Quantum Physics

A Quantum Algorithm for Molecular Dynamics Simulation

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Quantum computers could potentially simulate the dynamics of systems such as polyatomic molecules on a much larger scale than classical computers. We investigate a general quantum computational algorithm that simulates an arbitrary nonrelativistic, Coulombic many-body system in three dimensions. We use a simple discretized model of Schrodinger evolution and discuss detailed constructions of the time evolution operators involved. The algorithm is implemented in MATLAB and tested against both analytical solutions and classical methods, which suggests that it can be adapted for electronic structure calculations, chemical reaction simulations, and the like.

Comments:	15 pages, 6 figures; current version contains more references, more numerics, and better exposition
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