## Optimal Controlled Phasegates for Trapped Neutral Atoms at the Quantum Speed Limit

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Quantum Computation with Ultracold Trapped Atoms Theoretical Model and Optimization Method Two Calcium Atoms as Short Internuclear Distance Two Atoms at Long Distance under Strong Dipole Interaction

# Prologue: Quantum Computation

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## Classical Computing: 4-Bit Full Adder



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# A Single Qubit

## Definition of a Single Qubit

$$\left|\Psi\right\rangle_{1q} = \alpha_0 \left|0\right\rangle + \alpha_1 \left|1\right\rangle$$

with

$$|\alpha_0|^2 + |\alpha_1|^2 = 1$$

## Vector Representation

$$|0
angle = \begin{pmatrix} 1\\ 0 \end{pmatrix}$$
  $|1
angle = \begin{pmatrix} 0\\ 1 \end{pmatrix}$   $|\Psi
angle_{1q} = \begin{pmatrix} lpha_0\\ lpha_1 \end{pmatrix}$ 

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## Two Qubits

## Definition of a Two-Qubit System

$$|\Psi\rangle_{2g} = \alpha_{00} |00\rangle + \alpha_{01} |01\rangle + \alpha_{10} |10\rangle + \alpha_{11} |11\rangle$$

with

$$\begin{array}{l} |00\rangle \equiv |0\rangle \otimes |0\rangle & |01\rangle \equiv |0\rangle \otimes |1\rangle \\ |10\rangle \equiv |1\rangle \otimes |0\rangle & |11\rangle \equiv |1\rangle \otimes |1\rangle \end{array}$$

In general,  $\left|\Psi\right\rangle_{2a}$  can be entangled, i.e. it cannot be written as a product state

$$\left(\alpha_{0}^{(1)}\left|0\right\rangle + \alpha_{1}^{(1)}\left|1\right\rangle\right) \otimes \left(\alpha_{0}^{(2)}\left|0\right\rangle + \alpha_{1}^{(2)}\left|1\right\rangle\right)$$

Vector Representation

$$|00\rangle = \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix} \quad |01\rangle = \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix} \quad |10\rangle = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix} \quad |11\rangle = \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix} \quad |\Psi\rangle_{1q} = \begin{pmatrix} \alpha_{00}\\\alpha_{10}\\\alpha_{01}\\\alpha_{11} \end{pmatrix}$$

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## One and Two Qubit Gates

1 Qubit Gate: Hadamard2 Qubit Gate: CNOT
$$|\Psi\rangle_{1q,i} \xrightarrow{H} |\Psi\rangle_{1q,t}$$
 $|\Psi\rangle_{2q,i} \xrightarrow{CNOT} |\Psi\rangle_{2q,t}$  $|\Psi\rangle_{1q,i} \xrightarrow{-H} |\Psi\rangle_{1q,t}$  $|\Psi\rangle_{2q,i} \xrightarrow{V} |\Psi\rangle_{2q,t}$  $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} |\Psi\rangle_{1q,i} = |\Psi\rangle_{1q,t}$  $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} |\Psi\rangle_{2q,i} = |\Psi\rangle_{2q,t}$ 

**Optimal Controlled Phasegates for Trapped Neutral Atoms** 

 $\left|\Psi\right\rangle_{2q,i} \xrightarrow{CNOT} \left|\Psi\right\rangle_{2q,t}$ 

 $|\Psi\rangle_{2q,t}$ 

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## Quantum Circuits



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## Quantum Circuits



Figure 10.16. Quantum circuit for measuring the generators of the Steane code, to give the error syndrome. The top six qubits are the ancilla used for the measurement, and the bottom seven are the code qubits.

from: Nielsen, Chuang: Quantum Information and Quantum Computation

## **Quantum Computation:**



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## Quantum Circuits



Figure 10.16. Quantum circuit for measuring the generators of the Steane code, to give the error syndrome. TI top six qubits are the ancilla used for the measurement, and the bottom seven are the code qubits.

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A few explicit points:

- Universal Gate Theorem: only single-qubit gates and (two-qubit) CNOT.
- Restrictions on quantum circuit due to unitarity
- Power of quantum computing:
   Quantum Parallelism
- But: complex wavefunctions cannot be measured → Clever algorithms like Shor-algorithm for prime decompositions
- General problem:
   Decoherence

# Quantum Computation with Ultracold Trapped Atoms

Implement a Controlled Phasegate on Calcium Atoms

## The Controlled Phasegate

## Controlled Phasegate

$$\mathbf{\hat{O}}(\chi) = \mathsf{CPHASE}(\chi) = \begin{pmatrix} e^{i\chi} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



- CPHASE( $\pi$ ) equivalent to CNOT  $\Rightarrow$  Universal Quantum Computing
- CPHASE is used in Quantum Fourier Transform

# Calcium Term Scheme - Qubit Encoding



## Calcium Term Scheme – Qubit Encoding



## Two-Qubit Gates on Trapped Neutral Atoms



- Low-Lying states in Alkaline-Earth atoms or Rydberg states
- Atoms in optical lattice or optical tweezers

## The Objective

#### Problem

- **QC** with atomic collisions: adiabaticity  $\Rightarrow$  slow.
- Strong interaction ⇒ fast gates?
  - only if ignoring motion.

#### Quantum Speed limit

- QSL: What is the maximum speed at which a quantum system can evolve?
- What limits on the gate duration can we find through optimization?
- How do gate durations depend on the interaction strength?

## The Objective

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## Outline

## arXiv:1103.6050

- Describe the system including the motional degree of freedom.
- Optimize for varying times / interaction strengths:
  - Two Calcium atoms at fixed distance (fixed interaction): vary *T*
  - **Theorem 1** For fixed *T*, two atoms with "artificial" dipole-dipole interaction  $V(R) = -C_3/R^3$ : vary  $C_3$

# Theoretical Model and Optimization Method

Two-Qubit-Hamiltonian, Optimization with Krotov

## System Hamiltonian



## System Hamiltonian



$$\begin{split} \hat{\mathbf{H}} &= \left( \hat{\mathbf{H}}_{1q} \otimes \mathbb{I}_{1q} + \mathbb{I}_{1q} \otimes \hat{\mathbf{H}}_{1q} \right) \otimes \mathbb{I}_{R} + \mathbb{I}_{1q} \otimes \mathbb{I}_{1q} \otimes \hat{\mathbf{H}}_{trap} + \hat{\mathbf{H}}_{int} \\ &= \sum_{i,k} |ik\rangle \langle ik| \otimes \left[ \hat{\mathbf{T}} + \hat{\mathbf{V}}_{trap}(R) + \hat{\mathbf{V}}_{BO}^{ik}(R) + \hat{\mathbf{E}}_{ik} \right] + \\ &+ \epsilon(t) \sum_{i \neq j,k} \left[ |ik\rangle \langle jk| + |ki\rangle \langle kj| \right] \otimes \hat{\boldsymbol{\mu}}_{ij} \end{split}$$

## System Hamiltonian



# The Logical Subspace

Full System Hamiltonian

$$\hat{\mathbf{H}} = \left( \hat{\mathbf{H}}_{1\mathsf{q}} \otimes \mathbb{1}_{1\mathsf{q}} + \mathbb{1}_{1\mathsf{q}} \otimes \hat{\mathbf{H}}_{1\mathsf{q}} \right) \otimes \mathbb{1}_{R} + \mathbb{1}_{1\mathsf{q}} \otimes \mathbb{1}_{1\mathsf{q}} \otimes \hat{\mathbf{H}}_{\mathsf{trap}} + \hat{\mathbf{H}}_{\mathsf{int}}$$

Dimension of Ĥ: 3 × 3 × N<sub>R</sub>
Dimension of Ô: 4

 $\Rightarrow$  How does that work...?

## The Logical Subspace

Full System Hamiltonian

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- Dimension of  $\hat{\mathbf{H}}$ :  $3 \times 3 \times N_R$
- Dimension of **Ô**: 4
- $\Rightarrow$  How does that work...?
  - 4 initial states:  $|ij\varphi_0\rangle = |ij\rangle \otimes |\varphi_0\rangle$ , i, j = 0, 1with  $\varphi_0(R)$  the vibrational ground state of the harmonic trap.
  - After pulse: projection onto logical subspace
    - There should be no population left in the auxiliary electronic states
    - The vibrational state after the pulse should again be  $|\varphi_0(R)\rangle$  (up to a phase factor)

## The Logical Subspace

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$$\hat{\mathbf{H}} = \left(\hat{\mathbf{H}}_{1\mathsf{q}} \otimes \mathbb{1}_{1\mathsf{q}} + \mathbb{1}_{1\mathsf{q}} \otimes \hat{\mathbf{H}}_{1\mathsf{q}}\right) \otimes \mathbb{1}_{R} + \mathbb{1}_{1\mathsf{q}} \otimes \mathbb{1}_{1\mathsf{q}} \otimes \hat{\mathbf{H}}_{\mathsf{trap}} + \hat{\mathbf{H}}_{\mathsf{int}}$$

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General concept! Having a logical subspace in a large Hilbert space of the physical system is quite common in implementations of quantum computation.

# **Optimal Control**

Generally: we have some "knobs" that we can turn to influence the dynamics of a system, and we want find the optimal way to turn them to reach a desired outcome.

E.g. Curling:



- the goal: bring the stone as close as possible to the target at time T
- "Static control": speed, direction, and spin of thrown rock
- "Dynamic control" (at every point in time): sweeping
  - where to sweep
  - how hard to sweep
- take into account physical constraints: boundaries of the playing field, sweeping speed and strength of players

## **Optimal Control**

Generally: we have some "knobs" that we can turn to influence the dynamics of a system, and we want find the optimal way to turn them to reach a desired outcome.



#### In Quantum Mechanics:

- Drive a quantum state from an initial to a target state (or unitary transformation)
- System dynamics given by Hamiltonian
- Control: some parameter in the Hamiltonian; in our case: amplitude of laser pulse over time.
- Take into account constraints, e.g. finite pulse amplitude
- $\Rightarrow$  iterative optimization algorithms

## Optimizing the Laser Pulse

## Target Functional

$$J = -\underbrace{\frac{1}{N}\mathfrak{Re}\left[\mathrm{tr}\left(\hat{\mathbf{0}}^{\dagger}\hat{\mathbf{U}}\right)\right]}_{F} + \int_{0}^{T}\frac{\alpha}{S(t)}\Delta\epsilon^{2}(t)\,\mathrm{d}t; \qquad \hat{\mathbf{0}} = \mathrm{CPHASE}_{e^{-i\hat{\mathbf{H}}(\epsilon(t))t}}$$

Krotov: pulse update  $\Delta \epsilon$ minimizing J

 $\Delta\epsilon\sim\mathfrak{Im}\left<\Psi_{bw}\left|\hat{\boldsymbol{\mu}}\right|\Psi_{fw}
ight>$ 

Palao, Kosloff, PRA 68, 062308 (2003)



## The Krotov Algorithm



- Propagate target state backward with guess pulse
- Calculate pulse update
- Propagate forward with updated pulse

## Measures of Merit

Fidelity F and cost functional J are not very informative.

Control over the Motional Degree of Freedom

$$\boldsymbol{F_{00}} = \left| \left\langle 00\varphi_0 \left| \hat{\boldsymbol{\mathsf{U}}}(\boldsymbol{\mathcal{T}}, 0; \boldsymbol{\epsilon}^{opt}) \right| 00\varphi_0 \right\rangle \right|^2$$

Does  $|00\rangle$  return to it's initial vibrational eigenstate?

#### Gate Phases

$$\phi_{00} = \arg\left(\left\langle 00\varphi_{0} \left| \hat{\mathbf{U}}(\mathcal{T}, 0; \epsilon^{opt}) \right| 00\varphi_{0} \right) \right\rangle\right)$$

What is the phase change relative to the initial state?

## Cartan Decomposition

## Local Two-Qubit Gate

$$\begin{array}{c} \overbrace{\phantom{a}} X \\ \hline X \\ \hline \end{array} \qquad \qquad \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \mathbb{1} \right) \left( \mathbb{1} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

Distinguish local two-qubit gate from non-local gate like CNOT, that cannot be decomposed this way! (cf. product states vs entangled states)

## Cartan Decomposition

## Zhang et al. PRA 67, 042313 (2003)

$$\hat{\mathbf{U}} = \hat{\mathbf{k}}_1 \hat{\mathbf{A}} \hat{\mathbf{k}}_2$$

- $\boldsymbol{\hat{k}}_1,~\boldsymbol{\hat{k}}_2:$  local operations;  $\boldsymbol{\hat{A}}:$  purely non-local operation
  - Only has entangling power
  - Cartan decomposition defines equivalence class of two-qubit gates ("Locally equivalent")

## Measures of Merit

Fidelity F and cost functional J are not very informative.

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$$\boldsymbol{F}_{00} = \left| \left\langle 00\varphi_0 \left| \hat{\boldsymbol{\mathsf{U}}}(\boldsymbol{\mathsf{T}}, 0; \boldsymbol{\epsilon}^{opt}) \right| 00\varphi_0 \right\rangle \right|^2$$

Does  $|00\rangle$  return to it's initial vibrational eigenstate?

#### Gate Phases

$$\phi_{00} = \arg\left(\left\langle 00\varphi_{0}\left|\hat{\mathbf{U}}(\mathcal{T},0;\epsilon^{opt})\right|00\varphi_{0}\right)\right\rangle\right)$$

What is the phase change relative to the initial state?

#### True Two-Qubit Phase

Cartan Decomposition leads to

$$\chi = \phi_{00} - \phi_{01} - \phi_{10} + \phi_{11}$$

Concurrence (Entanglement)  $C = |\sin \frac{\chi}{2}|$ 

# Two Calcium Atoms at Short Internuclear Distance

For which gate durations can we reach a high-fidelity CPHASE?

## Parameters of the Optimization





## Optimization Success over Pulse Duration



 $\Rightarrow$  For small T, vibrational purity is lost with increasing two-qubit phase  $\Rightarrow$  High two-qubit phase *and* high vibrational only for long pulse durations

System Dynamics for 800 ps Pulse



# The Reduced Optimization Scheme

	full	reduced
target	$egin{aligned}  00 angle  o e^{i(\phi+\phi_{ au})}  00 angle \  01 angle  o e^{i\phi_{ au}}  01 angle \  10 angle  o e^{i\phi_{ au}}  10 angle \  11 angle  o e^{i\phi_{ au}}  11 angle \end{aligned}$	$egin{aligned}  00 angle  ightarrow e^{i(\phi+\phi au)} \ket{00} \  0 angle  ightarrow e^{i\phi au/2} \ket{0} \end{aligned}$
gate phases	$\phi_{00} \ \phi_{10} = \phi_{01} \ \phi_{11}$	$= \phi_{00}$ $= \phi_0 + \phi_1$ $= 2\phi_1$
non-local phase	$\chi = \phi_{00} - \phi_{01} - \phi_{10} + \phi_{11}$	$\chi=\phi_{00}-2\phi_0$

# Two Atoms at Long Distance under Strong Dipole-Dipole Interaction

Can we avoid vibration with very short pulses, but very strong interaction?

## Parameters of the Optimization

- Fixed short pulse duration
   T = 1 ps, T = 0.5 ps
- Realistic lattice spacing with strong interaction  $\sim -\frac{C_3}{R^3}$

■ Vary C<sub>3</sub>:

- $C_3 = 1 \times 10^6$ Action over 1 ps for Calcium at d = 5 nm, scaled to d = 200 nm
- Increase by three orders of magnitude Action over 800 ps for Calcium at d = 5 nm, scaled to d = 200 nm





## Optimization Success over Dipole Interaction Strength



interaction strength  $C_3$  (atomic units)

 $\Rightarrow$  Increasing two-qubit-phase with increasing interaction strength

 $\Rightarrow$  For small T, vibrational purity is lost with increasing two-qubit phase

# Conclusions

## Conclusions



- Long gate duration can reach arbitrarily high fidelities.
- For short gate durations, the two-qubit phase is at the expense of the vibrational purity.
- If T < QSL, not all measures of merit can be fulfilled.
- Time scale for a successful gate is determined by  $\max(T_{int}, T_{vib})$ .

# Thanks!