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Quantum Grid Dynamics (QGD): a method for solving the molecular Schroedinger Equation in Cartesian coordinates via angular momentum projection operators

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Abstract

A method for solving the Schroedinger equation of N-atom molecules in 3N-3 Cartesian coordinates usually defined by Jacobi vectors is presented [1]. The separation and conservation of the total angular momentum is obtained not by transforming the Hamiltonian in internal curvilinear coordinates but instead, by keeping the Cartesian formulation of the Hamiltonian operator and projecting the initial wavefunction onto the proper irreducible representation angular momentum subspace. The increased number of degrees of freedom from 3N-6 to 3N-3, compared to previous methods for solving the Schroedinger equation, is compensated by the simplicity of the kinetic energy operator and its finite difference representations which result in sparse Hamiltonian matrices. A parallel code in fortran 95 has been developed and tested for model potentials of harmonic oscillators. Moreover, we compare data obtained for the three dimensional hydrogen molecule and the six dimensional water molecule with results from the literature. The availability of large clusters of computers with hundreds of CPUs and GBytes of memory, as well as the rapid development of distributed (Grid) computing, make the proposed method, which is unequivocally highly demanding in memory and computer time, attractive for studying Quantum Molecular Dynamics.Several gridification schemes are discusded [2].

References

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[2] S. C. Farantos, S. Stamatiadis, L. Lathouwers, and R. Guantes, Grid Enabled Molecular Dynamics: classical and quantum algorithms, In G. Maroulis, Th. Simos, editor, Lecture Series on Computer and Computational Sciences: Trends and Perspectives in Modern Computational Science, volume˜3, pages 35–50. VSP, 2005.

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