Femtosecond Quantum Control for Quantum Computing and Quantum Networks

Caroline Gollub

Outline

- Quantum Control

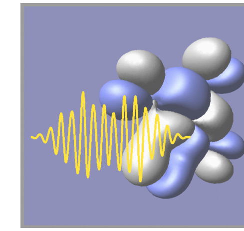
- Quantum Computing with Vibrational Qubits

    - 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

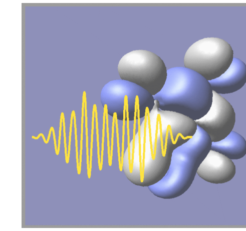
<u>theory:</u>
optimal control theory

<u>experiment:</u>
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

Outline



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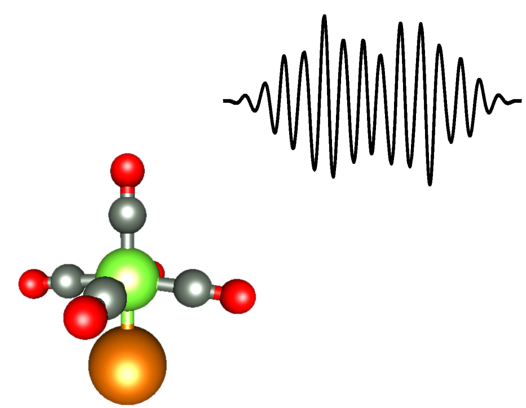
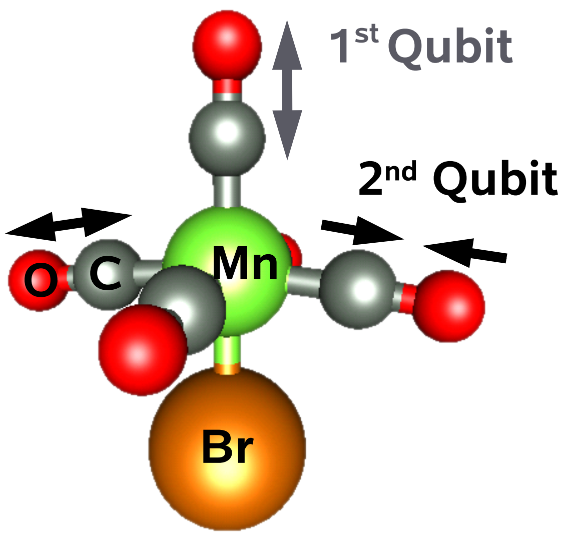
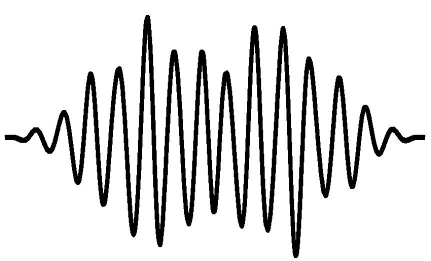


Molecular Quantum Computing

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:

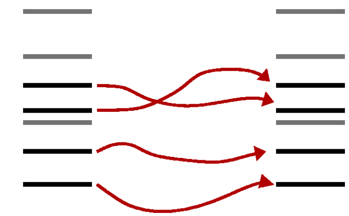
$$|00\rangle, |01\rangle, |10\rangle, |11\rangle$$

Tesch, de Vivie-Riedle, PRL **89**, 157901 (2002)

Optimal Control Theory

multi-target optimal control theory

global quantum gates



$$\mathbf{J}\left(\Psi_{ik}(t),\Psi_{fk}(t),\epsilon(t)\right)=F(\tau)\;-\alpha_0\int_0^T\frac{|\epsilon(t)|^2}{s(t)}dt$$

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

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

$$F_{\text{corr}}(\tau)=\sum_k^N\sum_l^N\langle\Phi_{fk}|\Psi_{ik}(T)\rangle\langle\Psi_{il}(T)|\Phi_{fl}\rangle$$

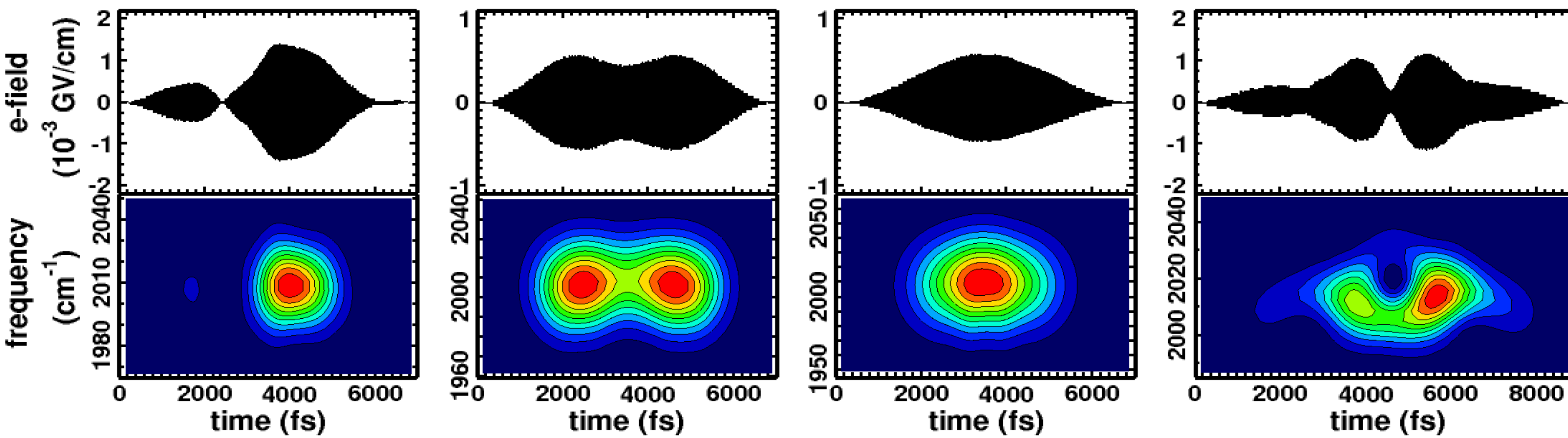
$$C_{\text{corr}}=\sum_l^N\langle\Psi_{il}(t)|\Psi_{fl}(t)\rangle$$

Tesch, de Vivie-Riedle, PRL **89**, 157901 (2002)

IR quantum gates

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

NOT	CNOT	Π	Hadamard



$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

Korff, Troppmann, de Vivie-Riedle, JCP **123**, 244509 (2005)

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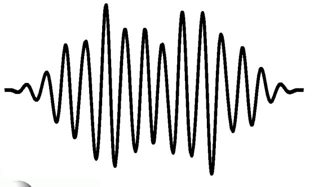
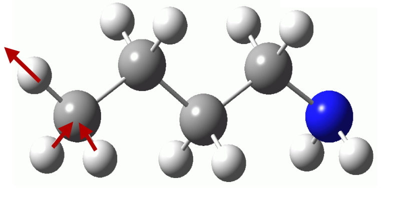


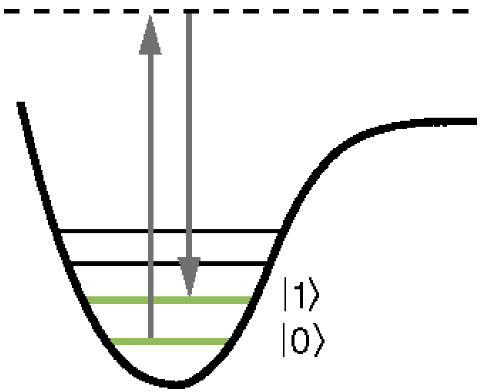


Raman Quantum Gates

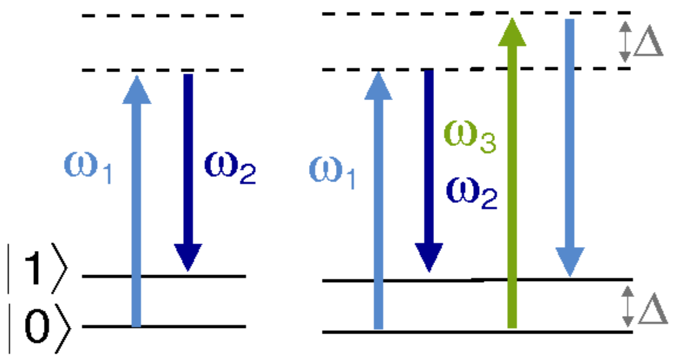
stimulated, non-resonant Raman quantum gates

strategy to optimize the two laser fields $\epsilon_1(t)$ and $\epsilon_2(t)$

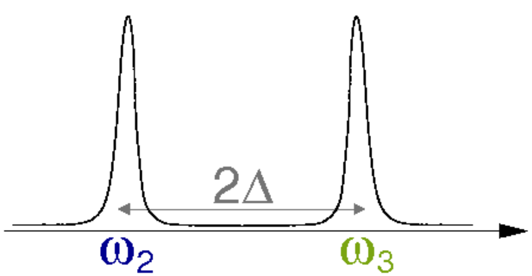
$$i\frac{\partial}{\partial t}\Psi(t) = \hat{H}_0\Psi(t) - \frac{1}{2}\varepsilon_1(t)\hat{\alpha}\varepsilon_2(t)\Psi(t)$$



optimization of
one laser pulse
possible with MTOCT



spectrum contains two
carrier frequencies



CG, Kowalewski, de Vivie-Riedle, PRL **41**, 073002 (2008)

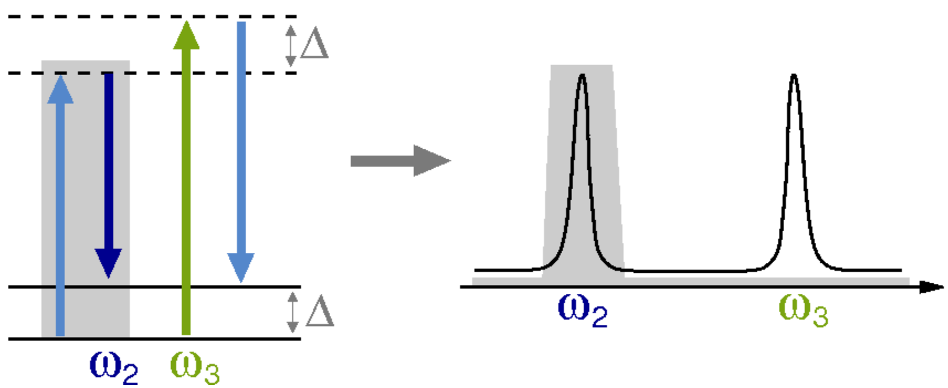
OCT with Frequency Filters

MTOCT for Raman transitions with frequency filter

$$J(\Psi_{ik}(t),\Psi_{fk}(t),\epsilon_1(t),\epsilon_2(t)) = \sum_{\mathbf{k}}\Bigg\{ |\langle\Psi_{ik}(T)|\Phi_{fk}\rangle|^2 - \sum_{l=1}^{2}\alpha_0\int_0^T \frac{|\epsilon_l(t)|^2}{s(t)}dt$$

$$-\,2\,Re\left[\langle\Psi_{ik}(T)|\Phi_{fk}\rangle\int_0^T\langle\Psi_{fk}(t)|\left[\frac{i}{\hbar}\left(\hat{H}_0-\frac{1}{2}\epsilon_1(t)\,\alpha\,\epsilon_2(t)\right)+\frac{\partial}{\partial t}\right]|\Psi_{ik}(t)\rangle dt\right]\Bigg\}$$

$$-\sum_{l=1}^{2}\gamma_l|F_l(\epsilon_l(t))|$$



CG, Kowalewski, de Vivie-Riedle, PRL **41**, 073002 (2008)

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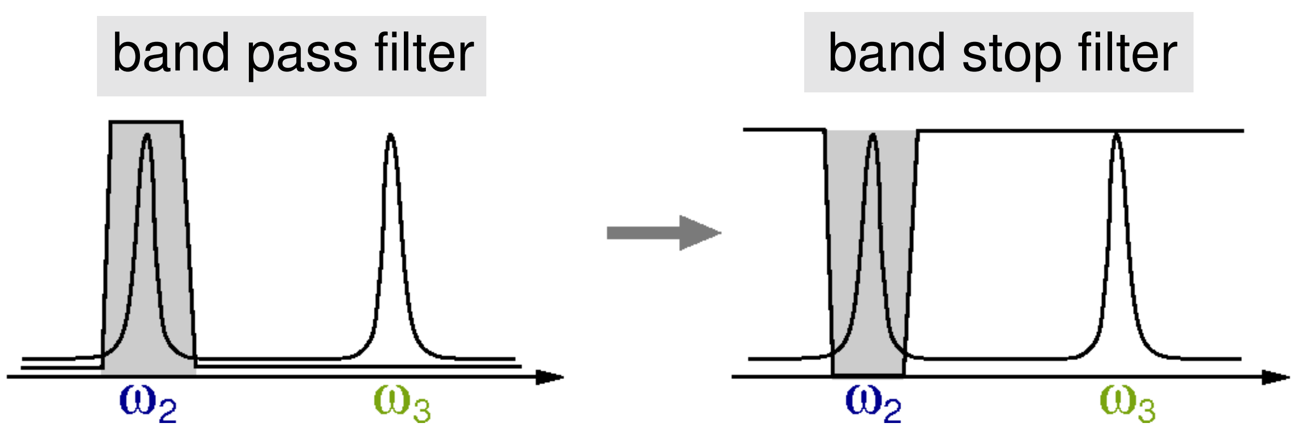
$$- 2\,Re\left[\langle\Psi_{ik}(T)|\Phi_{fk}\rangle \int_0^T \langle\Psi_{fk}(t)| \left[\frac{i}{\hbar}\left(\hat{H}_0 - \frac{1}{2}\epsilon_1(t)\,\alpha\,\epsilon_2(t)\right) + \frac{\partial}{\partial t}\right] |\Psi_{ik}(t)\rangle dt\right]\Bigg\}$$

$$- \sum_{l=1}^{2} \gamma_l |F_l(\epsilon_l(t))|$$



CG, Kowalewski, de Vivie-Riedle, PRL **41**, 073002 (2008)

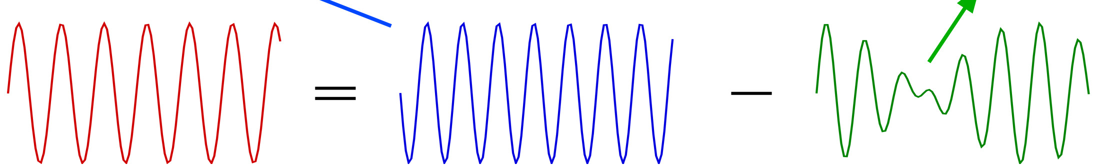
OCT with Frequency Filters

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:

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

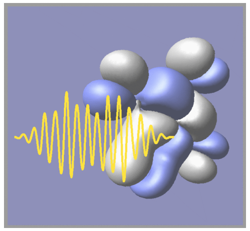


OCT output

Lagrange multiplier can be interpreted as a correction field

CG, Kowalewski, de Vivie-Riedle, PRL **41**, 073002 (2008)

OCT with Frequency Filters



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

$$\begin{aligned}\gamma'(t) = & \sum_k \Im[\langle \Phi_k(t,\epsilon^n)|\psi_k(t,\epsilon^n)\rangle \times \langle \Phi_k(t,\epsilon^n)|\hat{\mu}|\psi_k(t,\epsilon^n)\rangle] \\ \approx & \sum_k \Im[\langle \Phi_k(t,\epsilon^n)|\psi_k(t,\epsilon^{n+1})\rangle \times \langle \Phi_k(t,\epsilon^n)|\hat{\mu}|\psi_k(t,\epsilon^{n+1})\rangle]\end{aligned}$$

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

CG, Kowalewski, de Vivie-Riedle, PRL **41**, 073002 (2008)

Model System

properties of molecular candidates

- high Raman activities
- balanced anharmonicities

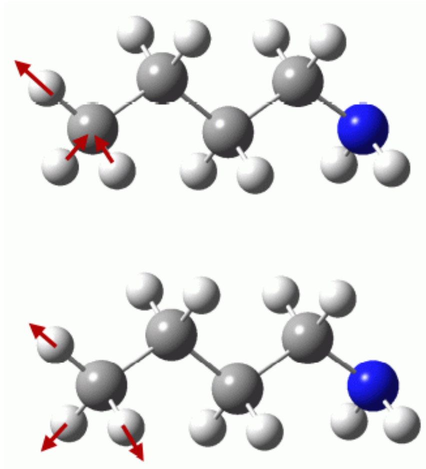
scanning several molecules with suitable Raman spectra

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

***n*-butylamine**

ω_1=3100 cm^{-1}, ω_2=3029 cm^{-1}

Δ_1=73 cm^{-1}, Δ_2=102 cm^{-1}, Δ_{12}=23 cm^{-1}

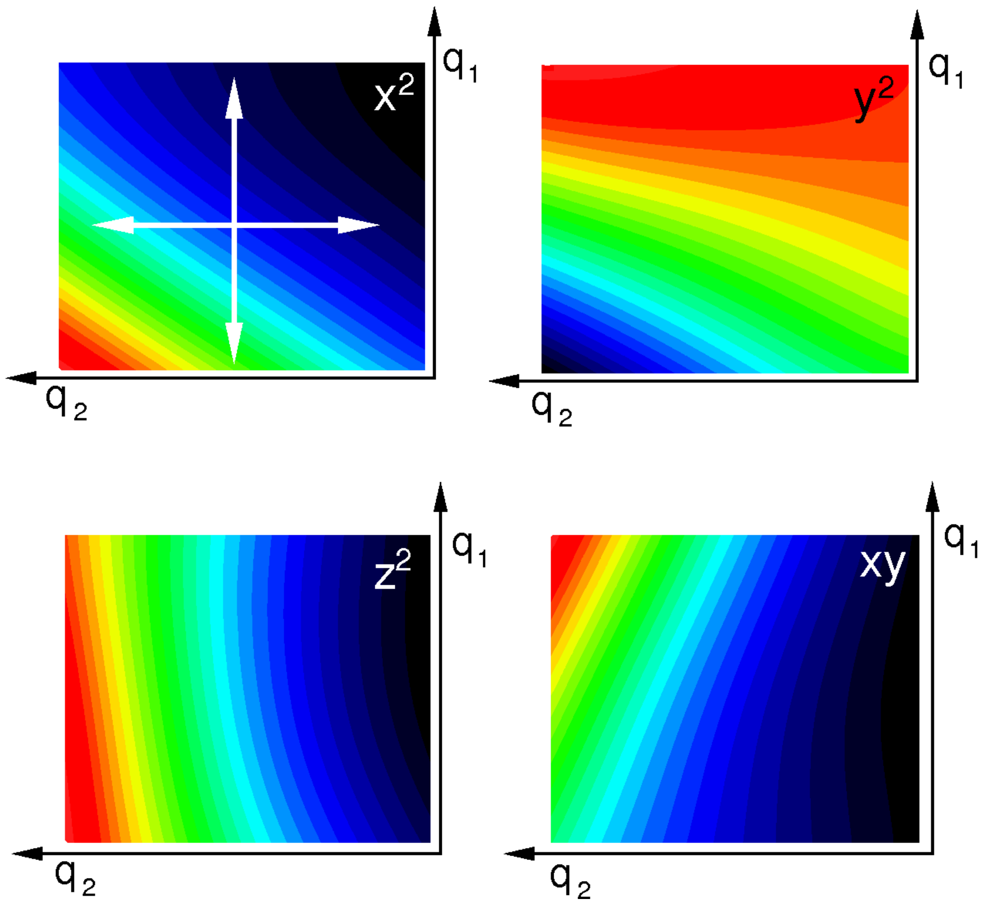


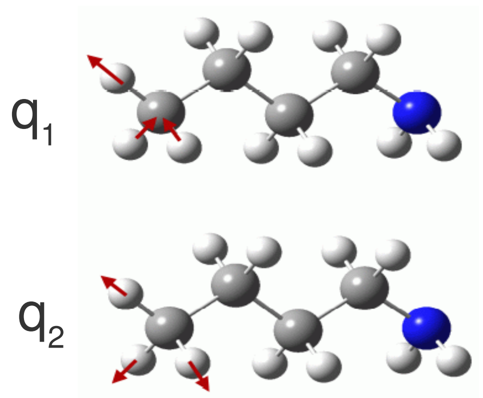
CG, Troppmann, de Vivie-Riedle, NJP **8**, 48 (2006)

Polarizability

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

suited components:

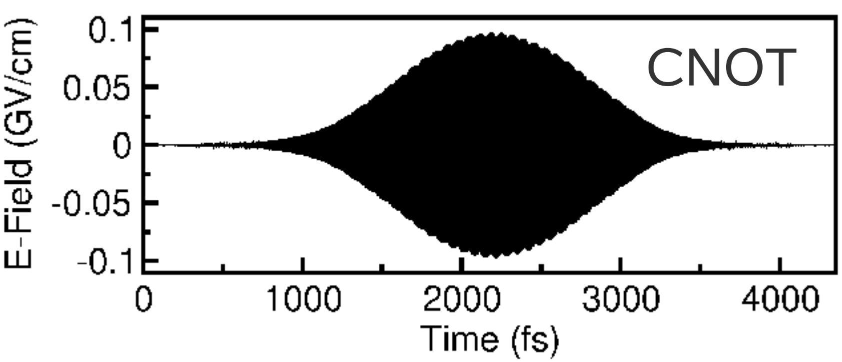


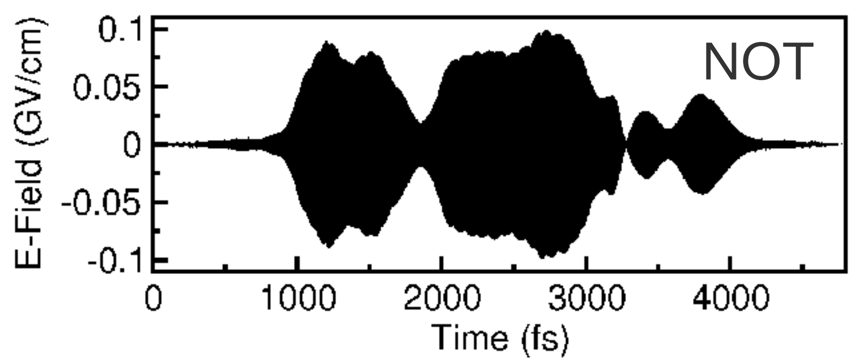


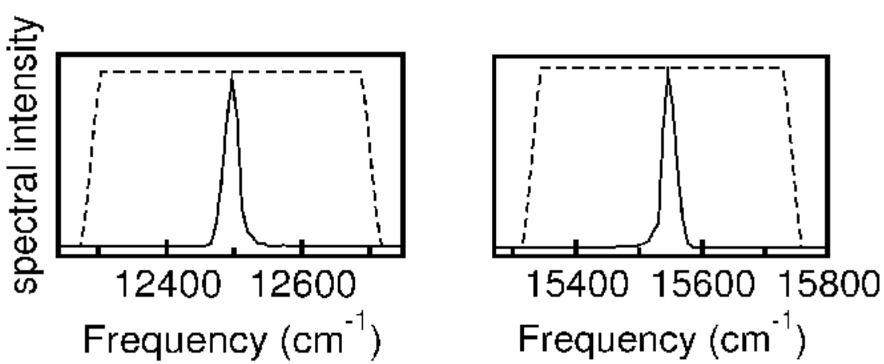
Vibrational Raman Quantum Gates

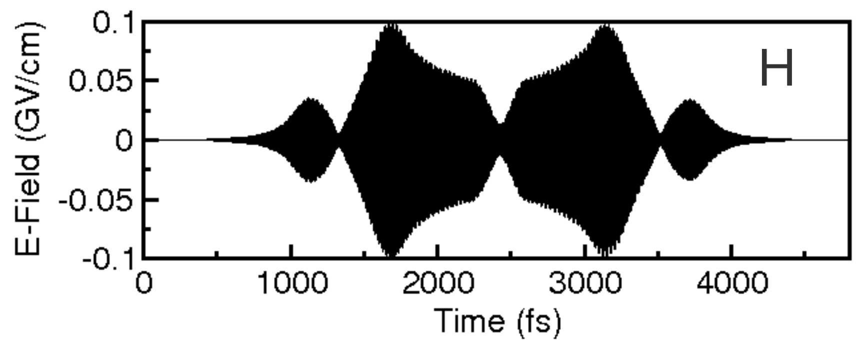
quantum gates with x-polarized laser fields

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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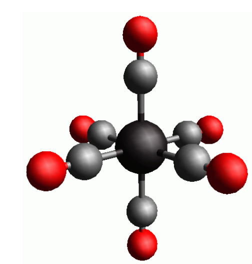
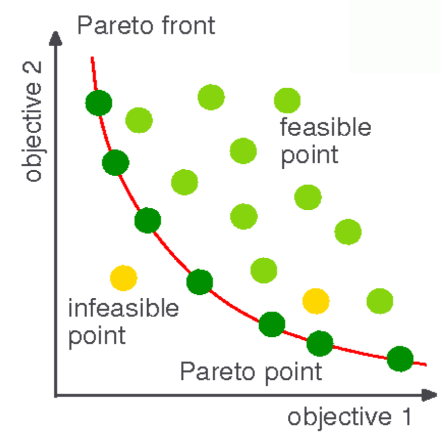
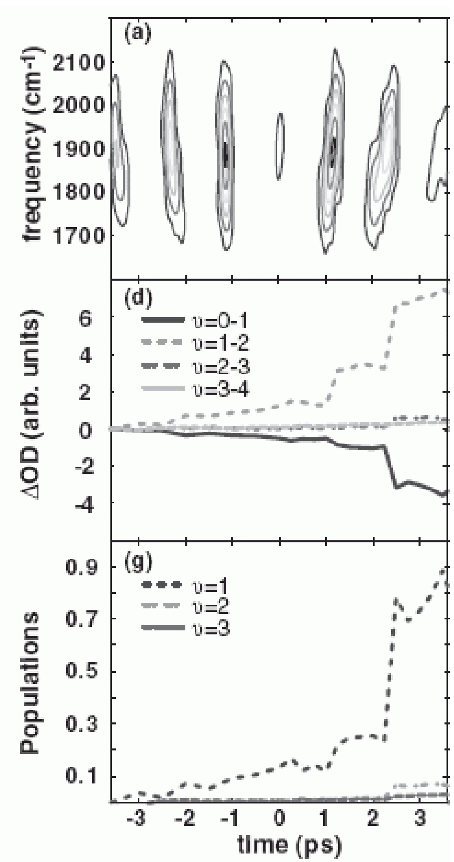
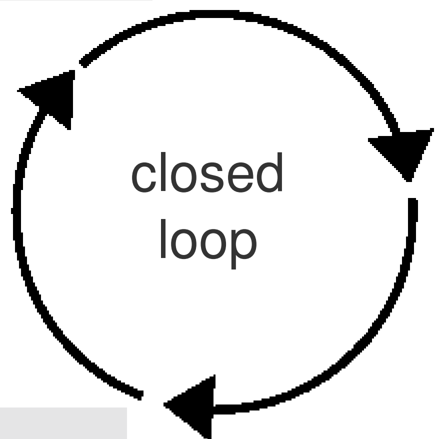




Control with Genetic Algorithms



algorithm (GA)



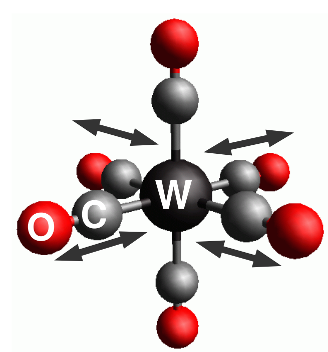
pulse shaper

experiment

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

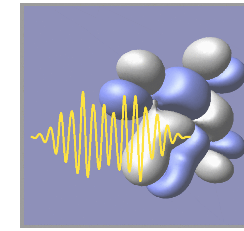
$$M_n(\omega_n^0) = T_n(\omega_n^0)\exp(i\phi_n(\omega_n^0))$$

$$\tilde{\varepsilon}_{\text{out}}(\omega) = M(\omega)\tilde{\varepsilon}_{\text{in}}(\omega)$$



D. Strasfeld, S. Shim,
M. Zanni, PRL **99**, 038102 (2007)

OCT versus GAs



<u>**optimal control theory**</u>	<u>**genetic algorithms**</u>
primarily in the time domain	frequency domain
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

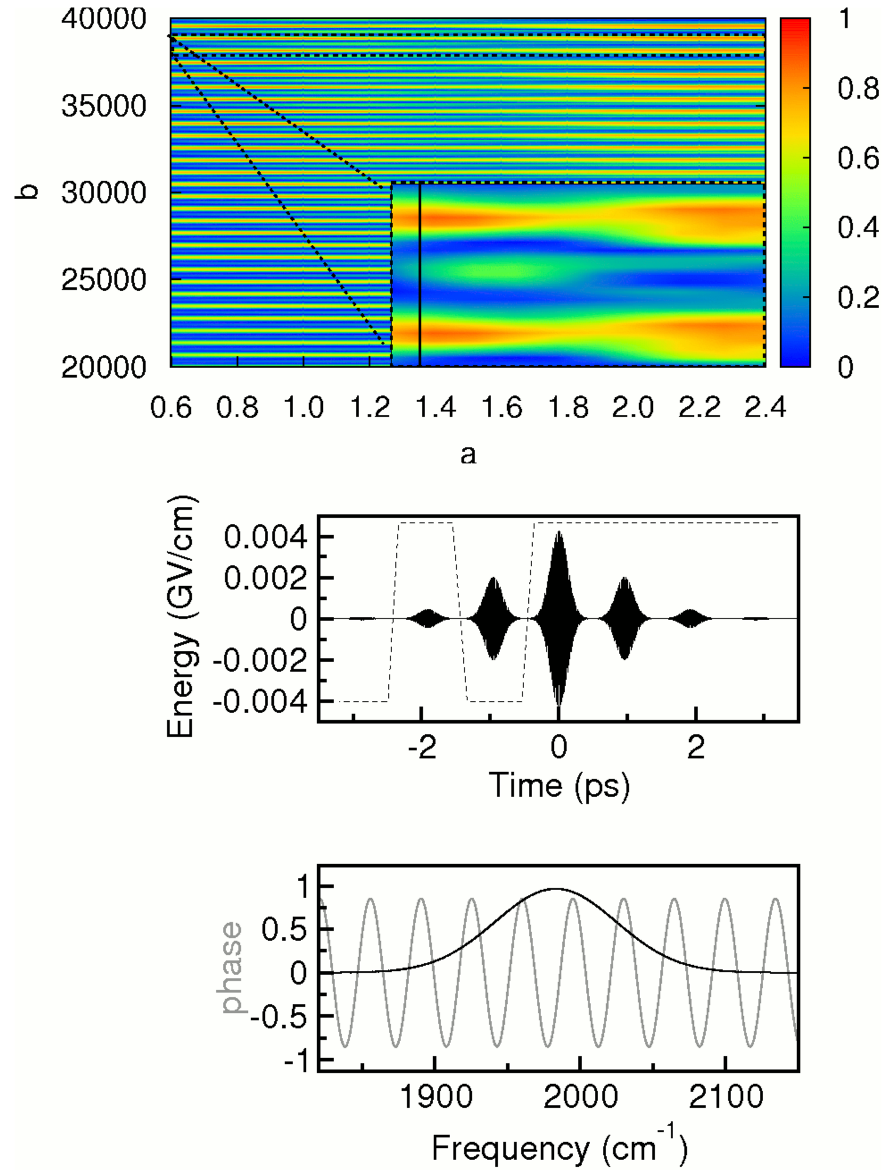
control landscape

for the excitation process from v=0 to v=1of 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

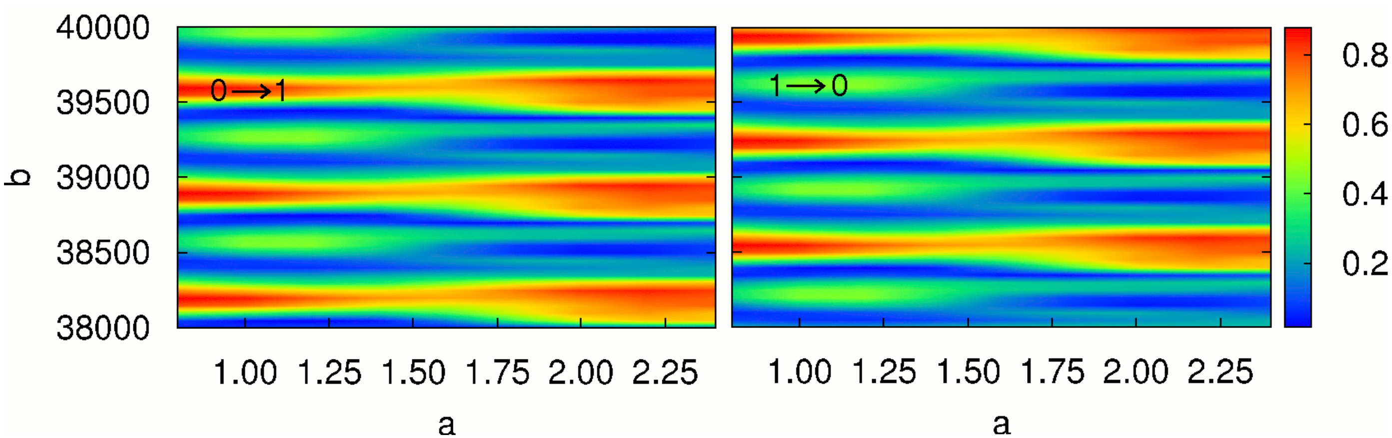


CG, de Vivie-Riedle, PRA **78**, 033424 (2008)

Parametrized Phase Functions

control landscapes

for a 1-qubit NOT gate with sinusoidal phase modulation

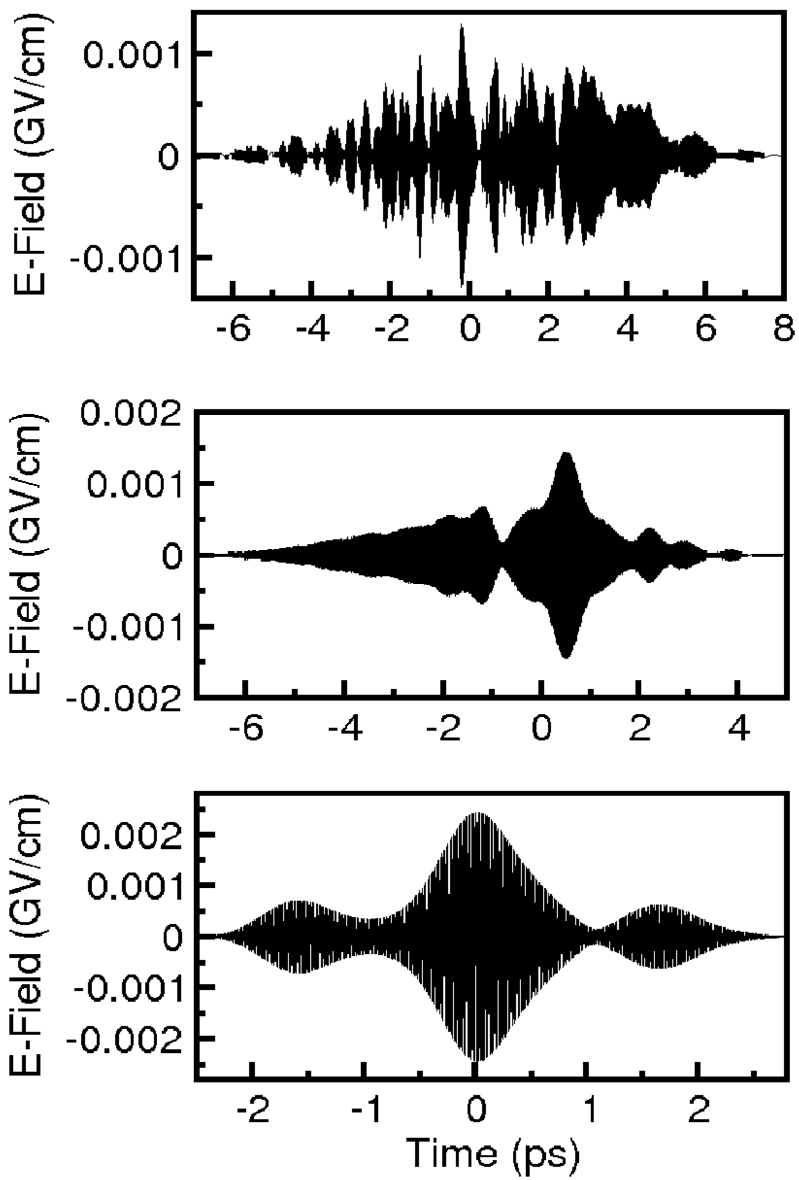


➡ control landscapes counter each other

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

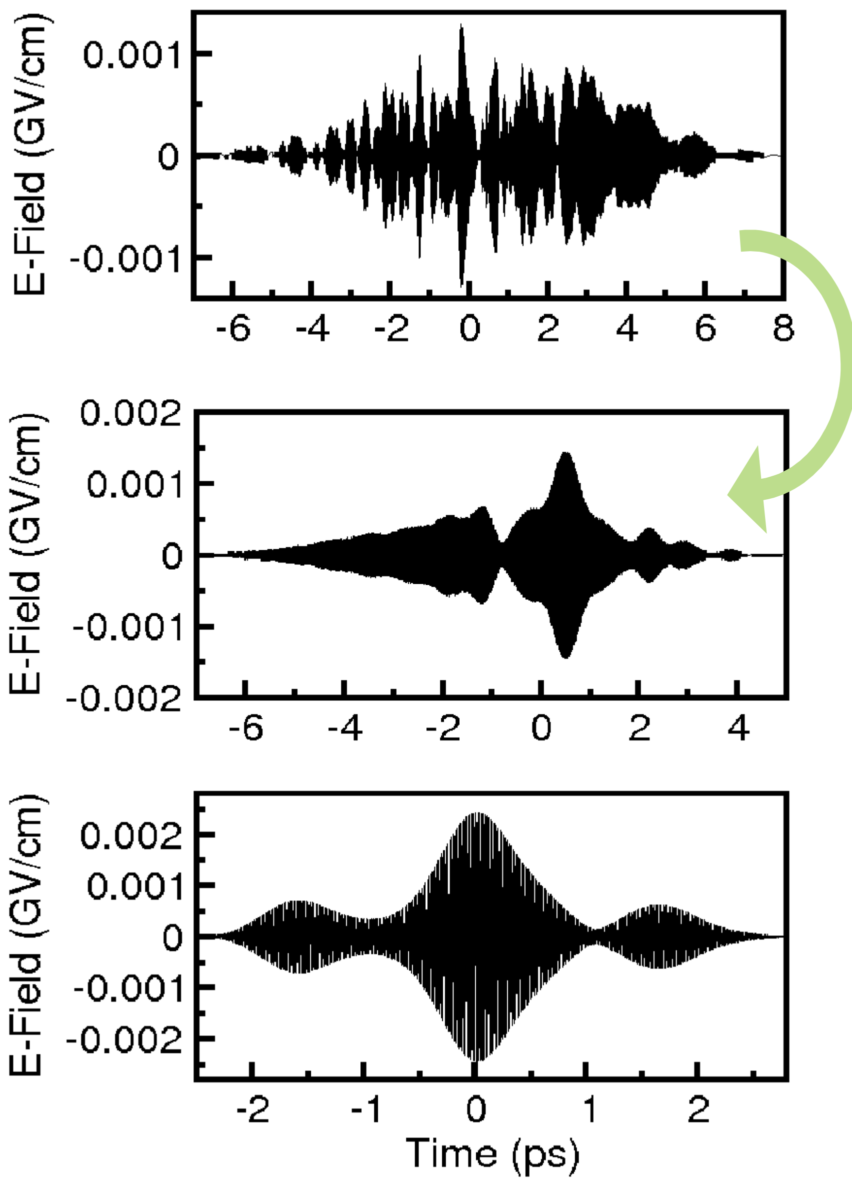


NOT gate laser pulses from GA calculations (efficiencies > 99%)

FL-pulse from experiment

CG, de Vivie-Riedle, PRA **78**, 033424 (2008)

Pixeled Phase Functions



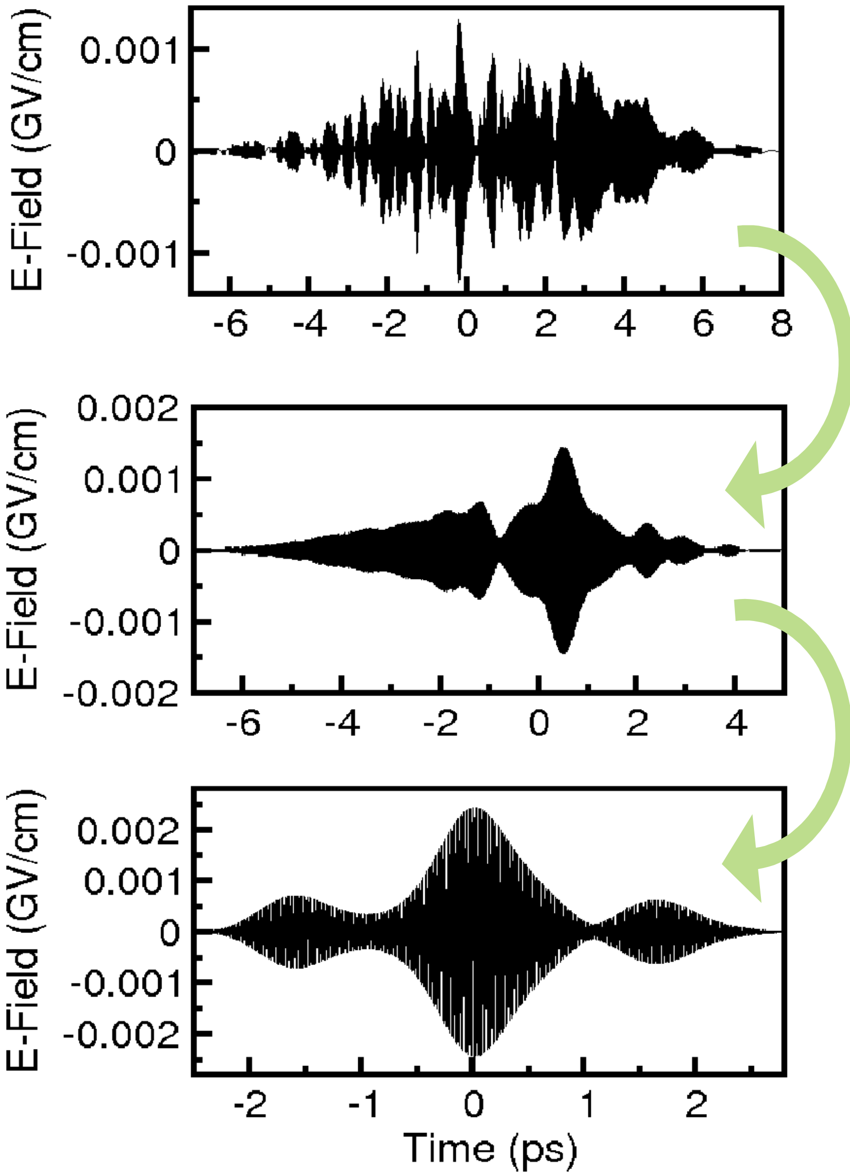
NOT gate laser pulses from GA calculations (efficiencies > 99%)

FL-pulse from experiment

elongation of FL-pulse duration (~amplitude shaping)

CG, de Vivie-Riedle, PRA **78**, 033424 (2008)

Pixeled Phase Functions



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

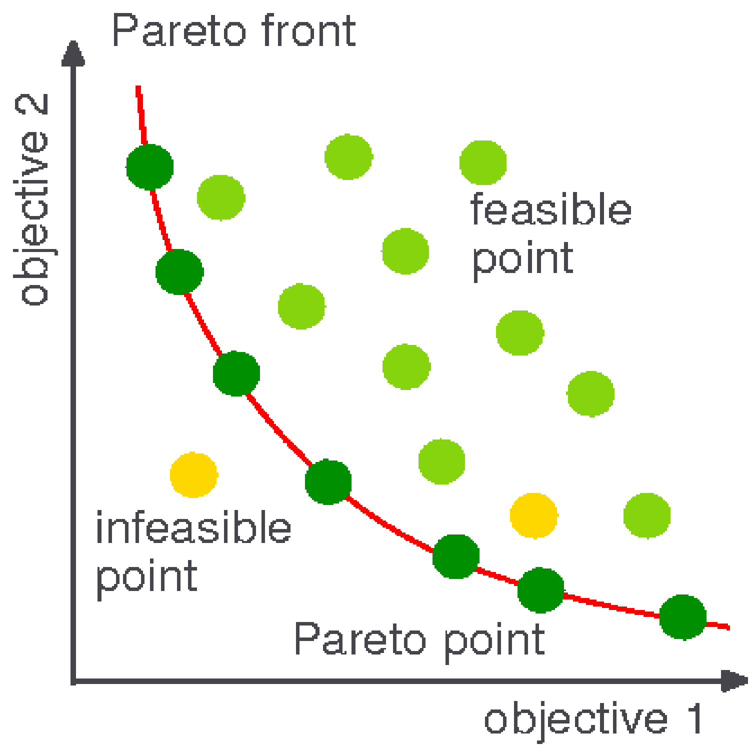
FL-pulse from experiment

elongation of FL-pulse duration (~amplitude shaping)

limitation of the phase range from [-π,+π] to [-0.1π, +0.1π]

CG, de Vivie-Riedle, PRA **78**, 033424 (2008)

Multi-Objective GAs



multi-objective / multi-criteria optimization

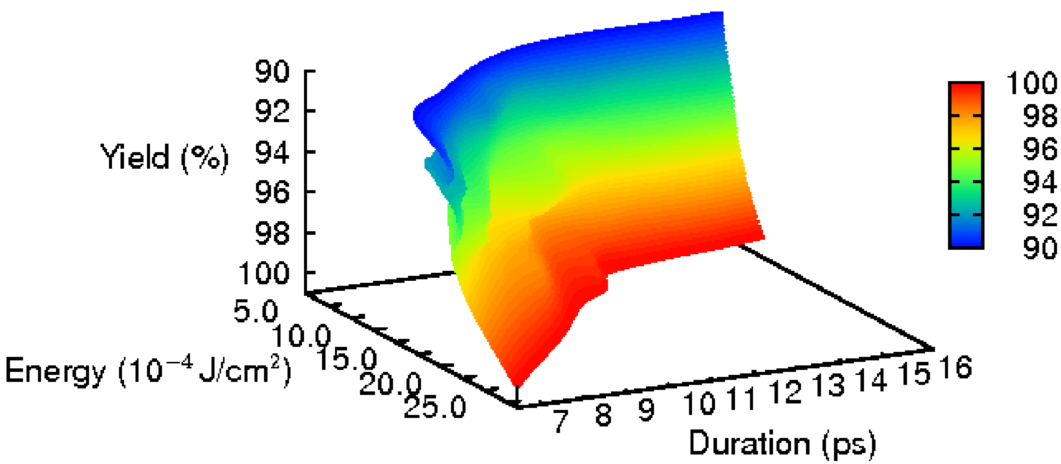
<u>Pareto fronts</u>
minimum requirements on the pulse properties

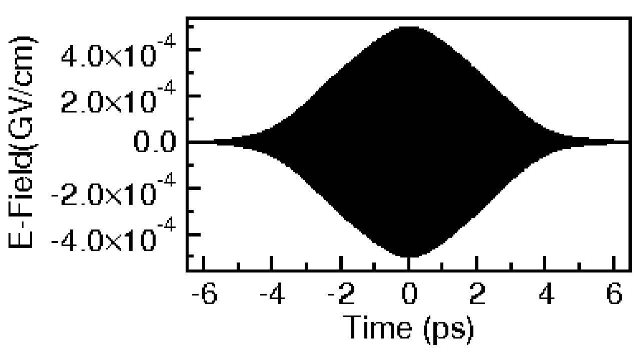
<u>control objectives</u>
- efficiency
- pulse duration
- pulse intensity

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

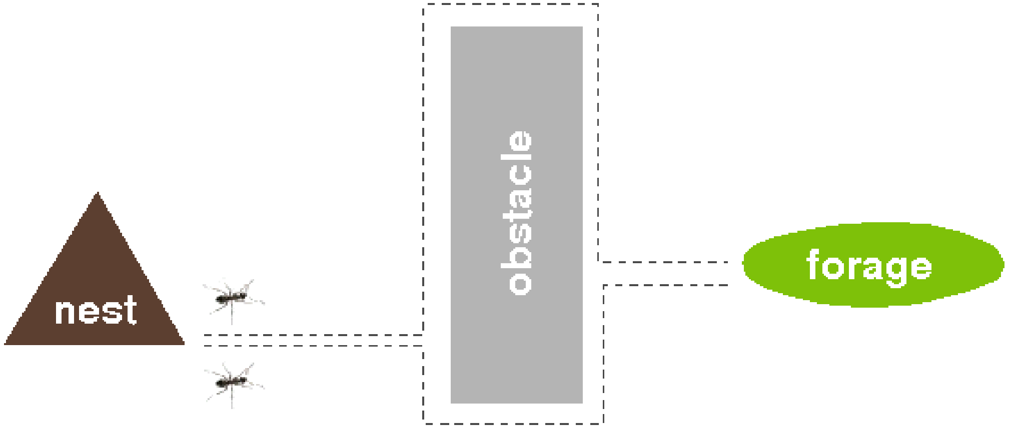
inspired by the behavior of real ant colonies
discrete, combinatorial optimization problems
belongs to the research field of swarm intelligence, which is part of AI

→ pheromone acts as biochemical information
for the ants in a colony: collective memory

Ant Colony Algorithm

in nature: ants reach forage on the direct track

due to the connection between pheromone deposition and search of favorable paths

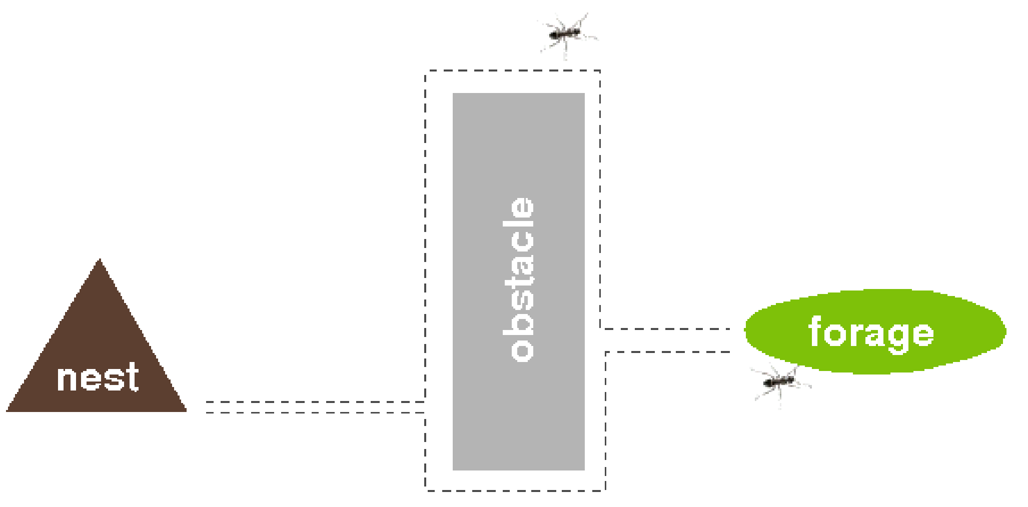


initially each ant chooses randomly one path

Ant Colony Algorithm

in nature: ants reach forage on the direct track

due to the connection between pheromone deposition and search of favorable paths

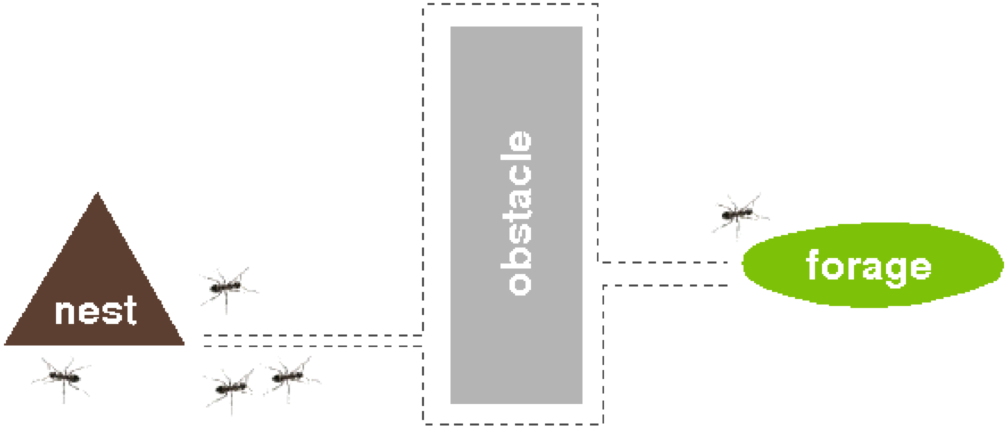


ant on shortest track reaches food source earlier and ...

Ant Colony Algorithm

in nature: ants reach forage on the direct track

due to the connection between pheromone deposition and search of favorable paths



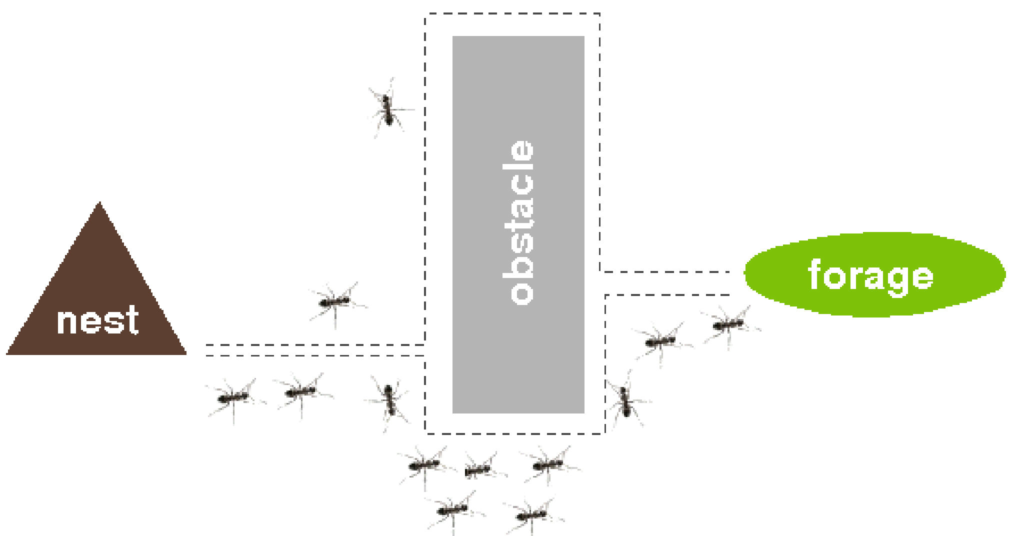
... deposits phermone earlier on the way back to the nest

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 (phase)

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

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

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

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

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

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

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

CG, de Vivie-Riedle, PRA, accepted

Modified ACO Algorithm (phase)

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

pheromone trail (updated in each iteration)

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

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

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

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

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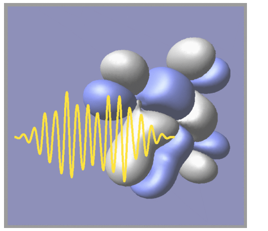
CG, de Vivie-Riedle, PRA, accepted

Modified ACO Algorithm (phase)



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

visibility function (constant)

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

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

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

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

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

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

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

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

probability function:
first iteration

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

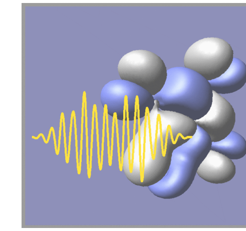
$$\tau^{\phi_i}(\Delta\phi_i, t+1) = \rho\tau^{\phi_i}(\Delta\phi_i, t) + (1-\rho)\Delta\tau^{\phi_i}(\Delta\phi_i)$$

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

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

CG, de Vivie-Riedle, PRA, accepted

Modified ACO Algorithm (phase)



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

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

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

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

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

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

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

CG, de Vivie-Riedle, PRA, accepted

Modified ACO Algorithm (phase)

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

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

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

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

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

trail update

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

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

CG, de Vivie-Riedle, PRA, accepted

Modified ACO Algorithm (phase)

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

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

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

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

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

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

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

CG, de Vivie-Riedle, PRA, accepted

Modified ACO Algorithm (phase)

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

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

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

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

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

process efficiency

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

CG, de Vivie-Riedle, PRA, accepted

Modified ACO Algorithm (phase)

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

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

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

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

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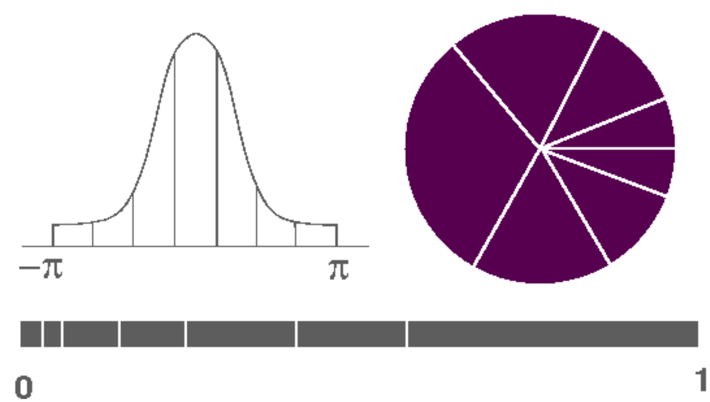
$$\Delta\tau^{\phi_i,k}(\Delta\phi_i) = \frac{Y^k}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{\Delta\phi_i-\Delta\phi_i^k}{\sigma}\right)^2}$$

implementation of the probability function:

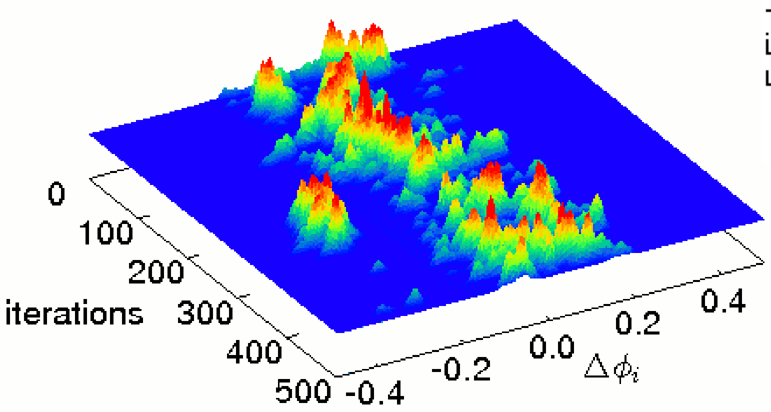
phase jump between two pixels are generated with a roulette wheel selection algorithm (fitness proportionate selection)



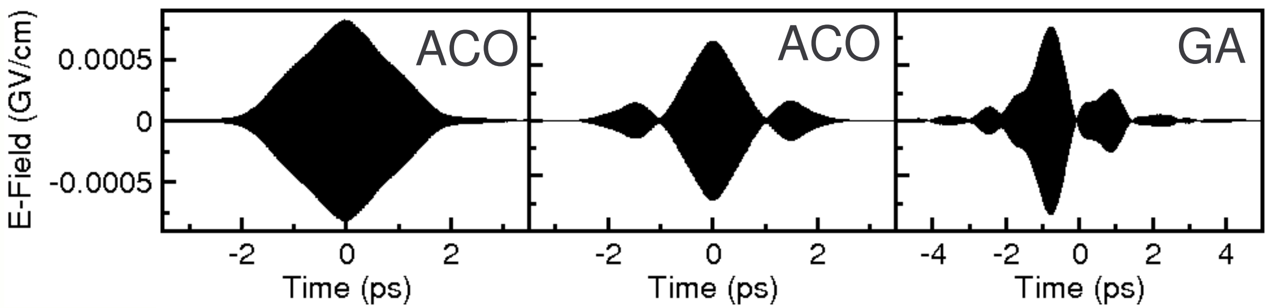
CG, de Vivie-Riedle, PRA, accepted

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 neccessary phase jumps
    - but avoiding strong fluctuations
- result: shorter and simple structured pulses

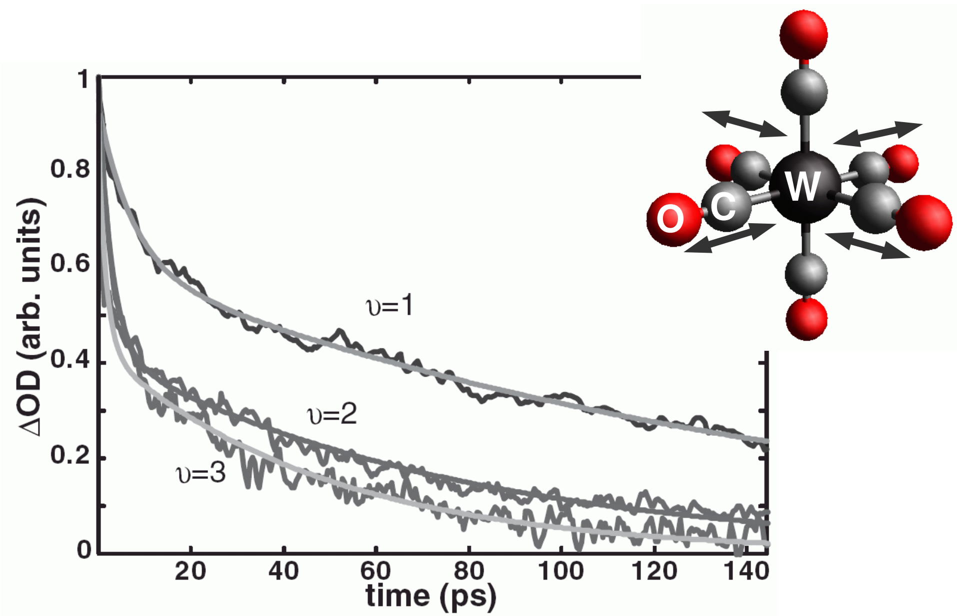
CG, de Vivie-Riedle, PRA, accepted

Outline

- Quantum Control
- Quantum Computing with Vibrational Qubits
    - Concept & IR-gates and MTOCT
    - Raman Quantum Computing
    - Control with Genetic Algorithms
    - Control with ACO
    - Dissipation
- Quantum Networks
- Conclusion & Outlook

Vibrational Relaxation

measured vibrational lifetimes



D. Strasfeld, S. Shim, M. Zanni, PRL **99**, 038102 (2007)

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

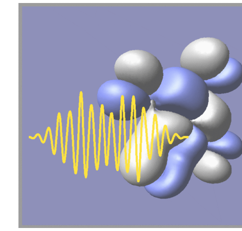
propagation in the density matrix formalism:
Lindblad approach & SPO propagator

$$\boldsymbol{\rho}(t_j) = \mathbf{U}_{\mathrm{coh}}^{(\mathcal{H})}\,\mathbf{T}^{\mathcal{H}\to\mathcal{L}}\left(\mathbf{V}^{(\mathcal{L})}\,e^{\mathcal{L}_D^{\mathrm{diag}(\mathcal{L})}\Delta t}\,\mathbf{V}^{-1(\mathcal{L})}\,\boldsymbol{\rho}^{(\mathcal{L})}(t_i)\right)\mathbf{T}^{\mathcal{L}\to\mathcal{H}}\,\mathbf{U}_{\mathrm{coh}}^{\dagger(\mathcal{H})}$$

$$\mathbf{U}_{\mathrm{coh}} = e^{-i\mathbf{H}\frac{\Delta t}{2}}\,\mathbf{X}^{\dagger}\,e^{i\boldsymbol{\mu}^{\mathrm{diag}}\epsilon(t_i)\Delta t}\,\mathbf{X}\,e^{-i\mathbf{H}\frac{\Delta t}{2}}$$

$$\mathcal{L}_D(\boldsymbol{\rho}(t)) = \sum_{i=0}\left\{\mathrm{C}_i\boldsymbol{\rho}\mathrm{C}_i^{\dagger} - \frac{1}{2}\left[\mathrm{C}_i^{\dagger}\mathrm{C}_i, \boldsymbol{\rho}\right]_+\right\}$$

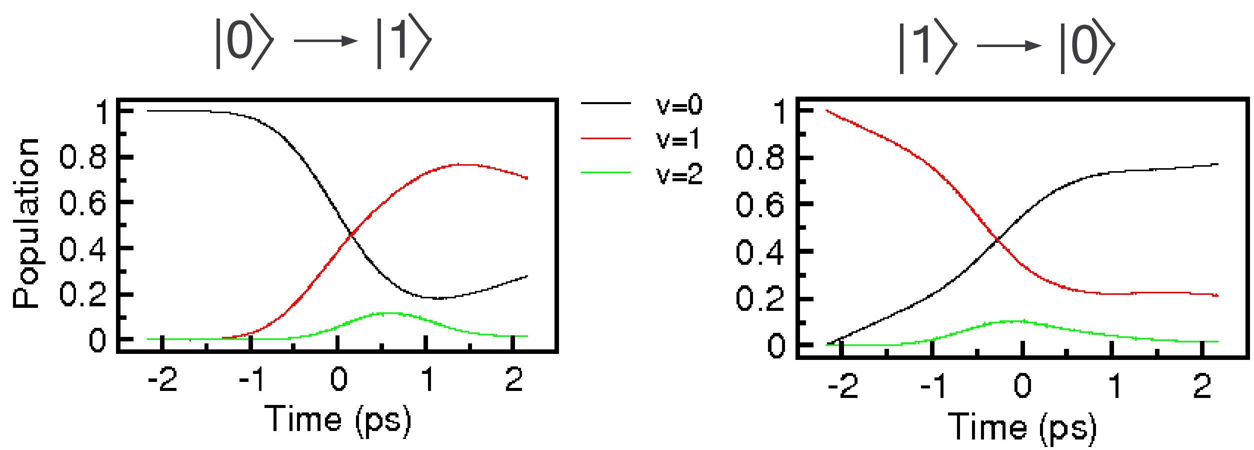
Vibrational Relaxation



$W(CO)_6$

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

NOT gate: maximum ~75% efficiency



$MnBr(CO)_5$

exponential decay of the A_1 mode with T_1> 200 ps

➡ realization of highly efficient quantum gates possible

first quantum gate experiments in progress!

Outline

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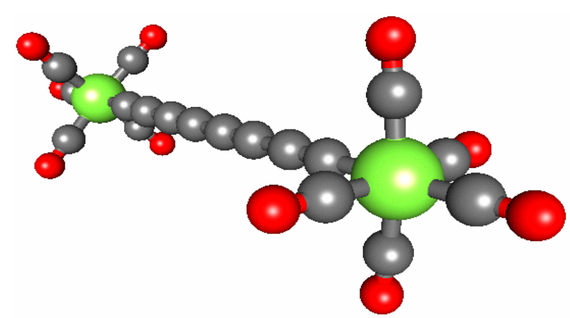
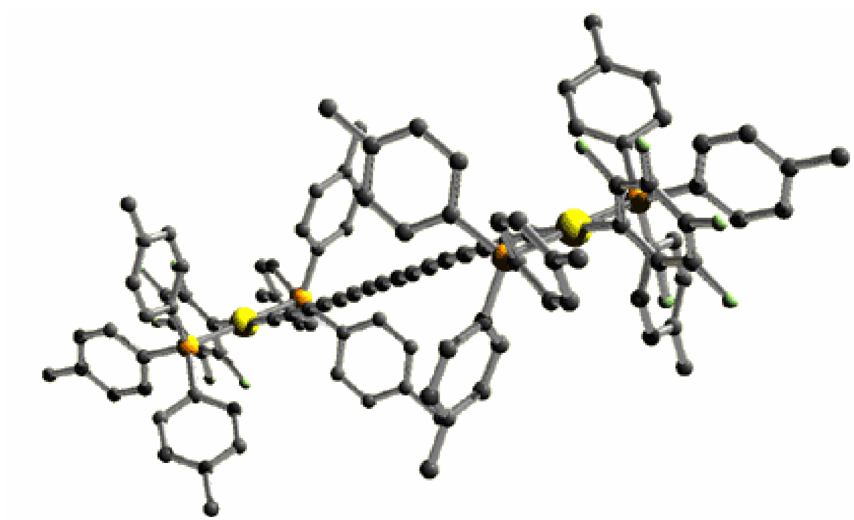
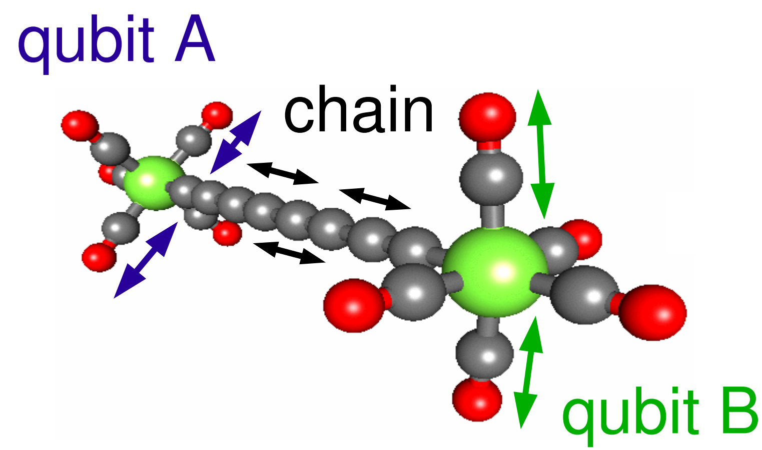


Setup

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



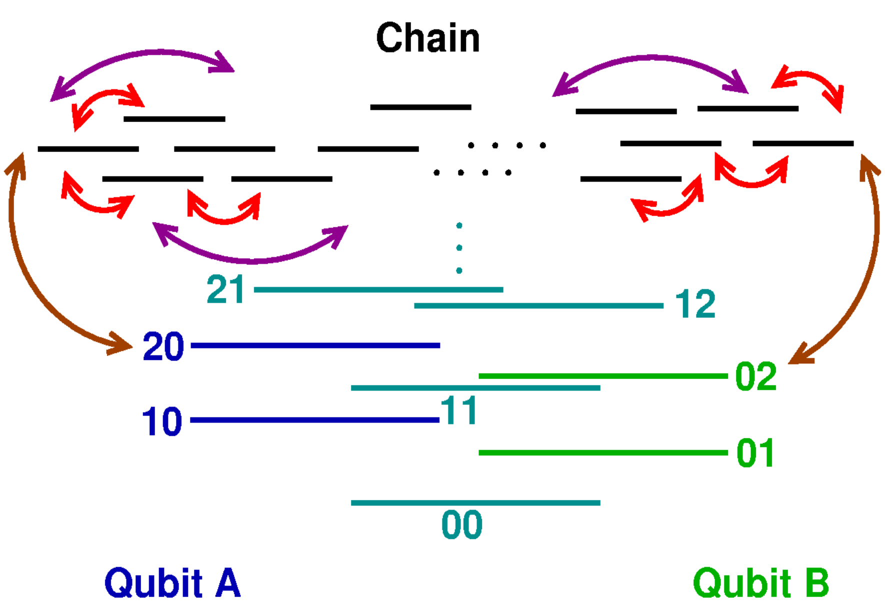
Prof. Gladysz,
Stahl et al., Angew. Chem.
Int. Ed. 41



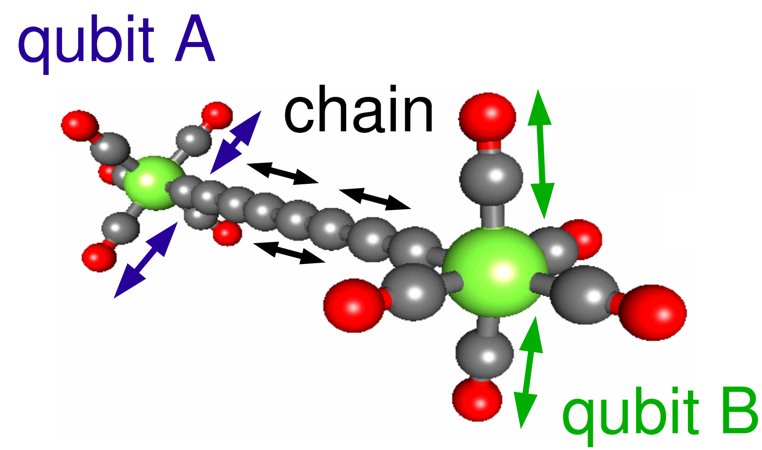
model system:
states of kinetically coupled local,
oscillators (chain) and qubit system
eigenstates

Setup

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



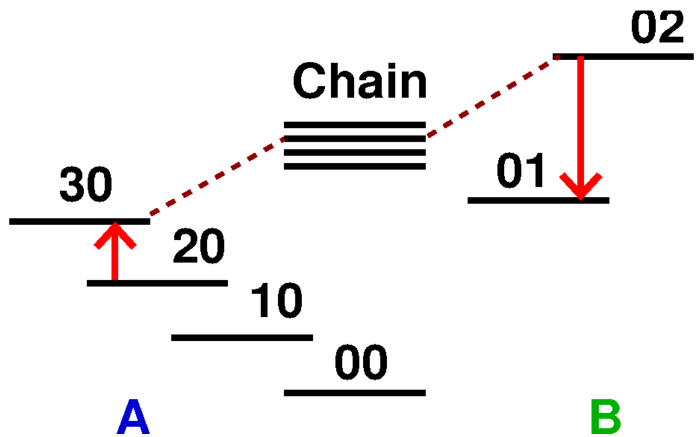
$$|00\rangle \equiv |0 - chain - 0\rangle$$



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

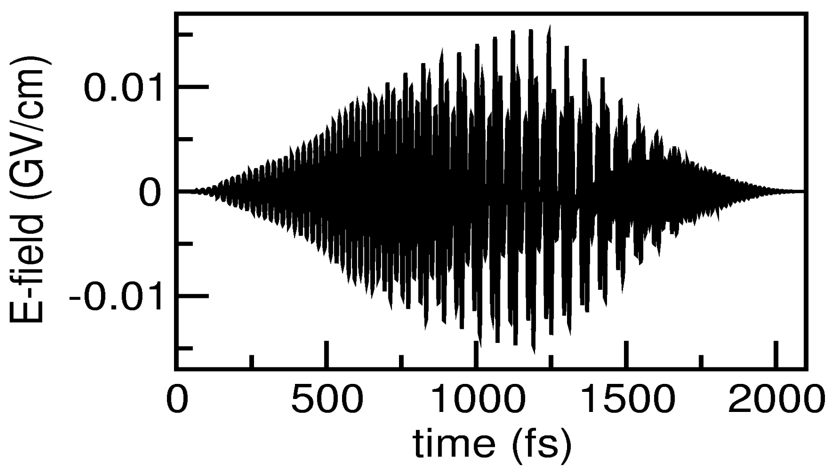
approximation: only one overtone of the normal mode, defining the qubits, couples to the chain

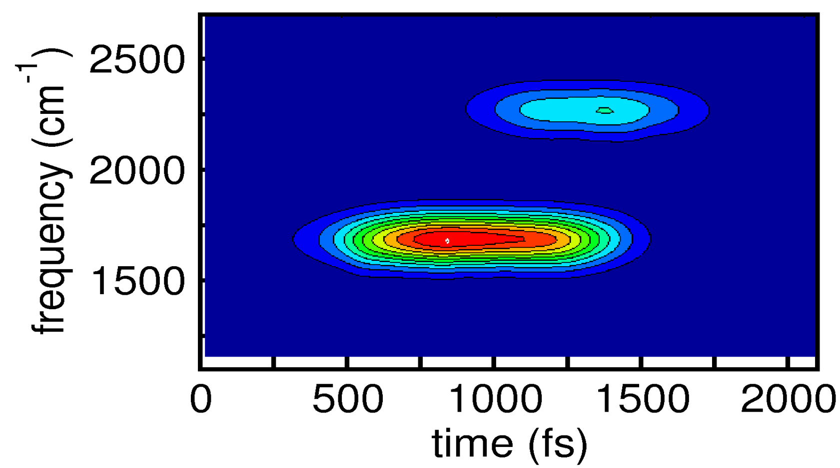
Information Transfer



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

diagonalization of Hamiltonian
normal mode representation

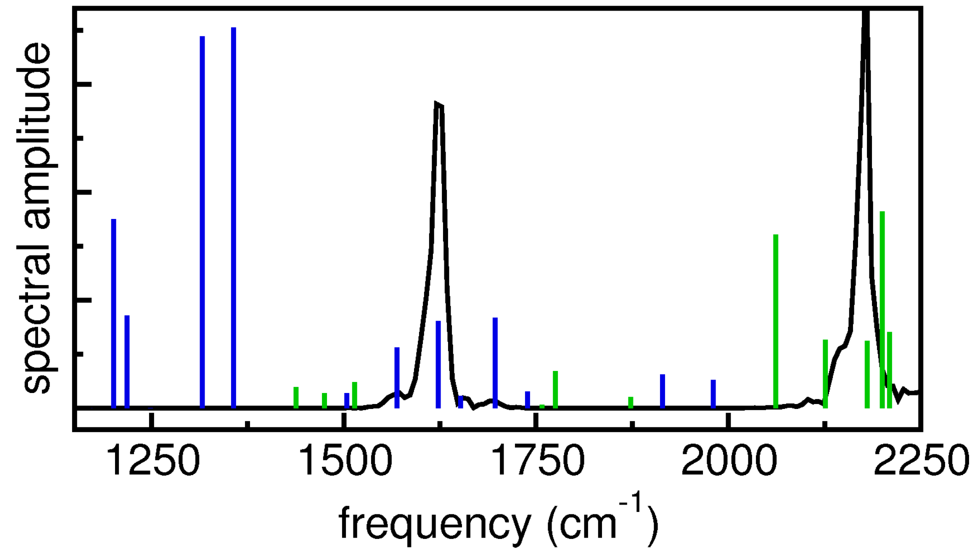


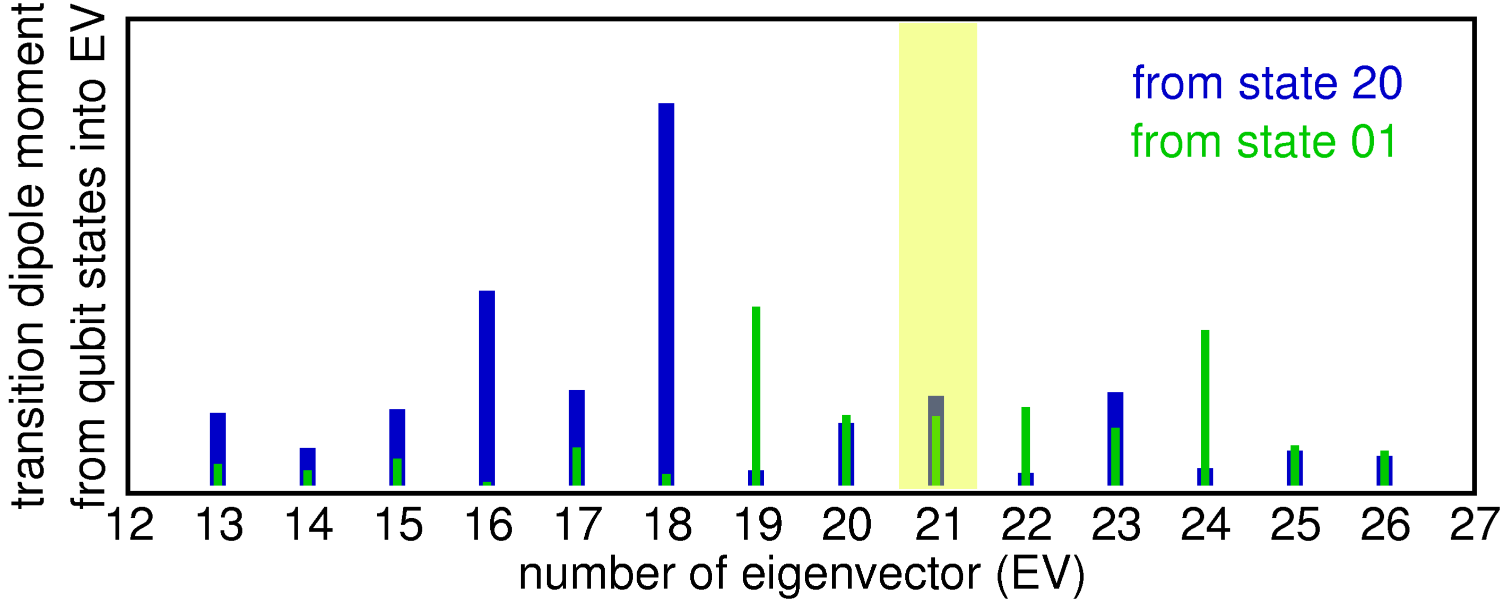


Quantum Channels

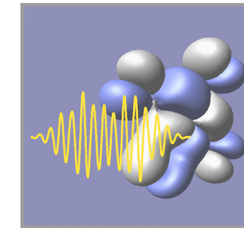
state transfer via different channels possible

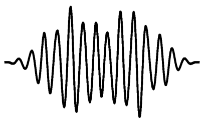
most suited channels:
similar transition probability in EV from both qubit systems

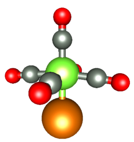




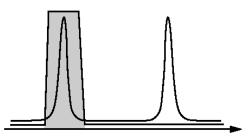
Conclusion & Outlook



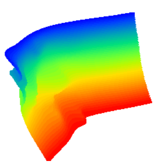




- molecular quantum computing with vibrational qubits
  IR quantum gates
  Raman quantum gates

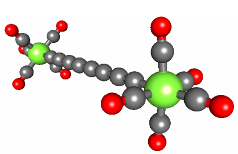


- OCT with frequency filters

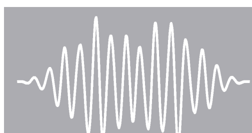


- matching solution subspaces of OCT and GA calculations
- ACO formalism for quantum control experiments

- 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?

thank you to:

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Martin Zanni
David Strasfeld

funding:
DFG Normalverfahren
MAP