EFFECTIVE POTENTIAL APPROACH TO THE SIMULATION OF LARGE PARA-HYDROGEN CLUSTERS AND DROPLETS

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The quantum simulation of large molecular system is a formidable task. We explore the use of effective potentials based on the Feynman path centroid variable in order to simulate large quantum clusters at a reduced computational cost. This centroid can be viewed as the "most classical" variable of a quantum system. Earlier work has shown that one can use a pairwise centroid pseudo-potential to simulate the quantum dynamics of hydrogen in the bulk phase at 25 K and 14 K.[a] Bulk hydrogen, however, freezes below 14 K and we rather focus on nanodroplets in the very low temperature regime in order to study the superfluid behaviour of hydrogen. The calculation of the effective potential will be discussed along with its use in the context of molecular dynamics simulations. Centroid structural properties will be presented and compared to the results of path integral Monte Carlo simulations. We will present an approach for de-convoluting centroid structural properties in order to obtain real space results for hydrogen clusters of a wide range of sizes. The extension of the approach to the treatment of confined hydrogen will be discussed.

[a] M. Pavese and G.A. Voth, *Chem. Phys. Lett.* **249**, 231 (1996).