Saturation properties of helium drops using a gaussian potential model

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ECT* Workshop

Open Quantum Systems: From atomic nuclei to ultracold atoms and quantum optics

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Universal behavior in few-body systems

Scales

- short-range interactions $\rightarrow r_0$
- natural energy scale $E_n \approx \hbar^2/mr_0^2$

- shallow states $\rightarrow$ large scattering length $a >> r_0$
- unnatural energy scale $E_s \approx \hbar^2/ma^2$

Limits

This two scales define two limits:

- scaling limit: $r_0 \rightarrow 0$ (Thomas collapse)
- unitary limit: $a \rightarrow \infty$ (Efimov states)
- in both cases the ratio $r_0/a \rightarrow 0$

Universal behavior in few-body systems

Two-body scattering: Low energy limit

In the low energy limit: $k \to 0$, the s-wave phase-shift is determined by the effective range expansion:

$$k \cot \delta_0 = -1/a + \frac{1}{2} r_{eff} k^2$$

with r_{eff} the effective range. For shallow states we can extend this low energy expansion to the complex plane $k \to i\kappa$ remembering that $\kappa \cot \delta_0 = i\kappa$

$$\kappa = 1/a + \frac{1}{2} r_{eff} \kappa^2$$

from which

$$\hbar^2 \kappa^2 / m = E_s = \hbar^2 / m a^2 \left(1 + \frac{r_{eff}}{a} + \ldots \right)$$

Universal behavior in few-body systems

Examples

- The helium dimer (as given by the TTY potential):
  $E_d = 1.309$ mk
  $a = 188.78$ a.u.
  $r_{eff} = 13.845$ a.u.
  $E(a, r_{eff}) = 1.311$ mk
- The deuteron:
  $E_d = 2.225$ MeV
  $a^1 = 5.419 \pm 0.007$ fm
  $r^1_{eff} = 1.753 \pm 0.008$ a.u.
  $E(a, r_{eff}) = 2.223$ fm

Gaussian potential model

$$V(r) = V_0 e^{-(r/r_0)^2}$$

with V_0 and r_0 fixed to describe a and E_d

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Gaussian potential model

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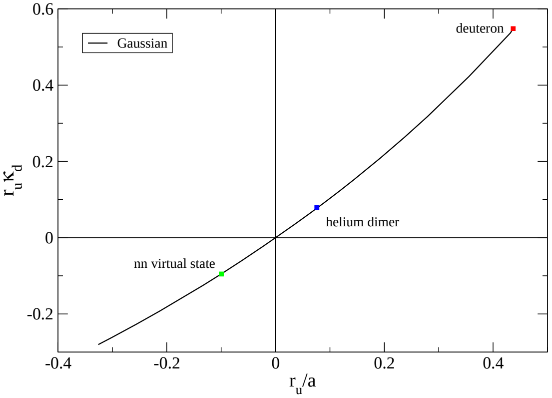
Universal behavior in few-body systems

- When a shallow state exists, a Gaussian potential gives a reasonable description of the low energy regime, bound and scattering states.



The three-boson system

Zero-Range Equations: Efimov spectrum

$$E_3^n/(\hbar^2/ma^2) = \tan^2\xi$$

$$\kappa_* a = e^{\pi(n-n_*)/s_0} e^{-\Delta(\xi)/2s_0} / \cos\xi$$

- The ratio E_3^n/E_2 defines the angle ξ
- The three-body parameter κ_* defines the energy of the system at the unitary limit $E_u = \hbar^2\kappa_*^2/m$
- The product $\kappa_* a$ is a function of ξ governed by the universal function $\Delta(\xi)$
- The universal function $\Delta(\xi)$ is obtained by solving the STM equations (Faddeev equation in the zero-range limit) and is the same for all levels n

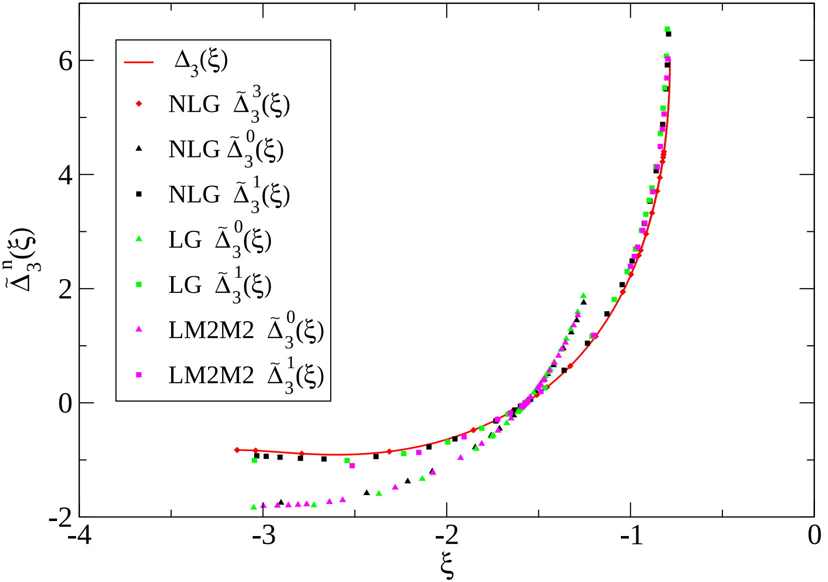
The three-boson system

Finite-Range Equations: Gaussian spectrum

$$E_3^n/E_2 = \tan^2 \xi_n$$

$$\kappa_*^n/\kappa_d = e^{\pi(n-n_*)/s_0} e^{-\widetilde{\Delta}_n(\xi_n)/2s_0} / \cos \xi$$

- The ratio E_3^n/E_2 defines the angle ξ_n
- The three-body parameter κ_*^n defines the energy of the system at the unitary limit $E_u = \hbar^2(\kappa_*^n)^2/m$
- The product $\kappa_*^n a$ is a function of ξ_n governed by the level function $\widetilde{\Delta}(\xi_n)$
- The level function $\widetilde{\Delta}(\xi)$ is obtained by solving the Schrödinger equation in the desired region.


$\Delta_3(\xi)$
NLG $\tilde{\Delta}_3^3(\xi)$
NLG $\tilde{\Delta}_3^0(\xi)$
NLG $\tilde{\Delta}_3^1(\xi)$
LG $\tilde{\Delta}_3^0(\xi)$
LG $\tilde{\Delta}_3^1(\xi)$
LM2M2 $\tilde{\Delta}_3^0(\xi)$
LM2M2 $\tilde{\Delta}_3^1(\xi)$
$\tilde{\Delta}_3^n(\xi)$
ξ
6
4
2
0
-2
-4
-3
-2
-1
0

Using $\widetilde{\Delta}_0(\xi)$

The three-body parameter κ_* for the helium trimer

- The ratio κ_*/κ_d is a function of ξ ($E_3/E_2 = \tan^2\xi$)
- To determine ξ we use experimental results $E_3 = 126$mK and $E_2 = 1.3$mK. Accordingly $\tan^2\xi = 97.0$
- This value of ξ is introduced in the gaussian level function

$$[\kappa_/\kappa_d]^{exp} = [\kappa_/\kappa_d]^{gaussian} = e^{-\widetilde{\Delta}_0(\xi)/2s_0}/\cos\xi$$

and

$$[\kappa_*]^{exp} = 1/\kappa_d^{exp}\left(e^{-\widetilde{\Delta}_0(\xi)/2s_0}/\cos\xi\right)$$

- application to the helium trimer: $[\kappa_*]^{exp} = 0.044a_0^{-1}$

The value of a_-

Finite-Range Equations at $\xi = -\pi$

We define the energy length as $a_B = \sqrt{\hbar^2/mE_2}$. At the angle $\xi = -\pi$ the three body energy is $E_3 = 0$. Therefore the equations are:

$$E_3^n/E_2 = 0$$

$$\kappa_* a_B^- = -e^{-\widetilde{\Delta}(-\pi)/2s_0} = -2.483$$

atomic species with van der Waals tail

The helium trimer as example:

$$a_B^- = -2.483/\kappa_* = -56.4a_0$$

$$a_- = r_B + a_B^- = -49a_0$$

$$a_-/\ell \approx -49/5.1 = -9.6$$

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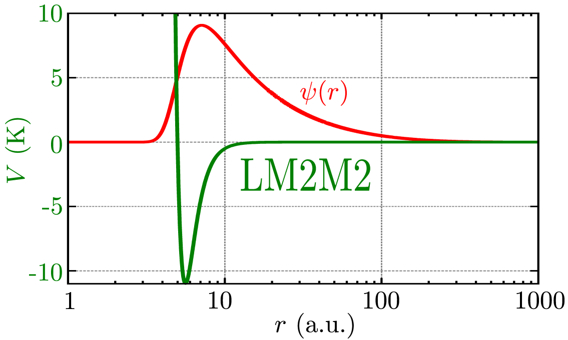
The Helium-Helium system

- The He-He system has been extensively studied in the ’80
- Many realistic potententials have been constructed as for example the Aziz LM2M2 potential



Ground state properties of helium drops

- The Aziz potential has been used to calculate the ground state energies of drops with $3 \leq N \leq \infty$
- For example in V.R. Pandharipande et al., PRL 50, 1676 (1983) using the GFMC method (The Aziz HFDHE2 potential)
- The motivations for that study were twofold:
  i) To compare theoretical results using potential models with experimental data
  ii) To analyze extrapolation formulas from calculations with fix number of atoms to the infinite system
- The E/N experimental value of liquid Helium (-7.14K) was well described. The calculations predicted -7.11K or -7.02K from an extrapolation using results in the range $20 \leq N \leq 112$

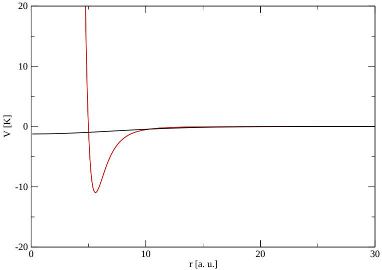
Soft Two-Body Gaussian Potential

Effective low-energy soft potential

- $V(r) = V_0 \; \mathrm{e}^{-r^2/r_0^2}$
- Fix V_0, r_0 to reproduce a and E_2

$V_0 = -1.2344$ K, $r_0 = 10.0$ a.u.

	Gaussian	LM2M2
a_0 (a.u.)	189.41	189.42
r_{eff} (a.u.)	13.81	13.84
E_2 (mK)	-1.303	-1.303



The helium trimer

Problems in the three-body sector

	Soft-Gaussian	LM2M2
$E_3^{(0)}$ (mK)	-150.4	-126.4
$E_3^{(1)}$ (mK)	-2.467	-2.271

Introducing a three-body-soft potential

$$W(\rho_{ijk}) = W_0 \, e^{-2\rho_{ijk}^2/\rho_0^2} \quad (\rho_{ijk}^2 \propto r_{ij}^2 + r_{jk}^2 + r_{ki}^2)$$

potential	$E_{3b}^{(0)}$ (mK)	$E_{3b}^{(1)}$ (mK)
LM2M2	-126.4	-2.265
gaussian	-150.4	-2.467
(W_0 [K], ρ_0 [a.u.])		
$(1.474, 10)$	-126.4	-2.292
$(0.721, 12)$	-126.4	-2.295
$(0.422, 14)$	-126.4	-2.299

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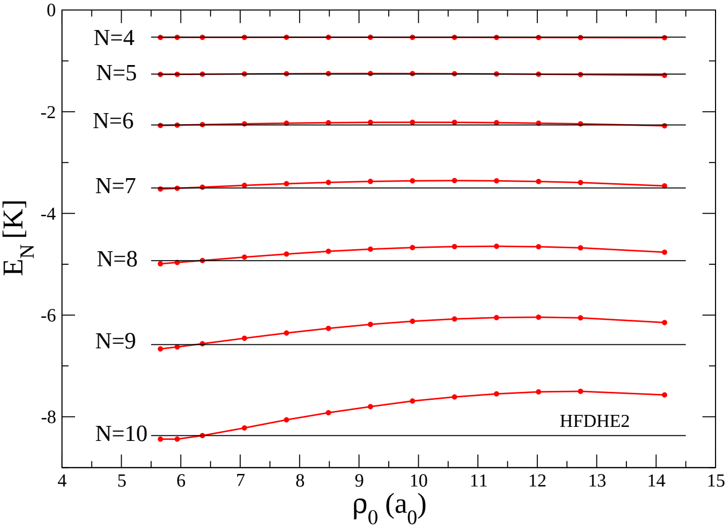
Propagation of universal behavior with N

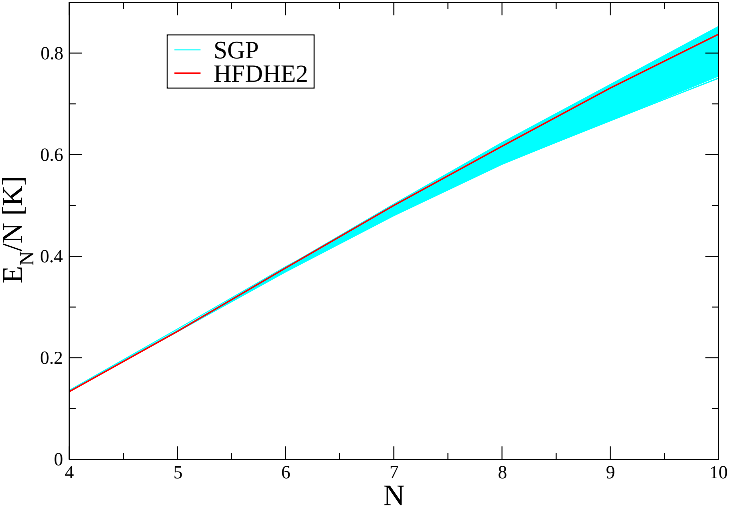
Saturation properties of helium drops

- We define a soft potential model to describe E_3
- It consists in a two- plus a three-body term $V = V(i,j) + W(i,j,k)$
- $V(i,j) = V_0 e^{-r_{ij}^2/r_0^2}$
- $W(i,j,k) = W_0 e^{-\rho_{ijk}^2/\rho_0^2}$
- W_0 is determined from E_3
- ρ_0 is taken as a parameter
- E/N is calculated for increasing values of N as a function the ρ_0
- the saturation properties are determined from a liquid drop formula:
  $E_N/N = E_v + E_s x + E_c x^2$ with $x = N^{-1/3}$
- In general drops with N around 100 is sufficient to determine E_v and E_s

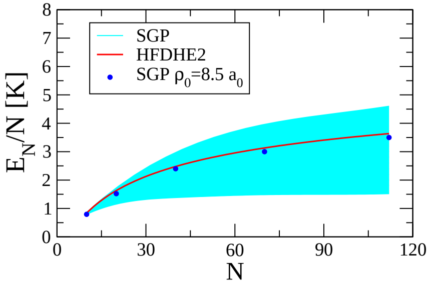
drops with $N \leq 10$

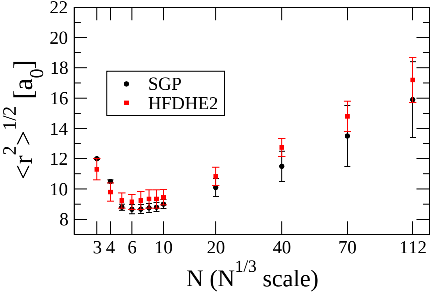


drops with $N \leq 10$

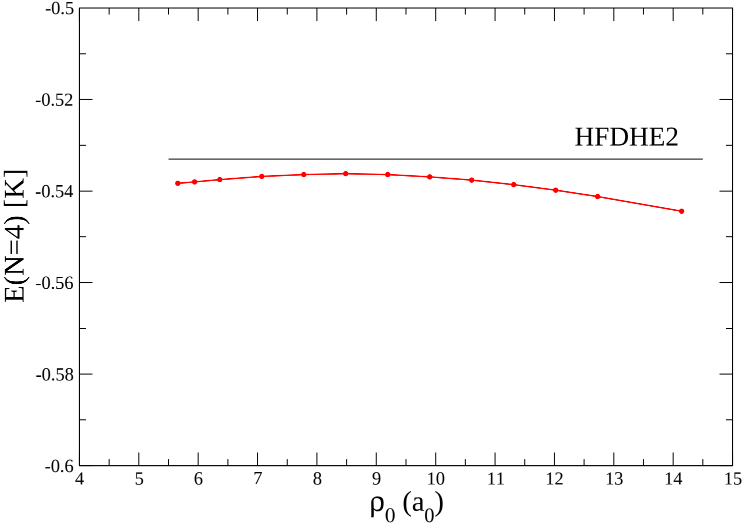


drops with $N \leq 112$





drops with $N = 4$



Propagation of universal behavior with N

Saturation properties of helium drops

- Using the appropriate value of ρ_0
- we obtain (in K):
  $E_N/N = 6.79 - 18.0x + 9.98x^2$
- To be compared to the results of the HFDHE2 potential:
  $E_N/N = 7.02 - 18.8x + 11.2x^2$
- The experimental result is 7.14 K
- for the surface tension $t = E_s/4\pi r_0^2(\infty)$
  the experimental value is 0.29 KA^2
  with the gaussian soft potential the result is 0.27 KA^2
- Since the potential model is determined only from the two, three and four body sector, we can conjeture that the saturation energy can be extracted from E_2, E_3 and E_4
- Accordingly we can think in a different expansion of E_N/N

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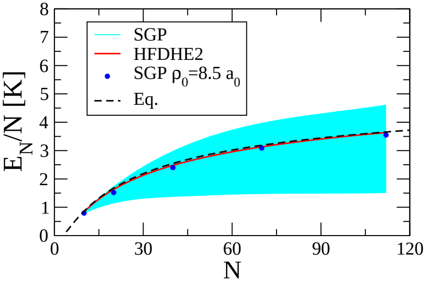
- For example we propose the following formula:

$$\frac{E_N}{N} = E_v^{(0)} \frac{1-(3/N)^{1/4}}{1+\frac{3E_4}{4E_3}(3/N)} ,$$



- From the equation:

$$\frac{E_N}{N} = E_v^{(0)} \frac{1-(3/N)^{1/4}}{1+\frac{3E_4}{4E_3}(3/N)}$$

- The saturation energy $E_v^{(0)}$ can be determined using a single value of E_N/N
- using the $N = 4$ value we obtain

$$\frac{E_v^{(0)}}{E_4} = 3.602\left(1+\frac{9E_4}{16E_3}\right)$$

- Using the GFMC ratio $E_4/E_3 = 4.55$, it results $E_v^{(0)}/E_4 = 3.602$
- This analysis suggests the possibility of describing $E_v^{(0)} = \xi_4 E_4$ at the unitary limit with ξ_4 a universal number?

Conclusions

- Helium drops have been studied using soft gaussian two- and three-body potentials
- The range and depth of the two-body gaussian have been fixed by a and E_2.
- The depth of the three-body gaussian was fixed by the trimer energy. Its range was taken as a parameter
- The soft potential has to follow the original potential in the description of the drops.
- However the original potential is a two-body interaction: the potential energy increases as the number of pairs
- The potential energy of the soft potential has an attractive two-body term which increases as the number of pairs and a repulsive three-body term increasing as the number of triplets

Conclusions

- The range of the three-body interaction has been taken as a parameter to set the total energy as close as possible to the original one
- Using this argument we have extended the leading order description to $N \to \infty$
- Moreover a four-body interaction seems not necessary at leading order