **35**, 169 (2004).

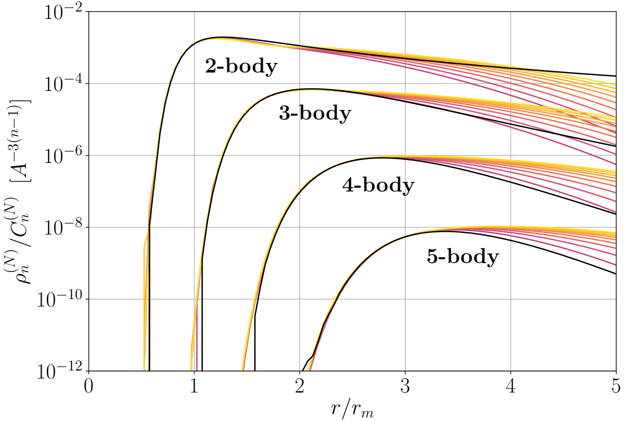
Lattice EFT calculations Lee, Phys. Rev. A **73**, 063204 (2006).

$B_N/B_{N-1} \xrightarrow{N\to\infty} 8.567$ Hammer and Son, ibid.

DMC-STM **BB** and Petrov, New J. Phys. **20**, 023045 (2018)

$$B_N/B_2 \approx 8.567^N \exp(c_1 + c_2/N), \quad c_1 = -2.06(4)\ c_2 = -8(2)$$

Results: n-body density function

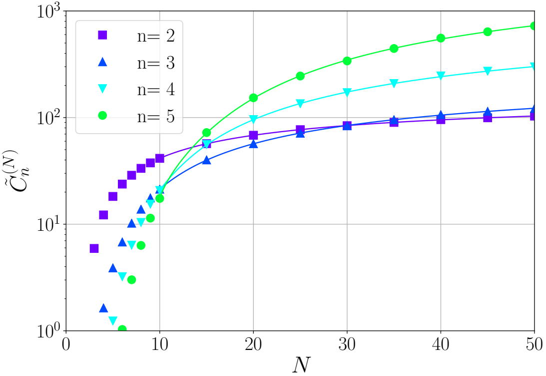


Black line: the reference density ρ_n

Colored lines: the densities for $N = 10, 15, 20 \ldots 50$ (from dark to light)

Results: n-body contact

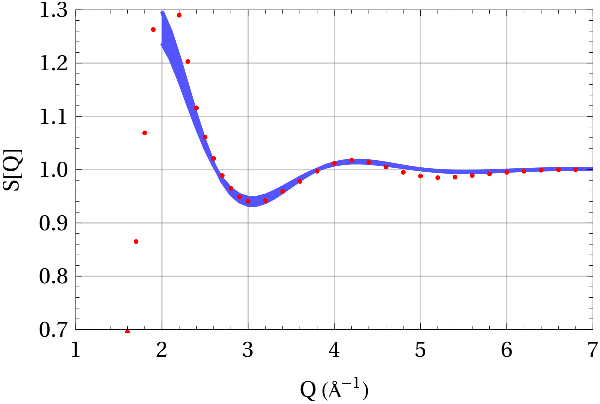
$$\tilde{C}_n^{(N)} = \tilde{C}_n^{\infty} + \alpha_n N^{-1/3} + \beta_n N^{-2/3} + \ldots; \; \tilde{C}_n^{(N)} \equiv C_n^{(N)}/N$$



Asymptotic values for ^{4}He droplets:

n	2	3	4	5
$\tilde{C}_n^{\infty}$	230 ± 25	500 ± 60	1800 ± 300	5900 ± 1000

Results: The structure factor



Experimental data: Svensson *et al.*, PRB **21**, 3638 (1980)
Blue band: theory for contact values of $\tilde{C}_2^\infty \in (200, 250)$

Conclusion

- The generalized contact formalism was applied to study short-range correlations in ^{4}He clusters.
- Using VMC and DMC calculations, we show the emergence of universal n-body short-range correlations
- The values of the n-body contacts were evaluated numerically for $n \leq 5$.
- A good agreement was found to measurements of the structure factor of liquid ^{4}He at high momenta.

BB, Valiente and Barnea, arXiv:1901.11247 (2019)

BB and Petrov, New J. Phys. **20**, 023045 (2018)
BB, Eliyahu and van Kolck, PRA **94**, 052502 (2016)
BB, Kirscher, Konnig, Valderrama, Barnea, and van Kolck, PRL **122**, 143001 (2019)
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Conclusion

- The generalized contact formalism was applied to study short-range correlations in ^{4}He clusters.
- Using VMC and DMC calculations, we show the emergence of universal n-body short-range correlations
- The values of the n-body contacts were evaluated numerically for $n \leq 5$.
- A good agreement was found to measurements of the structure factor of liquid ^{4}He at high momenta.

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