Quantum simulation: statics and dynamics

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Introduction

Introduction

- What is quantum simulation?
- Techniques: phase estimation
- Techniques: phase kickback
- Experiment 1: Ground state energy of H_2 in a minimal basis
- Quantum lattice gas methods
- Experiment 2: Simulating *zitterbewegung* in trapped ions

What is quantum simulation?

"Simulating a quantum system with a controllable laboratory system underlying the same mathematical model". (Gerritsma *et. al* arxiv:0909.0674v1)

- Lab system has fixed, finite capabilities in terms of initialization, evolution, measurement
- Want to compute $\langle\psi|\hat{A}|\psi\rangle$ for some target state $|\psi\rangle$, some target observable $\hat{A}$
- Initialize lab system in some state
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- Lab system = universal quantum computer: quantum simulation algorithms

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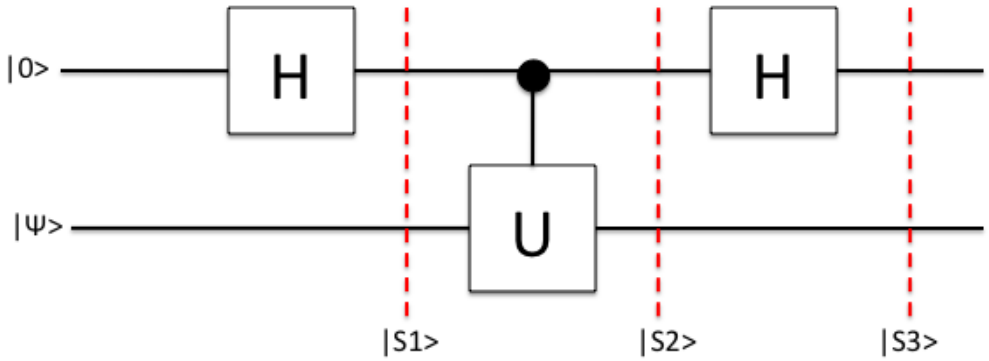
- Measure some set of observables (e.g qubit states 0,1) to obtain information about $\hat{A}$
- Lab system = universal quantum computer: quantum simulation algorithms
- If lab system = target system: we call that experiment!

Techniques: phase estimation



$$U|\psi\rangle = e^{-i\phi}|\psi\rangle$$
$$|S1\rangle = |+\rangle|\psi\rangle$$
$$= \frac{1}{\sqrt{2}}\left[|0\rangle|\psi\rangle + |1\rangle|\psi\rangle\right]$$

$$|S2\rangle = \frac{1}{\sqrt{2}}[|0\rangle|\psi\rangle + e^{-i\phi}|1\rangle|\psi\rangle]$$
$$|S3\rangle = \frac{1}{2}[(1+e^{-i\phi})|0\rangle + (1-e^{-i\phi})|1\rangle]|\psi\rangle$$

Measure high qubit:

$$Prob(0) = |1+e^{-i\phi}|^2/2 = 1+\cos\phi$$
$$Prob(1) = |1-e^{-i\phi}|^2/2 = 1-\cos\phi$$

From phase estimation to energy measurement

Suppose that we can estimate $\arccos(\langle\sigma_z\rangle/2) = \phi$ to fixed precision. Let U be the time evolution operator of a system for time t:

$$U = \exp(-it\hat{H}/\hbar) \qquad \phi = tE/\hbar$$

suppose the energy scale is such that $E/\hbar < 1$ so that we can write $E/\hbar$ as a binary fraction:

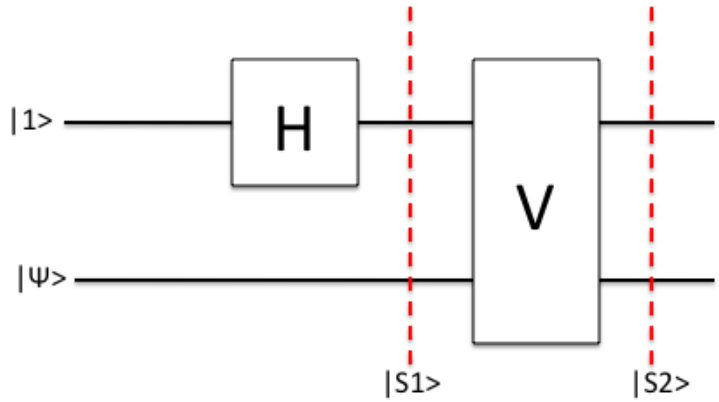
$$E/\hbar = 0.E_2E_4E_8E_{16}\cdots = \frac{E_2}{2} + \frac{E_4}{4} + \frac{E_8}{8} + \frac{E_{16}}{16} + \ldots$$

then choose $t = 2\pi 2^n$ so that:

$$\phi = N2\pi + \pi E_{2^n}/2 + \ldots \tag{1}$$

and we can repeat this calculation to estimate E one bit at a time.

Techniques: phase kickback

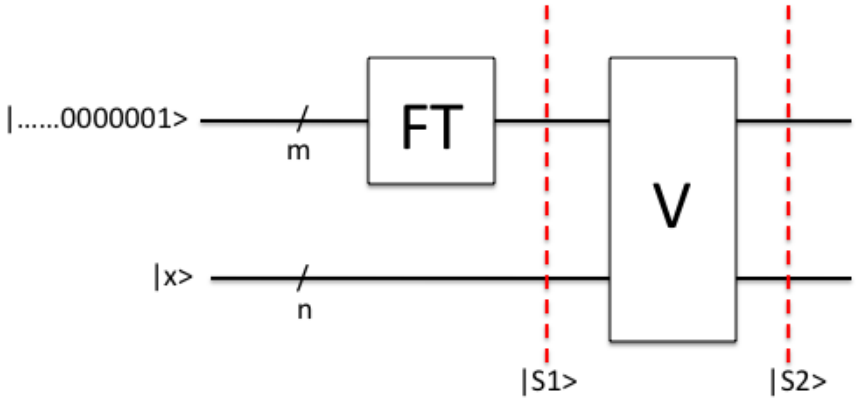


Action of V is
$V|a,b\rangle = |a, b \oplus V(a)\rangle$
Implemented by classical circuit
Consider $V(0) = 0,\ V(1) = 1$

$$|S1\rangle = \alpha(|00\rangle - |01\rangle) + \beta(|10\rangle - |11\rangle)$$
$$\mapsto |S2\rangle = \alpha(|00\rangle - |01\rangle) + \beta(|11\rangle - |10\rangle)$$
$$= |-\rangle \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} |\psi\rangle$$

Here phase kickback has been used to apply the diagonal unitary $e^{i\pi V}$ to the wavefunction. The cost is the classical cost of computing V.

Techniques: phase kickback



Action of V is
$V|a,b\rangle = |a, b \oplus V(a)\rangle$
On n state qubits and m ancillae.
$V : \{0,1\}^n \mapsto \{0,1\}^m$

$$|S1\rangle = |x\rangle \sum_{y=0}^{2^m-1} e^{2\pi i y/2^m}|y\rangle \mapsto |S2\rangle = |x\rangle \sum_{y=0}^{2^m-1} e^{2\pi i y/2^m}|y \oplus V(x)\rangle$$

$$= e^{-i2\pi V(x)/2^m}|x\rangle \sum_{y=0}^{2^m-1} e^{2\pi i y/2^m}|y\rangle$$

Again phase kickback has been used to apply the diagonal unitary $e^{-i\pi V/2^m}$ to the wavefunction.

Statics and dynamics

Common steps

1. Define mapping of system state to qubit state $|\psi\rangle$

Statics (Kitaev, Abrams and LLoyd PRL 83 5162 (1999))

1. Define circuit for time evolution operator $\exp(-i\hat{H}t/\hbar)$
2. Prepare eigenstate $|\psi\rangle$
3. Phase estimate energy.

Dynamics (Wiesner, quant-ph/9603028, Zalka, Proc. Roy. Soc. A 454, 313, 1998)

1. Time evolution operator is
   $\exp -i(T+V)\delta t/\hbar \simeq \exp -iT\delta t/\hbar \exp -iV\delta t/\hbar$
2. T is diagonal in $\hat{p}$ basis. V is diagonal in $\hat{x}$ basis
3. Can efficiently transform between $\hat{p}$ and $\hat{x}$ using QFT.
4. Use phase kickback to apply T and V operators.

Two recent experiments

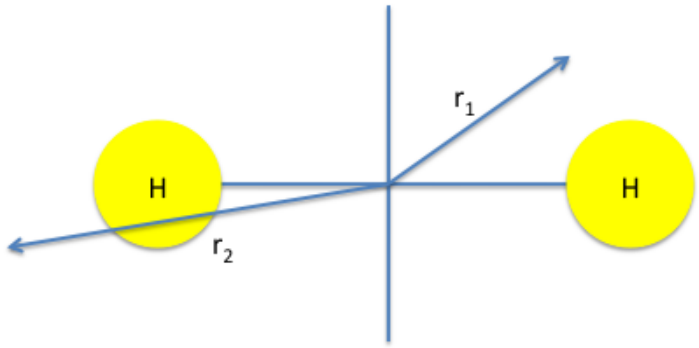
Calculation of ground state energy of H_2 in photonic quantum computer

"Towards quantum chemistry on a quantum computer" B.P. Lanyon, J. D. Whitfield, G. G. Gillett, M. E. Goggin, M. P. Almeida, I. Kassal, J. D. Biamonte, M. Mohseni, B. J. Powell, M. Barbieri, A. Aspuru-Guzik, A.G. White. arxiv:0905.0887v3 To appear in *Nature Chemistry*

Quantum Simulation of *zitterbewegung* in a trapped ion

"Quantum simulation of the Dirac equation" R. Gerritsma, G. Kirchmair, F. Zahringer, E. Solano, R. Blatt, C. F. Roos . arxiv:0909.0674v1

Quantum chemistry



Hamiltonian

$$\hat{H}^{mol} = \hat{T}_e + \hat{T}_Z + \hat{V}_{ZZ}(L_{pq}) + \hat{V}_{ee}(r_{ij}) + \hat{V}_{eZ}(R_{pi})$$

Born-Oppenheimer:

$$\hat{H}^{elec} = \hat{T}_e + \hat{V}_{ee}(r_{ij}) + \hat{V}_{eZ}(R_{pi})$$

Basis Sets

For two separated H, each will be in the $1s$ state: $|\psi\rangle = |1s\rangle|1s'\rangle$. Make one-particle orbitals that are eigenstates of spatial parity:

$$|g\rangle = |1s\rangle + |1s'\rangle \quad |u\rangle = |1s\rangle - |1s'\rangle \tag{2}$$

Now the two electrons can occupy 2 spin states in 2 orbitals, giving 6 two electron basis states, antisymmetrized to respect exchange.

Minimal basis H_2

Symmetry, symmetry, symmetry!

Spatial symmetry: which basis elements are parity invariant?

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Spatial symmetry: which basis elements are parity invariant?
Two g's or two u's:

$$m_s = 0 \quad |\Phi_1\rangle = |g\uparrow g\downarrow| = 2^{-1/2}(|g\uparrow g\downarrow\rangle - |g\downarrow g\uparrow\rangle)$$
$$|\Phi_6\rangle = |u\uparrow u\downarrow| = 2^{-1/2}(|u\uparrow u\downarrow\rangle - |u\downarrow u\uparrow\rangle)$$

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Remaining states are antisymmetric under parity:

$$m_s = 1 \quad |\Phi_3\rangle = |g\uparrow u\uparrow| = 2^{-1/2}(|g\uparrow u\uparrow\rangle - |u\uparrow g\uparrow\rangle)$$

$$m_s = 0 \quad |\Phi_3\rangle = |g\uparrow u\downarrow| = 2^{-1/2}(|g\uparrow u\downarrow\rangle - |u\uparrow g\downarrow\rangle)$$
$$|\Phi_4\rangle = |g\downarrow u\uparrow| = 2^{-1/2}(|g\downarrow u\uparrow\rangle - |u\uparrow g\downarrow\rangle)$$

$$m_s = -1 \quad |\Phi_3\rangle = |g\uparrow u\uparrow| = 2^{-1/2}(|g\downarrow u\downarrow\rangle - |u\downarrow g\downarrow\rangle)$$

Subspaces do not mix: two 2×2 matrix eigenvalue problems.

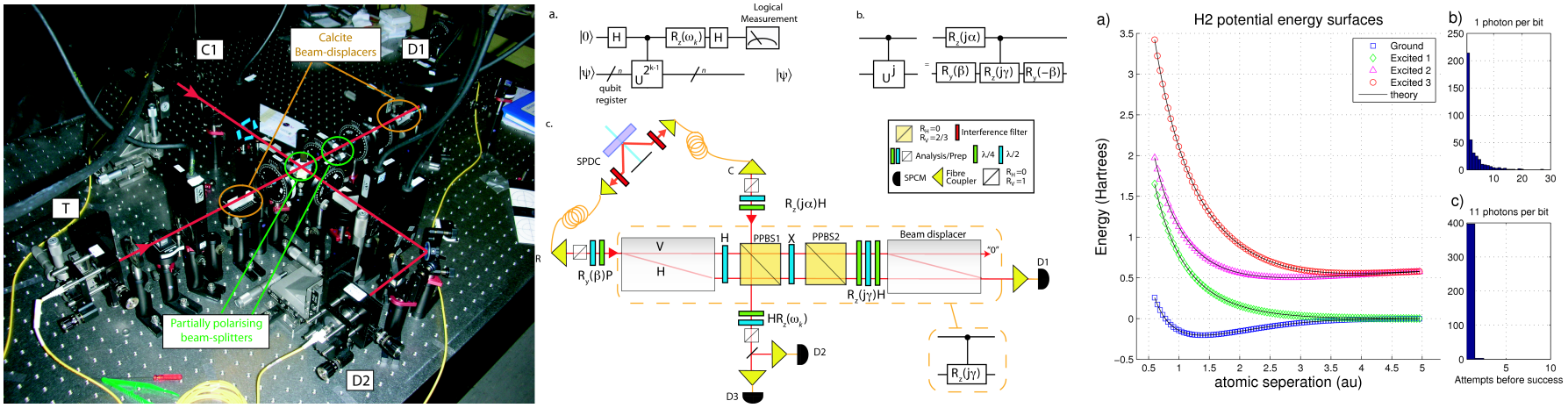


Figure: First quantum chemistry experiment executed on a prototype quantum computer. Two entangled photons are generated by parametric down conversion and processed using quantum optics. The simultaneous detection of the photons reveals the molecular energy of the hydrogen molecule eigenstates encoded on one of the two photons by means of the quantum phase estimation algorithm. **Left:** The experimental setup is a quantum optical information processor. **Center:** Scheme for the experimental setup and quantum algorithm. **Right:** Potential energy curves for the different states of molecular hydrogen in the minimal STO-3G basis set. The quantum computer setup is able to obtain more than 20 binary digits of precision, and therefore, the answer lies visually on top of the numerical result obtained by a classical computer.

A roadmap for quantum simulation?

Vintage quantum chemistry

Electronic wave functions

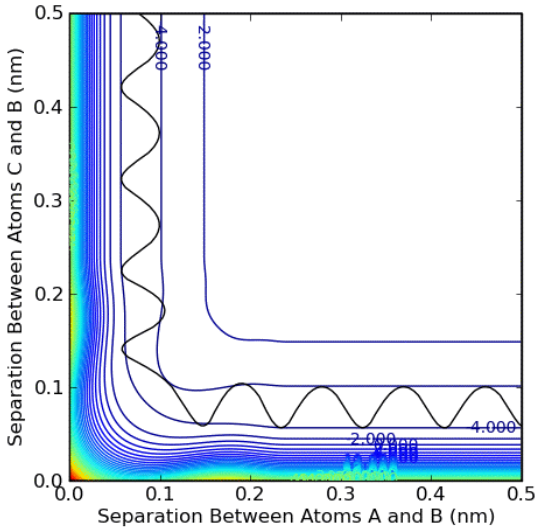
I. A general method of calculation for the stationary states of any molecular system

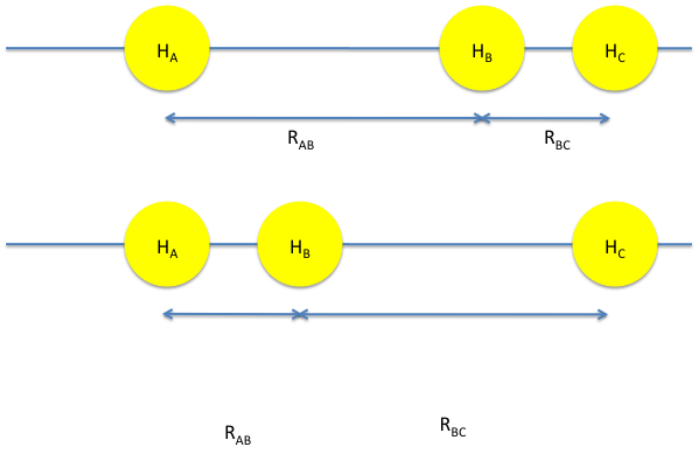
By S. F. Boys, *Theoretical Chemistry Department, University of Cambridge**

(*Communicated by Sir Alfred Egerton, F.R.S.—Received* 31 *August* 1949)

Year	Calculation	Citation	Qubits
1933	H_2	H. M. James, A. S. Coolidge, J. Chem. Phys, **1**, 825, (1933)	1
1950	Be	S. F. Boys, Proc. Roy. Soc. of London. Series A, bf 201, 125 (1950)	3, 4
1952	He	G. R. Taylor, R. G. Parr, Proc. U. S. Natl. Acad. Sci, (38), 154, (1952)	2
1955	He	H. Shull, P.-O. Lowdin, J. Chem. Phys, **23**, 1565 (1955)	2, 3
1956	BH, H_2O	S. F. Boys, G. B. Cook, C. M. Reeves, I. Shavitt, Nature **178**, 1207, (1956)	5, 7
1957	LiH, BeH^+	J. Miller *et al.*, J. Chem. Phys, **27**, 1385 (1957)	3 – 5
1960	Be	R. E. Watson, Phys. Rev. **119**, 170, (1960)	6
1960	CH_2	J. M. Foster, S. F. Boys, Rev. Mod. Phys. **32**, 305 (1960)	19
1963	H_2	S. Hagstrom, H. Shull, Rev. Mod. Phys. **35**, 624, (1963).	3 – 6
1966	HeH, Li_2	C. F. Bender, E. R. Davidson, J. Phys. Chem. **70**, 2675 (1966),	3
1967	H_2O	R. Mcweeny, K. A. Ohno, Proc. Roy. Soc. **A255**, 367 (1967)	10
1968	Be	C. F. Bunge, Phys. Rev. **168**, 92, (1968).	11
1970	H_2O	R. P. Hosteny *et al.* Chem. Phys. Lett. **7**, 325, (1970)	23

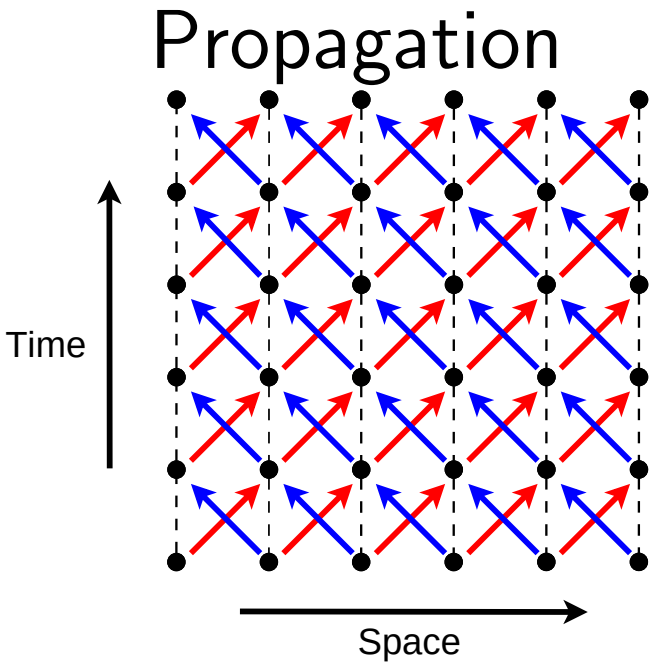
Dynamics

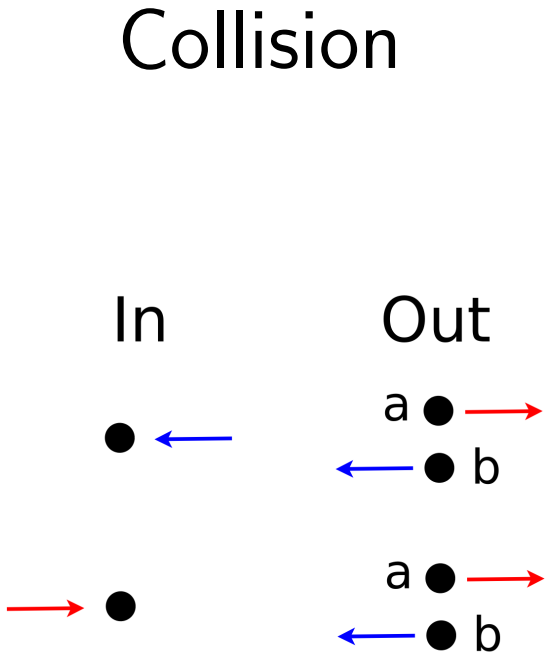




Suppose one has the solution to the electronic structure problem: energy as a function of nuclear coordinates. Imagine moving the nuclei around adiabatically on that potential energy surface. Semiclassical methods do well if curvature of surface small compared to wavepacket localization (E. Heller, Time-dependent approach to semiclassical dynamics, J. Chem. Phys. 1975 vol. 62 (4) pp. 1544-1555). Figure by D. Harrington, BMC '09

Quantum lattice gases

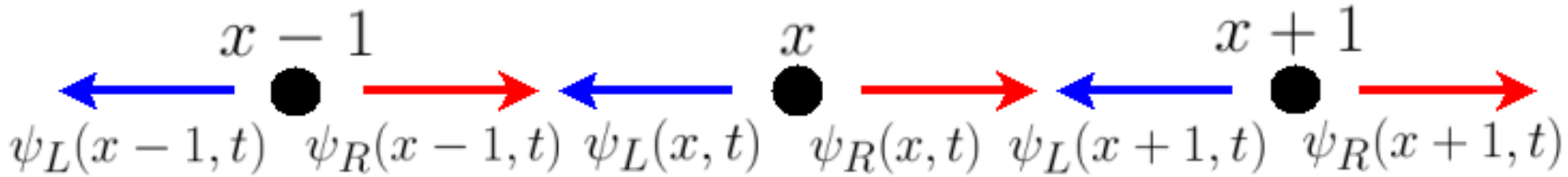




$$x-1 \qquad x \qquad x+1$$

$$\psi_L(x-1,t)\ \ \psi_R(x-1,t)\ \ \psi_L(x,t)\ \ \psi_R(x,t)\ \ \psi_L(x+1,t)\ \ \psi_R(x+1,t)$$

A General Quantum Lattice-Gas Model



Time Evolution Implemented By:

$$\begin{pmatrix} \psi_L(x,t+1) \\ \psi_R(x,t+1) \end{pmatrix} = p \begin{pmatrix} a & b \\ b & a \end{pmatrix} \begin{pmatrix} \psi_L(x+1,t) \\ \psi_R(x-1,t) \end{pmatrix}$$

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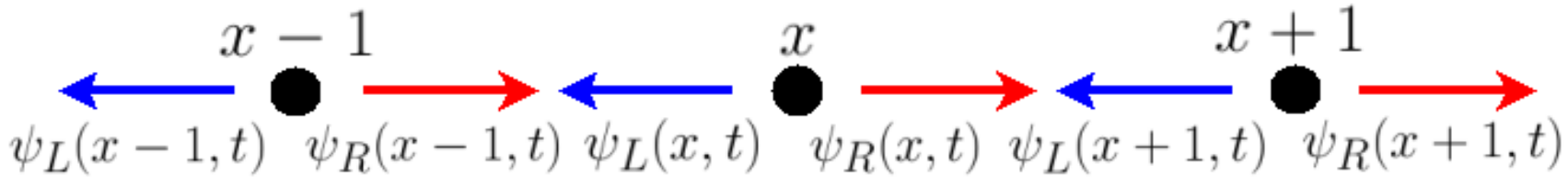

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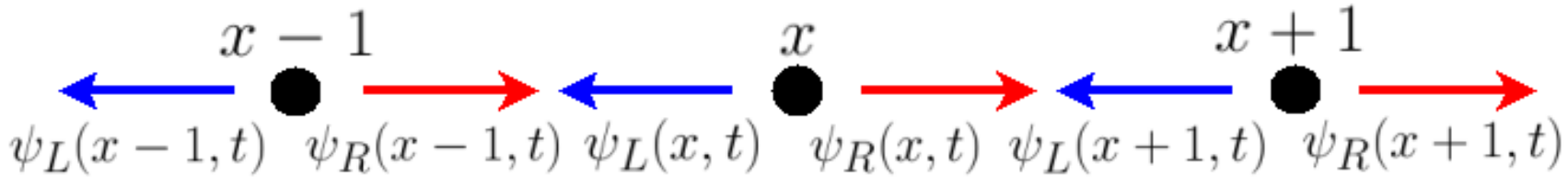

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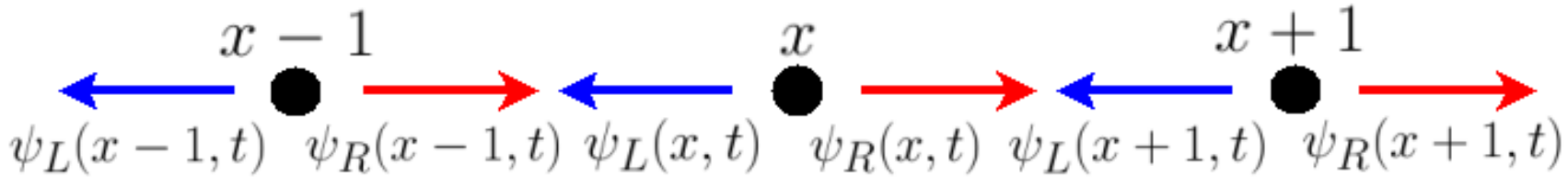

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- p is a phase
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  - $a^2 - b^2 = 1$
  - $|a|^2 + |b|^2 = 1$
  - $a\overline{b} + b\overline{a} = 0$
  - $\mathrm{Re}(a\overline{b}) = 0$

Model Comparisons

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- Meyer's model (J. Stat. Phys **85**,551; Phys. Rev. E **55**, 5261; Int. J. Mod. Phys. C **8**, 1997):
  - $p = 1$
  - $a = \cos\theta$
  - $b = i \sin\theta$
  - $m = \tan\theta$
  - $|\psi_{total}|^2 = |\psi_L|^2 + |\psi_R|^2$

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  - $m = \tan\theta$
  - $|\psi_{total}|^2 = |\psi_L|^2 + |\psi_R|^2$
- Boghosian and Taylor's model (Int. J. Mod. Phys. C **8**, 705 and Phys. Rev. E **57**, 54):
  - $p = e^{i\frac{\phi}{2}}$
  - $a = \cos\frac{\phi}{2}$
  - $b = i\sin\frac{\phi}{2}$
  - $m = \tan\frac{\phi}{2}$
  - $|\psi_{total}|^2 = |\psi_L - \psi_R|^2$

Dispersion Relation

In the general model:

$$\omega = \arccos\left(a(\cos\left(\pm k\right))\right) - \arg\left[p\right]$$

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In the Boghosian-Taylor parameterization, if we take the limit $\omega \ll \phi$, $k \ll \phi$, dispersion relation reduces to:

$$\omega = \frac{k^2}{2\tan\frac{\phi}{2}} = \frac{k^2}{2m},$$

Dispersion Relation

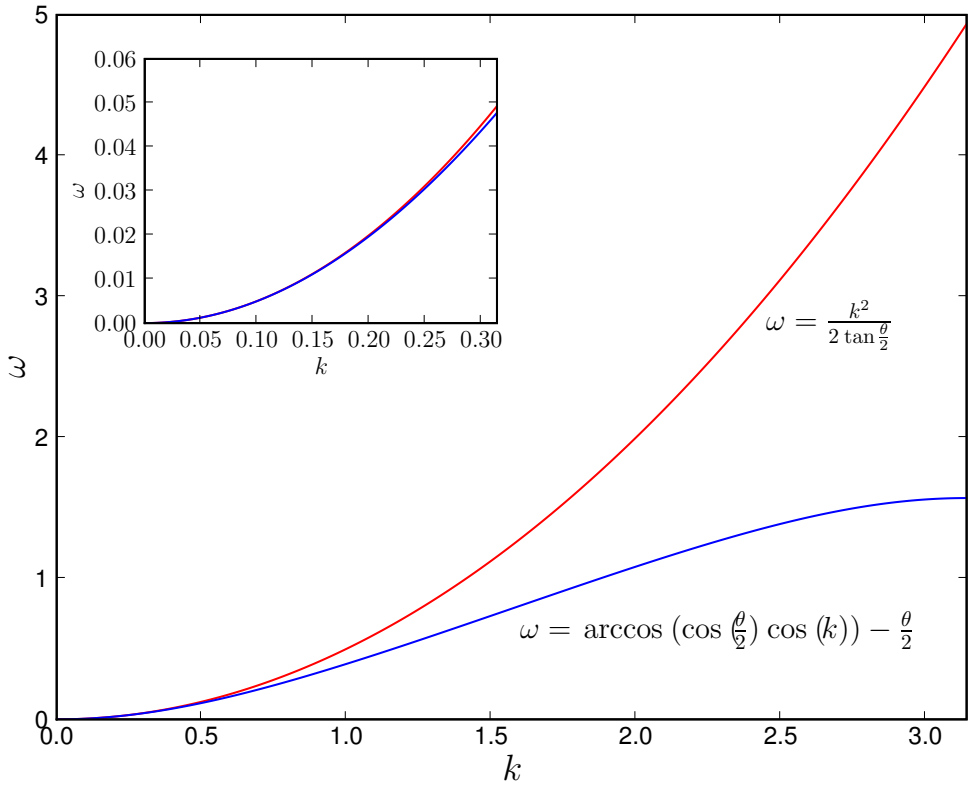
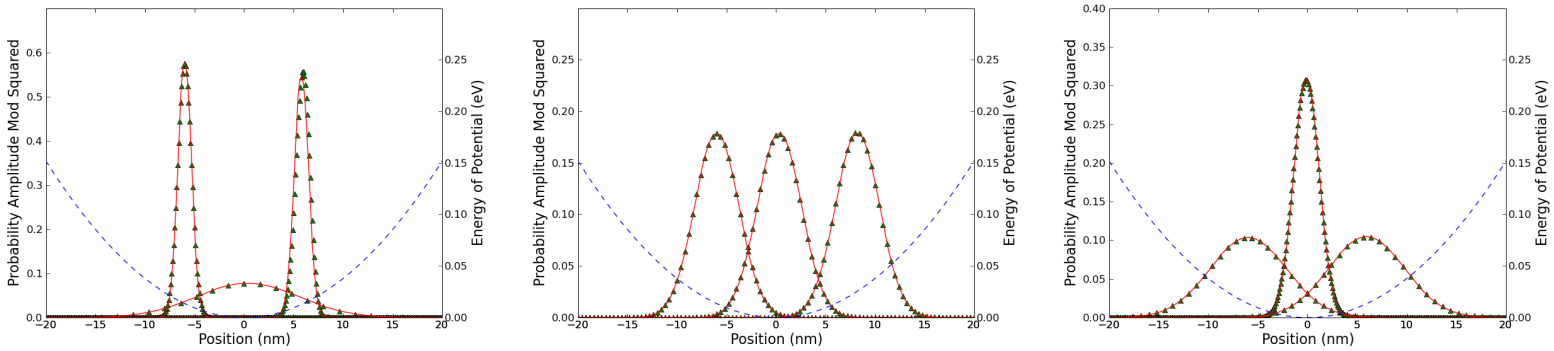


Figure: Dispersion of the Boghosian-Taylor model and the theoretical dispersion of nonrelativistic Quantum Mechanics with a focus on the small ω, small k limit.

Validating method for SHM



(a) (b) (c)

Figure: The dashed (blue) line represents the potential. The solid (red) line represents the analytic solution. The triangles (green) represent the lattice gas solution. The times are at $t = 0$ fs, $t = 69.10$ fs, and $t = 274.26$ fs. In the case of $t = 138.21$ fs, only a subset of the lattice solutions were plotted for clarity. Figure by Andrew O'Hara, HC '09

Scattering in Morse potential in QLGA

Peter - show a movie here!

Experiment 2: Dirac dynamics in trapped Ions

1-D Dirac equation

$$i\hbar\partial_t\psi = (c\hat{p}\sigma_x + mc^2\sigma_z)\psi \tag{3}$$

Phenomena: Klein paradox, *zitterbewegung* ("trembling motion"), negative energy eigenstates.

Zitterbewegung

Rapid oscillations of expectation value of position due to interference between positive and negative energy solutions.
For electron the zitterbewegung amplitude is $R_{ZB} \sim 10^{-12}$ m, and the frequency is 10^{21} Hz. That's picometer and zeptosecond length and time scales. Not observed yet.

Experiment 2: Dirac dynamics in trapped Ions: Lamata et. al. PRL 253005 (2007), Gerritsma et. al arxiv:0909.0674

Calcium ion in a linear Paul (quadrupole) trap

Bispinor states : $|0\rangle = |S_{1/2}, m = 1/2\rangle$ and $|0\rangle = |D_{5/2,m=3/2}\rangle$
Couple with laser at 729 nm
Hamiltonian:

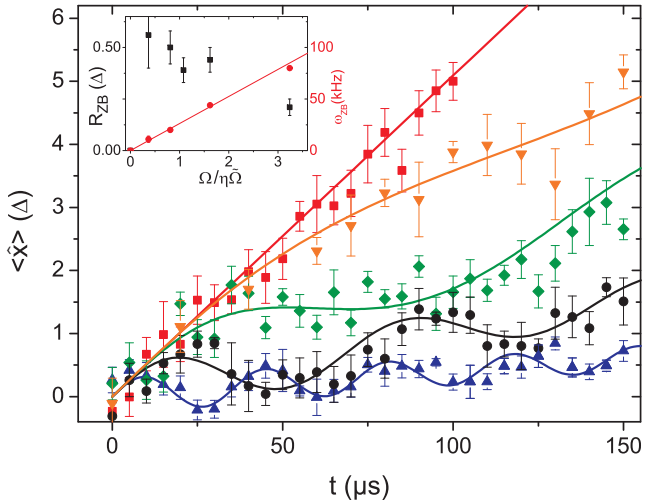
$$H = (2\eta\Delta\tilde{\Omega}\hat{p}\sigma_x + \hbar\Omega\sigma_z) \tag{4}$$

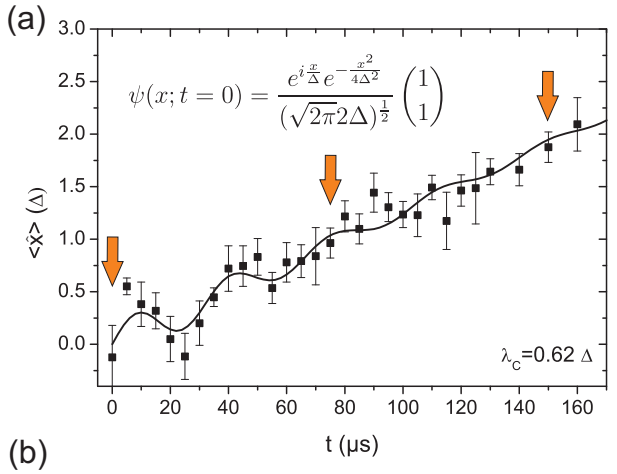
Jaynes-Cummings + optical Stark shift

Length and timescales

For $\eta = 0.06$, $\Delta = \sqrt{\hbar/2m_{Ca}\omega_{ax}} \simeq 1$ nm, $\omega_{ax} = 2\pi \times 1.36$ MHz.
$\tilde{\Omega} = 2\pi \times 68kHz$ and $0 < \Omega \leq 2\pi \times 13$ kHz
Identify $c = 2\eta\Delta\tilde{\Omega} = 0.052\Delta/\mu s \simeq 0.5\mathring{A}/\mu s$ ($\simeq 10^{-11}$ of $c = 3\mathring{A}$/attosecond)
$mc^2 = \hbar\Omega$ (about 10^{-16} the mass of an electron)

Results of Gerritsma et. al: arxiv:09090674





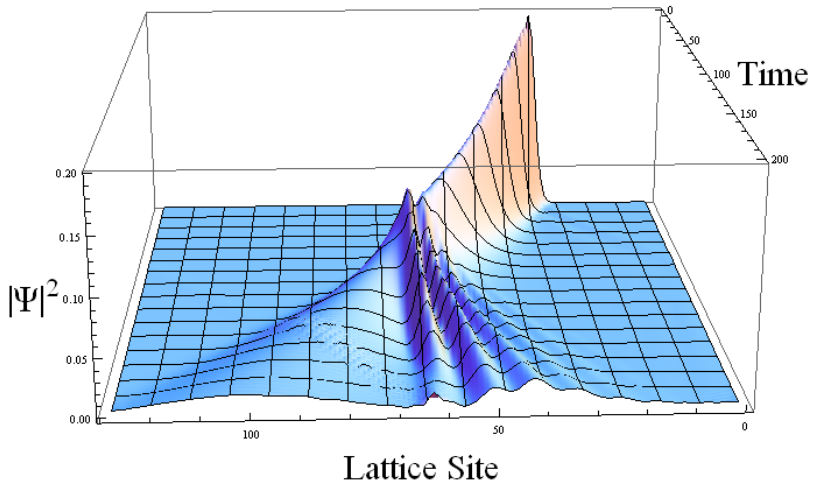
Relativistic Scattering and the Klein Paradox

Three regimes

- $0 < V_1 < E - m$
- $E - m < V_2 < E + m$
- $E + m < V_3$

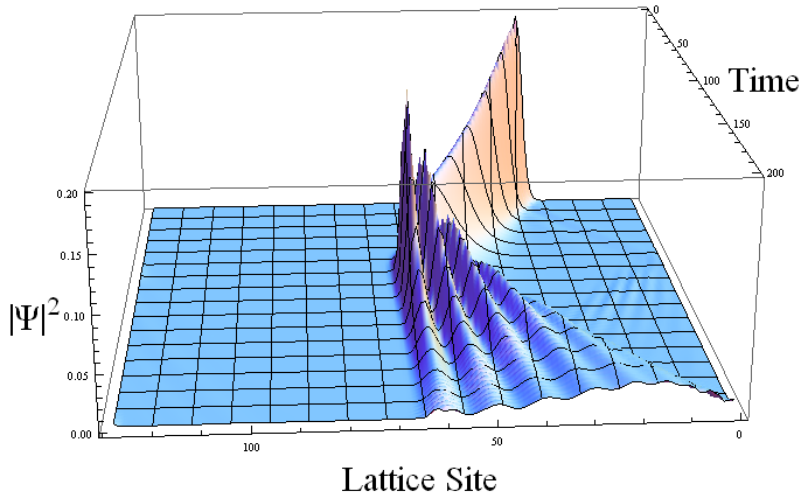
First two cases are the same as for nonrelativistic scattering.
Third case results in the Klein paradox

Relativistic Scattering: V_1



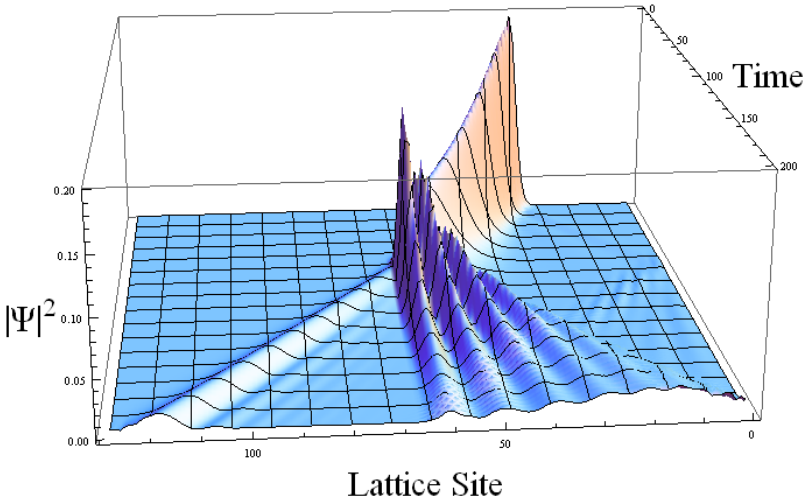
The above graph shows the $0 < V < E - m$ scenario of the Klein paradox. The origin is in the right, back corner. Parameters for the model were set so the lattice size was 128, $\theta = \frac{\pi}{3}$, and $k = \frac{\pi}{4}$. The initial binomial width was set to 32 spacings, the packet began at site 32 and the barrier was located at site 64 with a value of $\frac{\pi}{21}$.

Relativistic Scattering: V_2



The above graph shows the $E - m < V < E + m$ scenario of the Klein paradox. The origin is in the right, back corner. Parameters for the model were set so the lattice size was 128, $\theta = \frac{\pi}{3}$, and $k = \frac{\pi}{4}$. The initial binomial width was set to 32 spacings, the packet began at site 32 and the barrier was located at site 64 with a value of $\frac{\pi}{4}$.

Relativistic Scattering: V_3



The above graph shows the $E + m < V$ scenario of the Klein paradox. The origin is in the right, back corner. Parameters for the model were set so the lattice size was 128, $\theta = \frac{\pi}{3}$, and $k = \frac{\pi}{4}$. The initial binomial width was set to 32 spacings, the packet began at site 32 and the barrier was located at site 64 with a value of $\frac{5\pi}{6}$.

Conclusions

- Can perform interesting simulations of quantum systems on quantum computers
- Simplest cases are now within reach of experiment
- Historical development of classical simulation of quantum mechanics provides a potential roadmap for experiment
- Many interesting theoretical questions: state preparation for molecules (Kitaev, Webb arxiv:0801.0342, Wang, Ashab, Nori arxiv:0902.1419, Ward, Kassal, Aspuru-Gusik arxiv:0812.2681), alternatives to Jordan-Wigner, efficient quantum computation of potential functions....

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That's all, folks!

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