CALCULATION OF EXCITATIONS OF SUPERFLUID HELIUM NANODROPLETS

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Band shapes of vibrational and electronic excitation spectra of dopants solvated in superfluid helium nanodroplets are often attributed to phonon- and roton-like excitations. Quantum Monte Carlo techniques as well as time-dependent density-functional theory have previously been used to estimate the energies and momenta of the lowest few excitations in this finite superfluid. A general study of excitations in helium nanodroplets, however, is lacking at present, in particular for higher angular momentum states. We use normal mode analysis of time-dependent bosonic density-functional theory to compute the energies and shapes of single excitations of undoped and doped helium nanodroplets. Our calculations in spherical symmetry can deal with excitations of arbitrary angular momentum, and take into account backflow effects. The functionals employed are calibrated to give correct results for bulk superfluid helium at zero temperature.