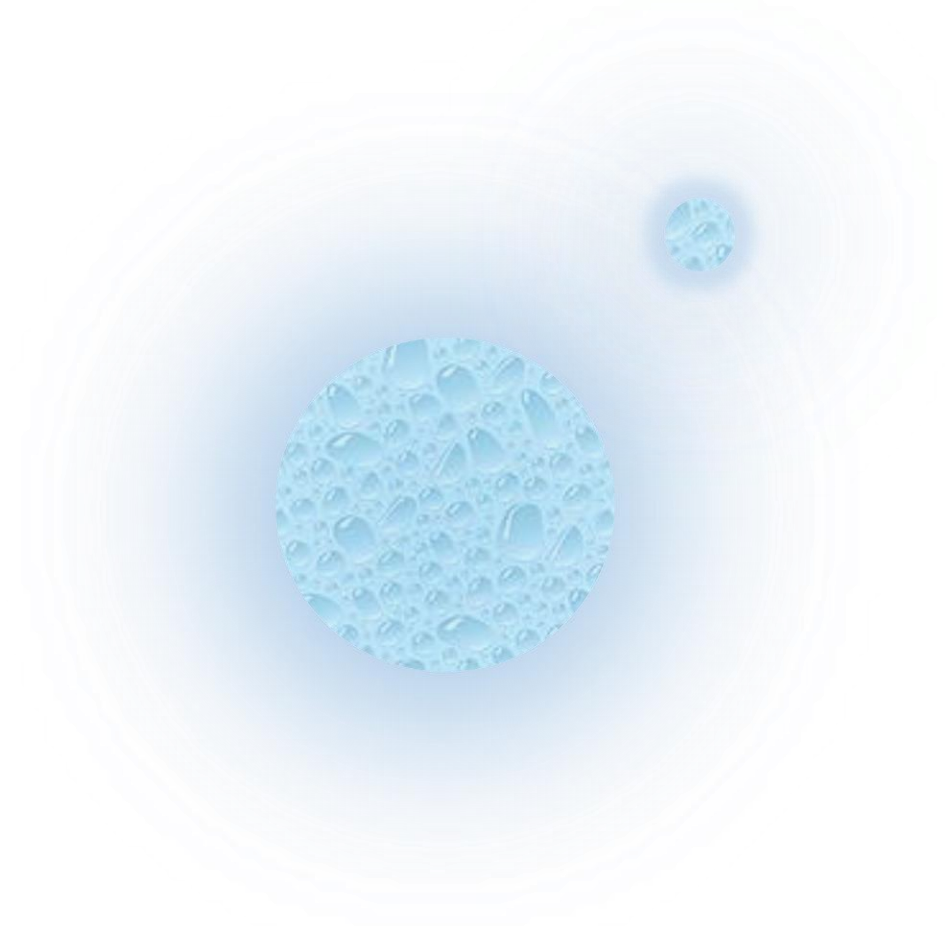
Hyperspherical Cluster Model for Bosons:

Application to Sub-Threshold Halo States in Helium Drops



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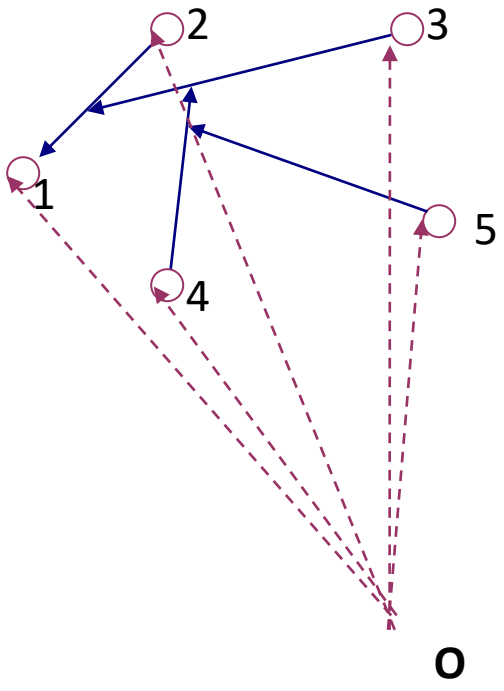
Co-ordinates in the A-body system:



- Individual: $\boldsymbol{r}_1, \boldsymbol{r}_2, \ \ldots \ \boldsymbol{r}_A$

- Jacobi $$\boldsymbol{\xi}_i = \sqrt{\frac{i}{i+1}}\left(\frac{1}{i}\sum_{i=1}^{j}\boldsymbol{r}_j - \boldsymbol{r}_{i+1}\right)$$

- Hyperspherical: **hyperradius** ρ, **hyperangles** $\theta_1, \theta_2, \ldots \theta_{3A-4}$

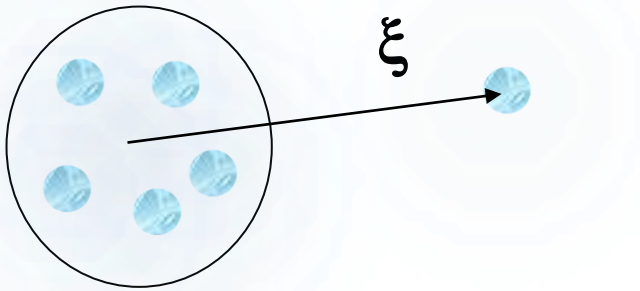
$$\begin{aligned}
\xi_1 &= \rho \sin\theta_{3A-4} \cdots \sin\theta_2 \sin\theta_1 , \\
\xi_2 &= \rho \sin\theta_{3A-4} \cdots \sin\theta_2 \cos\theta_1 , \\
&\cdots \\
\xi_{3A-4} &= \rho \sin\theta_{3A-4} \cos\theta_{3A-5} , \\
\xi_{3A-3} &= \rho \cos\theta_{3A-4} .
\end{aligned}$$

$$\rho^2 = \sum_{i=1}^{A-1}\boldsymbol{\xi}_i^2 = \sum_{i=1}^{A}\boldsymbol{r}_i^2 - \boldsymbol{R}_A^2 = \frac{1}{A}\sum_{i<j}^{A}\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)^2$$

Hyperspherical Cluster Harmoncs basis

A = (A-1) + 1

N.K. Timofeyuk, Phys. Rev. C **76**, 044309 (2007)
N.K. Timofeyuk, Few-Body Syst. **64**, 29 (2023)



Symmetrised product of the hyperspherical harmonics associated with A-1 and hyperangular function that depend on relative separation between A-1 and the last particle:

$$\mathcal{Y}_{K\gamma}(\hat{\boldsymbol{\rho}}) = \mathcal{N}_{K\gamma}^{-1}\ \mathcal{S}\left[Y_{K_c\gamma_c}(\hat{\boldsymbol{\rho}}_c)\ \times \varphi_{K_c\nu l}(\theta_1, \hat{\xi}_1)\right]_{LM}$$

$$\mathcal{S} = \frac{1}{A^{1/2}}\left(1 + \sum_{i=1}^{A-1} P_{iA}\right)$$

$$\varphi^{(n)}_{K_c\nu lm}(\theta, \hat{\xi}) = N^{(n)}_{K_c\nu l}\ \cos^l\theta \sin^{K_c}\theta\ P_\nu^{K_c+\frac{n-5}{2}, l+\frac{1}{2}}(\cos 2\theta) Y_{lm}(\hat{\xi})$$

$$N^{(n)}_{nK_cl} = \left(\frac{2\nu!\,(2\nu + K_c + l + (n-2)/2)\Gamma(\nu + K_c + l + (n-2)/2)}{\Gamma(\nu + l + 3/2)\,\Gamma(\nu + K_c + (n-3)/2)}\right)^{1/2}$$

$\rho_c, \theta_1, \theta_2, \ldots \theta_{3A-7}$

$\rho^2 = \rho_c^2 + \xi^2$

$\xi = \rho \sin\theta$

$\rho_c = \rho \cos\theta$

HCH are eigenfunctions of the angular part of the kinetic energy operator

$$\Delta_{\hat{\rho}}\mathcal{Y}_{K\gamma}(\hat{\boldsymbol{\rho}}) = -K(K + 3A - 5)\mathcal{Y}_{K\gamma}(\hat{\boldsymbol{\rho}})$$

Expansion of the many-body wave function onto HCH basis is the same as in general expansion onto hyperspherical harmonics basis

$$\Psi(\boldsymbol{\rho}) = \rho^{-\frac{n-1}{2}} \sum_{K\gamma} \chi_{K\gamma}(\rho) Y_{K\gamma}(\hat{\rho})$$

$$\left(-\frac{d^2}{d\rho^2} + \frac{\mathcal{L}_K(\mathcal{L}_K+1)}{\rho^2} - \frac{2m}{\hbar^2}\left(E - V_{K\gamma,K\gamma}(\rho)\right)\right)\chi_{K\gamma}(\rho) = -\frac{2m}{\hbar^2} \sum_{K'\gamma' \neq K\gamma} V_{K\gamma,K'\gamma'}(\rho)\chi_{K'\gamma'}(\rho)$$

$$\mathcal{L}_K = K + \frac{n-3}{2}$$

To calculate hyperradial potentials $V_{K\gamma,K'\gamma'}(\rho) = \langle Y_{K\gamma}(\hat{\rho}) | \hat{V} | Y_{K'\gamma'}(\hat{\rho}) \rangle$

one needs to know

- Extended versions of the Raynal-Revai coefficients
- Fractional parentage coefficients to extract particles from the core A-1

Application to helium drops with A = 5,6,8,10

Soft gaussian two-body potential

*M. Gattobigio, A. Kievsky, M. Viviani, Phys. Rev. A **84**, 052503 (2011)*

$$V_{ij}(r) = V_0 \exp\left(-\frac{r^2}{a_0^2}\right)$$

$$V_0 = -1.227 \text{ K}$$

$$a_0 = 10.03 \text{ a.u.}$$

$$\hbar^2/m = 41.281307 \text{ (a.u.)}^2\text{K}$$

Convergence of g.s. energies for single-gaussian potentials greatly improves with *A*

*(N.K. Timofeyuk, Phys. Rev. A **86**, 032507 (2012))*

$K_c = 0$ approximation

$$\mathcal{Y}_\nu(\hat{\boldsymbol{\rho}}) = \mathcal{N}_\nu^{-1}\mathcal{S}\left[Y_0(\hat{\rho}_c)\varphi^{(n)}_{0\nu 0}(\theta_1, \hat{\xi}_1)\right]$$

	$A=5$				$A=6$			
	g.s.		1ex		g.s.		1ex	
$K_{\max}$	HH	HCM	HH	HCM	HH	HCM	HH	HCM
0	1.9131	1.9131	0.64284	0.64284	3.7731	3.7731	2.0107	2.0107
4	1.9412	1.9366	0.74601	0.73503	3.8076	3.8024	2.0109	2.1260
6	1.9441	1.9381	0.77879	0.75940	3.8099	3.8034	2.1662	2.1448
8	1.9450	1.9385	0.80247	0.77666	3.8108	3.8038	2.1886	2.1606
10	1.9452	1.9386	0.81388	0.78694	3.8109	3.8038	2.1964	2.1672
12	1.9452	1.9386	0.82087	0.79250	3.8109	3.8038	2.2008	2.1706
14	1.9452	1.9386	0.82484	0.79608	3.8109	3.8038	2.2027	2.1723
16			0.82723	0.79817			2.2036	2.1731
18			0.82867	0.79949			2.2040	2.1736
20			0.82958	0.80032			2.2041	2.1738
22			0.83015	0.80085			2.2042	2.1739
24			0.83050	0.80119			2.2042	2.1740

	$A=8$				$A=10$			
	g.s.		1ex		g.s.		1ex	
$K_{\max}$	HH	HCM	HH	HCM	HH	HCM	HH	HCM
0	9.7159	9.7159	7.1217	7.1217	18.855	18.854	15.551	15.551
4	9.7607	9.7551	7.2720	7.2568	18.908	18.902	15.709	15.695
6	9.7623	9.7557	7.2882	7.2685	18.909	18.902	15.720	15.703
8	9.7632	9.7560	7.3053	7.2794	18.910	18.902	15.734	15.711
10	9.7633	9.7560	7.3089	7.2822	18.910	18.902	15.736	15.712
12	9.7633	9.7561	7.3108	7.2834	18.910	18.902		15.713
14	9.7633	9.7561		7.2839				15.713
16				7.2840				
18				7.2841				

Overlap of two wave functions that differ by one particle:

$$\langle A-1|A_{g.s.}\rangle$$

$$\langle A-1|A^{*}\rangle$$

$$I(\boldsymbol{r}) = \sqrt{A}\langle \Psi_{A-1}(1,\ldots,A-1)|\Psi_A(1,\ldots,A-1,A)\rangle$$

are called:

- **overlap integrals** (or **overlap functions**) in nuclear physics
- **Dyson orbitals** in atomic and molecular physics

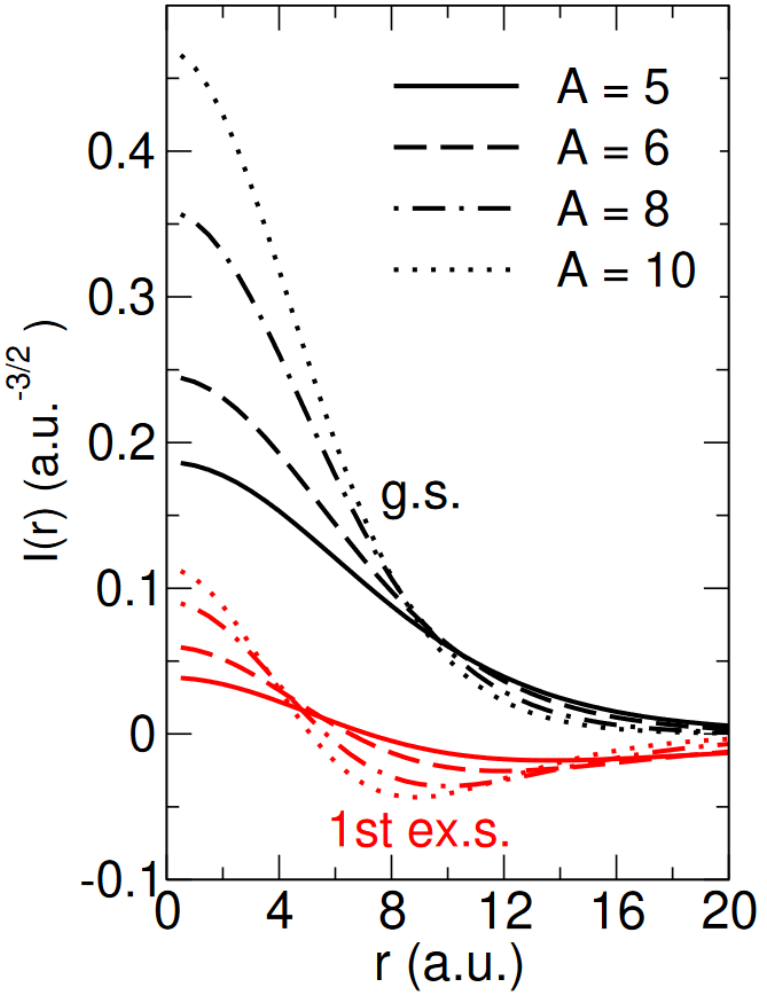
Used for:

- *Nuclear physics*: one-nucleon removal reaction like transfer, knockout and radiative nucleon capture
- *Atomic physics*: photoelectron spectroscopy and *(e, 2e)* ionization experiments

In $K_c = 0$ approximation

$$I(r) = \mu^{3/4} \sum_{\nu=0}^{\nu_{\max}} N_{0\nu 0}^{(n)} \sqrt{\mathcal{N}_\nu} \times \int_0^\infty d\rho_c \frac{\rho_c^{\frac{n-4}{2}} \chi_0^{(A-1)}(\rho_c)\, \chi_\nu^{(A)}\left(\sqrt{\rho_c^2+\mu r^2}\right)}{\left(\rho_c^2+\mu r^2\right)^{\frac{n-1}{2}}} P_\nu^{\frac{n-5}{2},\frac{1}{2}}\left(\frac{\mu r^2-\rho_c^2}{\mu r^2+\rho_c^2}\right)$$

$$\mu = (A-1)/A$$



Asymptotic behaviour of single-particle overlaps:

in the case of neutral particles and s-wave orbital momentum

$$I_{as}(r) = C\,\frac{\exp(-\kappa r)}{r}$$

Asymptotic Normalization Coefficient (ANC)

$$\kappa = \sqrt{2\mu(E_A - E_{A-1})/\hbar}$$

ANCs determine peripheral processes involving one particle

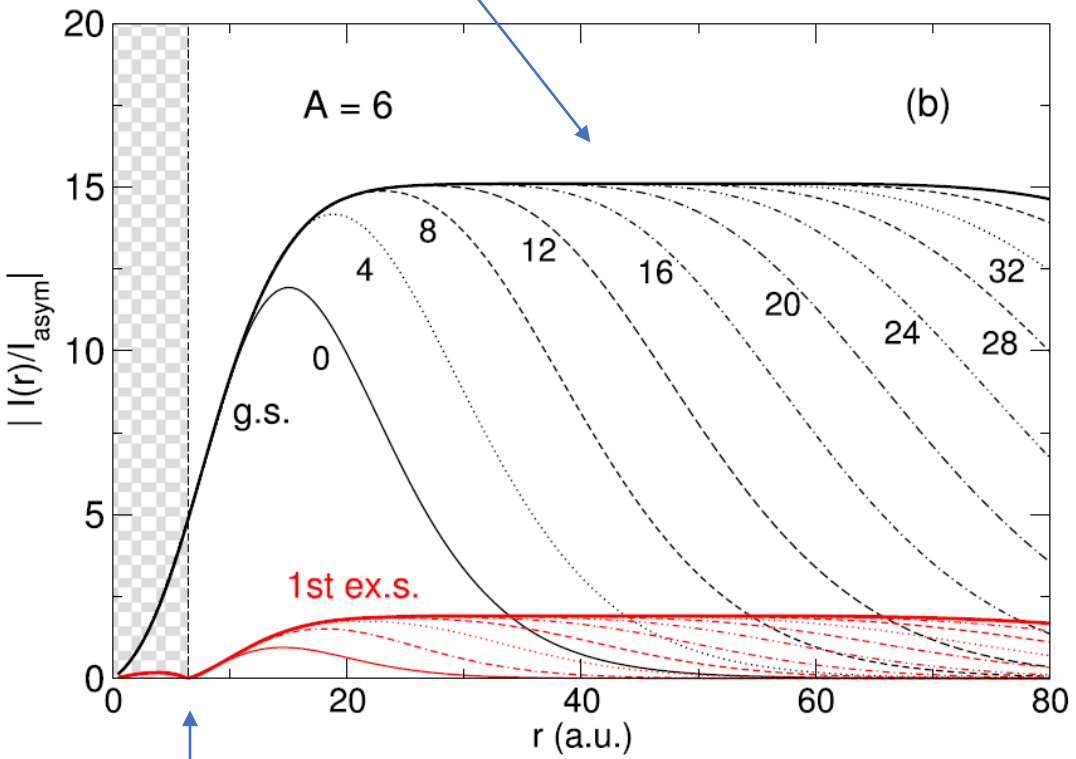
Examples from nuclear physics:

- radiative proton capture
- many transfer reactions

$$\frac{I(r)}{I_{as}(r)}$$

$$\langle A-1|A_{g.s.}\rangle$$

$$\langle A-1|A^*\rangle$$



r.m.s. radius of A=6 system

Where does the valence particle stay?

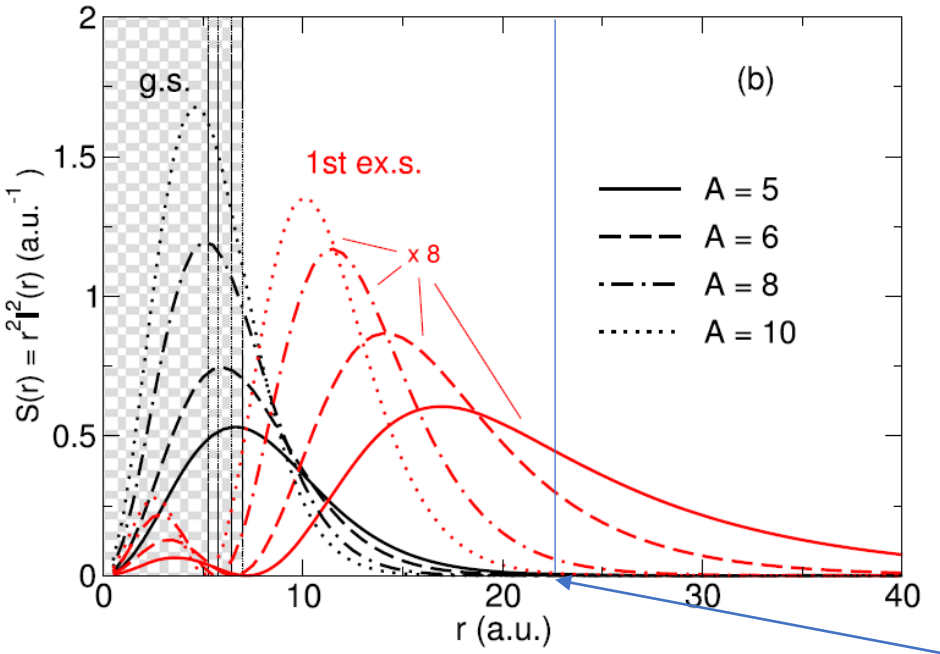
Probability density $P(r)$ to find the particle at location r

$$P(r) = \frac{r^2 I^2(r)}{\int_0^\infty dr\, r^2 I^2(r)}$$

Contribution to the r.m.s. radius of the valence orbit:

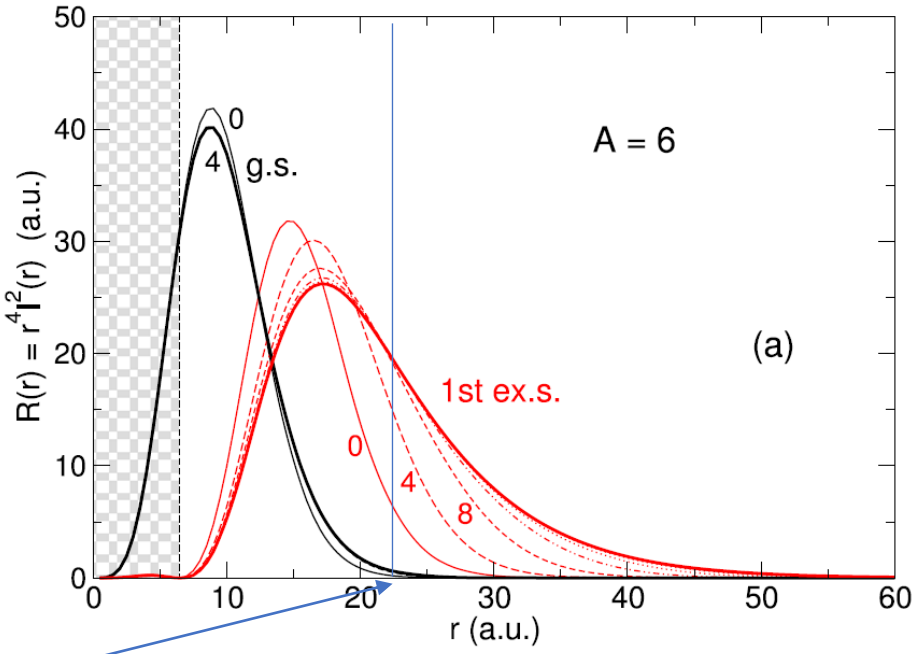
$$R(r) = r^4 I^2(r)$$

Position of maximum in $R(r)$ gives the r.m.s. radius of the orbit.



$\langle A-1|A_{g.s.}\rangle$

$\langle A-1|A^*\rangle$



Asymptotics starts here

First exited states are two-body molecules. Are they halos?

Spectroscopic factors

$$S = \int_0^\infty dr\, r^2 I^2(r)$$

- can be related to occupancies of the single-particle orbitals of the many-body system
- can be interpreted as the numbers of ($A-1$) subsystems in a chosen state inside A
- In atomic physics *SFs* are related with the probability of a selected ionization channel and are often called probability factors or pole strengths

$A-1$	$A=5$		$A=6$		$A=8$		$A=10$	
	g.s.	1ex	g.s.	1ex	g.s.	1ex	g.s.	1ex
g.s.	4.67	1.36	5.74	1.32	7.78	1.25	9.79	1.21
1ex	0.11	1.39	0.17	3.31	0.16	5.85	0.14	8.03
2ex		0.03	0.02	0.25	0.01	0.30	0.01	0.27
3ex	0.01	0.09		0.01		0.04		0.02
4ex	0.01	0.13		0.02		0.01		
5ex	0.02	0.15		0.02				
6ex	0.02	0.15		0.03				
7ex	0.02	0.13		0.03				
8ex	0.02	0.12		0.03				
9ex	0.02	0.10		0.03				
10ex	0.02	0.08		0.03				
11ex	0.01	0.07		0.03				
12ex	0.01	0.05		0.03				
13ex	0.01	0.04		0.02				
14ex	0.01	0.03		0.02				
15ex	0.01	0.02		0.02				
sum	4.97	3.94	5.93	5.21	7.95	7.45	9.94	9.53
max	5	5	6	6	8	8	10	10

Sum rules: for any selected state of A

$$\sum_{\text{all } i \text{ in } A-1} S_i = A$$

Conclusions

- Hyperspherical Cluster Harmonics basis can be used to restore correct long-range behaviour of particles

- HCM predicts molecular structure of first excited states in helium drops where one atom stays far apart from the rest.

However:

Conclusions are done for a single-gaussian He-He potential only, which does not provide saturation with increasing number of atoms . Including 3-body force (3BF) is needed. More HHs for the core is needed if 3BF are to be included.

Questions for future:

- Will halo structure of excited states in helium drops survive for realistic potentials? Is this structure universal? How it behave at unitary limit?

- Can HCH be used for scattering calculations?