Microscopic Description of Resonance in the Brownian Motion of Hydrophobic Nanoparticle in Harmonic Potential Trap

JAE HYUN PARK, Gyeongsang National University — Harmonic potential has been popular for the trapping of micro- and nanoparticles (e.g. optical tweezer). With the rapid development of harmonic potential trapping technology, its application is nowadays being extended to explore the fundamental nature in the random thermal fluctuation of particles in order to confirm the classical theory of Brownian motion. In this study, using extensive molecular dynamics simulations, we investigate the molecule-level features of dynamic response of hydrophobic C$_{60}$ nanoparticle in harmonic potential trap with water medium. The time-averaged magnitudes of random fluctuation are measured for various trap stiffness and then the virtual mass, the amount of fluid moving together with particle, is extracted from curve fitting. The fluctuation is proportional to the inverse of trap stiffness. The virtual mass is mostly originated from the first hydration shell around the particle and it is not influenced by the stiffness. The resonance in frequency domain is observed as a result of coloured noise in the motion. The effect of stiffness on the resonance is weaker than that on the magnitude of fluctuation because the motion of particle is partially dissipated in the RDF valley between the first and the second hydration shell.

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