STRUCTURAL TRANSITION OF SMALL QUANTUM CLUSTER

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Recent experimental advances offer new information across many different time scales of interest, ranging from submillisecond slow macroscopic structural transitions to subpicosecond electronic rearrangements, and femtosecond nonadiabatic dynamics. In order to describe these phenomena, one should adopt quantum mechanics, which cost too much. In contrast to quantum dynamics, classical dynamics methods are routinely used to study complex chemical problems that can involve many thousands of particles, such as protein folding and docking. In proteins, the Amino I modes are of such high frequency that the quantum effects cannot be neglected, even if the experiments are performed at room temperature. Thus, quantum effects, such as zero point energy, tunneling, and resonance, are essential, and cannot be avoided.

Rencently, we have developed a quantal cumulant dynamics (QCD) in order to treat large quantum systems with low costs [1-7]. The key ideas are that a coordinate shift operator acting on a potential operator is introduced and that a cumulant expansion technique is applied to evaluate the expectation value of the shift operator. In the presentation, we derive the coupled equations of motion of coordinates, momenta, cumulants that consist of symmetric-ordered products of the coordinate and the momentum fluctuation operators. We apply the methodology to describe quantum nature of structural transitions of Morse clusters. We have evaluated a Lindemann index of small quantum clusters and observed quantum isotope effects on their melting behavior. The quantum effects shallow the potential and elongate the equilibrium distance of the Morse potential. These features result in increase of transition temperatures of freezing and melting toward those of classical ones.

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