Implementation of a Calcium Phasegate

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Part I

Why?

Outline

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

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad |\Psi\rangle_{1q} = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}$$

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

$$|00\rangle \equiv |0\rangle \otimes |0\rangle \qquad |01\rangle \equiv |0\rangle \otimes |1\rangle$$
$$|10\rangle \equiv |1\rangle \otimes |0\rangle \qquad |11\rangle \equiv |1\rangle \otimes |1\rangle$$

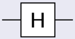
Vector Representation

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

One and Two Qubit Gates

1 Qubit Gate: Hadamard

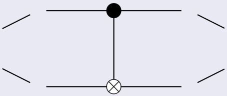
$$|\Psi\rangle_{1q,i} \xrightarrow{H} |\Psi\rangle_{1q,t}$$

$|\Psi\rangle_{1q,i}$  $|\Psi\rangle_{1q,t}$

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}|\Psi\rangle_{1q,i} = |\Psi\rangle_{1q,t}$$

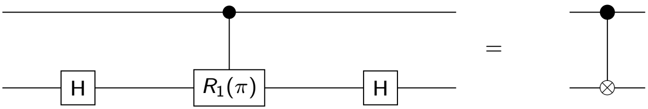
2 Qubit Gate: CNOT

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

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

$$\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}|\Psi\rangle_{2q,i} = |\Psi\rangle_{2q,t}$$

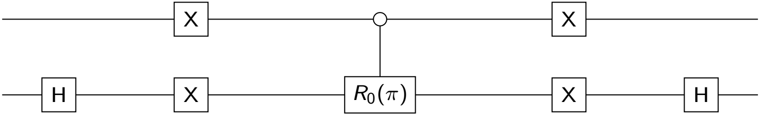
Quantum Circuits



$$\mathbf{1} \otimes \hat{H} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \cdot \mathbf{1} \otimes \hat{H} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

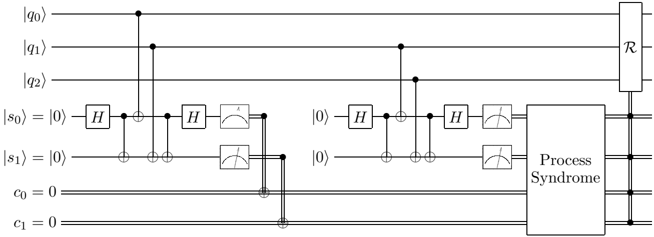
CNOT from Phasegate

=

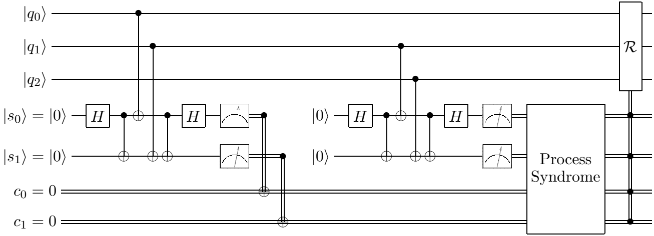


$$= \mathbf{1} \otimes \hat{H} \cdot (\hat{X} \otimes \mathbf{1} \cdot \mathbf{1} \otimes \hat{X}) \cdot \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \cdot (\hat{X} \otimes \mathbf{1} \cdot \mathbf{1} \otimes \hat{X}) \cdot \mathbf{1} \otimes \hat{H}$$

Complicated Gates from One- and Two-Qubit Gates



Complicated Gates from One- and Two-Qubit Gates



Replacing Gates

In a complicated circuit involving multi-qubit gates, we can replace these gates with a series of one- and two-qubit gates

Universal Gate Theorem

Theorem

Single Qubit and CNOT gates are universal: every quantum circuit can be constructed using only single qubit gates and the two-qubit CNOT gate.

The Controlled Phasegate

Two-Qubit Controlled Phasegate

$$\hat{O} = \begin{pmatrix} e^{i\phi} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Benefits of the Controlled Phasegate

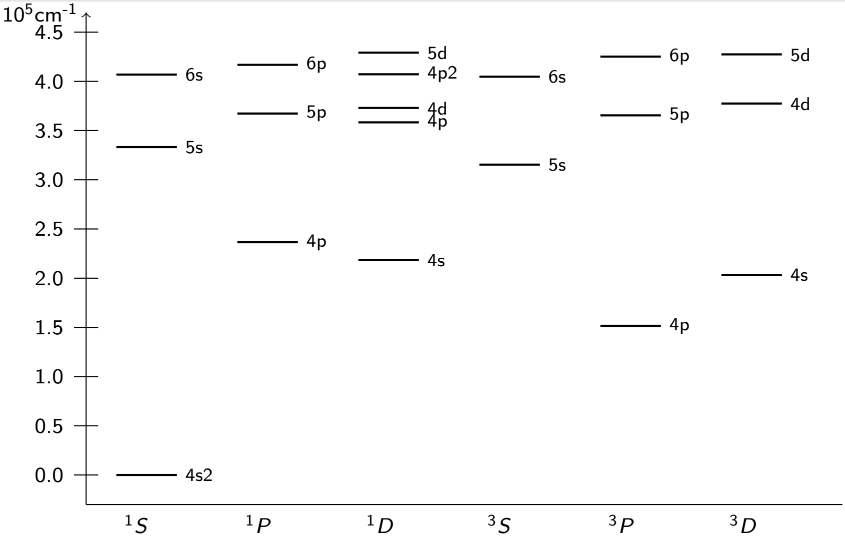
- Depending on ϕ, the Controlled Phasegate can emulate other gates.
- For $\phi = \pi$, it can emulate a CNOT.
- For $\phi = \pi/2$, it can emulate a SWAP.
- For $\phi = \phi'/n$, the gate can be repeated n times to achieve a total phase of ϕ'.

Part II

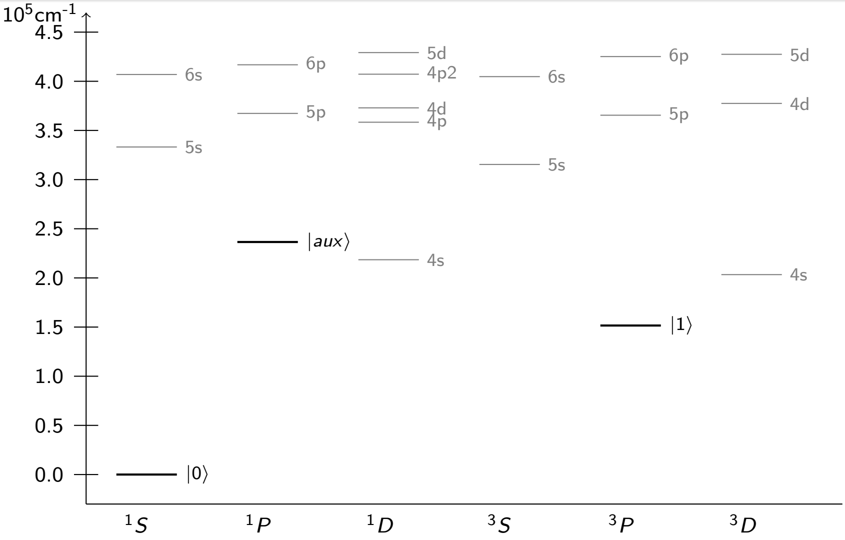
What?

Outline

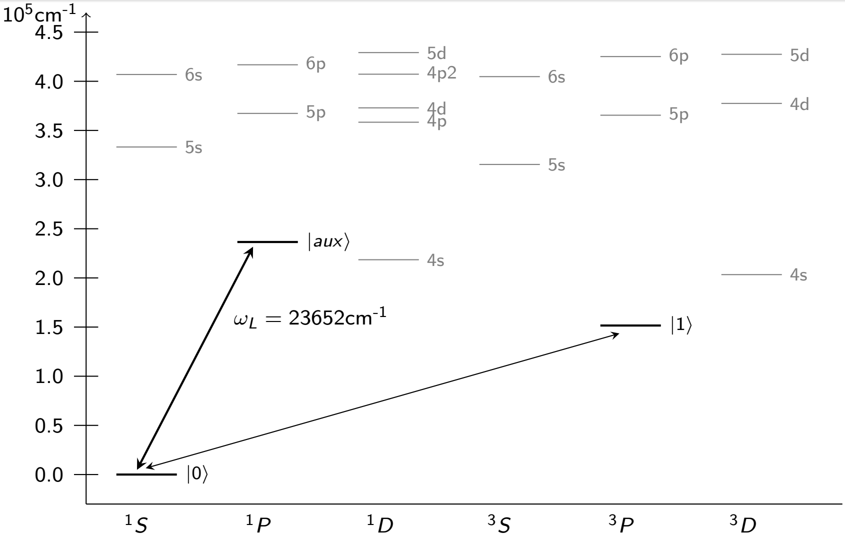
Calcium Term Scheme



Calcium Term Scheme



Calcium Term Scheme



One-Qubit Hamiltonian

Field Free Hamiltonian

$$\hat{H}_{1q}^{(0)} = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_{\text{aux}} \end{pmatrix}$$

Field Hamiltonian

$$\hat{H}_{1q} = \begin{pmatrix} E_0 & 0 & \mu\epsilon(t) \\ 0 & E_1 & 0 \\ \mu^*\epsilon(t) & 0 & E_{\text{aux}} \end{pmatrix}$$

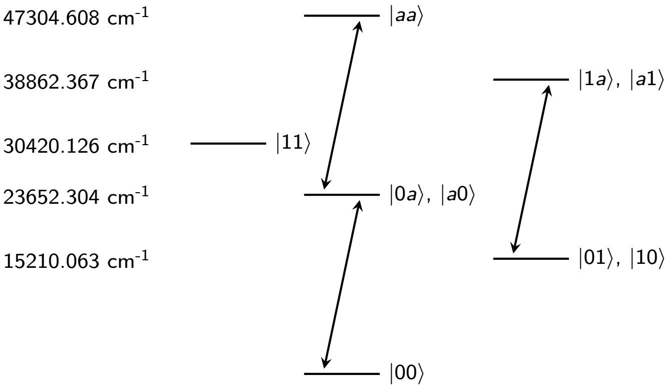
Logical Two-Qubit Hamiltonian

$$\hat{H}_{2q} = \hat{H}_{1q} \otimes \mathbf{1} + \mathbf{1} \otimes \hat{H}_{1q}$$

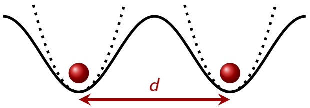
$$= \begin{pmatrix} E_0^0 & \cdot & \mu\epsilon & & & & \mu\epsilon & \cdot & \cdot \\ \cdot & E_1^0 & \cdot & & & & \cdot & \mu\epsilon & \cdot \\ \mu\epsilon & \cdot & E_{\text{aux}}^0 & & & & \cdot & \cdot & \mu\epsilon \\ & & & E_0^1 & \cdot & \mu\epsilon & & & \\ & & & \cdot & E_1^1 & \cdot & & & \\ & & & \mu\epsilon & \cdot & E_{\text{aux}}^1 & & & \\ \mu\epsilon & \cdot & \cdot & & & & E_0^{\text{aux}} & \cdot & \mu\epsilon \\ \cdot & \mu\epsilon & \cdot & & & & \cdot & E_1^{\text{aux}} & \cdot \\ \cdot & \cdot & \mu\epsilon & & & & \mu\epsilon & \cdot & E_{\text{aux}}^{\text{aux}} \end{pmatrix},$$

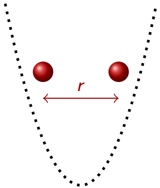
with $E_i^j \equiv E_i + E_j$

Logical Two-Qubit System



Atoms in the Optical Lattice

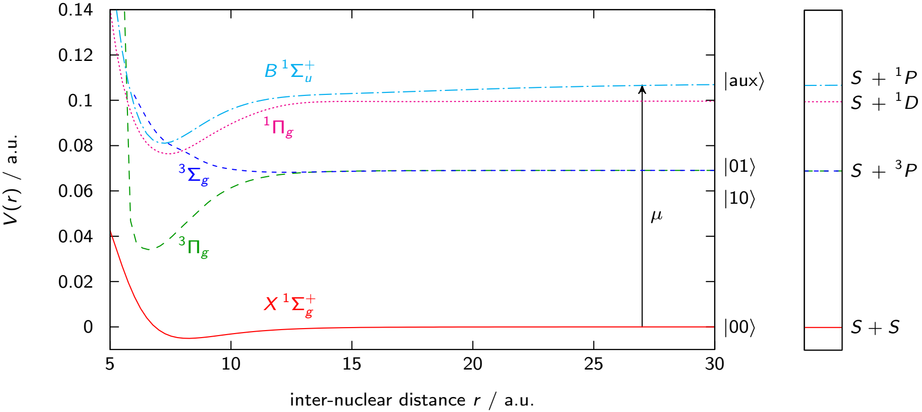




Wavefunction Including the Motional Degree of Freedom

$$|\Psi(r)\rangle_{2q} = \Psi(r) \otimes \sum_{i,j=\{0,1\}} a_{ij} \, |ij\rangle$$

Interaction (Born-Oppenheimer) Potentials



Full Two-Qubit Hamiltonian

$$\hat{H}_{2q}(r) = \begin{pmatrix} \hat{T} + \hat{V}_0^0(r) + \hat{V}_{\text{trap}}(r) & & \hat{\mu}\epsilon(t) & \\ & \ddots & & \ddots \\ \hat{\mu}\epsilon(t) & & \hat{T} + \hat{V}_{\text{aux}}^0(r) + \hat{V}_{\text{trap}}(r) & \\ & \ddots & & \ddots \end{pmatrix}$$

Optimization of Full Unitary Transformations

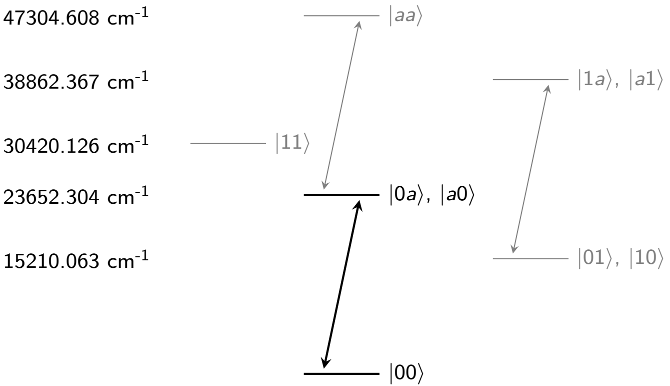
$$
\begin{aligned}
|\Psi(r)\rangle_{00}\,,\ \epsilon(t) &\quad \overset{!}{\longrightarrow} \quad e^{i\phi}\,|\Psi(r)\rangle_{00} \\
|\Psi(r)\rangle_{01}\,,\ \epsilon(t) &\quad \overset{!}{\longrightarrow} \quad |\Psi(r)\rangle_{01} \\
|\Psi(r)\rangle_{10}\,,\ \epsilon(t) &\quad \overset{!}{\longrightarrow} \quad |\Psi(r)\rangle_{10} \\
|\Psi(r)\rangle_{11}\,,\ \epsilon(t) &\quad \overset{!}{\longrightarrow} \quad |\Psi(r)\rangle_{11} \quad \text{(guaranteed)}
\end{aligned}
$$

Objective

Find a pulse $\epsilon(t)$ that transforms the basis states into transformed states within a given time window $[0, T]$. This pulse will transform any state $|\Psi(r)\rangle$ according to the unitary transformation

$$
\hat{O} = \begin{pmatrix} e^{i\phi} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
$$

Reduced Two-Level System



Reduced Hamiltonian and Target

Hamiltonian for Reduced System

$$\hat{H}_{2q,\text{red}}(r) = \begin{pmatrix} \hat{T} + \hat{V}_0^0(r) + \hat{V}_{\text{trap}}(r) & \hat{\mu}\epsilon(t) \\ \hat{\mu}\epsilon(t) & \hat{T} + \hat{V}_{\text{aux}}^0(r) + \hat{V}_{\text{trap}}(r) \end{pmatrix}$$

Reduced System Optimization Target

$$|\Psi(r)\rangle_{00}\,,\ \epsilon(t) \quad \stackrel{!}{\longrightarrow} \quad e^{i\phi}\ |\Psi(r)\rangle_{00}$$

Is this enough?

One-Qubit Phase

$$R_0(\phi_0) \otimes \mathbf{1} \cdot \mathbf{1} \otimes R_0(\phi) = \begin{pmatrix} e^{2i\phi_0} & 0 & 0 & 0 \\ 0 & e^{i\phi_0} & 0 & 0 \\ 0 & 0 & e^{i\phi_0} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{aligned} |\Psi(r)\rangle_{00}\,,\ \epsilon(t) &\longrightarrow e^{i\chi_{00}}\ |\Psi(r)\rangle_{00} \\ |\Psi(r)\rangle_{01}\,,\ \epsilon(t) &\longrightarrow e^{i\chi_{00}/2}\ |\Psi(r)\rangle_{01} \\ |\Psi(r)\rangle_{10}\,,\ \epsilon(t) &\longrightarrow e^{i\chi_{00}/2}\ |\Psi(r)\rangle_{10} \\ |\Psi(r)\rangle_{11}\,,\ \epsilon(t) &\longrightarrow |\Psi(r)\rangle_{11} \end{aligned}$$

Non-interaction Target

Hamiltonian for Reduced System

$$\hat{H}_{2q,\mathrm{red}}(r) = \begin{pmatrix} \hat{T} + \hat{V}_0^0(r) + \hat{V}_{\mathrm{trap}}(r) & \hat{\mu}\epsilon(t) \\ \hat{\mu}\epsilon(t) & \hat{T} + \hat{V}_{\mathrm{aux}}^0(r) + \hat{V}_{\mathrm{trap}}(r) \end{pmatrix}$$

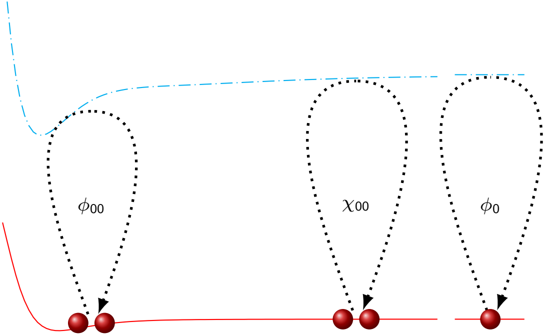
Reduced System Optimization Target

$$|\Psi(r)\rangle_{00}\,,\ \epsilon(t) \quad \stackrel{!}{\longrightarrow} \quad e^{i\phi}\ |\Psi(r)\rangle_{00}$$

$$|0\rangle\,,\ \epsilon(t) \quad \stackrel{!}{\longrightarrow} \quad |0\rangle$$

$$|00\rangle \quad \longrightarrow \quad e^{i\phi_{00}+2\phi_0}\ |00\rangle\,; \qquad \phi_{00} : \text{true interaction phase}$$

Interacting and Non-Interacting Contributions to the Phase



Part III

How?

Outline

Numerics

- Discretization of time grid and spatial grid
- Mapping
- Numerical Calculation of Eigensystem
- IO/Analysis: Expectation values, population, etc.

Chebychev Propagation

- Time Evolution: $\Psi(r,t) = \Psi(r,0)\, e^{-i\hat{H(\epsilon)}t}$
- Polynomial Expansion: $e^{-i\hat{H}t} = \sum_{n=0}^{N} a_n P_n(\hat{H(\epsilon)})$
- Renormalization: $\hat{H}' = \frac{1}{\Delta E}\left(\hat{H} - (\frac{\Delta E}{2} + V_{\text{min}}) \cdot \mathbf{1}\right)$
- Chebychev-Propagation: $e^{-i\hat{H}t} = e^{-i(\frac{\Delta E}{2} + V_{min})t} \sum \left[a_n(\frac{\Delta E}{2} t)\ \phi_n(-i\hat{H}')\right]$
- a_n, $\phi_n(-i\hat{H}')$ from recursion

OCT Formulas

Optimization Functional

$$J = -F(\{\Psi(T)\}) + \int_{t=0}^{T} \frac{\alpha_0}{s(t)} \Delta\epsilon^2(t)\,\mathrm{d}t$$

Field Update

$$\Delta\epsilon(t) = \frac{s(t)}{2\alpha_0} \Im \left[\sum_{k=1}^{N} \left\langle \Psi_{ik} \middle| \hat{O}^\dagger \, \hat{U}^\dagger(t, T; \epsilon^{(0)}) \, \hat{\mu} \, \hat{U}(t, 0; \epsilon^{(1)}) \middle| \Psi_{ik} \right\rangle \right]$$

OCT Formulas

Optimization Functional

$$J = -F(\{\Psi(T)\}) + \int_{t=0}^{T} \frac{\alpha_0}{s(t)} \Delta\epsilon^2(t)\,\mathrm{d}t$$

Field Update

$$\Delta\epsilon(t) = \frac{s(t)}{2\alpha_0}\,\Im\left[\sum_{k=1}^{N} \overbrace{\langle\Psi_{ik}|\hat{O}^\dagger}^{=\langle\Psi_{tk}|}\,\hat{U}^\dagger(t,T;\epsilon^{(0)})\,\hat{\mu}\,\hat{U}(t,0;\epsilon^{(1)})|\Psi_{ik}\rangle\right]$$

OCT Formulas

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Field Update

$$\Delta\epsilon(t) = \frac{s(t)}{2\alpha_0} \Im \left[\sum_{k=1}^{N} \underbrace{\overbrace{\left\langle \Psi_{ik} \right|}^{=\left\langle \Psi_{tk} \right|} \hat{O}^{\dagger} \hat{U}^{\dagger}(t, T; \epsilon^{(0)})}_{\underset{\epsilon^{(0)}}{\longleftarrow} \left\langle \Psi_{tk} \right|} \hat{\mu}\, \hat{U}(t, 0; \epsilon^{(1)}) \left| \Psi_{ik} \right\rangle \right]$$

OCT Formulas

Optimization Functional

$$J = -F(\{\Psi(T)\}) + \int_{t=0}^{T} \frac{\alpha_0}{s(t)} \Delta\epsilon^2(t)\,\mathrm{d}t$$

Field Update

$$\Delta\epsilon(t) = \frac{s(t)}{2\alpha_0}\,\Im\left[\sum_{k=1}^{N} \overbrace{\langle\Psi_{ik}|\hat{O}^\dagger}^{=\langle\Psi_{tk}|} \hat{U}^\dagger(t,T;\epsilon^{(0)})\,\hat{\mu}\,\hat{U}(t,0;\epsilon^{(1)})|\Psi_{ik}\rangle\right]$$

$$\underbrace{\langle\Psi_{ik}|\hat{O}^\dagger \hat{U}^\dagger(t,T;\epsilon^{(0)})}_{\xleftarrow[\epsilon^{(0)}]{} \langle\Psi_{tk}|} \qquad \underbrace{\hat{U}(t,0;\epsilon^{(1)})|\Psi_{ik}\rangle}_{|\Psi_{ik}\rangle \xrightarrow[\epsilon^{(1)}]{}}$$

OCT Formulas

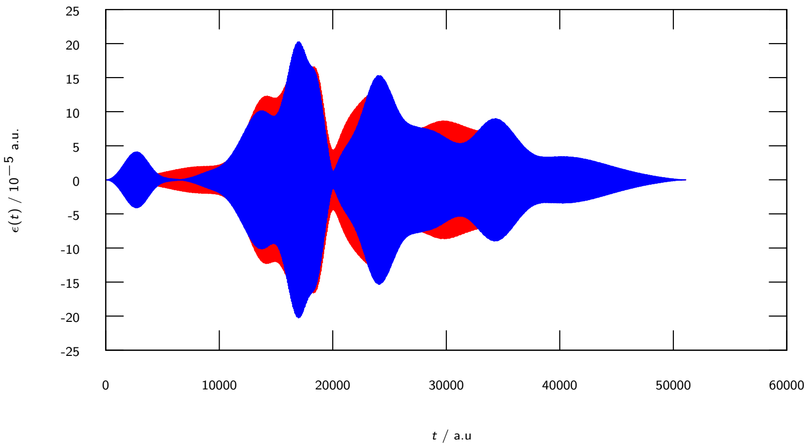
Optimization Functional

$$J = -F(\{\Psi(T)\}) + \int_{t=0}^{T} \frac{\alpha_0}{s(t)} \Delta\epsilon^2(t)\, \mathrm{d}t$$

Field Update

$$\Delta\epsilon(t) = \frac{s(t)}{2\alpha_0} \Im \left[\sum_{k=1}^{N} \underbrace{\overbrace{\langle \Psi_{ik}|}^{=\langle \Psi_{tk}|} \hat{O}^\dagger \hat{U}^\dagger(t, T; \epsilon^{(0)})}_{\xleftarrow[\epsilon^{(0)}]{} \langle \Psi_{tk}|} \hat{\mu}\, \underbrace{\hat{U}(t, 0; \epsilon^{(1)}) |\Psi_{ik}\rangle}_{|\Psi_{ik}\rangle \xrightarrow[\epsilon^{(1)}]{}} \right]$$

Guess Pulse and Optimized Pulse



OCT Algorithm

t_0 $\quad t = t_0 + dt \quad \cdots \quad t = T - dt \quad T = t_0 + nt \cdot dt$

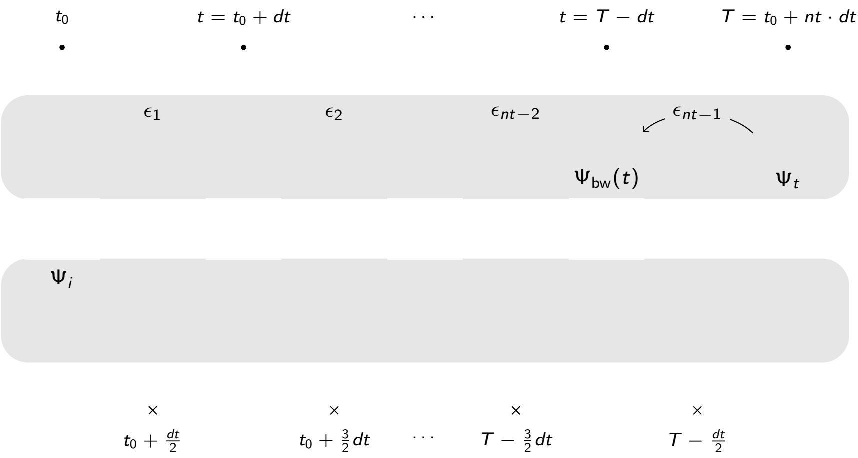
$\epsilon_1 \quad \epsilon_2 \quad \epsilon_{nt-2} \quad \epsilon_{nt-1}$

Ψ_t

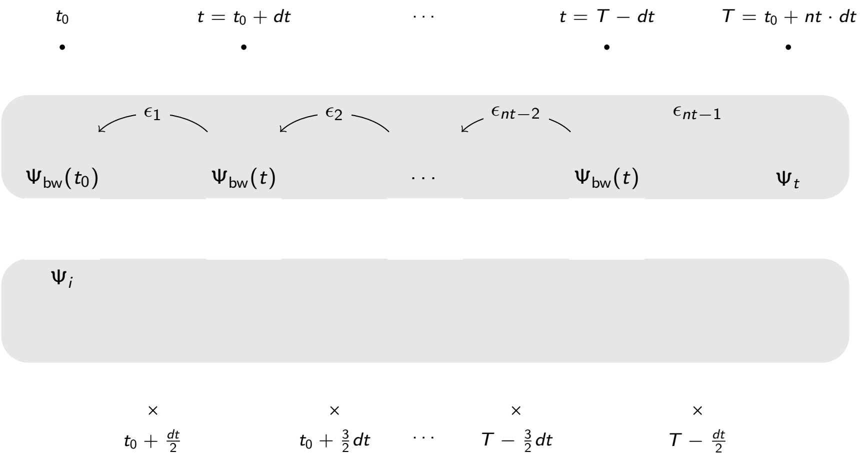
Ψ_i

$t_0 + \frac{dt}{2} \quad t_0 + \frac{3}{2}dt \quad \cdots \quad T - \frac{3}{2}dt \quad T - \frac{dt}{2}$

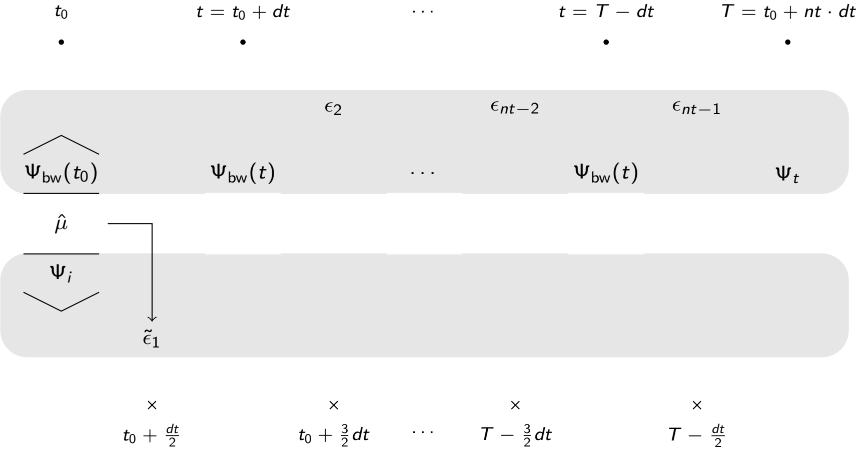
OCT Algorithm



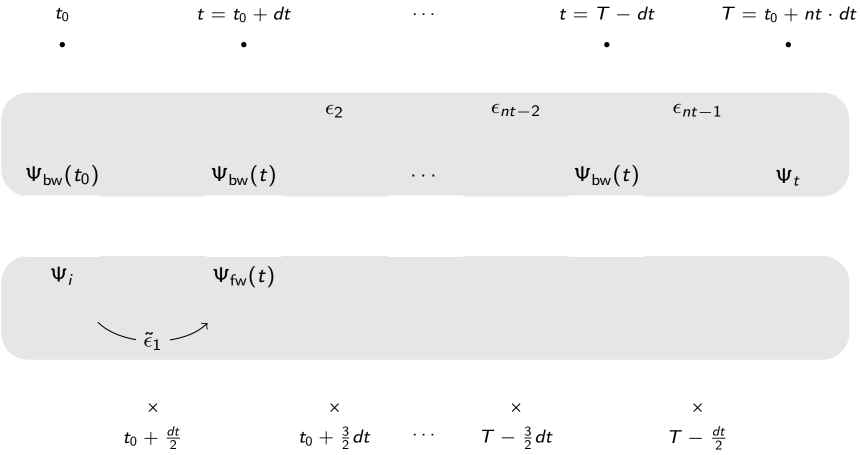
OCT Algorithm



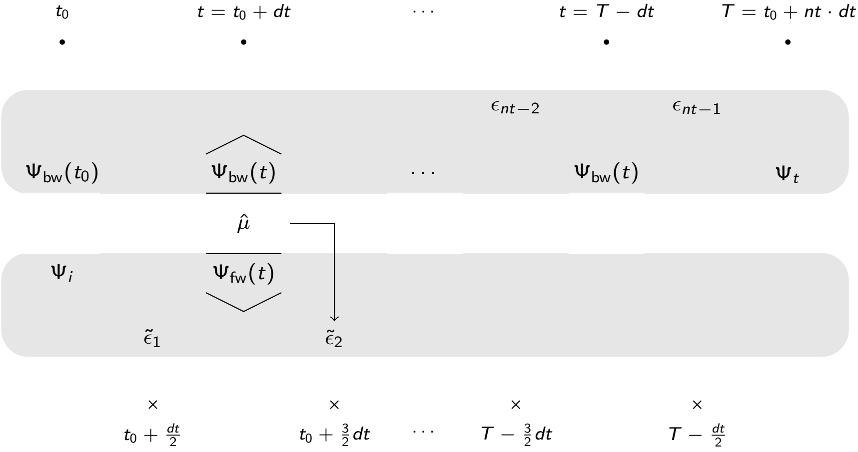
OCT Algorithm



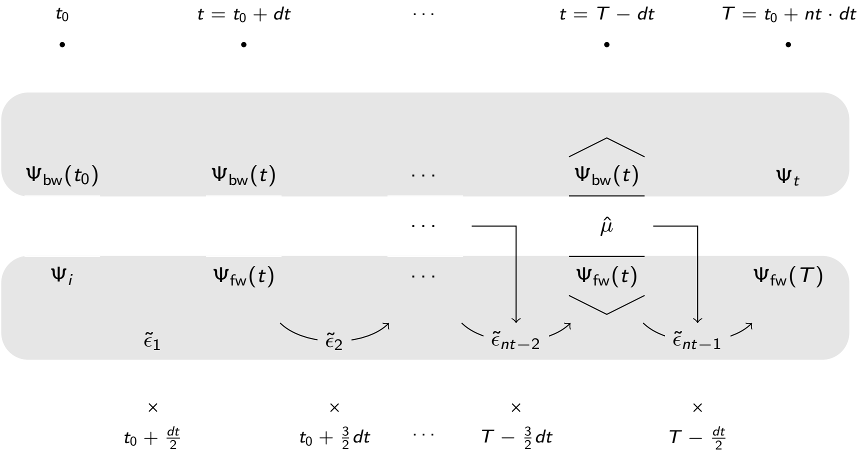
OCT Algorithm



OCT Algorithm



OCT Algorithm



OCT Algorithm

t_0 $\quad$ $t = t_0 + dt$ $\quad$ $\cdots$ $\quad$ $t = T - dt$ $\quad$ $T = t_0 + nt \cdot dt$

$\Psi_{\text{bw}}(t_0)$ $\quad$ $\Psi_{\text{bw}}(t)$ $\quad$ $\cdots$ $\quad$ $\Psi_{\text{bw}}(t)$ $\quad$ Ψ_t

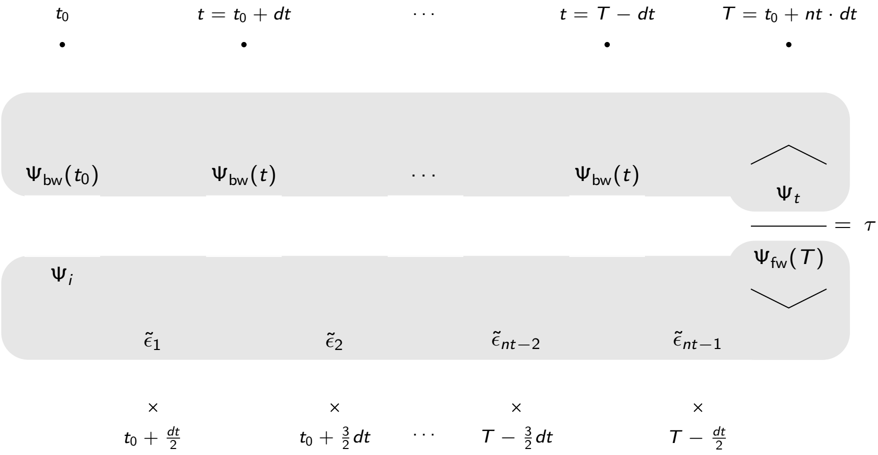
Ψ_i $\quad$ $\Psi_{\text{fw}}(T)$

$\tilde{\epsilon}_1$ $\quad$ $\tilde{\epsilon}_2$ $\quad$ $\tilde{\epsilon}_{nt-2}$ $\quad$ $\tilde{\epsilon}_{nt-1}$

$\times$ $\quad$ $\times$ $\quad$ $\times$ $\quad$ $\times$

$t_0 + \frac{dt}{2}$ $\quad$ $t_0 + \frac{3}{2}dt$ $\quad$ $\cdots$ $\quad$ $T - \frac{3}{2}dt$ $\quad$ $T - \frac{dt}{2}$

OCT Algorithm



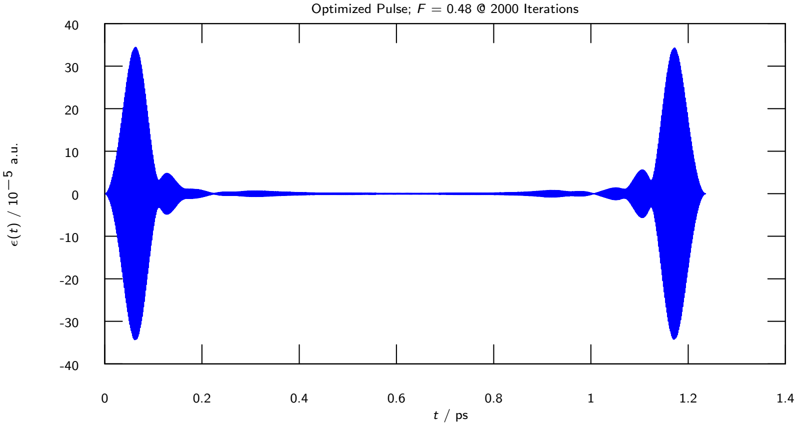
Part IV

Results

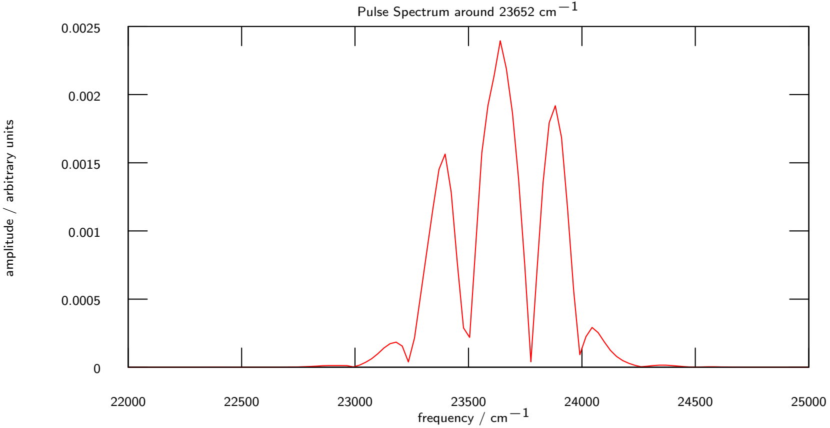
Outline

1 ps Pulse in Reduced System

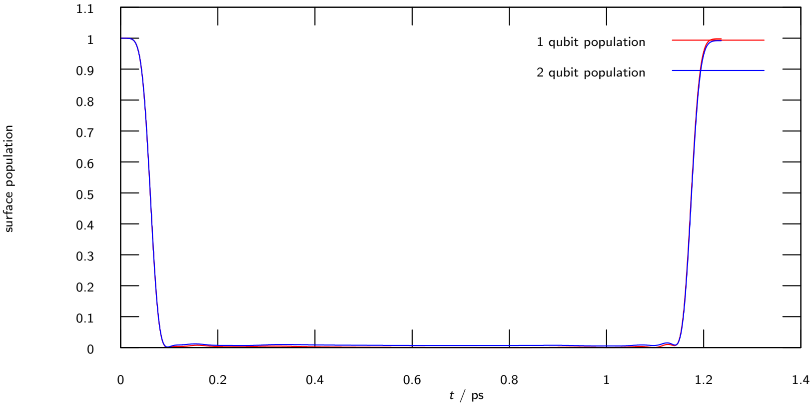
Optimized Pulse



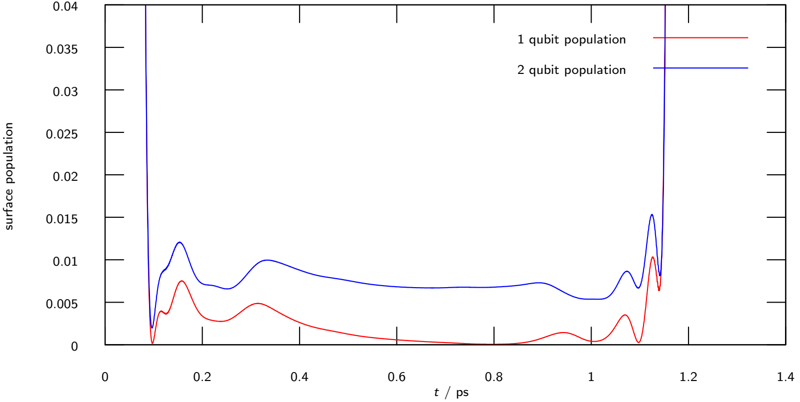
Optimized Pulse Spectrum



Population


1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
surface population
1 qubit population
2 qubit population
0
0.2
0.4
0.6
0.8
1
1.2
1.4
t / ps

One and Two-Qubit Population



Plotting the Phase Dynamics

One-Qubit System

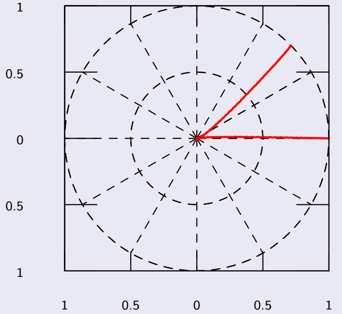
- $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \longrightarrow \begin{pmatrix} a_0 \\ a_a \end{pmatrix}$
- One-Qubit Phasegate if $a_a = 0$ and $a_0 \in \mathbb{C}$
- Plot a_0 in complex plane: points on unit circle represent phase gate.

Two-Qubit System

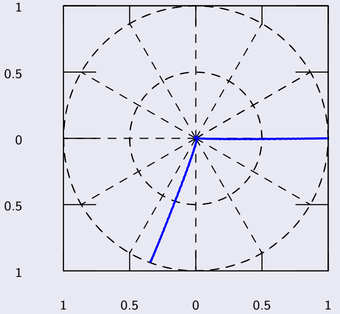
- $\begin{pmatrix} \Psi_{0,i}(r) \\ 0 \end{pmatrix} \longrightarrow \begin{pmatrix} \Psi_0(r) \\ \Psi_a(r) \end{pmatrix}$
- *Average* relative phase: $\phi = \text{ph}\left(\langle \Psi_{0,i} | \Psi_0 \rangle\right)$
- Population: $a_0^2 = |\Psi_0|^2$
- Plot $a_0^2 e^{i\phi}$ in complex plane: points on unit circle represent (average) phase gate.

Phase Dynamics

One-Qubit System

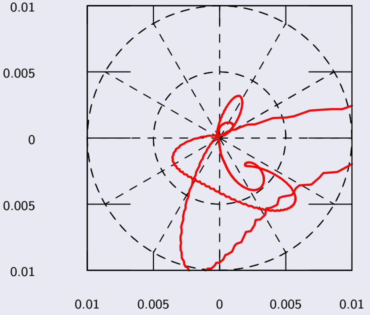


Two-Qubit System

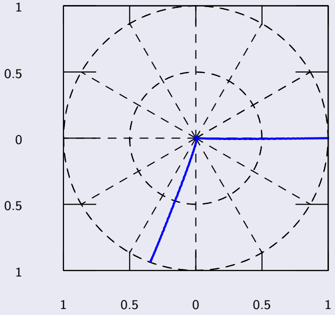


Phase Dynamics during Depopulated Period

One-Qubit System

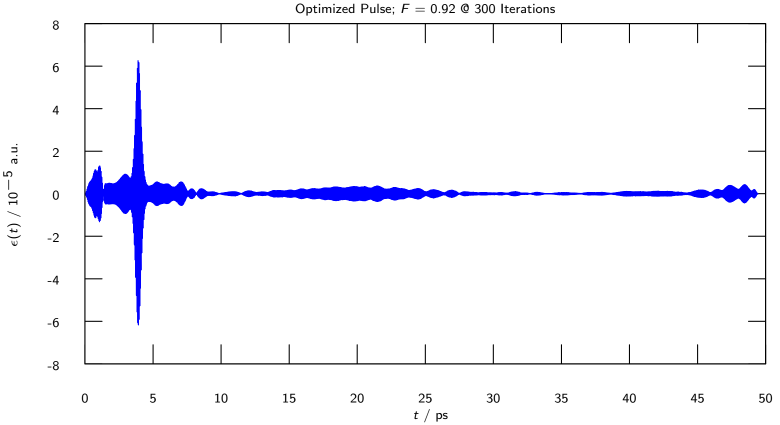


Two-Qubit System

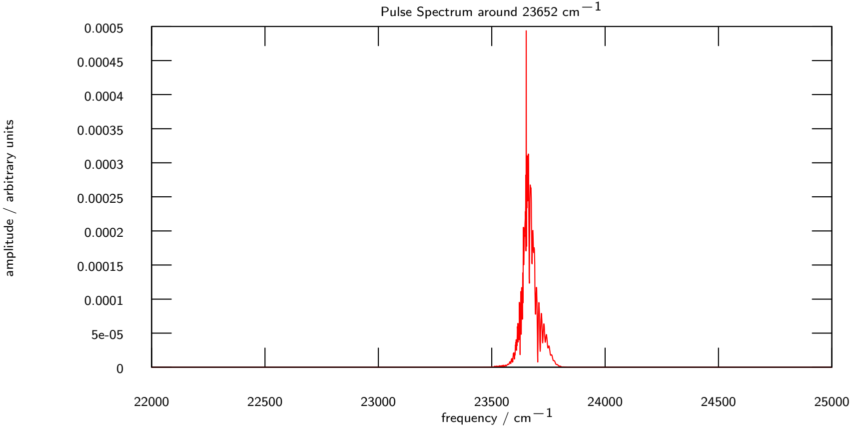


50 ps Pulse in Reduced System

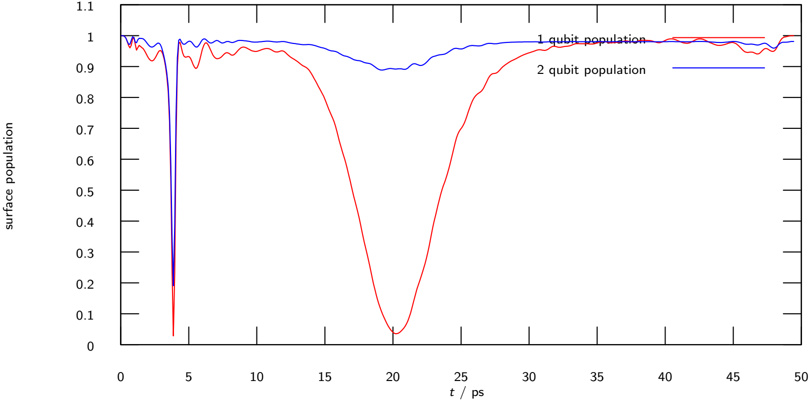
Optimized Pulse



Optimized Pulse Spectrum

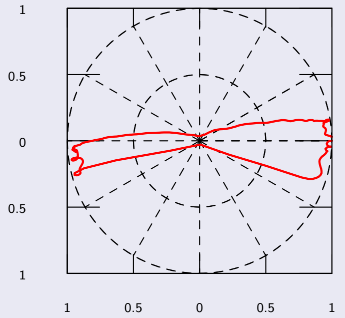


Population

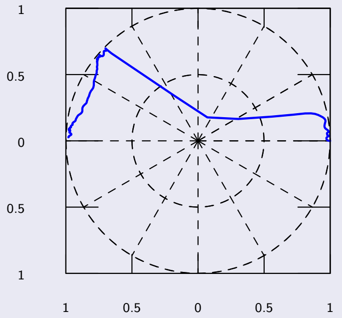

1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
surface population
0
5
10
15
20
25
30
35
40
45
50
t / ps
1 qubit population
2 qubit population

Phase Dynamics

One-Qubit System

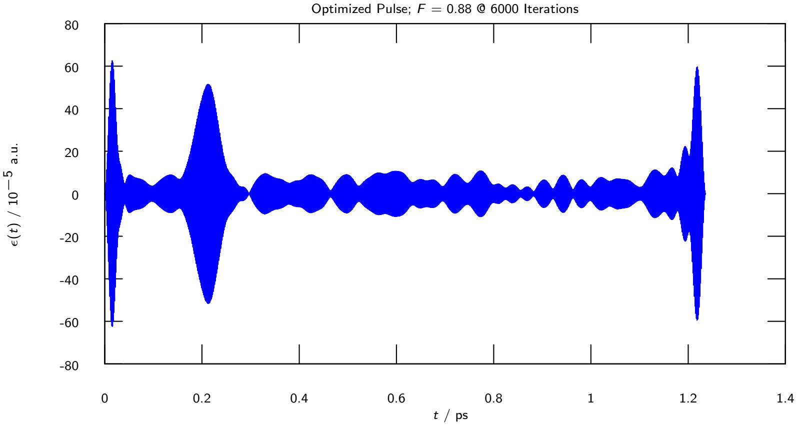


Two-Qubit System

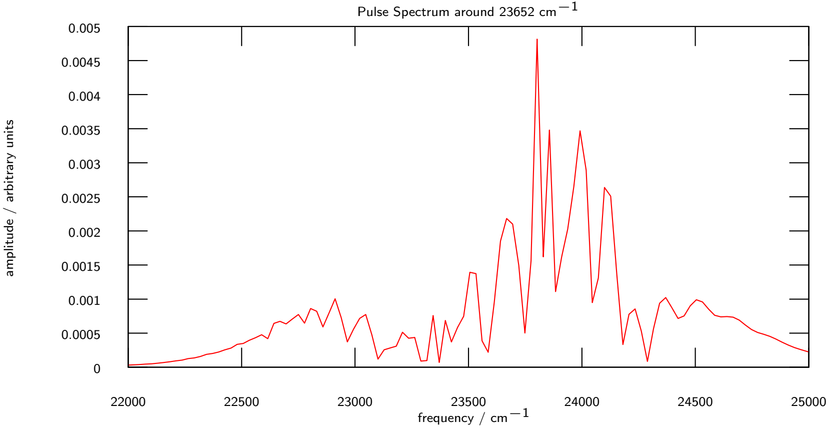


1 ps Pulse for $\pi/2$ Phase Gate in Reduced System

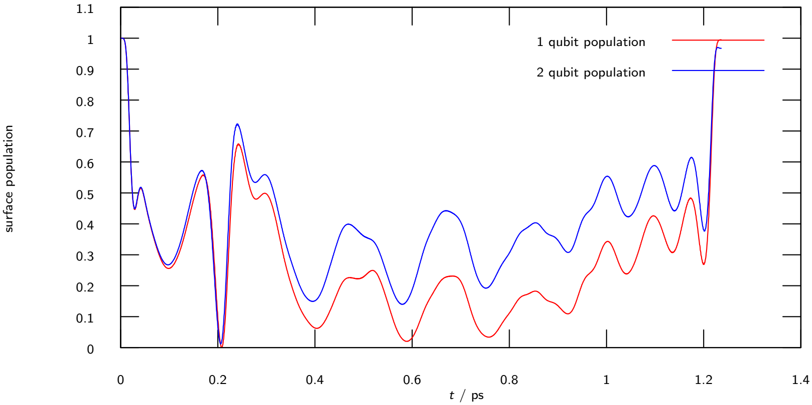
Optimized Pulse



Optimized Pulse Spectrum

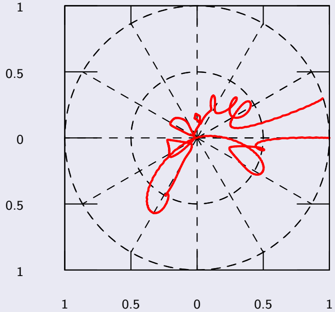


Population

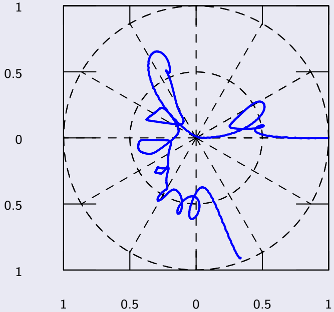

1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
surface population
1 qubit population
2 qubit population
0
0.2
0.4
0.6
0.8
1
1.2
1.4
t / ps

Phase Dynamics

One-Qubit System

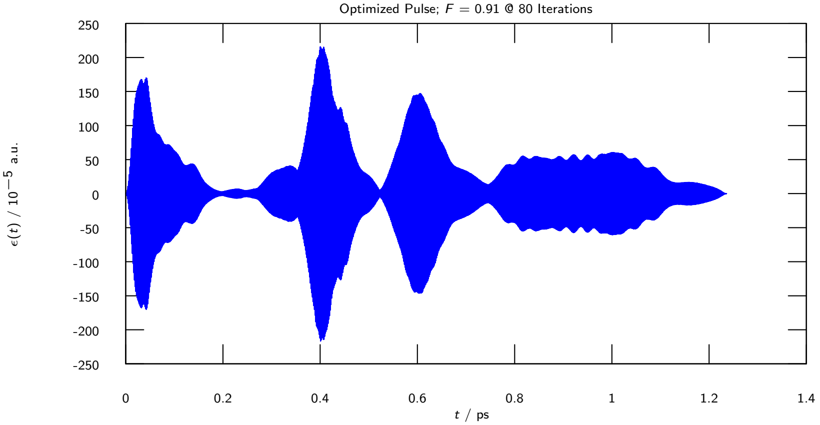


Two-Qubit System

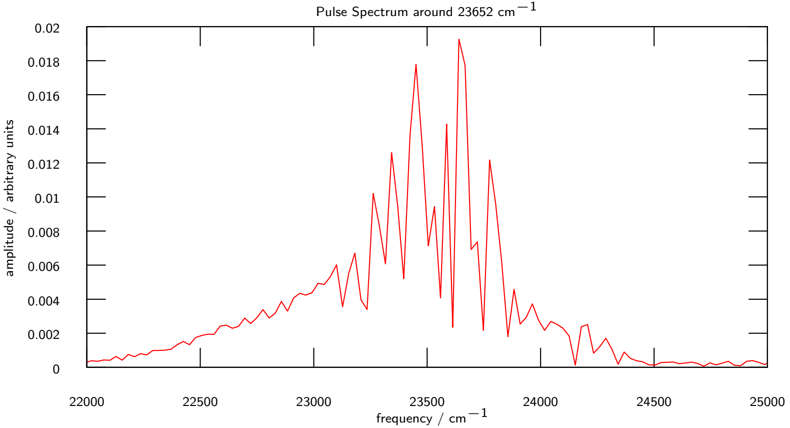


1 ps Pulse in Full System

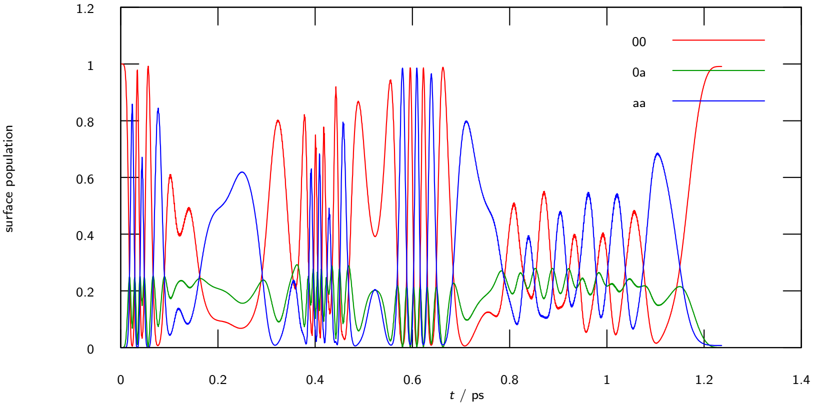
Optimized Pulse



Optimized Pulse Spectrum

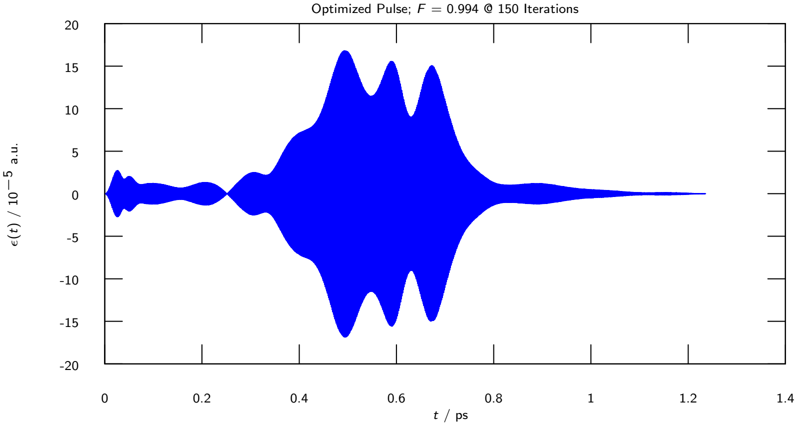


Population

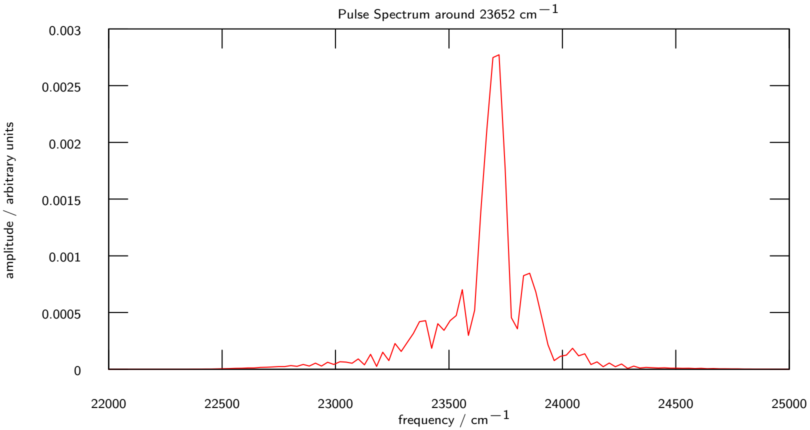

surface population
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2
1.4
t / ps
00
0a
aa

1 ps Pulse for $\pi/2$ Phase Gate in Full System

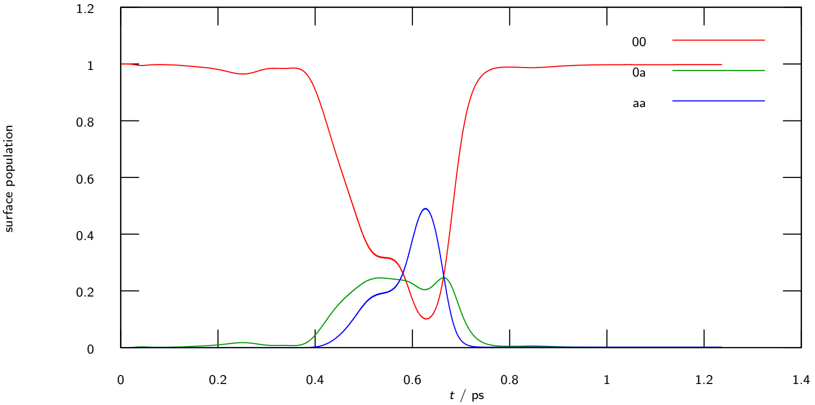
Optimized Pulse



Optimized Pulse Spectrum



Population


1.2
1
0.8
0.6
0.4
0.2
0
surface population
0
0.2
0.4
0.6
0.8
1
1.2
1.4
t / ps
00
0a
aa

- How can we get a fidelity of 1?
- Why does OCT go to pulses of such radically different pulses in similar situations? How can we explore the search space more effectively?
- Further analysis: Compare behavior of optimized pulses in different systems.
- Ultimate goal: much larger values for d, at equal time scales.
- Problem: numerical complexity.

Thank You!