Development of *Ab Initio* Anharmonic Algorithms

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ABSTRACT

One of the central challenges in Chemical Physics is that the vibrational Hamiltonian of a given molecular system is not known and the construction of the vibrational Hamiltonian requires performing computational expensive electronic structure calculations. The second challenge is known as "curse of dimensionality" that severally limits the size of the quantum systems that can be solved. Our group has been working on developing "*Ab Initio* Anharmonic Algorithms" (A^3) to simulate and to gain further insight of vibrational coupling in the proton transfer processes.

To fully describe the quantum dynamics of a solvated hydronium will require treating all 33 degrees of freedom (DoF). Even if one assumes that only the 12 DoF of the central H_3O^+ are important remain as a numerical challenging task. Our A^3 codes work with Cartesian coordinates make the construction of kinetic energy operator (KEO) a trivial task. Furthermore, we have developed a set of code to construct potential energy operator (PEO) with different resolutions that can balance computational costs and accuracy. Very recently, we are working to integrate A^3 with Cytnx to transfer PEO into Matrix Product Operator (MPO) form and to use DMRG tools to solve time independent Schrödinger equations with up to 12 DoF of the central H_3O^+.

REFERENCE STYLE

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KEYWORDS

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