Rotational Superfluidity in Small Helium Droplets

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The first minimum appearing in molecular rotational constants as a function of helium droplet size has been previously associated with the onset of superfluidity in these finite systems. We investigate this relationship by bosonic density functional theory calculations of classical molecular rotors (OCS, N_2O, CO and HCN) interacting with the surrounding helium. The calculated rotational constants are in fair agreement with the existing experimental data, demonstrating the applicability of the theoretical model. By inspecting the spatial evolution of the global phase and density, the increase in the rotational constant after the first minimum is shown to correlate with continuous coverage of the molecule by helium and appearance of angular phase coherence rather than completion of the first solvent shell. We assign the observed phenomenon to quantum phase transition between a localized state and one-dimensional superfluid, which represents the onset of rotational superfluidity in small helium droplets.