MOLECULAR ROTATION IN SUPERFLUID $^4$He NANODROPLETS: THE VALIDITY OF A HYDRODYNAMIC MODEL

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In order to accurately predict the effective moments of inertia ($I_{\rm eff}$) of linear molecules rotating in superfluid $^4$He droplets, we have recently devised a superfluid hydrodynamic model. In the present implementation, the helium density profile induced by the He-molecule interaction potential is first calculated at the Density Functional level, and then used as the input of the hydrodynamic equation for the irrotational motion of a viscousless fluid. The kinetic energy of the fluid ($E_{\rm k}$) is then used to calculate $I_{\rm eff}$ via: $E_{\rm k} = \frac{1}{2}\Delta I\,\omega^2$, where $\omega$ is the angular velocity of the molecule, and $\Delta I$ is the difference between $I_{\rm eff}$ and the moment of inertia of the bare molecule.[a] The model relies on the assumption that the density of the fluid in the rotating frame of reference is independent of $\omega$ and can therefore be calculated in the limit of a static molecule (adiabatic following approximation). The validity of this approximation, and its first-order corrections will be discussed. The advantages and limitations of Density Functional Theory for calculating the true helium density will also be addressed, in a comparison with Quantum Monte Carlo results which recently became available for HCN and its oligomers.[b]

[a] C. Callegari, A. Conjusteau, I. Reinhard, K.K. Lehmann, G. Scoles, and F. Dalfovo, Phys. Rev. Lett. **83**, 5058 (1999); *ibid.* **84**, 1848(E) (2000).
[b] E. Draeger and D. M. Ceperley, private communication.