

## Quantum Physics

# A Quantum Algorithm for Molecular Dynamics Simulation

Yale Fan

*(Submitted on 27 Jan 2009 (v1), last revised 4 Sep 2009 (this version, v3))*

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

Subjects: **Quantum Physics (quant-ph)**

Cite as: **arXiv:0901.4163v3 [quant-ph]**

## Submission history

From: Yale Fan [[view email](#)]

[\[v1\]](#) Tue, 27 Jan 2009 05:47:33 GMT (460kb,D)

[\[v2\]](#) Wed, 25 Mar 2009 05:31:35 GMT (157kb,D)

[\[v3\]](#) Fri, 4 Sep 2009 05:53:07 GMT (174kb,D)

*[Which authors of this paper are endorsers?](#)*

Link back to: [arXiv](#), [form interface](#), [contact](#).

## Download:

- [PDF](#)
- [Other formats](#)

Current browse context:

**quant-ph**

[< prev](#) | [next >](#)

[new](#) | [recent](#) | [0901](#)

## References & Citations

- [SLAC-SPIRES HEP](#)  
([refers to](#) | [cited by](#))
- [CiteBase](#)

## Bookmark([what is this?](#))

[CiteULike logo](#)

[Connotea logo](#)

[BibSonomy logo](#)

[Mendeley logo](#)

[Facebook logo](#)

[del.icio.us logo](#)

[Digg logo](#)

[Reddit logo](#)