Angular momentum effects on the Ne+(^{4}He)$_N$ → Ne@(^{4}He)$_{N'}$ + (N-N')^{4}He capture process and quantised vortex formation: a quantum-classical approach.

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Introduction

The properties of ^{4}He nanodroplets, such as superfluidity, chemical intertie and its ability to pick up almost any chemical specie makes these systems very interesting from the chemical perspective[1,2]. Here we present results on the theoretical study of the Ne+(^{4}He)$_N$ → Ne@(^{4}He)$_{N'}$ + (N-N')^{4}He pick up process taking into account the effects of the angular momentum introduced by the neon atom which approaches the nanodroplet with a certain impact parameter. Because of the capture, vortexes have been seen to be created.

Methodology: quantum-classical approach

^{4}He nanodroplet: phenomenological TDDFT[3] (Time Dependent Functional Theory):

$$i\hbar\frac{\partial}{\partial t}\Psi_{He}(\boldsymbol{R_{He}}) = \left[-\frac{\hbar^2}{2m_{He}}\nabla^2 + \frac{\partial \varepsilon_c[\rho_{He}]}{\partial \rho_{He}} + \int d\boldsymbol{R_{He}}\rho_{He}V_{He-Ne}(|\boldsymbol{R_{He}}-\boldsymbol{R_{Ne}}|)\right]\Psi_{He}(\boldsymbol{R_{He}})$$

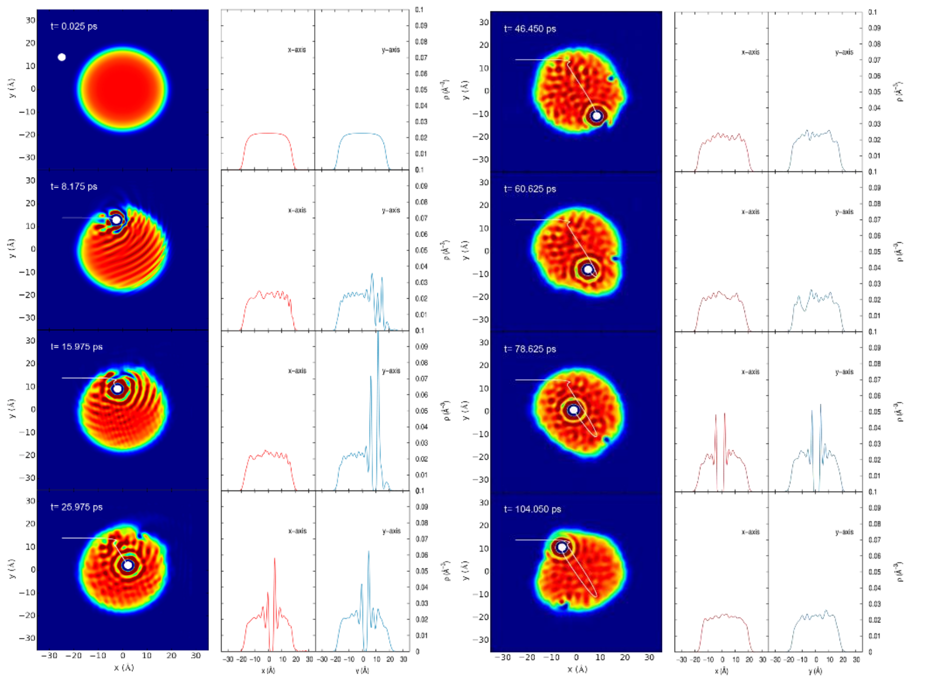
Ne atom: classical laws of motion:

$$m_{Ne}\ddot{\boldsymbol{R}}_{\boldsymbol{He}} = -\nabla_{Ne}\left[\int d\boldsymbol{R_{He}}\rho_{He}V_{He-Ne}(|\boldsymbol{R_{He}}-\boldsymbol{R_{Ne}}|)\right]$$

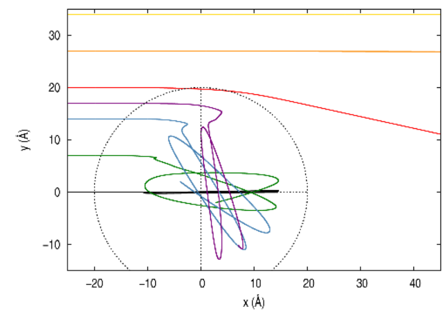
Mechanism

Droplet of N=500; Initial velocity, v_0=500 m/s: peak of the Maxwell distribution of gas Ne; Impact parameters, b=0, 7, 14, 17, 20, 27 and 34 Å.

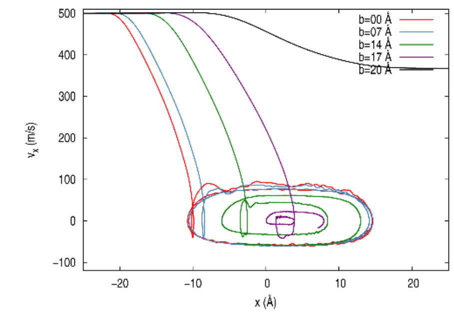
Helium density evolution with time (v_0=500 m/s; b=14 Å):



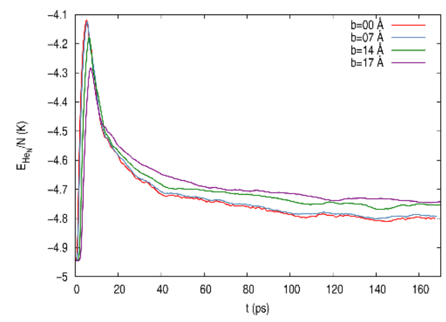
Ne atom trajectories: capture.

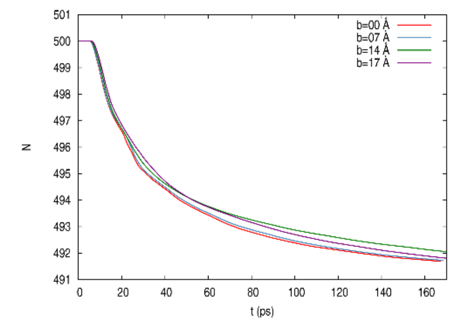


Phase space-like diagram: reaching Landau velocity inside nanodroplet.



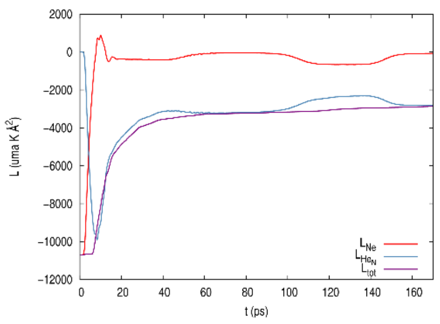
Helium nanodroplet energy and norm: excitation introduced by Ne is relaxed by evaporating helium density.



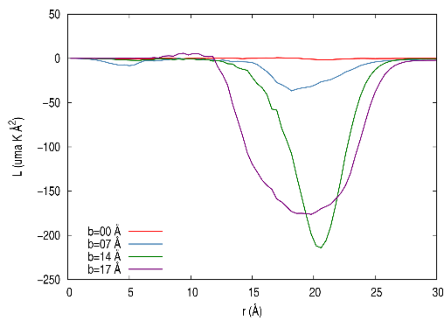


Angular momentum and quantised vortex formation

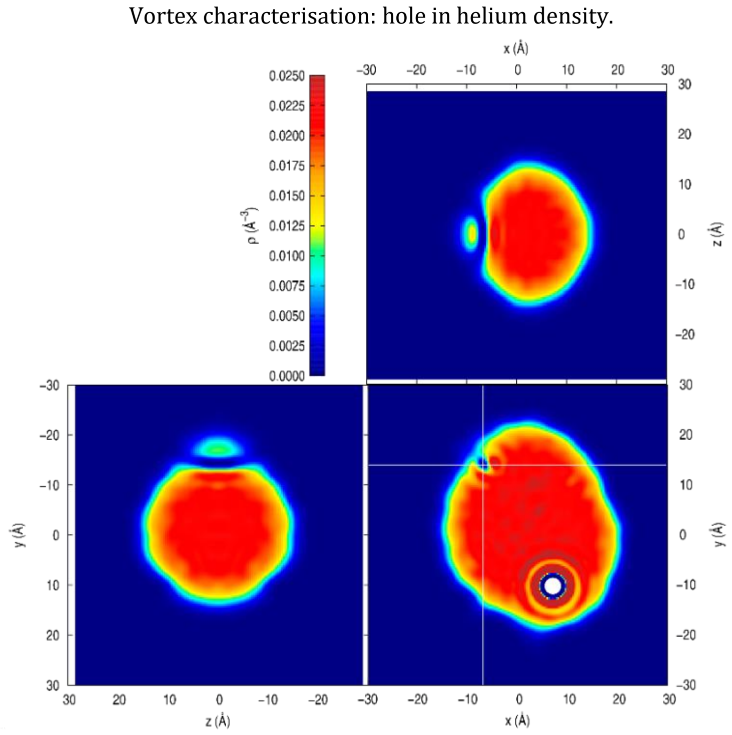
Droplet-atom angular momentum exchange



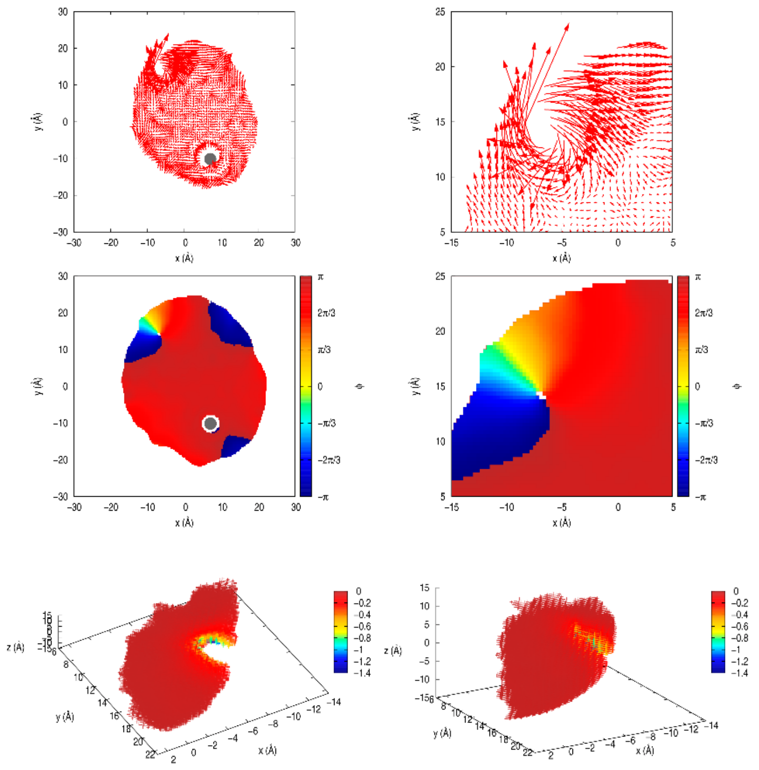
Droplet angular momentum radial distribution



Vortex characterisation: hole in helium density.



Vortex characterisation: velocity field, wave function phase and shape.



Conclusions

- Helium nanodroplets can capture a Ne atom with impact parameter up to the value of the radius of the nanodroplet.
- Ne travels inside the nanodroplet at Landau velocity indefinitely due to superfluidity.
- Excitation introduced by capture is relaxed by helium evaporation.
- There is an efficient energy exchange between Ne and the helium nanodroplet.
- A similar behaviour is seen for the angular momentum exchange.
- Angular momentum does not have important effects in the pick-up process.
- Remaining angular momentum is stored near the nanodroplet surface forming vortex in some cases.
- Vortexes can be seen as holes in the helium density or in the closed circulation of the wave function which is quantised.

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