Universal Short Range Correlations in Bosonic Helium Clusters

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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 governed 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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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: $a_\text{s} \approx -23.4$ fm, $a_\text{t} \approx 5.42$ fm, $R = \hbar/m_\pi c \approx 1.4$ fm.

Deuteron binding energy, 2.22 MeV, is close to $\hbar^2/m_\text{t}^2 \approx 1.4$ MeV.

$^4$He atoms: $a \approx 95$ Å $\gg r_\text{vdW} \approx 5.4$ Å.

Ultracold atoms near a Feshbach resonance,

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

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The contact $C$ measures the number of pairs of particles with small separations, $C = \int dR C(R)$.

The Contact - Tan’s Relations

Tan relations connects the contact $C$ with:

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

\[
n_\sigma(k) \longrightarrow \frac{C}{k^4}
\]

- The energy relation

\[
E = T + U + V
\]

The kinetic energy diverges

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

but the sum $T + U$ is regular

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T + U = \sum_\sigma \int \frac{dk}{(2\pi)^3} \frac{\hbar^2k^2}{2m} \left( n_\sigma(k) - \frac{C}{k^4} \right) + \frac{\hbar^2}{4\pi ma} C
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Density-Density correlator at short distances

\[ \langle n_1 \left( R + \frac{r}{2} \right) n_2 \left( R - \frac{r}{2} \right) \rangle \rightarrow \frac{1}{16\pi^2} \left( \frac{1}{r^2} - \frac{2}{ar} \right) C(R) \]

Adiabatic relation

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

Virial theorem For a system in a harmonic trapping potential,

\[ T + U - V = -\frac{\hbar^2}{8\pi ma} C \]

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Ultra cold gas of fermionic $^{40}\text{K}$

J. T. Stewart et al. PRL 104, 235301 (2010)
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Strong and Weak Universality

- **Wave function factorization:** when two particles approach each other,
  \[ \Psi \xrightarrow{r_{ij} \to 0} \phi_2(r_{ij}) A_{ij}(R_{ij}, \{r_k\}_{k \neq i,j}) \]

  \[ C \propto \sum_{ij} \langle A_{ij} | A_{ij} \rangle; \quad \langle A_{ij} | A_{ij} \rangle = \int \prod_{k \neq i,j} dr_k dR_{ij} | A_{ij}(R_{ij}, \{r_k\}_{k \neq i,j}) |^2 \]

- 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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- For finite-range potential, **weak universality** holds, \( \phi_2(r) \) is not sensitive to the system size or state.
quasi-deuteron model: $\sigma_A(\omega) = L^N A^Z \sigma_d(\omega)$

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

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

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

- The 1-body momentum distribution

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

- 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

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

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

\[ \Psi \xrightarrow{r_{ijk} \to 0} \phi_3(x_{ijk}, y_{ijk}) A_3^{(N)}(R_{ijk}, \{r_l\}_{l \neq i,j,k}) \]

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 $a \rightarrow \infty$, 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.
  

- Therefore, there is no need for four-body parameter at leading order.
  

- Same is true for 5- and 6-body clusters, also attached to an Efimov trimer.

\[ B_{3^*}/3 \text{ (mK)} \]

\[ B_N/N \text{ (mK)} \]

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
- **Variational Monte Carlo (VMC)**
  \[
  E_{\text{var}} = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0
  \]
  with $\Psi_T = \prod_{i<j} f(r_{ij})$, where
  \[
  f(r) = \exp \left( -\frac{(p_5 / r)^5}{r} - \frac{(p_2 / r)^2}{r} - p_1 r \right) / r^{p_0}.
  \]
- **Diffusion Monte Carlo (DMC):**
  \[
  \frac{\partial \Psi(r_1 \ldots r_N, \tau)}{\partial \tau} = (T + V - E_R) \Psi(r_1 \ldots r_N, \tau)
  \]
  is treated as a diffusion-reaction process for walkers, distributed according to $\Psi$. $\Psi$ converges to $\Psi_0$ and $E_R$ to $E_0$.
- $\Psi_T$, 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].

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<td>3</td>
<td>126.39</td>
<td>126.40</td>
<td>125.5(6)</td>
<td>124(2)</td>
<td>125.9(2)</td>
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<td>4</td>
<td>557.7</td>
<td>558.98</td>
<td>557(1)</td>
<td>558(3)</td>
<td>557.4(4)</td>
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<td></td>
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<td>1296(1)</td>
<td>1310(5)</td>
<td>1300(2)</td>
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<td>2309(3)</td>
<td>2308(5)</td>
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<td>6677(6)</td>
<td>6679(9)</td>
<td>6697(2)</td>
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<td>10</td>
<td></td>
<td></td>
<td>8495(7)</td>
<td>8532(10)</td>
<td>8519(3)</td>
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</table>

$B_3/B_2 = 16.522688(1)$

$B_4/B_2 = 197.3(1)$

Lattice EFT calculations

$B_N/B_{N-1} \xrightarrow{N \to \infty} 8.567$

DMC-STM

$B_N/B_2 \approx 8.567^N \exp(c_1 + c_2/N), \quad c_1 = -2.06(4) \quad c_2 = -8(2)$
Results: n-body density function

Black line: the reference density $\rho_n$
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:

<table>
<thead>
<tr>
<th>$n$</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
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<tr>
<td>$\tilde{C}_n^\infty$</td>
<td>230 ± 25</td>
<td>500 ± 60</td>
<td>1800 ± 300</td>
<td>5900 ± 1000</td>
</tr>
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Results: The structure factor

Experimental data: Svensson et al., PRB 21, 3638 (1980)
Blue band: theory for contact values of $\tilde{C}_2^\infty \in (200, 250)$
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, Eliyahu and van Kolck, PRA 94, 052502 (2016)
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