Femtosecond Quantum Control for Quantum Computing and Quantum Networks

Caroline Gollub
Outline

- Quantum Control

- Quantum Computing with Vibrational Qubits
  - Concept & IR-gates
  - Raman Quantum Computing
  - Control with Genetic Algorithms
  - Control with ACO
  - Dissipation

- Quantum Networks

- Conclusion & Outlook
Quantum Control

controlling quantum phenomena and intramolecular wave packet dynamics with shaped electric laser fields

theory: optimal control theory

experiment: closed-loop techniques with genetic algorithms

numerous successful demonstrations in various fields: biology, chemistry, physics

application requiring precise control of quantum systems: quantum information processing
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Molecular Quantum Computing

eigenstates of molecular vibrational normal modes encode the qubit states

logic operations (quantum gates):
specially shaped ultrashort laser pulses

calculated with optimal control theory

qubit basis:
\[ |00\rangle, |01\rangle, |10\rangle, |11\rangle \]

Tesch, de Vivie-Riedle, PRL 89, 157901 (2002)
Optimal Control Theory

multi-target optimal control theory

\[ J(\Psi_{ik}(t), \Psi_{fk}(t), \epsilon(t)) = F(\tau) - \alpha_0 \int_0^T \frac{|\epsilon(t)|^2}{s(t)} dt \]

\[ - \sum_{k}^{N} 2 \text{Re} \left[ C \int_0^T \langle \Psi_{fk}(t) | \frac{i}{\hbar} \left[ \hat{H}_0 - \mu \epsilon(t) \right] + \frac{\partial}{\partial t} | \Psi_{ik}(t) \rangle \right] dt \]

standard MTOCT

\[ F_{\text{std}}(\tau) = \sum_{k}^{N} |\langle \Phi_{fk} | \Psi_{ik}(T) \rangle|^2 \]

\[ C_{\text{std}} = \langle \Psi_{ik}(t) | \Psi_{fk}(t) \rangle \]

phase-correlated MTOCT

\[ F_{\text{corr}}(\tau) = \sum_{k}^{N} \sum_{l}^{N} \langle \Phi_{fk} | \Psi_{ik}(T) \rangle \langle \Psi_{il}(T) | \Phi_{fl} \rangle \]

\[ C_{\text{corr}} = \sum_{l}^{N} \langle \Psi_{il}(t) | \Psi_{fl}(t) \rangle \]

Tesch, de Vivie-Riedle, PRL 89, 157901 (2002)
IR quantum gates

universal set of IR quantum gates for the 2-qubit system MnBr(CO)$_5$

\[
\begin{align*}
\text{NOT} & : \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
\end{pmatrix} \\
\text{CNOT} & : \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
\end{pmatrix} \\
\Pi & : \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1 \\
\end{pmatrix} \\
\text{Hadamard} & : \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & -1 & 0 \\
0 & 1 & 0 & -1 \\
\end{pmatrix}
\end{align*}
\]
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Raman Quantum Gates

stimulated, non-resonant Raman quantum gates
strategy to optimize the two laser fields $\epsilon_1(t)$ and $\epsilon_2(t)$

\[
i \frac{\partial}{\partial t} \Psi(t) = \hat{H}_0 \Psi(t) - \frac{1}{2} \epsilon_1(t) \hat{\alpha} \epsilon_2(t) \Psi(t)
\]

optimization of one laser pulse possible with MTOCT

spectrum contains two carrier frequencies

CG, Kowalewski, de Vivie-Riedle, PRL 41, 073002 (2008)
MTOCT for Raman transitions with frequency filter

\[
J(\Psi_{ik}(t), \Psi_{fk}(t), \epsilon_1(t), \epsilon_2(t)) = \sum_k \left\{ |\langle \Psi_{ik}(T) | \Phi_{fk} \rangle|^2 - \sum_{l=1}^{2} \alpha_0 \int_0^T \frac{|\epsilon_l(t)|^2}{s(t)} dt \right. \\
\left. - 2 \Re \left[ \langle \Psi_{ik}(T) | \Phi_{fk} \rangle \int_0^T \langle \Psi_{fk}(t) | \left[ \frac{i}{\hbar} \left( \hat{H}_0 - \frac{1}{2} \epsilon_1(t) \alpha \epsilon_2(t) \right) + \frac{\partial}{\partial t} \right] |\Psi_{ik}(t)\rangle dt \right] \right\} \\
- \sum_{l=1}^{2} \gamma_l |F_l(\epsilon_l(t))| \right]
\]
MTOCT for Raman transitions with frequency filter

\[ J(\Psi_{ik}(t), \Psi_{f_k}(t), \epsilon_1(t), \epsilon_2(t)) = \sum_k \left\{ \left| \langle \Psi_{ik}(T) | \Phi_{f_k} \rangle \right|^2 - \sum_{l=1}^{2} \alpha_0 \int_{0}^{T} \frac{|\epsilon_l(t)|^2}{s(t)} dt \right\} \]

\[ - 2 \text{Re} \left[ \langle \Psi_{ik}(T) | \Phi_{f_k} \rangle \int_{0}^{T} \langle \Psi_{f_k}(t) | \left[ \frac{i}{\hbar} \left( \hat{H}_0 - \frac{1}{2} \epsilon_1(t) \alpha \epsilon_2(t) \right) + \frac{\partial}{\partial t} \right] | \Psi_{ik}(t) \rangle dt \right] \]

\[ - \sum_{l=1}^{2} \gamma_l |F_l(\epsilon_l(t))| \]
Finite Impulse Response filters (FIR) realized as a band stop Fourier-filter

\[ F(\epsilon(t)) = \sum_{j=0}^{N} c_j \epsilon(t - j\Delta t) \]

new field calculated with the Krotov iteration scheme:

\[ \epsilon^{n+1}(t) = \epsilon^n(t) - \frac{s(t)}{2\alpha_0} \left( \gamma(t) - \sum_k \Im[\langle \Phi_k(t, \epsilon^n) | \Psi_k(t, \epsilon^{n+1}) \rangle \times \langle \Phi_k(t, \epsilon^n) | \hat{\mu} | \Psi_k(t, \epsilon^{n+1}) \rangle] \right) \]

Lagrange multiplier can be interpreted as a correction field

CG, Kowalewski, de Vivie-Riedle, PRL 41, 073002 (2008)
Finite Impulse Response filters (FIR) realized as a band stop Fourier-filter

\[ F(\epsilon(t)) = \sum_{j=0}^{N} c_j \epsilon(t - j \Delta t) \]

prediction of the Lagrangian correction field

\[ \gamma'(t) = \sum_k \Im \left[ \langle \Phi_k(t, \epsilon^n) | \psi_k(t, \epsilon^n) \rangle \times \langle \Phi_k(t, \epsilon^n) | \hat{\mu} | \psi_k(t, \epsilon^n) \rangle \right] \]

\[ \approx \sum_k \Im \left[ \langle \Phi_k(t, \epsilon^n) | \psi_k(t, \epsilon^{n+1}) \rangle \times \langle \Phi_k(t, \epsilon^n) | \hat{\mu} | \psi_k(t, \epsilon^{n+1}) \rangle \right] \]

after the filter operation \[ \gamma(t) = \mathcal{F}^{-1} [f'(\omega) \cdot \mathcal{F} (\gamma'(t))] \]

only the unwanted components remain in the Lagrangian and are subtracted from the original OCT output
Model System

properties of molecular candidates

- high Raman activities
- balanced anharmonicities

scanning several molecules with suitable Raman spectra

(ab initio calculation [DFT: b3lyp/6-31++G**] of spectra and anharmonicities)

\[ \omega_1 = 3100 \text{ cm}^{-1}, \omega_2 = 3029 \text{ cm}^{-1} \]
\[ \Delta_1 = 73 \text{ cm}^{-1}, \Delta_2 = 102 \text{ cm}^{-1}, \Delta_{12} = 23 \text{ cm}^{-1} \]

CG, Troppmann, de Vivie-Riedle, NJP 8, 48 (2006)
Polarizability

ab initio calculation of the polarizability [DFT: b3lyp/6-31++G**]

suited components:
Vibrational Raman Quantum Gates

quantum gates with x-polarized laser fields

carrier frequency: 800 nm
Application Prospects

**general:**

- reliable predictions of experimental laser fields: limited spectral bandwidth
- simplification of theoretical pulse shapes

**molecular physics and beyond:**

- multi-color, multi-photon processes: e.g. CARS
- preparation of cold molecules by photoassociation
- atom transport in optical lattices
- fast and robust gate operations with trapped ions and NMR-qubits
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Control with Genetic Algorithms


\[ \phi(\omega) = \sum_{i} a_i \sin(b_i \omega + c_i) \]

\[ M_n(\omega_n^0) = T_n(\omega_n^0) \exp(i\phi_n(\omega_n^0)) \]

\[ \tilde{\varepsilon}_{\text{out}}(\omega) = M(\omega) \tilde{\varepsilon}_{\text{in}}(\omega) \]
## OCT versus GAs

<table>
<thead>
<tr>
<th><strong>optimal control theory</strong></th>
<th><strong>genetic algorithms</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>primarily in the time domain</strong></td>
<td><strong>frequency domain</strong></td>
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</table>

### OCT specific parameters
- penalty factor, shape functions

### GA specific parameters
- mutations, crossing-over, replacement factor, generations, population

### Laser pulse
- guess laser field, explicitly pulse duration

### Laser pulse and mask function
- FWHM of FL-pulses, carrier frequency, maximum energy, number of pixels, pixel width
Parametrized Phase Functions

control landscape

for the excitation process from $v=0$ to $v=1$ of the $T_{1u}$ mode in $W(CO)_6$

sinusoidal phase modulation ($i=1$)

$$\phi(\omega) = \sum_i a_i \sin(b_i \omega + c_i)$$

scanning the parameters $a$ and $b$
Parametrized Phase Functions

control landscapes

for a 1-qubit NOT gate with sinusoidal phase modulation

control landscapes counter each other

parametrized wave functions lead to simple pulse structures, but are not flexible enough for quantum gate implementations

CG, de Vivie-Riedle, PRA 78, 033424 (2008)
Pixeled Phase Functions

NOT gate laser pulses from GA calculations (efficiencies > 99%)

FL-pulse from experiment

CG, de Vivie-Riedle, PRA 78, 033424 (2008)
Pixeled Phase Functions

NOT gate laser pulses from GA calculations (efficiencies > 99%)

FL-pulse from experiment

elongation of FL-pulse duration (~amplitude shaping)

CG, de Vivie-Riedle, PRA 78, 033424 (2008)
NOT gate laser pulses from GA calculations (efficiencies > 99%)

FL-pulse from experiment

elongation of FL-pulse duration (~amplitude shaping)

limitation of the phase range from $[-\pi, +\pi]$ to $[-0.1\pi, +0.1\pi]$

CG, de Vivie-Riedle, PRA 78, 033424 (2008)
Multi-Objective GAs

multi-objective / multi-criteria optimization

Pareto fronts
minimum requirements on
the pulse properties

control objectives
- efficiency
- pulse duration
- pulse intensity

CG, de Vivie-Riedle, NJP 11, 013019 (2009)
Multi-Objective GAs

3D-Pareto front of a CNOT gate in MnBr(CO)$_5$

multi-objective / multi-criteria optimization

Pareto fronts
minimum requirements on
the pulse properties

control objectives
• efficiency
• pulse duration
• pulse intensity

solution subspaces of OCT and GA match

CG, de Vivie-Riedle, NJP 11, 013019 (2009)
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Ant Colony Algorithm

alternative approach for optimization strategy in closed-loop experiments
parametrized and pixeled mask functions: advantages and shortcomings

**Ant Colony Optimization metaheuristic**
introduced by Dorigo, Di Caro and Gambardella

inspired by the behavior of real ant colonies
discrete, combinatorial optimization problems
belongs to the research field of swarm intelligence, which is part of AI

pheromone acts as biochemical information
for the ants in a colony: collective memory
in nature: ants reach forage on the direct track due to the connection between pheromone deposition and search of favorable paths

initially each ant chooses randomly one path
Ant Colony Algorithm

in nature: ants reach forage on the direct track due to the connection between pheromone deposition and search of favorable paths

ant on shortest track reaches food source earlier and ...
Ant Colony Algorithm

in nature: ants reach forage on the direct track due to the connection between pheromone deposition and search of favorable paths

... deposits phermone earlier on the way back to the nest more ants follow the track with the higher concentration of pheromone
Ant Colony Algorithm

in nature: ants reach forage on the direct track
due to the connection between pheromone deposition and search of favorable paths

... after some time (almost) the whole ant colony uses of the shortest track
Modified ACO Algorithm

\[ p^{\phi_i}(\Delta \phi_i, t) = (1 - \beta)\tau^{\phi_i}(\Delta \phi_i, t) + \beta \eta^{\phi}(\Delta \phi_i) \]

\[ p^{\phi_i}(\Delta \phi_i, 0) = \eta^{\phi}(\Delta \phi_i) \]

\[ \eta^{\phi}(\Delta \phi_i) = N \eta^{\phi} \frac{1}{\sigma^{\phi} \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma^{\phi}} \right)^2} \]

\[ \tau^{\phi_i}(\Delta \phi_i, t + 1) = \rho \tau^{\phi_i}(\Delta \phi_i, t) + (1 - \rho) \Delta \tau^{\phi_i}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i}(\Delta \phi_i) = N \tau^{\phi_i} \sum_k \Delta \tau^{\phi_i,k}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i,k}(\Delta \phi_i) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi_i^k}{\sigma} \right)^2} \]

probability function: gives the probability that an ant will choose a certain value for the \( i \)-th phase jump in iteration \( t \)
Modified ACO Algorithm

\[ p^{\phi_i}(\Delta \phi_i, t) = (1 - \beta)\tau^{\phi_i}(\Delta \phi_i, t) + \beta \eta^{\phi}(\Delta \phi_i) \]

\[ p^{\phi_i}(\Delta \phi_i, 0) = \eta^{\phi}(\Delta \phi_i) \]

\[ \eta^{\phi}(\Delta \phi_i) = N \eta^{\phi} \frac{1}{\sigma_{\phi} \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma_{\eta}} \right)^2} \]

\[ \tau^{\phi_i}(\Delta \phi_i, t + 1) = \rho \tau^{\phi_i}(\Delta \phi_i, t) + (1 - \rho) \Delta \tau^{\phi_i}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i}(\Delta \phi_i) = N \tau_{\phi} \sum_k \Delta \tau^{\phi_i,k}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i,k}(\Delta \phi_i) = \frac{\gamma^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi_i^k}{\sigma} \right)^2} \]

pheromone trail (updated in each iteration)

probability function:
gives the probability that an ant will choose a certain value for the \( i \)-th phase jump in iteration \( t \)
Modified ACO Algorithm

Visibility function (constant)

\[ p^{\phi_i}(\Delta \phi_i, t) = (1 - \beta) \tau^{\phi_i}(\Delta \phi_i, t) + \beta \eta^{\phi}(\Delta \phi_i) \]

Probability function:
gives the probability that an ant will choose a certain value for the \( i \)-th phase jump in iteration \( t \)

\[ p^{\phi_i}(\Delta \phi_i, 0) = \eta^{\phi}(\Delta \phi_i) \]

\[ \eta^{\phi}(\Delta \phi_i) = N \eta^{\phi} \frac{1}{\sigma_{\phi}^{\phi} \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma_{\phi}^{\phi}} \right)^2} \]

\[ \tau^{\phi_i}(\Delta \phi_i, t + 1) = \rho \tau^{\phi_i}(\Delta \phi_i, t) + (1 - \rho) \Delta \tau^{\phi_i}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i}(\Delta \phi_i) = N \tau^{\phi_i} \sum_k \Delta \tau^{\phi_i,k}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i,k}(\Delta \phi_i) = \frac{\gamma^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi_i^k}{\sigma} \right)^2} \]

CG, de Vivie-Riedle, PRA, accepted
Modified ACO Algorithm (phase)

\[ p^\phi_i(\Delta \phi_i, t) = (1 - \beta)\tau^\phi_i(\Delta \phi_i, t) + \beta \eta^\phi(\Delta \phi_i) \]

**visibility function**

\[ p^\phi_i(\Delta \phi_i, 0) = \eta^\phi(\Delta \phi_i) \]

\[ \eta^\phi(\Delta \phi_i) = N \eta^\phi \frac{1}{\sigma^\phi \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma^\phi} \right)^2} \]

**probability function:**

first iteration

\[ \tau^\phi_i(\Delta \phi_i, t + 1) = \rho \tau^\phi_i(\Delta \phi_i, t) + (1 - \rho) \Delta \tau^\phi_i(\Delta \phi_i) \]

\[ \Delta \tau^\phi_i(\Delta \phi_i) = N \tau^\phi_i \sum_k \Delta \tau^\phi_i,k(\Delta \phi_i) \]

\[ \Delta \tau^\phi_i,k(\Delta \phi_i) = \frac{Y^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi_i^k}{\sigma} \right)^2} \]

CG, de Vivie-Riedle, PRA, accepted
Modified ACO Algorithm

\[ p^{\phi_i}(\Delta \phi_i, t) = (1 - \beta)\tau^{\phi_i}(\Delta \phi_i, t) + \beta \eta^{\phi}(\Delta \phi_i) \]

\[ p^{\phi_i}(\Delta \phi_i, 0) = \eta^{\phi}(\Delta \phi_i) \]

\[ \eta^{\phi}(\Delta \phi_i) = N\eta^{\phi} \frac{1}{\sigma^{\phi} \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma^{\eta}} \right)^2} \]

\[ \tau^{\phi_i}(\Delta \phi_i, t + 1) = \rho \tau^{\phi_i}(\Delta \phi_i, t) + (1 - \rho) \Delta \tau^{\phi_i}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i}(\Delta \phi_i) = N\tau^{\phi_i} \sum_k \Delta \tau^{\phi_i, k}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i, k}(\Delta \phi_i) = \frac{Y^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi^k_i}{\sigma} \right)^2} \]

visibility function:
normal distribution centered at a phase difference of zero guarantees low phase variation
Modified ACO Algorithm

\[ p^{\phi_i}(\Delta\phi_i, t) = (1 - \beta)\tau^{\phi_i}(\Delta\phi_i, t) + \beta\eta^{\phi}(\Delta\phi_i) \]

\[ p^{\phi_i}(\Delta\phi_i, 0) = \eta^{\phi}(\Delta\phi_i) \]

\[ \eta^{\phi}(\Delta\phi_i) = N^{\phi} \frac{1}{\sigma^{\phi} \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta\phi_i}{\sigma^{\phi}} \right)^2} \]

\[ \tau^{\phi_i}(\Delta\phi_i, t + 1) = \rho\tau^{\phi_i}(\Delta\phi_i, t) + (1 - \rho)\Delta\tau^{\phi_i}(\Delta\phi_i) \]

\[ \Delta\tau^{\phi_i}(\Delta\phi_i) = N^{\tau_i} \sum_k \Delta\tau^{\phi_i,k}(\Delta\phi_i) \]

\[ \Delta\tau^{\phi_i,k}(\Delta\phi_i) = \frac{\chi^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta\phi_i - \Delta\phi_i^k}{\sigma} \right)^2} \]

trail persistence constant can be varied between 0 and 1

phermone trail:
initial phermone trail is a uniform probability function, but updated in each iteration

trail update

CG, de Vivie-Riedle, PRA, accepted
Modified ACO Algorithm

$$p^{\phi_i}(\Delta \phi_i, t) = (1 - \beta)\tau^{\phi_i}(\Delta \phi_i, t) + \beta \eta^{\phi}(\Delta \phi_i)$$

$$p^{\phi_i}(\Delta \phi_i, 0) = \eta^{\phi}(\Delta \phi_i)$$

$$\eta^{\phi}(\Delta \phi_i) = N\eta^{\phi} \frac{1}{\sigma^\phi \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma^\phi} \right)^2}$$

$$\tau^{\phi_i}(\Delta \phi_i, t + 1) = \rho \tau^{\phi_i}(\Delta \phi_i, t) + (1 - \rho)\Delta \tau^{\phi_i}(\Delta \phi_i)$$

trail update:
summation over all $k$ ants,
normalization constant $N$

$$\Delta \tau^{\phi_i}(\Delta \phi_i) = N\tau_i^{\phi} \sum_k \Delta \tau^{\phi_i,k}(\Delta \phi_i)$$

$$\Delta \tau^{\phi_i,k}(\Delta \phi_i) = \frac{Y^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi_i^k}{\sigma} \right)^2}$$

CG, de Vivie-Riedle, PRA, accepted
Modified ACO Algorithm (phase)

\[ p^{\phi_i}(\Delta \phi_i, t) = (1 - \beta)\tau^{\phi_i}(\Delta \phi_i, t) + \beta \eta^{\phi}(\Delta \phi_i) \]

\[ p^{\phi_i}(\Delta \phi_i, 0) = \eta^{\phi}(\Delta \phi_i) \]

\[ \eta^{\phi}(\Delta \phi_i) = N^{\eta^\phi} \frac{1}{\sigma^{\eta^\phi} \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma^{\eta^\phi}} \right)^2} \]

\[ \tau^{\phi_i}(\Delta \phi_i, t + 1) = \rho \tau^{\phi_i}(\Delta \phi_i, t) + (1 - \rho) \Delta \tau^{\phi_i}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i}(\Delta \phi_i) = N^{\tau^\phi_i} \sum_k \Delta \tau^{\phi_i,k}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i,k}(\Delta \phi_i) = \frac{Y^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi_i^k}{\sigma} \right)^2} \]

**contribution to trail update:**
normal distribution for each ant \(k\), with the learning rate \(Y(\text{ield})\) referring to the ant \(k\)

process efficiency

CG, de Vivie-Riedle, PRA, accepted
Modified ACO Algorithm (phase)

\[ p^{\phi_i}(\Delta \phi_i, t) = (1 - \beta) \tau^{\phi_i}(\Delta \phi_i, t) + \beta \eta^{\phi}(\Delta \phi_i) \]

\[ p^{\phi_i}(\Delta \phi_i, 0) = \eta^{\phi}(\Delta \phi_i) \]

\[ \eta^{\phi}(\Delta \phi_i) = N \eta^{\phi} \frac{1}{\sigma^{\phi} \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i}{\sigma^{\phi}} \right)^2} \]

\[ \tau^{\phi_i}(\Delta \phi_i, t + 1) = \rho \tau^{\phi_i}(\Delta \phi_i, t) + (1 - \rho) \Delta \tau^{\phi_i}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i}(\Delta \phi_i) = N \tau^{\phi}_i \sum_k \Delta \tau^{\phi_i, k}(\Delta \phi_i) \]

\[ \Delta \tau^{\phi_i, k}(\Delta \phi_i) = \frac{\chi^k}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left( \frac{\Delta \phi_i - \Delta \phi_i^k}{\sigma} \right)^2} \]

Implementation of the probability function:

Phase jump between two pixels are generated with a roulette wheel selection algorithm (fitness proportionate selection).

CG, de Vivie-Riedle, PRA, accepted
ACO Results

Evolution of the phase probability function for phase jumps between two neighboring pixels results for a NOT gate in $W(CO)_{6}$

- Tunable correlation of the pixel values
- Flexible approach:
  - Tolerating necessary phase jumps
  - But avoiding strong fluctuations
- Result: Shorter and simple structured pulses

CG, de Vivie-Riedle, PRA, accepted
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Vibrational Relaxation

measured vibrational lifetimes

biexponential decay with $T_1=150$ ps and $T_1=5.6$ ps


propagation in the density matrix formalism:
Lindblad approach & SPO propagator

\[
\rho(t_j) = U_{coh}^{(H)} T_{\mathcal{H} \rightarrow \mathcal{L}} \left( V^{(\mathcal{L})} e^{\mathcal{L}_D^{\text{diag}(\mathcal{L})} \Delta t} V^{-1(\mathcal{L})} \rho^{(\mathcal{L})(t_i)} \right) T_{\mathcal{L} \rightarrow \mathcal{H}} U_{coh}^{\dagger(\mathcal{H})}
\]

\[
U_{coh} = e^{-i\frac{\mathcal{H}}{2} \Delta t} X \dagger e^{i\mu_{\text{diag}} \mathcal{E}(t_i) \Delta t} X e^{-i\frac{\mathcal{H}}{2} \Delta t}
\]

\[
\mathcal{L}_D(\rho(t)) = \sum_{i=0} \left\{ C_i \rho C_i^\dagger - \frac{1}{2} [C_i^\dagger C_i, \rho]_+ \right\}
\]
**Vibrational Relaxation**

**W(CO)$_6$**
biexponential decay with $T_1 = 150$ ps and $T_1 = 5.6$ ps

NOT gate: maximum $\sim 75\%$ efficiency

**MnBr(CO)$_5$**
exponential decay of the $A_1$ mode with $T_1 > 200$ ps

$\rightarrow$ realization of highly efficient quantum gates possible

*first quantum gate experiments in progress!*
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Setup

- quantum information processing
- connection of qubits through molecular chains
- energy transfer through molecular chains

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model system: states of kinetically coupled local, oscillators (chain) and qubit system eigenstates
Setup

- quantum information processing
- connection of qubits through molecular chains
- energy transfer through molecular chains

\[
\ket{00} \equiv \ket{0 - \text{chain} - 0}
\]

approximation: only one overtone of the normal mode, defining the qubits, couples to the chain

model system: states of kinetically coupled local, oscillators (chain) and qubit system eigenstates
Information Transfer

laser pulse with two main frequencies induces population transfer via chain states

diagonalization of Hamiltonian normal mode representation
Quantum Channels

state transfer via different channels possible

most suited channels: similar transition probability in EV from both qubit systems
• molecular quantum computing with vibrational qubits
  IR quantum gates
  Raman quantum gates

• OCT with frequency filters

• matching solution subspaces of OCT and GA calculations

• ACO formalism for quantum control experiments

• highly efficient quantum gate operations in MnBr(CO)$_5$
  with vibrational relaxation

• quantum networks: qubits and molecular chains, state transfer

• outlook: first experimental realizations of vibrational quantum gates
Questions?

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