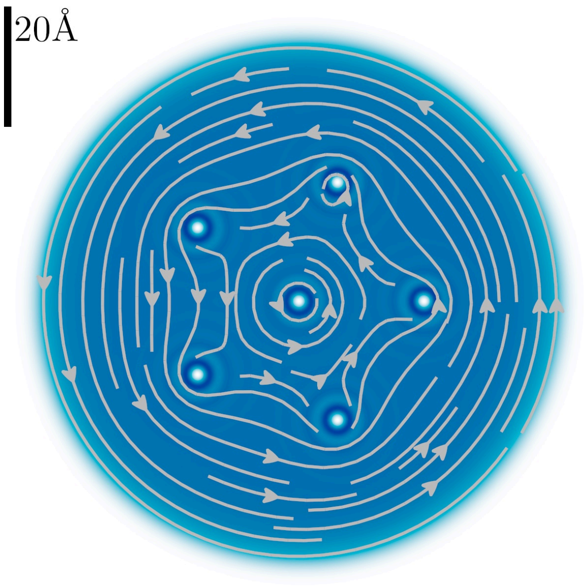
Superfluid ^{4}He nanodroplets: The many impurities, many vortices cornucopia



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Our goal: Within DFT, contribute to answer to some non-trivial questions:

- How impurities are captured by vortex lines inside a He droplet?

- How impurities clusterize inside a He droplet and how the process is affected by the presence of vortices?

- How superfluid He droplets "rotate"? Vortex arrays in ^{4}He droplets and in ^{3}He-^{4}He mixed droplets as well

(… plus results for normal ^{3}He droplets after the talk by Swetha Erukala)

Why DFT (static and time-dependent)?

- DFT emerges as a compromise between accuracy and numerical feasibility. Semi- or phenomenological method (as any other real-time approach!).

- Able to describe physical situations that more microscopic approaches are *-at present-* unable to. Firmly established with limitations of its own.

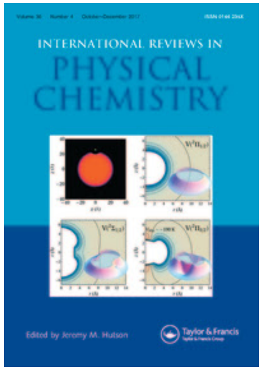
- Full self-consistent description.

- *An useful tool that allows for close interplay between theory and experiment*.

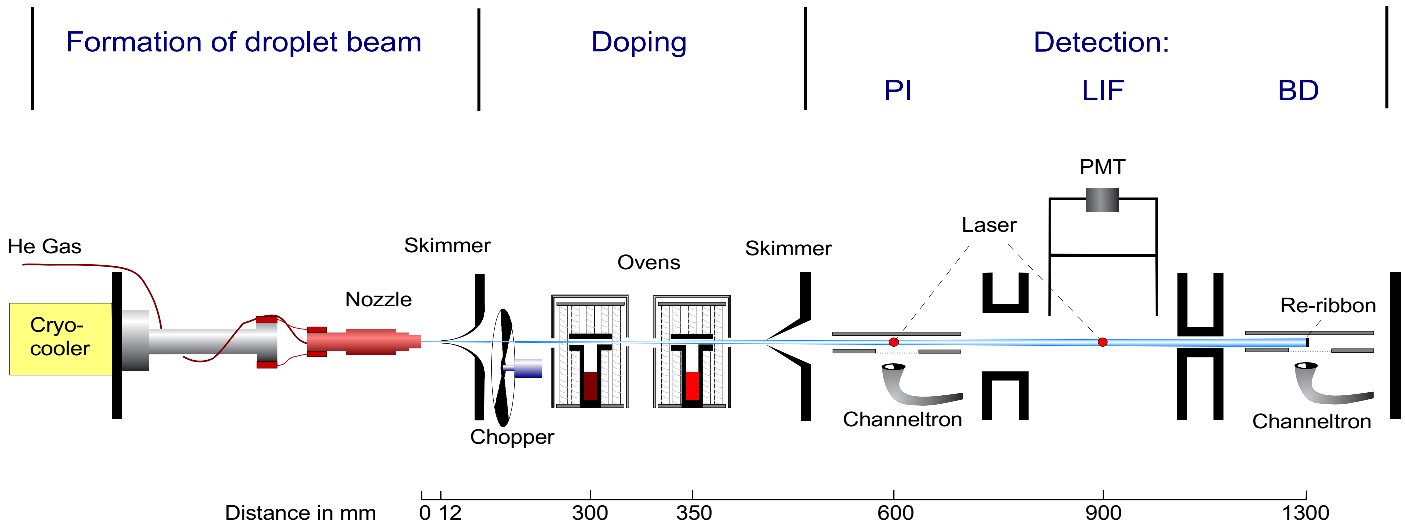
- Key ingredients: accurate functionals and He-impurity potentials

If interested, look at our recent review on the subject:

F. Ancilotto et al, Int. Rev. Phys. Chem. **36**, 621 (2017)



Where vortices are expected to be nucleated?



- Very large droplets can gain angular momentum due to inhomogeneous flow through the nozzle of the "helium machine".

Droplets there are believed to be in the normal, non-superfluid phase (T_{boil} =4.2K).
Rotation may lead to formation of quantized vortices in the droplets; mechanism effective for very large droplets.

- Also in the doping chambers: impurity capture may lead to vortex nucleation [Mateo et al, JCP **140**, 131101 (2014); Leal et al, PCCP **16**, 23206 (2014)]

Xe 200 m/s against $^{4}\mathrm{He}_{1000}$ hosting a vortex line

[Coppens et al, PCCP 19, 24805 (2017)]

“Pinball machine”effect: not necessarily a first-passage capture

- Bending and twisting excitations of the vortex line (Kelvin waves) accompanies the “capture” of the impurity.
- Orbiting around the vortex line, a different kind of impurity capture to have in mind.

Capture of several impurities

[Coppens et al, PCCP just submitted]

Time-consuming calculations: A systematic study hopeless

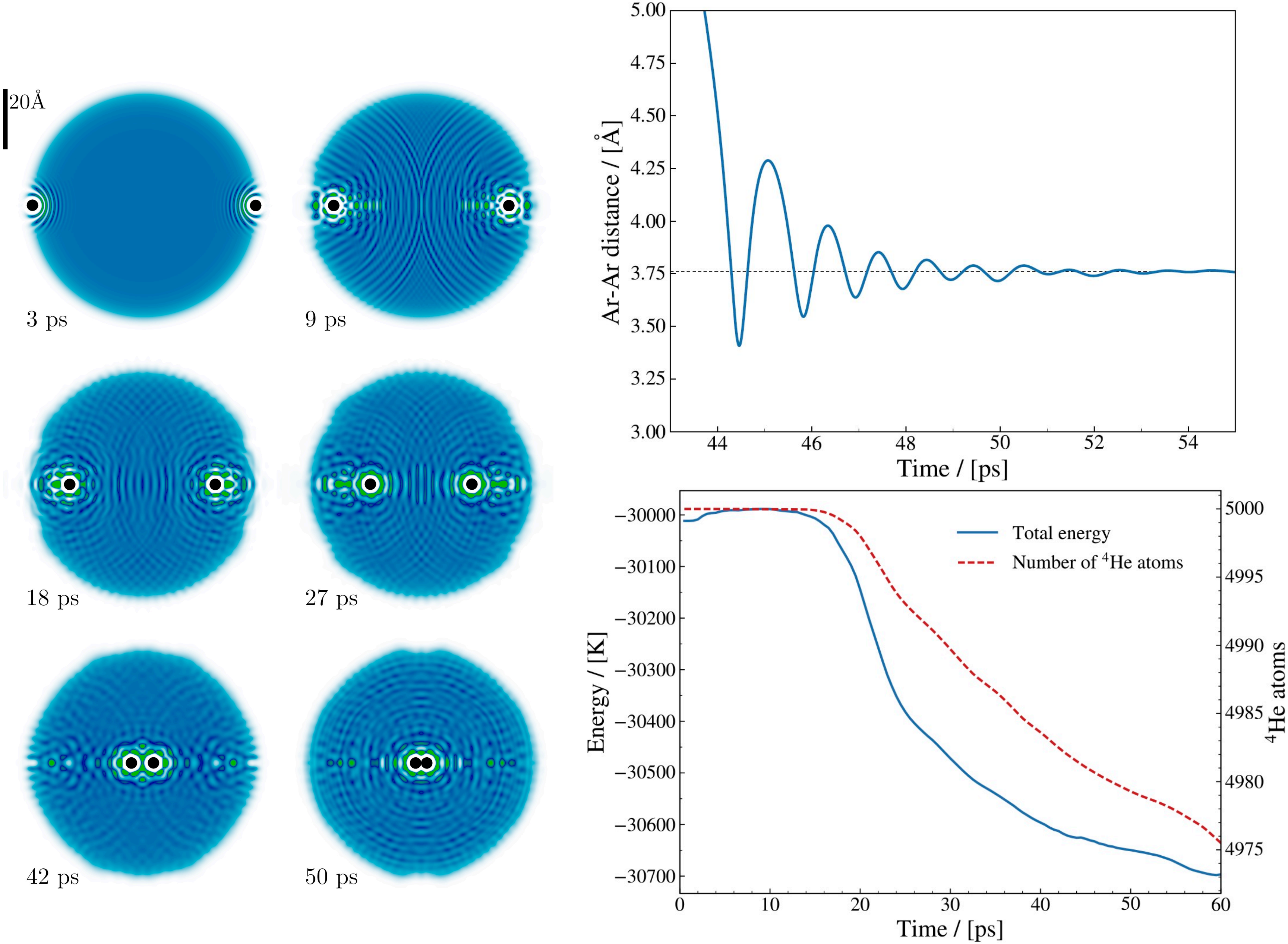
[Hauser et al, PCCP **17**, 10805 (2015)]

Hence, cases of study must be judiciously chosen.

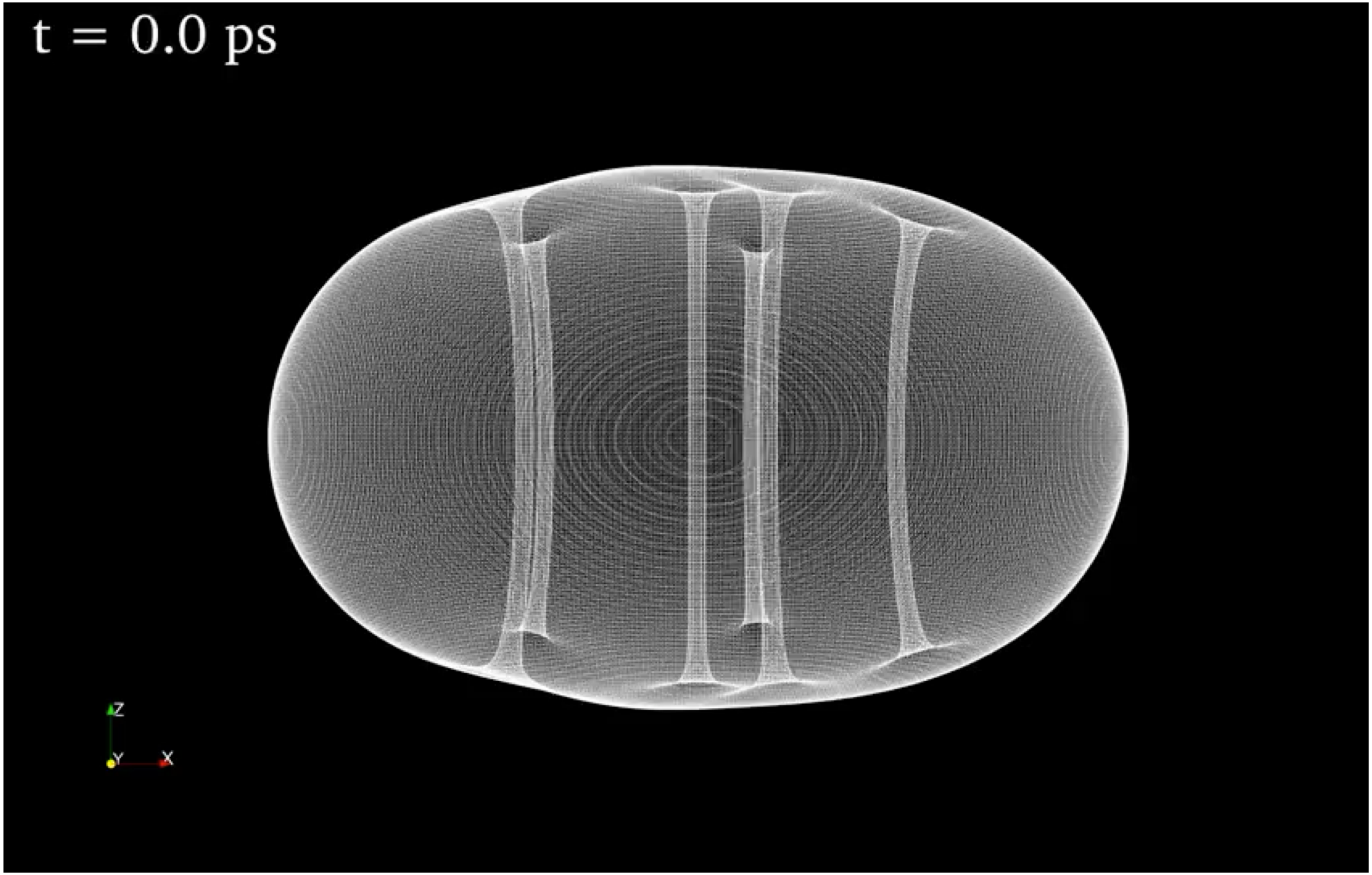
- Choose an interesting yet "simple" impurity (→ He-impurity and impurity-impurity pair potentials known, treat it as a classical particle, cluster structure fairly OK in the pair-sum approximation)
- Not too many impurities, nor too large a droplet, nor too many vortices.
- Rather "symmetric", L=0 initial droplet-impurities configurations
- Address simultaneous or sequential (delayed) captures

Our choice: 2 or 6 Ar atoms; n_v=6 vortex array, $^4He_{5000}$ droplet

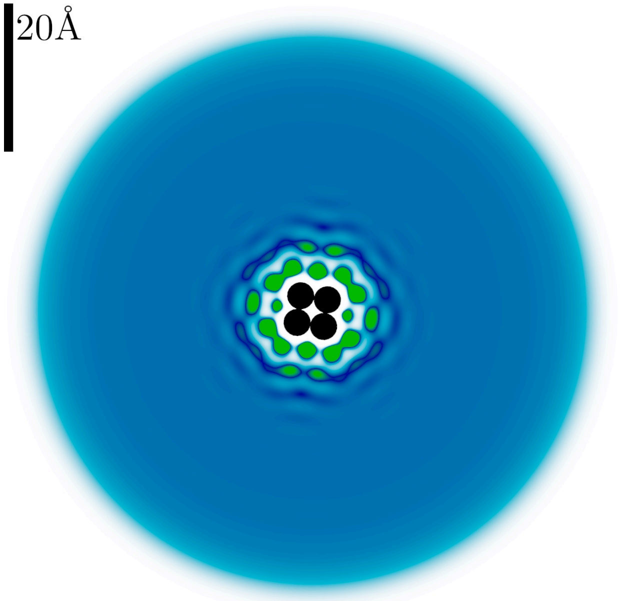
Two Ar atoms dimerize at 360 m/s (thermal velocity)



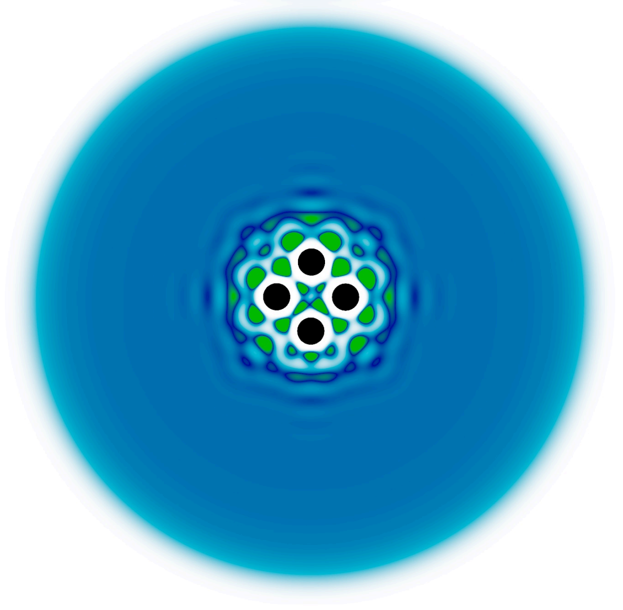
Influence of the presence of vortices (I)



Increasing the number of impurities



Solvation of the Ar_6 cluster pre-formed



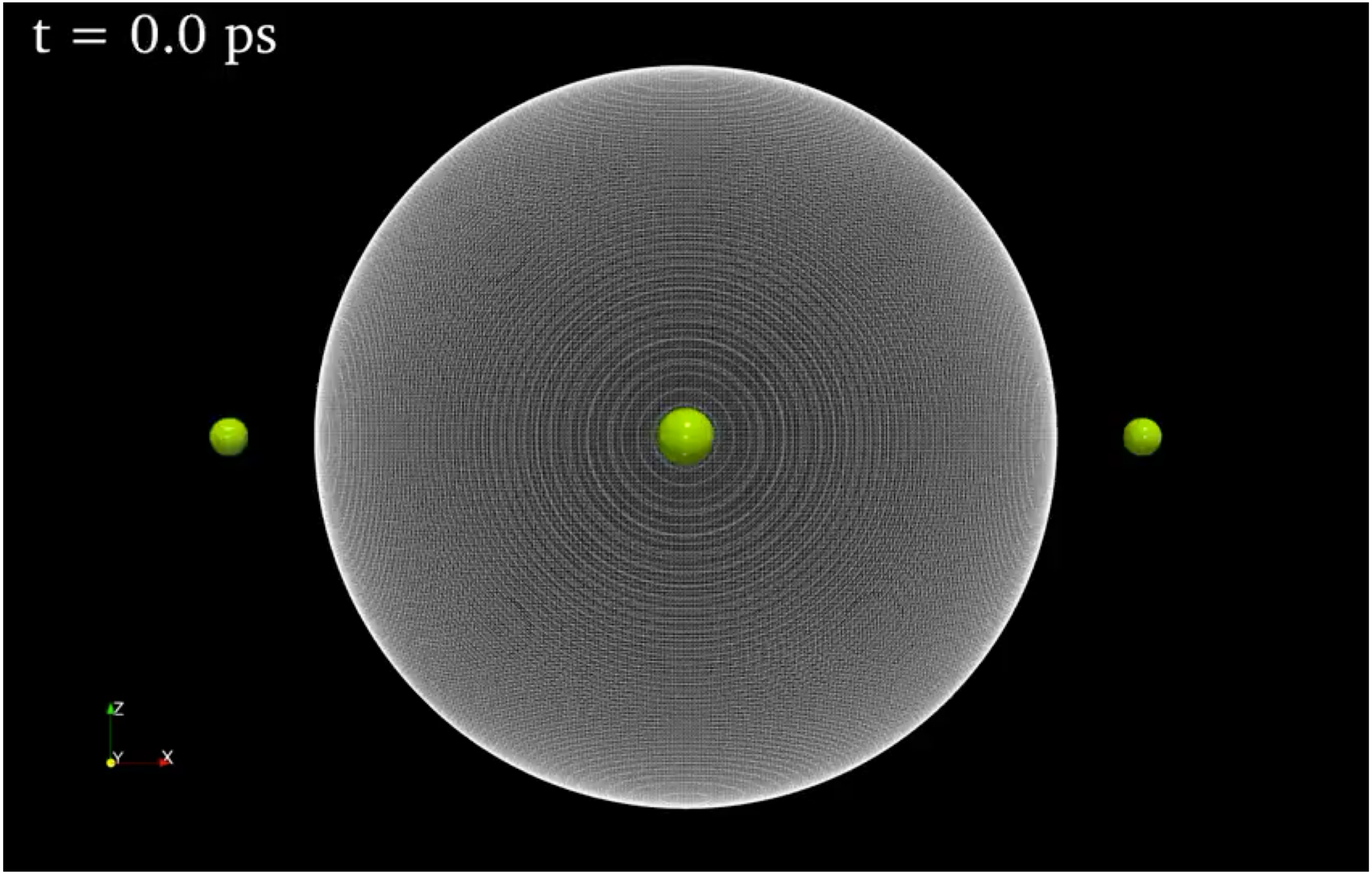
Clustering of 6 Ar atoms at 100 m/s hitting the droplet simultaneously along the Cartesian axes, t=125 ps:

Outcome:

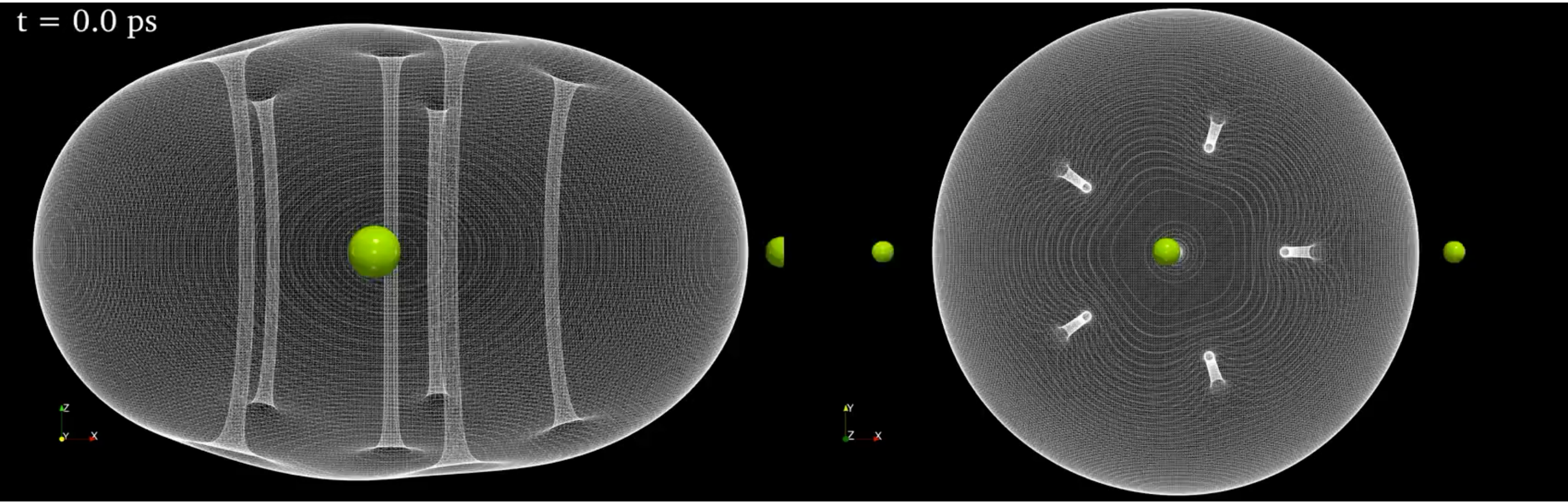
A loosely bound, stretched Ar_6 cluster is dynamically formed ("cage effect")

Artifact of the preparation?

Simultaneous vs sequential capture



Influence of the presence of a vortex array



(No time delay, superflow deflects impurities)

Some conclusions to have in mind:

- Dynamics has a crucial influence on the clustering process
- Impurity and droplet dynamics *are strongly coupled*
- Impurities are dynamically captured by vortices, *not a trivial point!*

(Ar binding energy to a vortex, 5 K; E_{kin} = 311 K at 360 m/s)

Positive message: Other less symmetric preparations of the capture process will lead to the clustering of impurities

"Rotating" superfluid droplets, a subtle issue…

Key difference between classical and superfluid ^{4}He droplets:

- Classical fluids are rather incompressible and viscous: droplets **eventually** rotate as rigid bodies:

$$\boldsymbol{\omega} = \mathbf{r} \times \mathbf{v} \quad \Rightarrow \quad \mathbf{v} = \boldsymbol{\omega} \times \mathbf{r} \quad \Rightarrow \quad \nabla \times \mathbf{v} = 2\,\boldsymbol{\omega}$$

- Superfluid ^{4}He **flows irrotationally**: $\nabla \times \mathbf{v} = 0$ **(potential flow)**

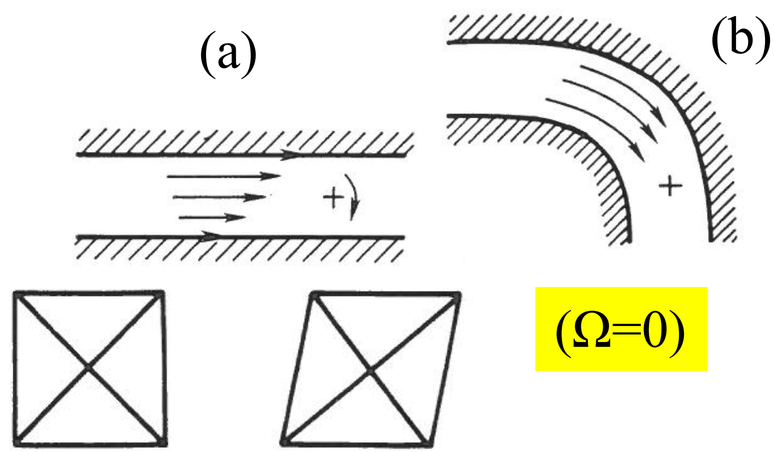
Vorticity $\boldsymbol{\Omega} = \nabla \times \mathbf{v}$ is zero for the superfluid (in absence of vortices)

How does a fluid rotate?

[D.J. Tritton, Am. J. Phys. **50**, 421 (1982); Donnelly, *Quantized vortices in He II*]

- Motion represented by a combination of translation, rotation and deformation of the fluid elements
- **Vorticity $\Omega = \nabla \times \mathbf{v}$ is a measure of fluid-element rotation** in a general situation in which they also undergo distortion
- **Rotation** is formulated in terms of local changes of orientation, and does not refer to the trajectory of the fluid element: important to distinguish between fluid element rotation and motion along a curved path: One may have irrotational flow $\nabla \times \mathbf{v} = 0$ with curved fluid element paths

(as around a linear vortex!!!)



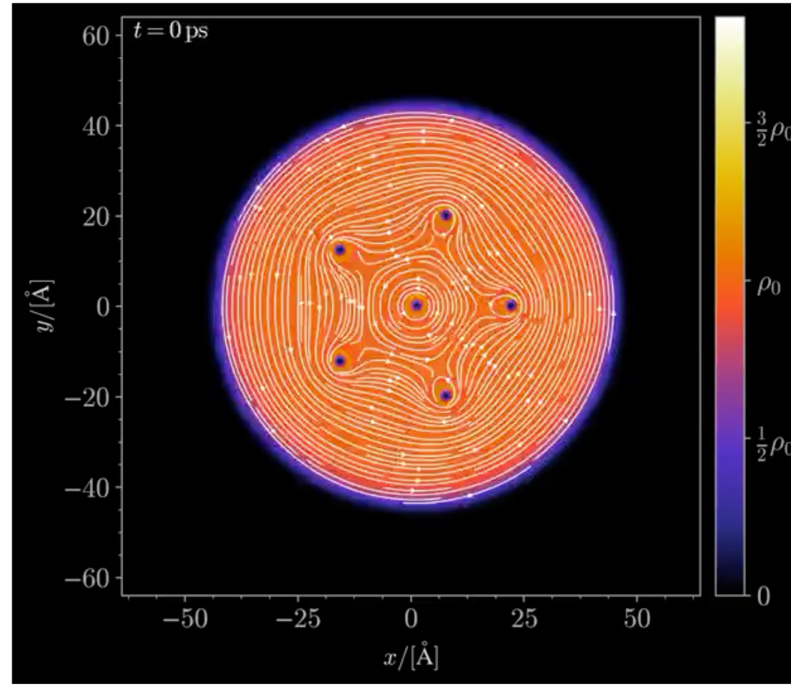
In
- a) A par of diagonals will rotate (simple shear flow)
- b) Orientation of diagonals does not change

($\Omega \neq 0$)

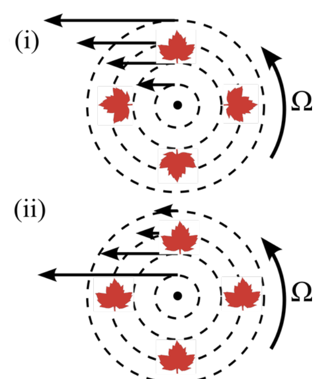
It is **very** important to keep in mind the distinction between vorticity and the curvature of streamlines

Potential flow superimposed on rigid-body rotation of the vortex cores (the magic of vortex arrays!)

Dancing vortices:



Only vortices



(i) Rigid body rotation

(ii) Quantum vortex

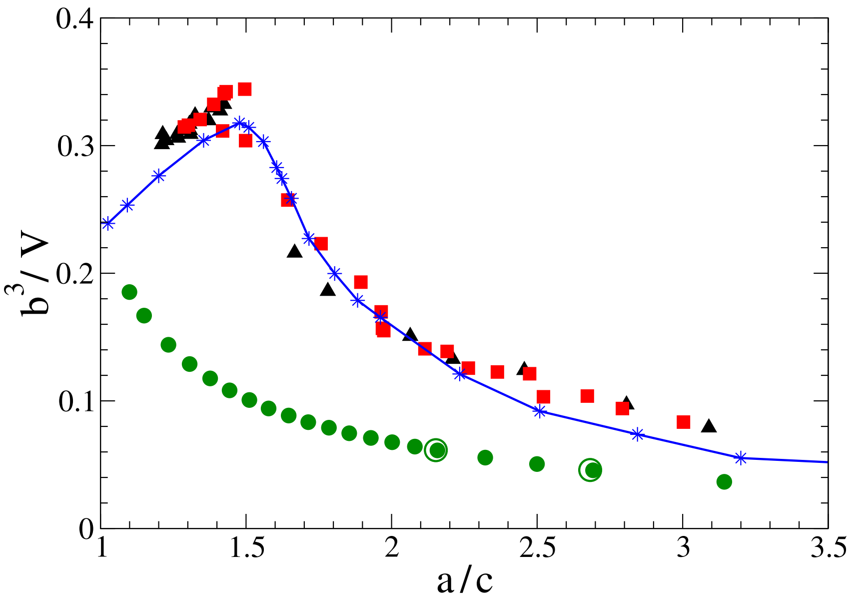
[Coppens et al, PCCP19, 24805 (2017)]

Vortices and capillary waves

Aspect-ratio curve

[Langbehn et al, PRL **121**, 255301 (2018)]

The appearance of the aspect-ratio curve, indirect evidence of the presence of vortices in spinning droplets



a) Rigid-body rotational appearance (as in the rotating bucket experiment: presence of a meniscus)

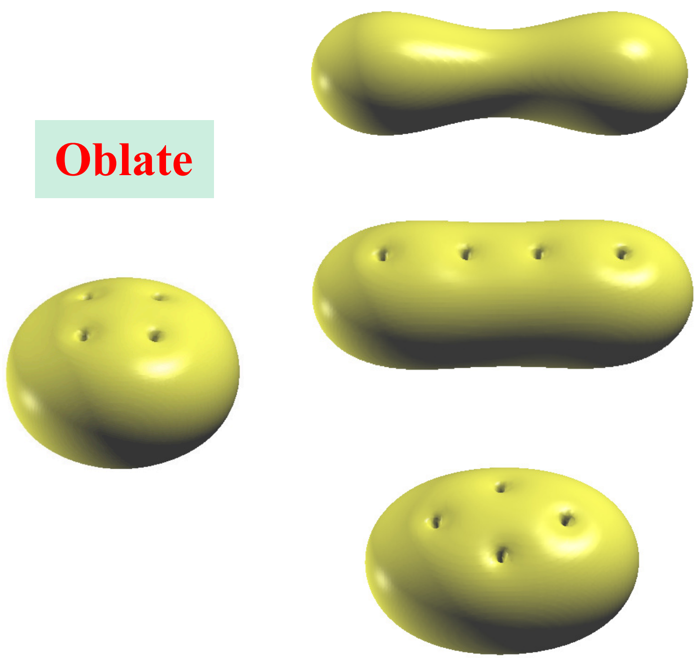
b) Makes it possible that oblate-like droplets "rotate" around a symmetry axis

c) Deformed vortex-free configurations may exist as stable objects where the angular momentum is stored as a **"giant capillary wave"**

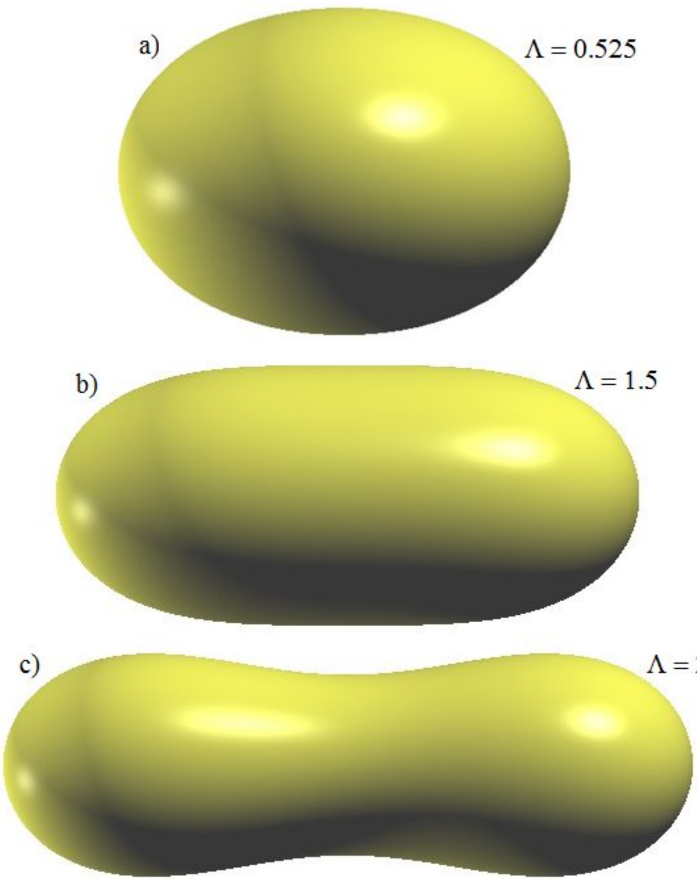
d) In prolate configurations, **capillary waves and vortices may/do coexist.**

Prolate configurations:

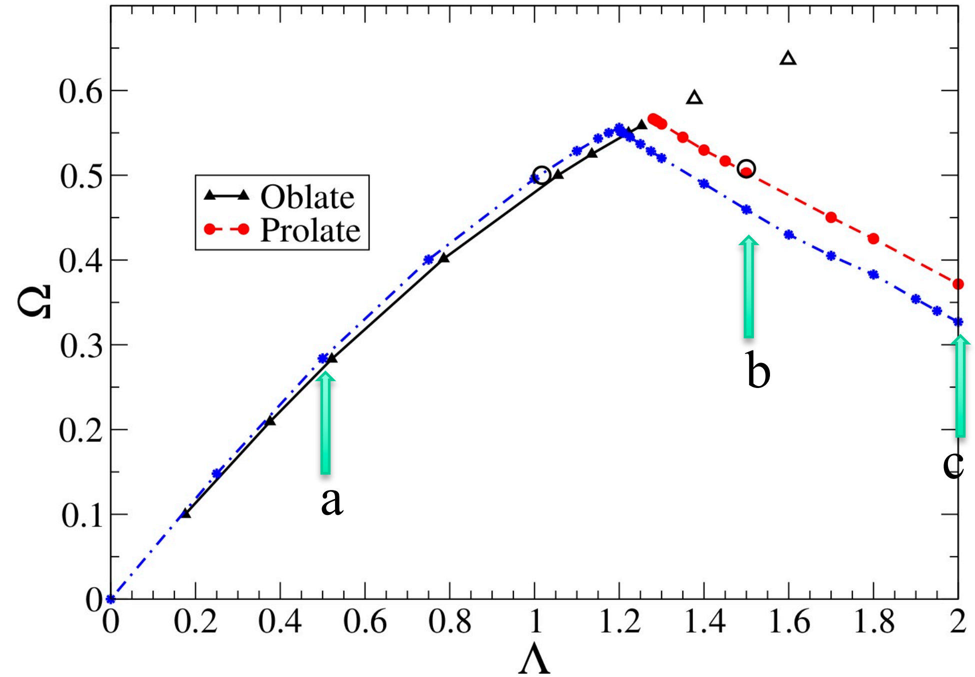
Oblate



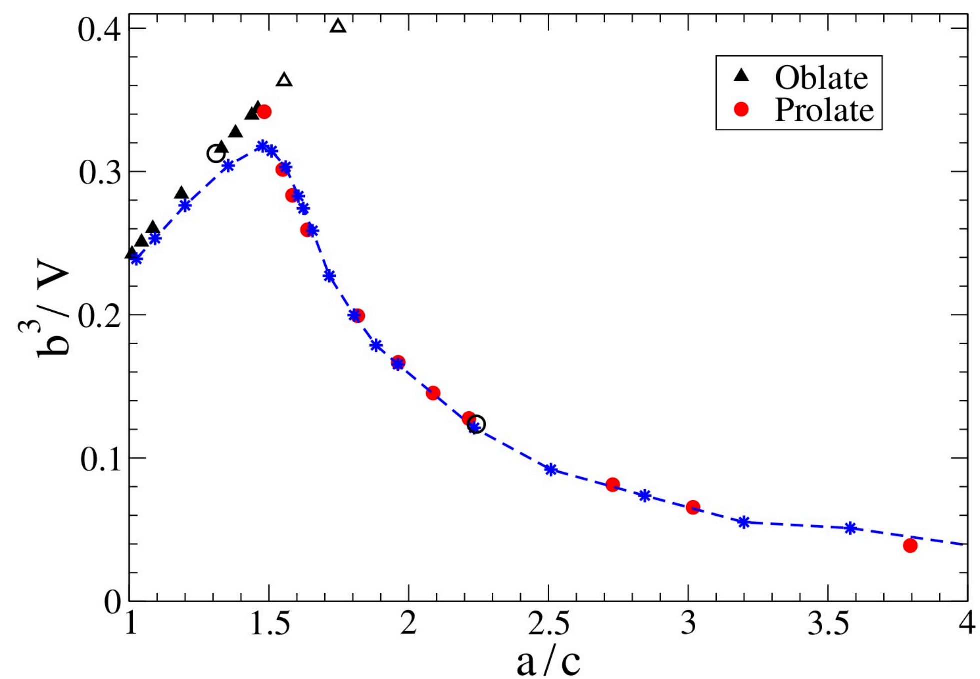
^{3}He



a)
Λ = 0.525
b)
Λ = 1.5
c)
Λ = 2



Oblate
Prolate
Ω
Λ
a
b
c
0
0.1
0.2
0.3
0.4
0.5
0.6
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2



Oblate
Prolate
b³/ V
a / c
0
0.1
0.2
0.3
0.4
1
1.5
2
2.5
3
3.5
4

Concluding remarks