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Selective mode analysis of nuclear quantum effects for liquid water using non-Markovian thermostats SRIRAM GANESHAN, MARIVI FERNÁNDEZ-SERRA, Stony Brook University — Simulating nuclear quantum effects in liquid water using both DFT and force fields has been an active area of research in recent years. Recently, Ceriotti et. al [1] introduced a comprehensive framework to use a custom-tailored Langevin equation with correlated-noise in the context of molecular-dynamics simulations. One of the interesting applications of these thermostats is that, such a framework can be used to selectively damp normal modes whose frequency falls within a prescribed range. In this work we study how the flexible force field models respond to the selective mode thermostating using the delta-like memory kernels. We apply this delta thermostat to the molecular dynamics of TIP4P/F water force field [2], a model explicitly fitted with the lack of zero point ionic vibrations. We address the question of whether thermostating each mode to its zero point temperature is enough to generate the nuclear quantum effects in water and similar systems. This work also provides a way to identify the dominant modes for which the quantum effects are important. [1] M. Ceriotti, G. Bussi, and M. Parrinello, Phys. Rev. Lett. 103, 030603 (2009). [2] S. Habershon, T. E. Markland, and D. E. Manolopoulos, J. Chem. Phys 131, 024501 (2009).

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