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

Michael Goerz

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

Classical Computing: 4-Bit Full Adder

Inside the CPU:

- **Bits:**
  - $0 \equiv$ low voltage
  - $1 \equiv$ high voltage

- **Calculations:**
  - logical functions of bits
  - mapped to electronic gates

  - Gates combine to more complex gates
  - Gates can be decomposed into NAND-gates

A Single Qubit

Definition of a Single Qubit

\[ |\psi\rangle_{1q} = \alpha_0 |0\rangle + \alpha_1 |1\rangle \]

with

\[ |\alpha_0|^2 + |\alpha_1|^2 = 1 \]

Vector Representation

\[ |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad |\psi\rangle_{1q} = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \]
Two Qubits

**Definition of a Two-Qubit System**

\[
|\Psi\rangle_{2q} = \alpha_{00} |00\rangle + \alpha_{01} |01\rangle + \alpha_{10} |10\rangle + \alpha_{11} |11\rangle
\]

with

\[
|00\rangle \equiv |0\rangle \otimes |0\rangle \quad |01\rangle \equiv |0\rangle \otimes |1\rangle \quad |10\rangle \equiv |1\rangle \otimes |0\rangle \quad |11\rangle \equiv |1\rangle \otimes |1\rangle
\]

In general, \(|\Psi\rangle_{2q}\) can be entangled, i.e. it cannot be written as a product state

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

**Vector Representation**

\[
|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad |\Psi\rangle_{1q} = \begin{pmatrix} \alpha_{00} \\ \alpha_{10} \\ \alpha_{01} \\ \alpha_{11} \end{pmatrix}
\]
### One and Two Qubit Gates

#### 1 Qubit Gate: Hadamard

\[
\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} |\psi\rangle_1, i = |\psi\rangle_1, t
\]

\[
|\psi\rangle_1, i \xrightarrow{H} |\psi\rangle_1, t
\]

#### 2 Qubit Gate: CNOT

\[
\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} |\psi\rangle_2, i = |\psi\rangle_2, t
\]

\[
|\psi\rangle_2, i \xrightarrow{CNOT} |\psi\rangle_2, t
\]
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Quantum Circuits

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  - Gates can be decomposed into NAND-gates

Quantum Computation:

- **Qubits:**
  - Eigenstates $|0\rangle$, $|1\rangle$
  - Superposition states $|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$

- **Calculations:**
  - logical functions of bits
    - mapped to electronic gates
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Quantum Computation

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Quantum Circuits

- Qubits:
  - Eigenstates $|0\rangle$, $|1\rangle$
  - Superposition states $|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$

- Calculations:
  - unitary transformations of qubits
  - mapped to quantum gates


Optimal Controlled Phasegates for Trapped Neutral Atoms
Quantum Computation: 

- Qubits:
  - Eigenstates \( |0\rangle, |1\rangle \)
  - Superposition states \( |\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle \)

- Calculations:
  - unitary transformations of qubits
  - mapped to quantum gates
  - Gates combine to more complex gates
  - Gates can be decomposed into single-qubit and CNOT

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
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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.

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

from: Nielsen, Chuang: Quantum Information and Quantum Computation
Quantum Computation with Ultracold Trapped Atoms

Implement a Controlled Phasegate on Calcium Atoms
The Controlled Phasegate

**Controlled Phasegate**

\[ \hat{O}(\chi) = \text{CPHASE}(\chi) = \begin{pmatrix} e^{i\chi} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]

**Controlled-Not**

\[ \text{CNOT} = \begin{array}{cccc} \text{H} & \text{X} & O(\pi) & \text{X} \\ \text{X} & \text{X} & \text{H} & \text{X} \end{array} \]

- CPHASE(\pi) equivalent to CNOT \Rightarrow Universal Quantum Computing
- CPHASE is used in Quantum Fourier Transform
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Calcium Term Scheme – Qubit Encoding

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**Calcium Term Scheme – Qubit Encoding**

\[ |0\rangle \quad |1\rangle \quad |\text{aux}\rangle \]

\( \omega_L = 23652\text{cm}^{-1} \)

Optimal Controlled Phasegates for Trapped Neutral Atoms
Two-Qubit Gates on Trapped Neutral Atoms

Calcium:

\[ \begin{align*}
\frac{1}{1} P_1 & \quad |a\rangle \\
\frac{1}{1} S_0 & \quad |0\rangle \\
\frac{1}{1} P_3 & \quad |1\rangle
\end{align*} \]

\[ \omega_L = 23652 \text{ cm}^{-1} \]

- 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 $\Rightarrow$ 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

Problem

- QC with atomic collisions: adiabaticity ⇒ 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?
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Outline

- Describe the system including the motional degree of freedom.
- Optimize for varying times / interaction strengths:
  1. Two Calcium atoms at fixed distance (fixed interaction):
     vary $T$
  2. 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

\[
\begin{align*}
\hat{H} &= \hat{H}_0 + \hat{H}_I \\
\hat{H}_0 &= \frac{1}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + V_0 (x_1, x_2) \\
\hat{H}_I &= \hat{P}_1 \hat{P}_2 \\
&= \frac{i}{\hbar} \left[ \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2} \right] + \frac{i}{\hbar} \left[ \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2} \right] + \frac{i}{\hbar} \left[ \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2} \right]
\end{align*}
\]

integrate out COM

\[
R_0 = d
\]
System Hamiltonian

\[ \hat{H} = \left( \hat{H}_{1q} \otimes 1_{1q} + 1_{1q} \otimes \hat{H}_{1q} \right) \otimes 1_R + 1_{1q} \otimes 1_{1q} \otimes \hat{H}_{\text{trap}} + \hat{H}_{\text{int}} \]

\[ = \sum_{i,k} |ik\rangle \langle ik| \otimes \left[ \hat{T} + \hat{V}_{\text{trap}}(R) + \hat{V}_{\text{BO}}(R) + \hat{E}_{ik} \right] + \]

\[ + \epsilon(t) \sum_{i \neq j,k} \left[ |ik\rangle \langle jk| + |ki\rangle \langle kj| \right] \otimes \hat{\mu}_{ij} \]
System Hamiltonian

\[ h = d x_1 x_2 \]

\[ R_0 = d \]

\[ |00\rangle, |01\rangle, |10\rangle, |11\rangle \]

\[ 47304.61 \text{ cm}^{-1}, 38862.37 \text{ cm}^{-1}, 30420.13 \text{ cm}^{-1}, 23652.30 \text{ cm}^{-1}, 15210.06 \text{ cm}^{-1}, 0.0 \text{ cm}^{-1} \]
Full System Hamiltonian

\[ \hat{H} = \left( \hat{H}_{1q} \otimes 1_{1q} + 1_{1q} \otimes \hat{H}_{1q} \right) \otimes 1_R + 1_{1q} \otimes 1_{1q} \otimes \hat{H}_{\text{trap}} + \hat{H}_{\text{int}} \]

- Dimension of \( \hat{H} \): \( 3 \times 3 \times N_R \)
- Dimension of \( \hat{O} \): 4

⇒ How does that work...?
Quantum Computation with Ultracold Trapped Atoms

Theoretical Model and Optimization Method

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The Logical Subspace

Full System Hamiltonian

\[
\hat{H} = \left( \hat{H}_1 \otimes 1_{1q} + 1_{1q} \otimes \hat{H}_1 \right) \otimes 1_R + 1_{1q} \otimes 1_{1q} \otimes \hat{H}_{\text{trap}} + \hat{H}_{\text{int}}
\]

- Dimension of \( \hat{H} \): \( 3 \times 3 \times N_R \)
- Dimension of \( \hat{O} \): 4

⇒ How does that work...?

- 4 initial states: \( |ij\varphi_0\rangle = |ij\rangle \otimes |\varphi_0\rangle \), \( i, j = 0, 1 \)
  with \( \varphi_0(R) \) 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

Full System Hamiltonian

\[ \hat{H} = \left( \hat{H}_{1q} \otimes 1_{1q} + 1_{1q} \otimes \hat{H}_{1q} \right) \otimes 1_R + 1_{1q} \otimes 1_{1q} \otimes \hat{H}_{\text{trap}} + \hat{H}_{\text{int}} \]

- Dimension of $\hat{H}$: $3 \times 3 \times N_R$
- Dimension of $\hat{O}$: 4

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

- 4 initial states: $|ij\varphi_0\rangle = |ij\rangle \otimes |\varphi_0\rangle$, $i, j = 0, 1$
  with $\varphi_0(R)$ the vibrational ground state of the harmonic trap.
- After pulse: projection onto logical subspace
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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 to 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 to 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

⇒ iterative optimization algorithms
Optimizing the Laser Pulse

Target Functional

\[ J = -\frac{1}{N} \text{Re} \left[ \text{tr} \left( \hat{O}^{\dagger} \hat{U} \right) \right] + \int_{0}^{T} \frac{\alpha}{S(t)} \Delta \epsilon^2(t) \, dt; \]
\[ \hat{O} = \text{CPHASE} \]
\[ \hat{U} = e^{-i \hat{H}(\epsilon(t)) t} \]

Krotov: pulse update \( \Delta \epsilon \)
minimizing \( J \)

\( \Delta \epsilon \sim \text{Im} \left< \psi_{bw} | \hat{\mu} | \psi_{fw} \right> \)

Palao, Kosloff,
PRA 68, 062308 (2003)
The Krotov Algorithm

- Propagate target state backward with guess pulse
- Calculate pulse update
- Propagate forward with updated pulse
Fidelity $F$ and cost functional $J$ are not very informative.

**Control over the Motional Degree of Freedom**

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

Does $|00\rangle$ return to its initial vibrational eigenstate?

**Gate Phases**

$$\phi_{00} = \text{arg} \left( \langle 00\varphi_0 | \hat{U}(T, 0; \epsilon_{opt}) | 00\varphi_0 \rangle \right)$$

What is the phase change relative to the initial state?
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**Theoretical Model and Optimization Method**

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## Cartan Decomposition

### Local Two-Qubit Gate

\[
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix} \otimes \mathbb{1} \otimes \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix} =
\begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}
\]

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

---

\[ \hat{U} = \hat{k}_1 \hat{A} \hat{k}_2 \]

\( \hat{k}_1, \hat{k}_2 \): local operations; \( \hat{A} \): purely non-local operation

- Only \( \hat{A} \) has entangling power
- Cartan decomposition defines equivalence class of two-qubit gates ("Locally equivalent")

---

Optimal Controlled Phasegates for Trapped Neutral Atoms
Measures of Merit

Fidelity $F$ and cost functional $J$ are not very informative.

Control over the Motional Degree of Freedom

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Does $|00\rangle$ return to its initial vibrational eigenstate?

Gate Phases

$$\phi_{00} = \arg \left( \left\langle 00 \varphi_0 \left| \hat{U}(T, 0; \epsilon_{opt}) \right| 00 \varphi_0 \right\rangle \right)$$

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)

$$C = \left| \sin \frac{\chi}{2} \right|$$
Two Calcium Atoms at Short Internuclear Distance

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

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Parameters of the Optimization

- Short internuclear distance
  \( \Rightarrow \) sufficient interaction

- Peak intensity \( \epsilon_0 \)
  to induce 1 Rabi cycle

- Pulse duration between \( T_{\text{int}}^{1\text{rad}} = 1.23 \text{ ps} \) and \( T_v = 800 \text{ ps} \)

\[ \begin{align*}
\frac{1}{T_{\text{int}}^{1\text{rad}}} & \quad |0a\rangle \\
d & \quad |00\rangle \\
\frac{\pi}{T_v} & \quad |00\rangle
\end{align*} \]
it increases rather slowly for larger local gate. However, for short gate durations, no control action of the exchange interaction leads indeed to a non-value of $\chi$ general shape. The non-local phase reaches the desired switch-on and switch-off excited state for the complete gate duration. This is not surprising since the wavepacket is not in the phase of the time that was roughly estimated to reach a non-local $\chi$ Fig. 4 can be understood as follows: The two-qubit phase arbitrarily close to one can be reached. The results shown in optimization is successful in the sense that fidelities are obtained. As the gate operation time approaches errors remaining larger than $10^{-3}$ within except for $\chi$ lied between the two limits $\Delta$ energy difference in the trap is estimated by considering the mean π and $a$ rated, i.e. non-interacting atoms in the where $E_0$ denotes the energy of two infinitely separated, Eq. (16), and vibrational fidelity, i.e., projection onto the vibrational time scale associated with the vibrational motion in the trap states. As the gate duration becomes comparable only once the pulse is long enough to resolve di $\Delta$lation of excited trap states after the gate can be avoided state and thus it cannot counteract the excitation. Population in the trap, optimization cannot identify the desired trap pulse returns the wavepacket to the electronic ground state, it has acquired significant vibrational energy. Since pulse returns the wave packet spending enough time in the excited state $\chi\approx 1$ for a non-local phase of $\approx 30 \text{ ps}$ and $50 \text{ ps}$ which are converged to $4 \text{ ps}$ for a non-local phase of $4 \text{ ps}$ and $\approx 7 \text{ during the course of iterations.}$ Optimization results for gate operation times vary $\chi\approx 7 \text{ during the course of iterations.}$ Optimization results for gate operation times vary.

$\Rightarrow$ 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

$$F = 0.999$$

$$\tau_{00} = \langle 00\varphi_0 | \hat{U}(T, 0; \epsilon^{opt}) | 00\varphi_0 \rangle$$
## The Reduced Optimization Scheme

<table>
<thead>
<tr>
<th>Target</th>
<th>Full</th>
<th>Reduced</th>
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<tbody>
<tr>
<td>$</td>
<td>00\rangle \rightarrow e^{i(\phi + \phi_T)}</td>
<td>00\rangle$</td>
</tr>
<tr>
<td>$</td>
<td>01\rangle \rightarrow e^{i\phi_T}</td>
<td>01\rangle$</td>
</tr>
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<td>$</td>
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<tr>
<td>$\phi_{10} = \phi_{01}$</td>
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<td>$\phi_{11}$</td>
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<tr>
<th>Non-local phase</th>
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<tr>
<td>$\chi = \phi_{00} - \phi_{01} - \phi_{10} + \phi_{11}$</td>
</tr>
<tr>
<td>$\chi = \phi_{00} - 2\phi_0$</td>
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</table>
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
  \[ T = 1 \text{ ps}, \quad T = 0.5 \text{ ps} \]

- Realistic lattice spacing with strong interaction
  \[ \sim - \frac{C_3}{R^3} \]

- Vary \( C_3 \):
  
  - \( C_3 = 1 \times 10^6 \)
    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

\[ \begin{align*}
|0a\rangle & \quad C_3 = 1 \times 10^6 \\
|00\rangle & \quad C_3 = 1 \times 10^9
\end{align*} \]
to realize the non-local phase, we expect to find high-electron density in the dipole-dipole interaction. This is because the requirement of a sufficiently strong interaction is such that such an interaction energy is sufficient for entropy production. The electron density has to be set to at least 250 kHz. This corresponds to a realistic optical lattice in the UV regime. In order to separate atoms by more, increasing its vibrational excitation. This results in the motional degree of freedom, with the vibrational frequency being at a typical distance of 4 nm. Based on the results of Sec. III A, we know that the interaction potential of two calcium atoms in a.u., resulting in an interaction energy of about 1 a.u. Just for comparison, the interaction energy for highly excited Rydberg states is about 3 a.u.

For small interaction strength, the dipole-dipole interaction potential is 3 a.u. However, increasing the interaction strength leads to a sufficiently strong interaction that is used in Sec. III A, the dipole-dipole interaction potential is 3 a.u., resulting in an interaction energy of about 1 a.u. Just for comparison, the interaction energy for highly excited Rydberg states is about 3 a.u. From 1 a.u. to 100 a.u., the optimization algorithm cannot resolve the eigenstates of the trap. Thus it cannot identify the motional degree of freedom, with the vibrational frequency being more, increasing its vibrational excitation. This results in the non-local phase of the state, with the vibrational frequency being at a typical distance of 4 nm.

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Increasing two-qubit-phase with increasing interaction strength

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 $\max (T_{int}, T_{vib})$. 

![Graph showing fidelity over pulse duration and interaction strength](image-url)
Thanks!