Quantum molecular computing: optimal control theory for unitary transformations

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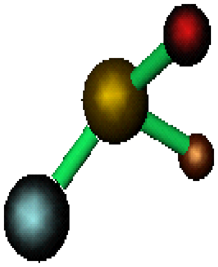

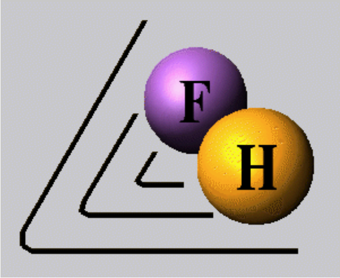

Quantum Information and Quantum Control Conference
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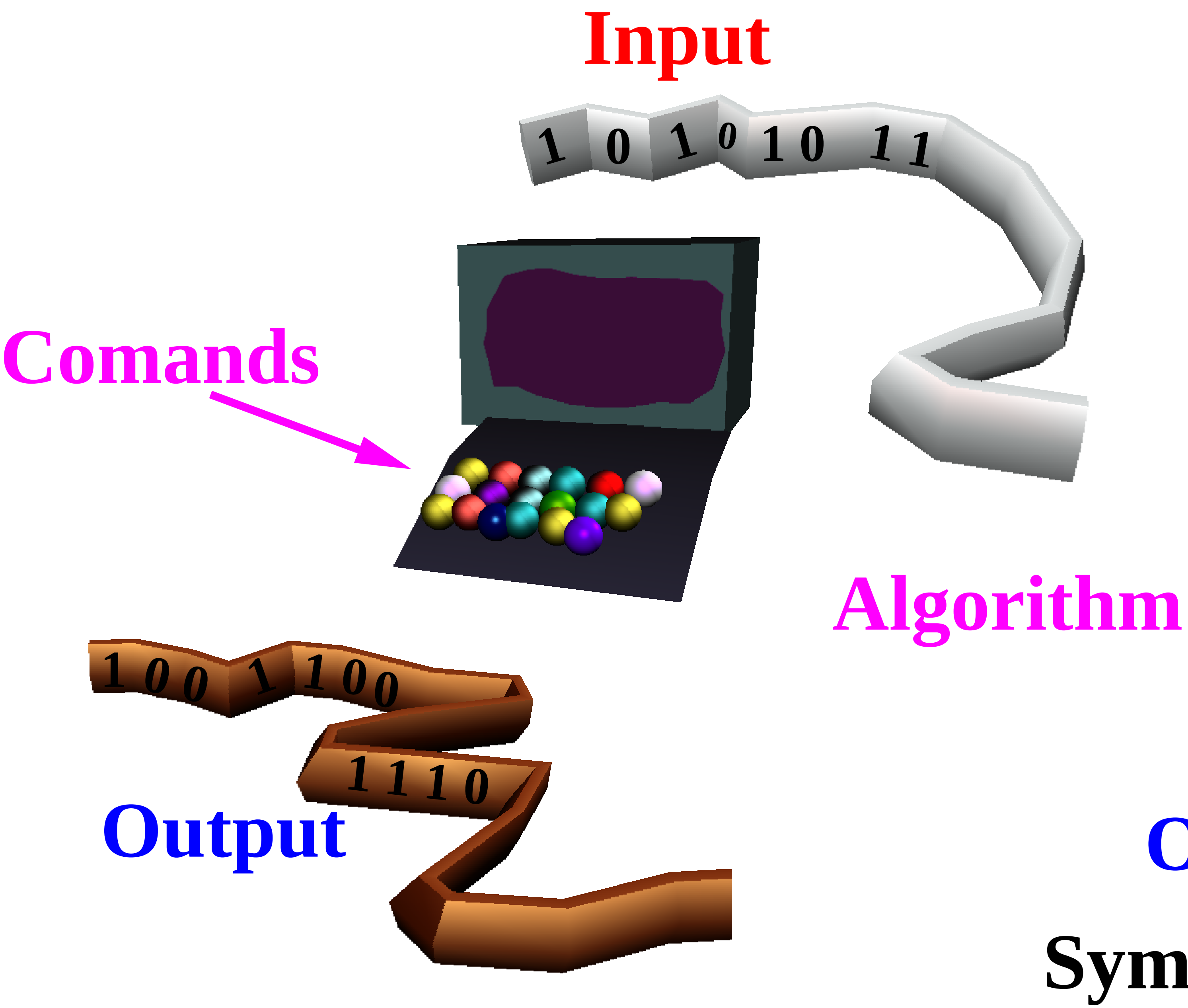
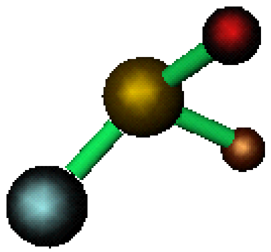
Universal computer



$$O = U\,I$$

Symbolically

The molecular computer



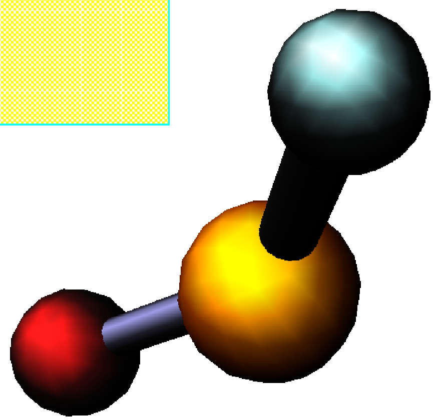
Input: writing into the molecular states.

Processing: executing an algorithm.

Output: reading out the result.

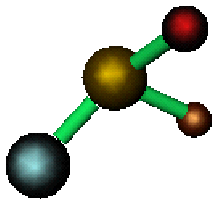
What are the relevant time scales ?

reading
writing
executing
coherence



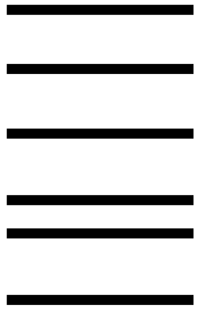
What are the resources required
and how do they scale with the computation task?

The molecular quantum computer



Input: writing into the molecular energy levels?

Algorithm = Unitary transformation



$$\boxed{\psi_{out} = U\psi_{in}}$$

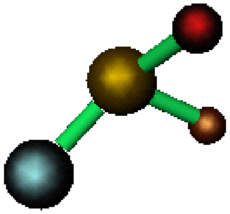
Output: written in place on the same molecular levels

The unitary transformation is generated by the Hamiltonian

$$\boxed{i\frac{dU}{dt} = H\,U} \qquad \text{if} \quad \mathbf{H} = H_0 + \mu\,\varepsilon(t)$$

If we control the field ε can we control the algorithm?

Reading and writing into molecular levels



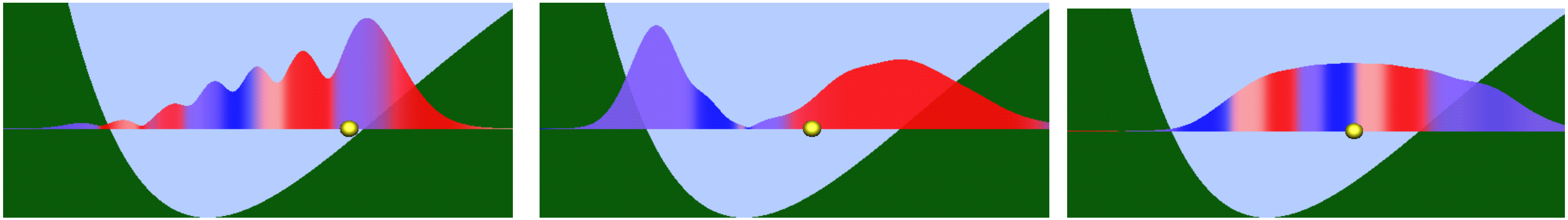
Writing into the relative phase of a wavepaket:

$$\Psi = \sum a_n e^{-i\phi_n} \psi_n$$

where: $H\psi_n = \varepsilon_n \psi_n$

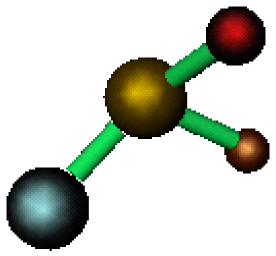
Ahn, Weinacht, Bucksbaum, Science *287* 463 (2000).

Starting from a preselected state, using pulse shaping techniques one can write into the amplitude and phase of atomic and molecular levels.



Three superpositions which differ only by the phases of the energy eigenvalues

Executing algorithms. We first consider a limited set of U's that are naturally mapped into the free evolution:



$$\text{if}: \boxed{i\frac{\partial\psi}{\partial t} = \mathbf{H}\psi} \qquad \psi(t) = \mathbf{U}_t\,\psi(0)$$

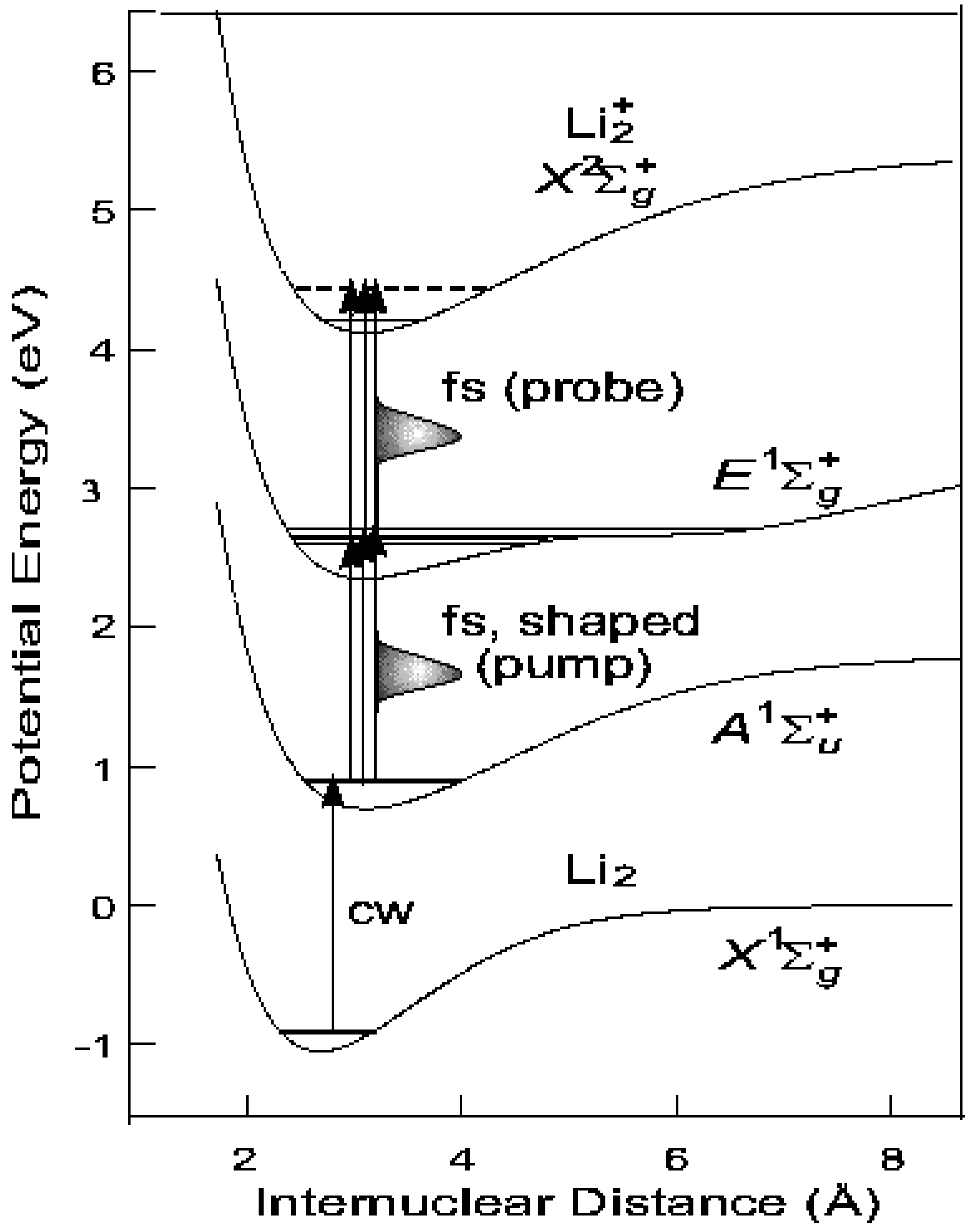
The unitary evolution operator becomes:

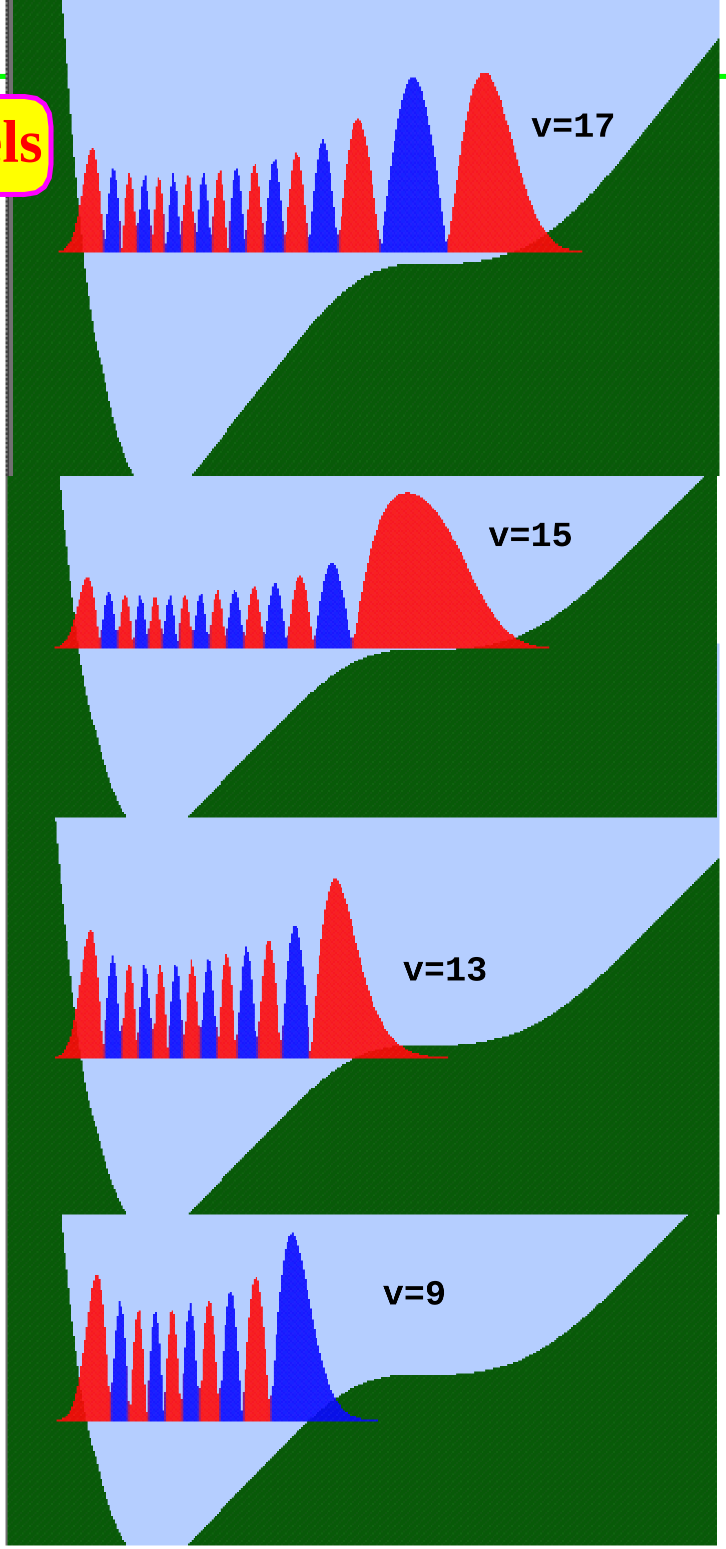
$$\boxed{\mathbf{U}_t = \mathbf{e}^{-i\mathbf{H}t}}$$

t can be used as a parameter

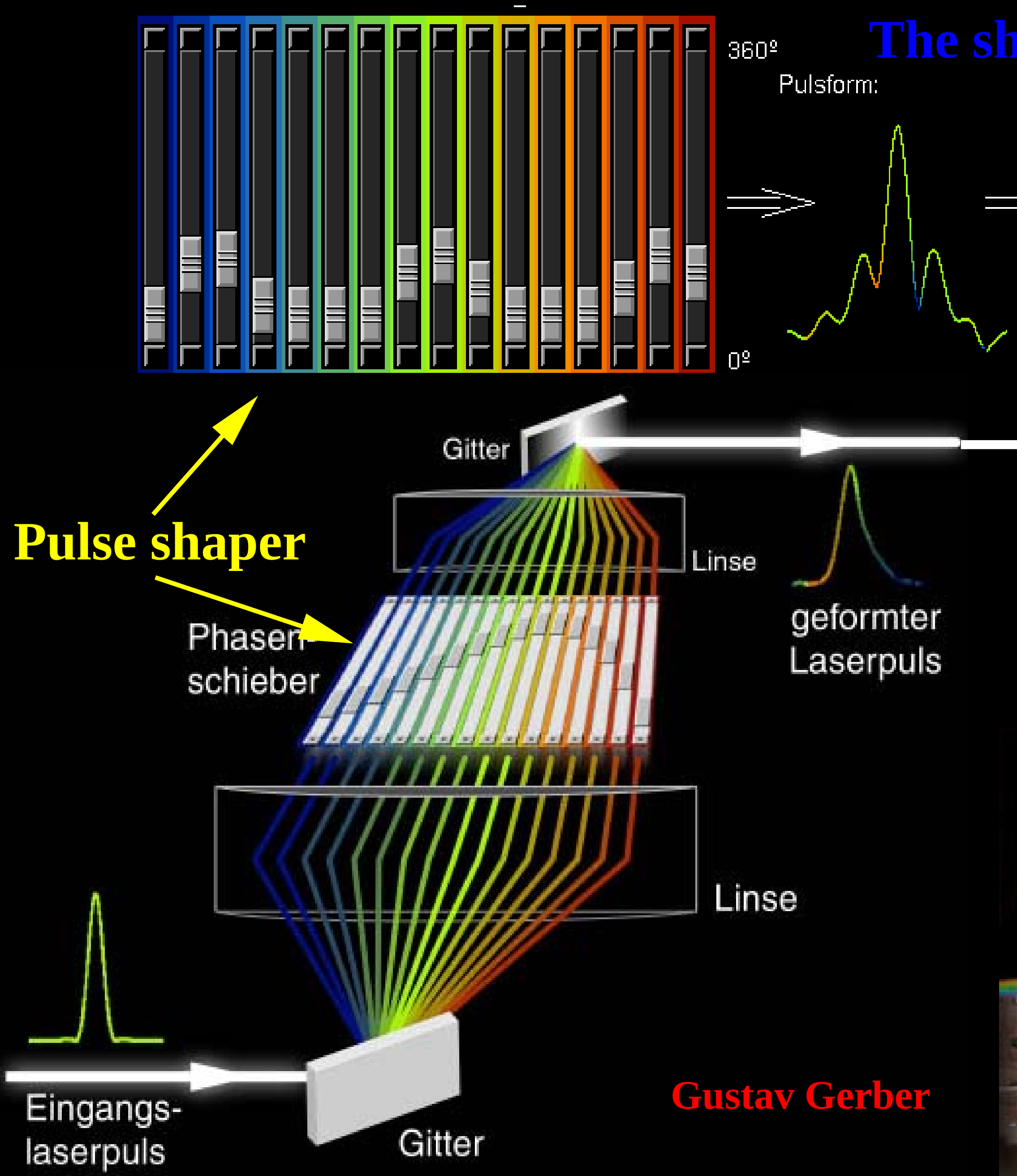
Example using the free rovibrational evolution on the E state of Li_2

The excitation scheme and a few vibrational levels





Input: writing into the molecular states.

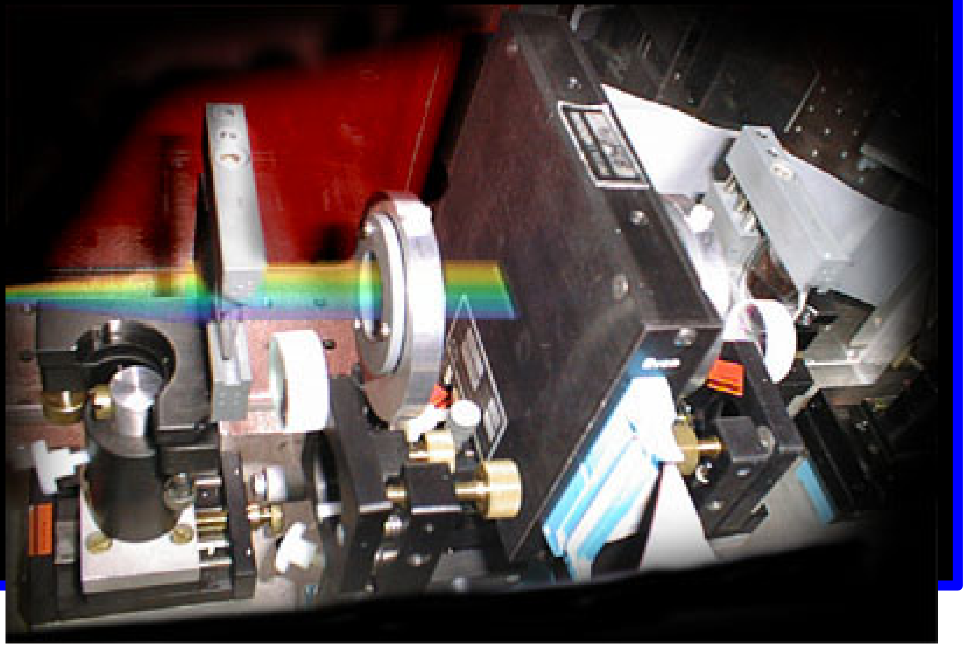


The shaped pulse in time

Pulse shaper

The molecules

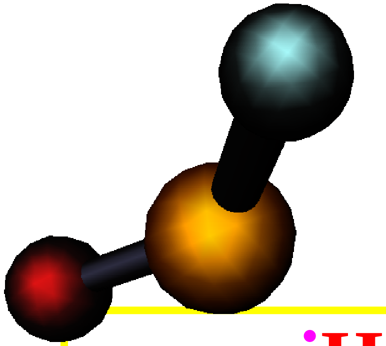
Spatial light Modulator



Gustav Gerber

http://www.physik.uni−wuerzburg.de/femto−welt/

Processing: executing an algorithm.



The algorithms in quantum computing are a full set
of unitary operations on the state space of the molecule

A unitary operator is already carried out by the free propagation: $U = e^{-iHt}$

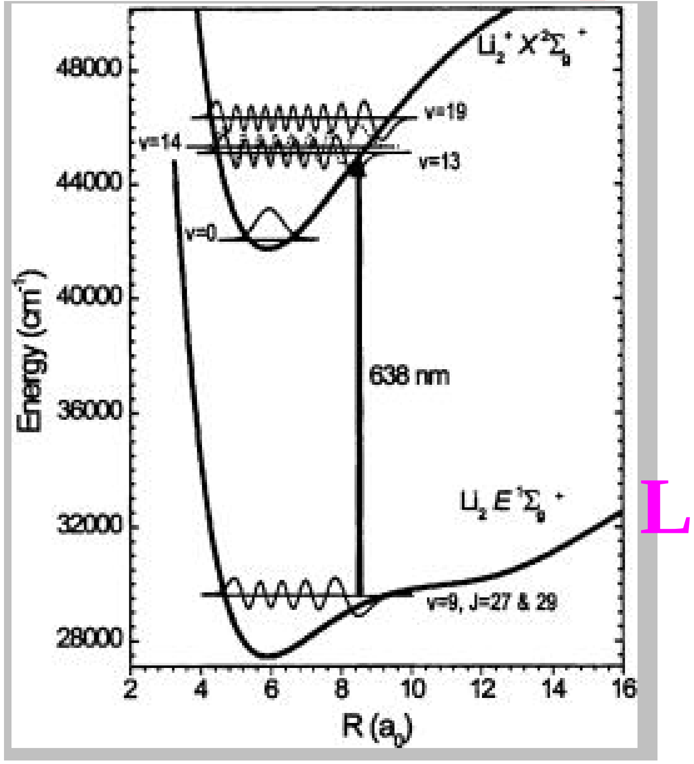
For the most simple cases the free propagation can execute the algorithm.

Implementation of the Deutsch−Jozsa Algorithm for Three−Qubit Functions

$$\hat{U} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & (-1)^{f(|0\rangle)} & 0 & 0 & \\ 0 & 0 & (-1)^{f(|1\rangle)} & 0 & \\ 0 & 0 & 0 & (-1)^{f(|2\rangle)} & \\ \vdots & & & & \ddots \end{pmatrix} \begin{pmatrix} 1 & -a_0 & -a_1 & -a_2 & \cdots \\ a_0 & 1 & 0 & 0 & \\ a_1 & 0 & 1 & 0 & \\ a_2 & 0 & 0 & 1 & \\ \vdots & & & & \ddots \end{pmatrix} .$$

Jiri Vala, Zohar Amitay, Bo Zhang, Stephen R. Leone, and Ronnie Kosloff PRA 66 062316 (2002)

Output: reading out the result.



The output of the computation is an ion signal at a preselected time delay of the probe pulse.

An ultrafast probe pulse is equivalent to a finite precisson position measurement

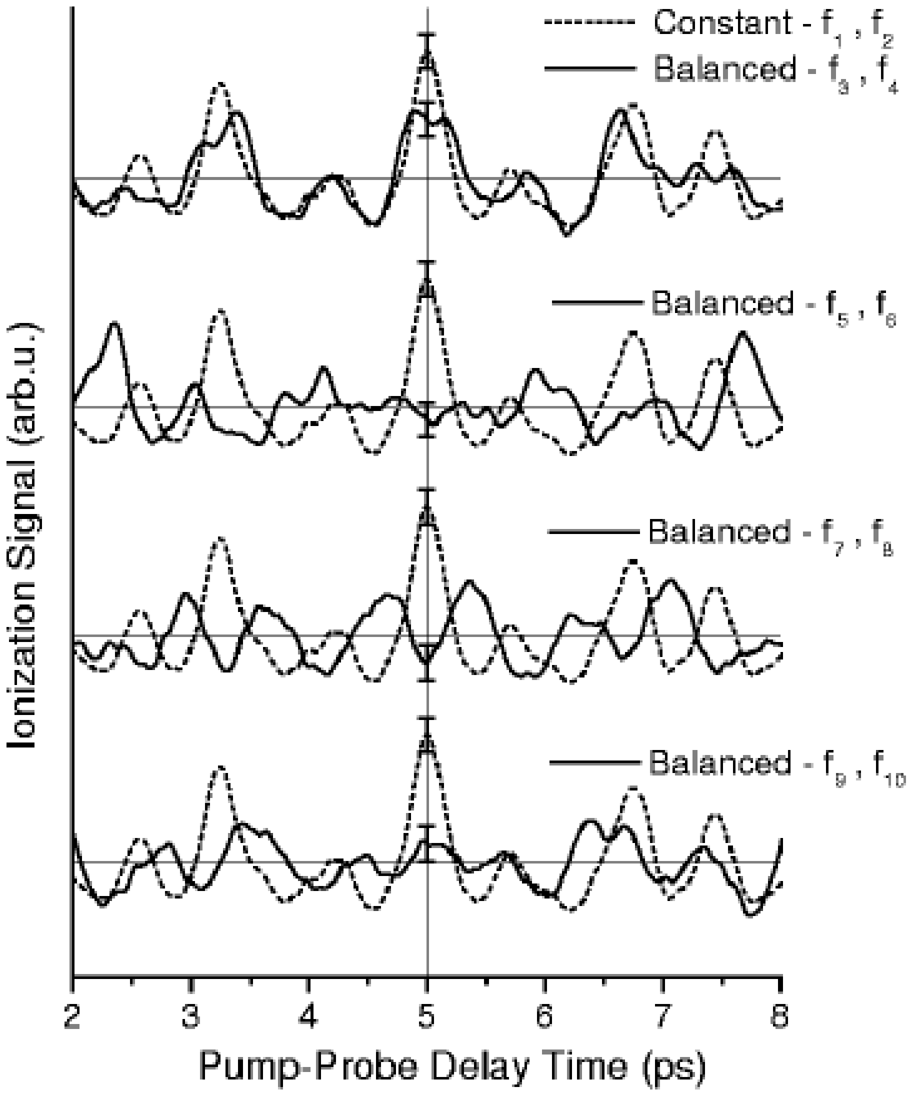
The ion signal is produced through a high lying Rydberg state (n~25).

Ultrafast spectroscopy of wavelength−dependent coherent photoionization cross sections of Li2 wave packets in the E1 state: The role of Rydberg states

Radoslaw Uberna, Zohar Amitay, Charles X. W. Qian, and Stephen R. Leone

The Journal of Chemical Physics, Vol. 114, No. 23, pp. 10311−10320, 15 June 2001

Implementation of the Deutsch−Jozsa Algorithm for Three−Qubit Functions on Li2



f1 ={0,0,0,0,0,0,0,0} constant

f2 ={1,1,1,1,1,1,1,1} constant

f3 ={1,0,0,1,1,0,1,0} balanced

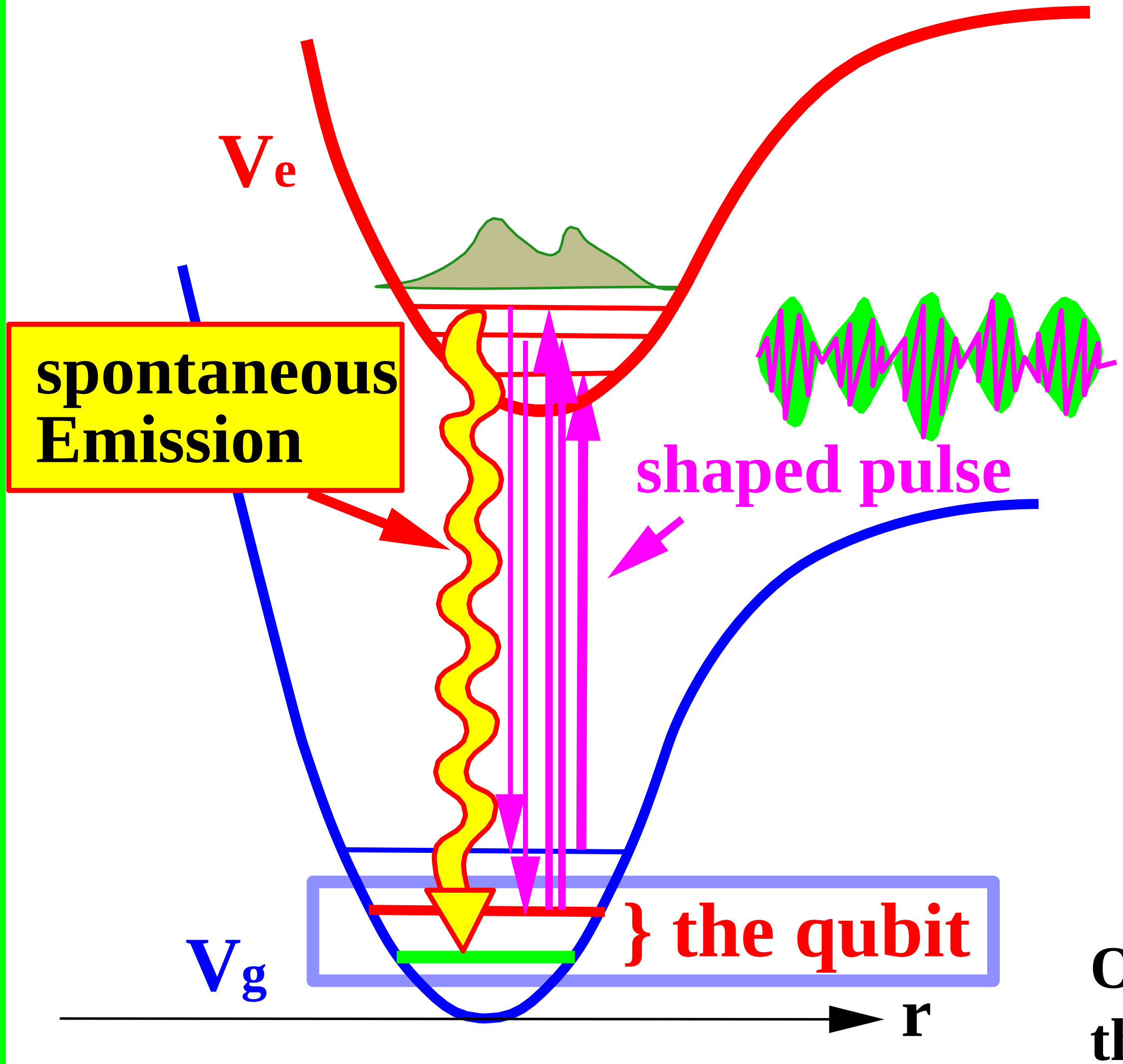
f4 ={1,1,0,0,1,0,1,0} balanced

•
•
•
•

Each function is mapped into a different Unitary transformation. One readout is sufficient to distinguish between the classes.

Jiri Vala, Zohar Amitay, Bo Zhang, Stephen R. Leone, and Ronnie Kosloff PRA 66 062316 (2002)

The real molecular computer problem: Can we carry out the algorithm in a congested molecular environment?



The basic molecular model

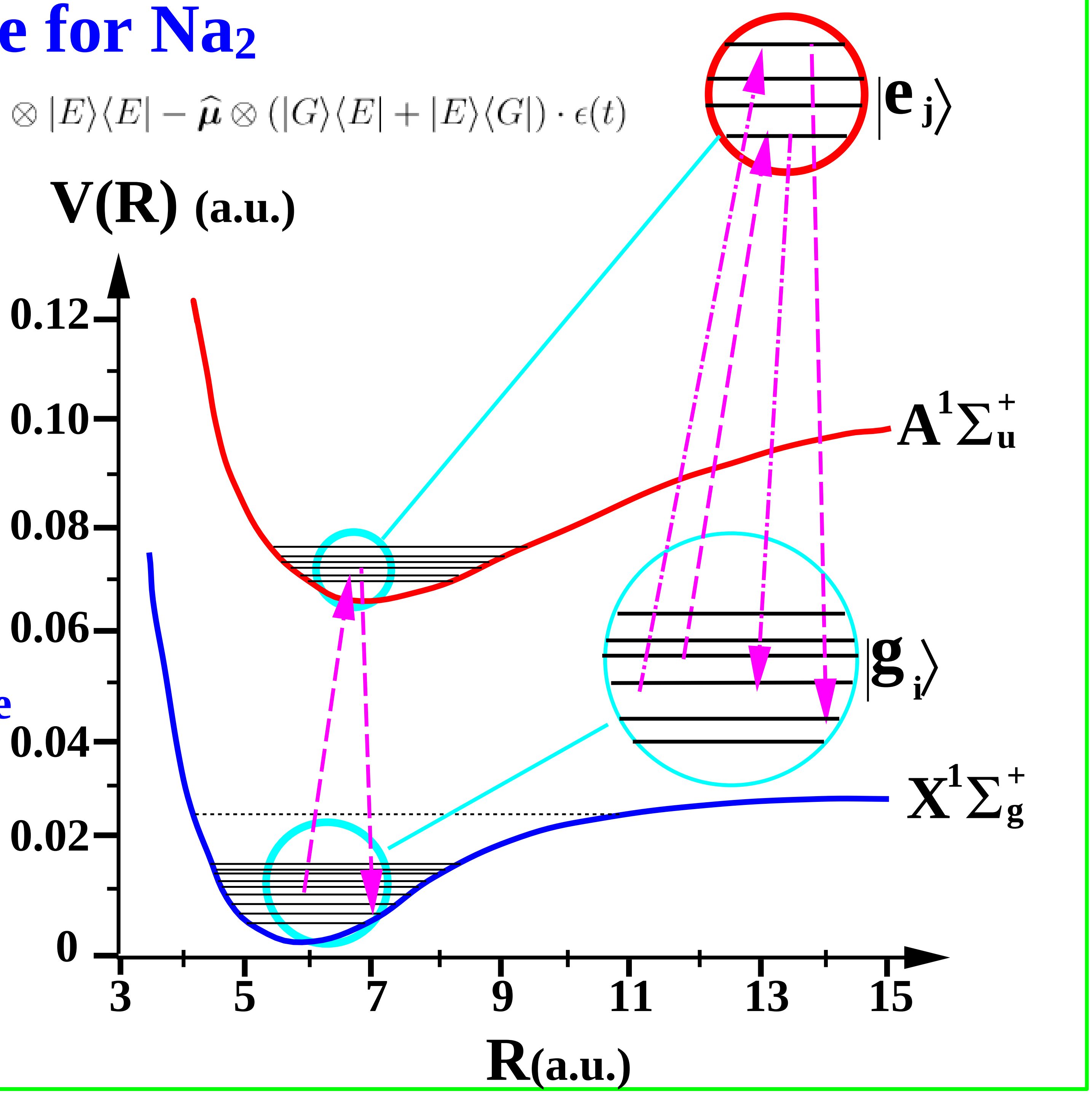
$$\mathbf{H} = \mathbf{H_g} \otimes |\mathbf{g}\rangle\langle\mathbf{g}| + \mathbf{H_e} \otimes |e\rangle\langle e| + \mu\varepsilon(\mathbf{t}) \otimes |\mathbf{e}\rangle\langle\mathbf{g}| + \mu\varepsilon^*(\mathbf{t}) \otimes |\mathbf{g}\rangle\langle\mathbf{e}|$$

$$\mathbf{H} = \begin{pmatrix} \mathbf{He} & \mu\varepsilon(\mathbf{t}) \\ \mu\varepsilon^*(\mathbf{t}) & \mathbf{Hg} \end{pmatrix}$$

Only a small fraction of the levels are used as registeres

Control scheme for Na_2

$$\widehat{\mathrm{H}} = \widehat{\mathrm{H}}_g \otimes |G\rangle\langle G| \; + \; \widehat{\mathrm{H}}_e \otimes |E\rangle\langle E| - \widehat{\boldsymbol{\mu}} \otimes (|G\rangle\langle E| + |E\rangle\langle G|) \cdot \epsilon(t)$$



The $X^1\Sigma_g^+$ ground state vibrational levels are used for registers

The excited $A^1\Sigma_u^+$ levels are used for auxiliary storage

Principles of coherent control

$i \rightarrow f$

I

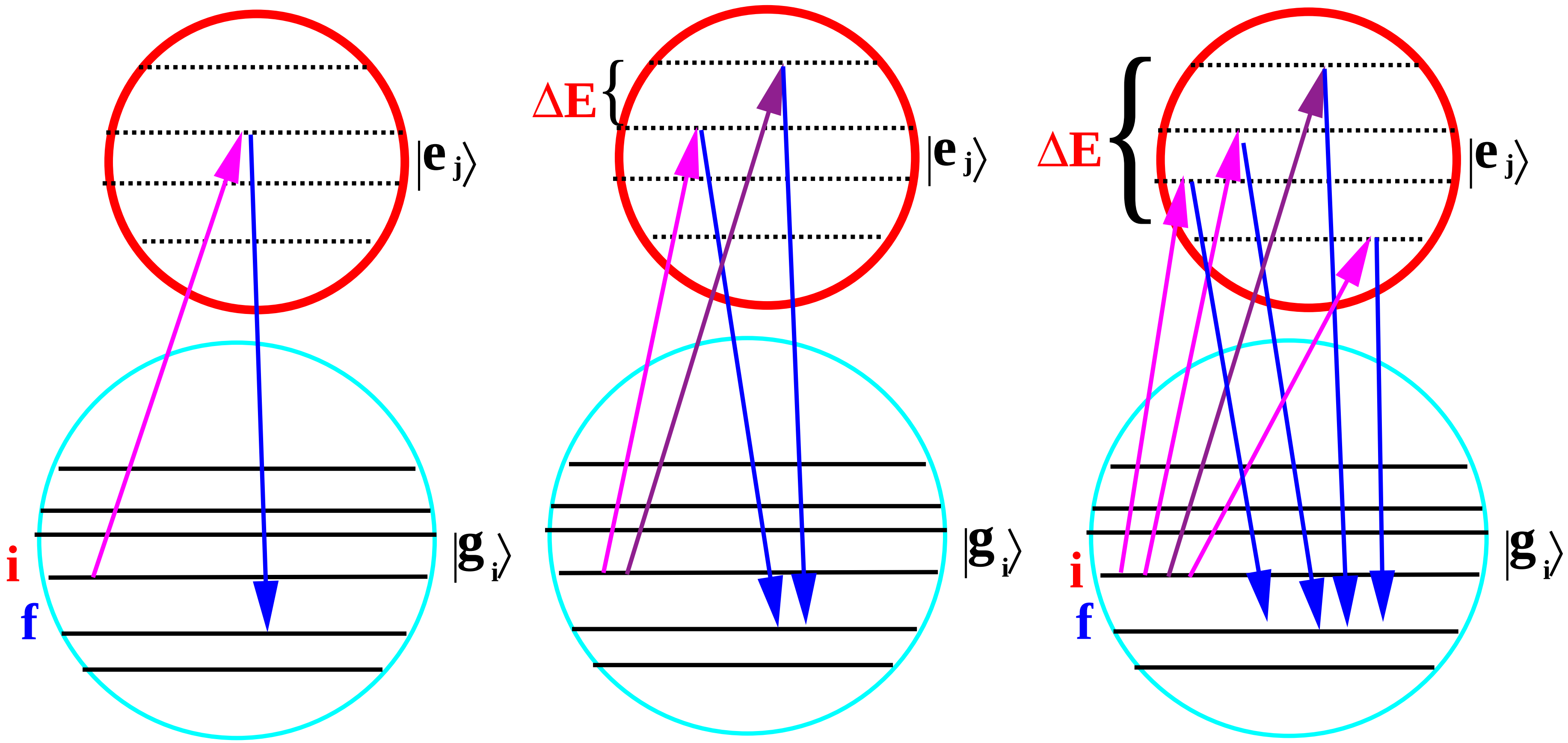
State−to−State Weak field

II

State−to−State Weak field
Coherent Control

III

State−to−State Weak field
More Coherent Control

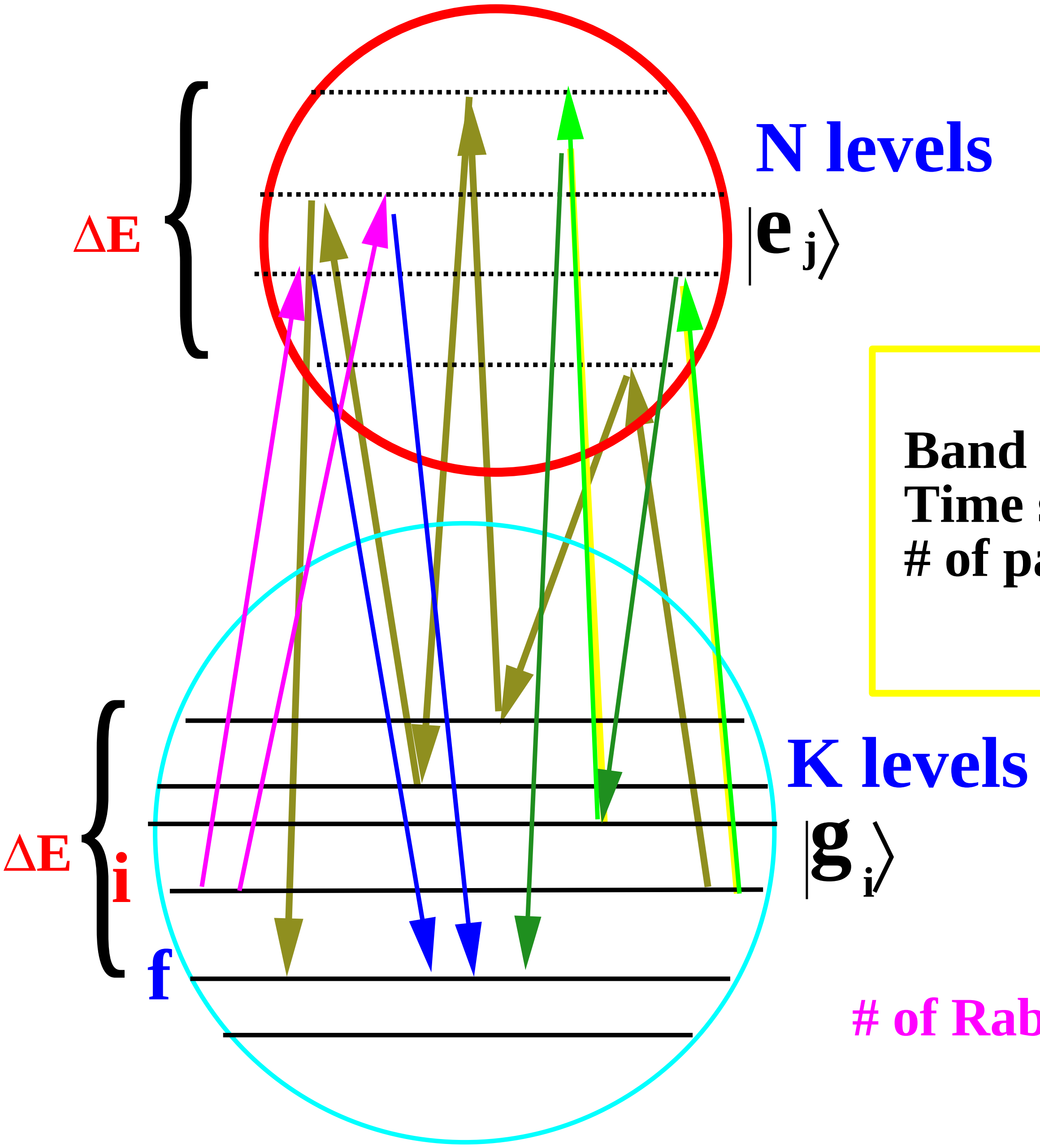


		I	II	III
Band width	ΔE	very small	vibratioanl spacing	N vibratioanl spacings
Time scale	Δt	adiabatic	vibrational period	vibrational period
# of paths		1	2	N

State−to−State strong field
More Coherent Control

$i \rightarrow f$

IV



resources

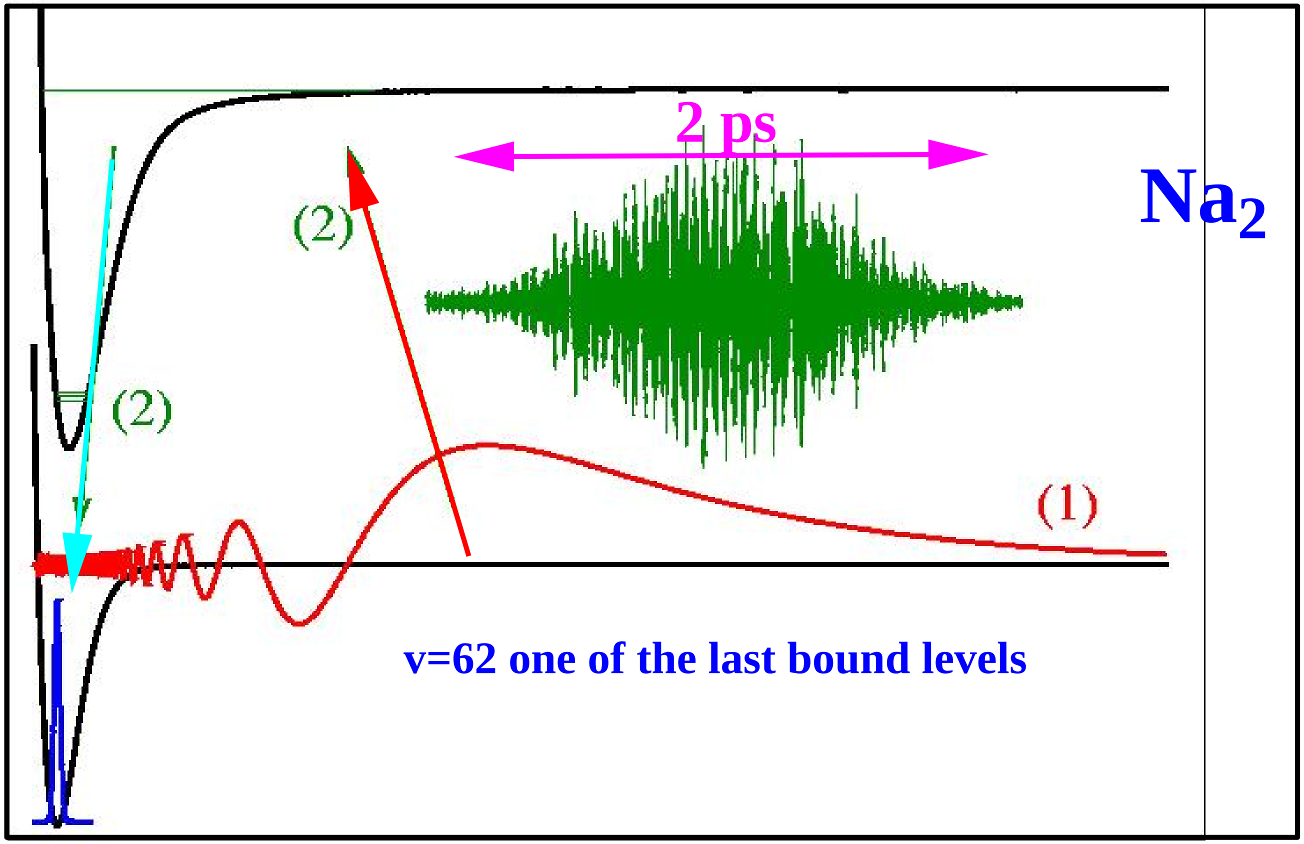
Band width	ΔE	N vibratioanl spacings
Time scale	Δt	t << vibrational period
# of paths		N K exponential with intensity

# of Rabi periods is linear with intensity

Example: State−to−State strong field $i \rightarrow f$

Making stable molecules from the last bound level

Transforming V=62 to v=0 in a period of 2 ps



v=0

period 210 fs

v=62

period 8 ps

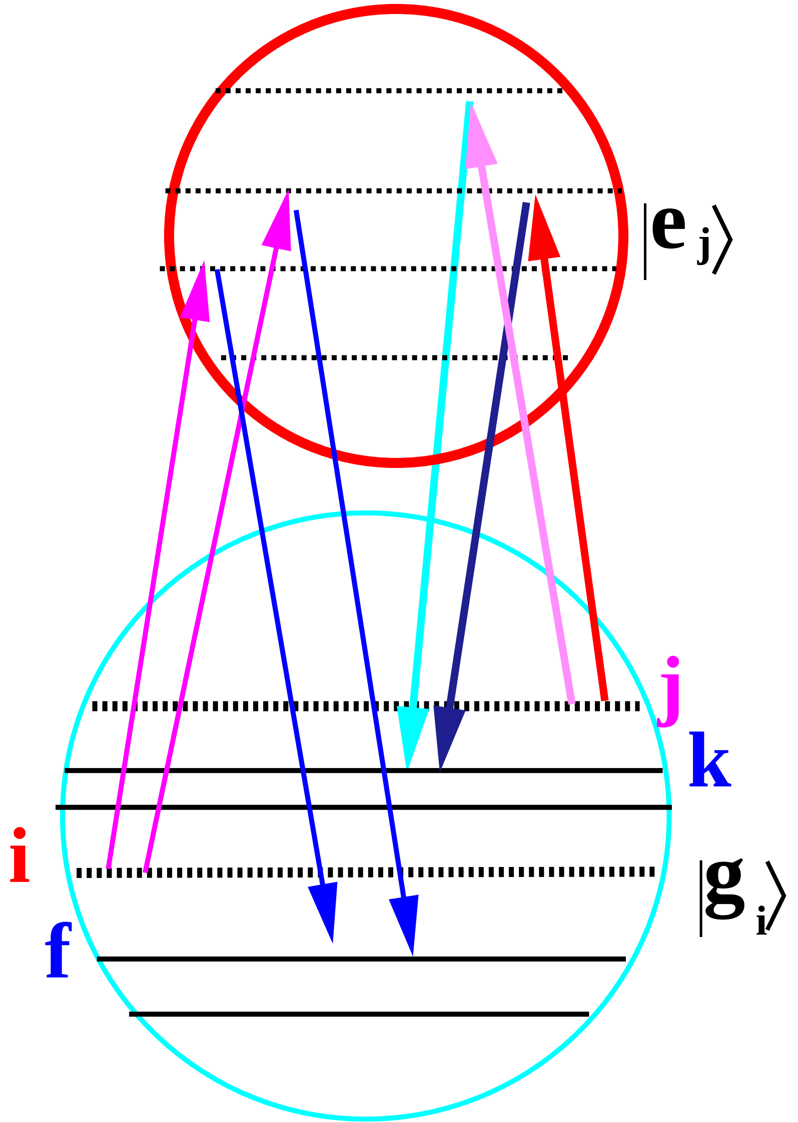
v=65

period 60 ps

Christiane P. Koch, José P. Palao, Ronnie Kosloff and Francoise Masnou−Seeuws
Stabilization of Ultracold Molecules Using Optimal Control Theory Phys. Rev. A, 70 013402 (2004).

Quantum computing

Multiple State−to−State Coherent Control



$i \rightarrow f$ simultaneous with $j \rightarrow k$

The quantum Compiler

Inversion Problem:

find the field that executes the task

$$H(t) = H_0 + \mu\varepsilon(t)$$

resources

For the execution:

Band width ΔE
Time scale Δt
Pulse energy

For the compiler:

How much computation resources are required to compile an m qubit general task.

The Quantum compiler

How can a molecule execute a general algorithm?

We need to control the Unitary evolution.

Input is $\Psi(0)$ output is $\Psi(t_f) = U(t_f)\Psi(0)$

Solution: molecular evolution subject to a control field

$$\boxed{H(t) = H_0+\mu\varepsilon(t) \qquad \frac{\partial U(t)}{\partial t} = -iH(t)U(t)\,, \qquad U(0)=I}$$

Given $O(t_f)$ we need to find the field $\varepsilon(t)$ for $0 < t < t_f$

A field needs to perform $i \rightarrow f$ transformation simultaneous with all other $j \rightarrow k$

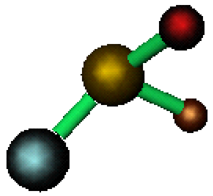
A problem of inversion solved by optimal control theory

$$\boxed{\text{Optimize } \tau = |\mathrm{Tr}\{O^{+}U(t_f)\}|}$$

The scalar product between the objective O and the evolution operator $U(t_f)$

José P. Palao and Ronnie Kosloff Optimal control theory for unitary transformations Phys. Rev. A, 68 062308 (2003).

The quantum Compiler



Global objective

O is the objective and **U** is the actual evolution operator

$$\tau = t_r\{O^{\dagger} \cdot U\} = \sum_{k=1}^{N} \langle \phi_k | O^{\dagger} U(\varepsilon, T) | \phi_k \rangle$$

τ defines how close to our goal we are. we can either use Real (τ) or $|\tau|^2$.

Simultaneous state to state objectives

$$\eta = \sum_{l=1}^{N} |\langle \phi_l | O^{\dagger} U(\varepsilon) | \phi_l \rangle|^2$$

Using Krotov's method the correction to the field becomes:

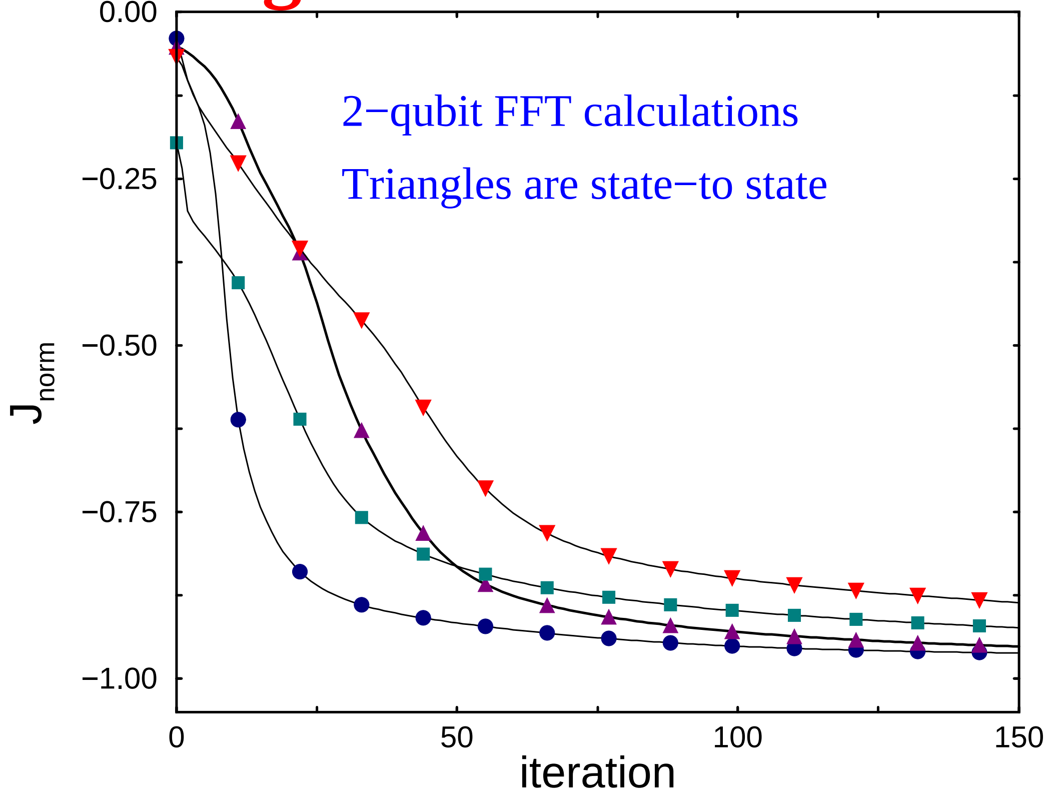
$$\Delta\varepsilon(t) = \frac{s(t)}{\lambda h} \sum_{k=1}^{N} a_k \langle \phi_k | O^{\dagger} U^{\dagger}(\varepsilon, t, T) \mu U(\varepsilon, 0, T) | \phi_k \rangle$$

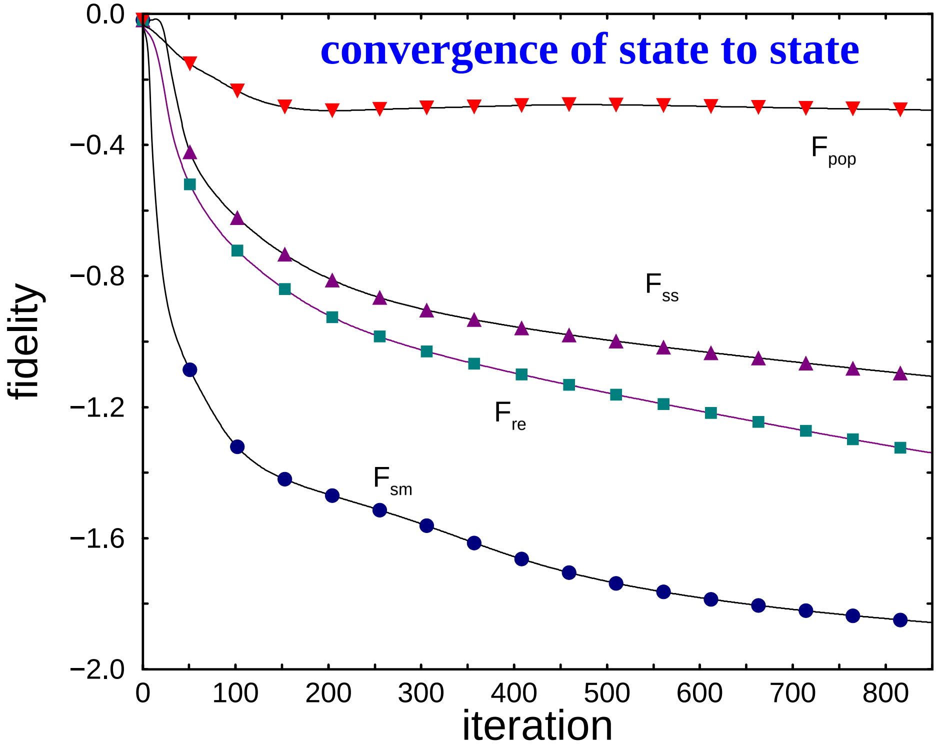
propagation
from final time

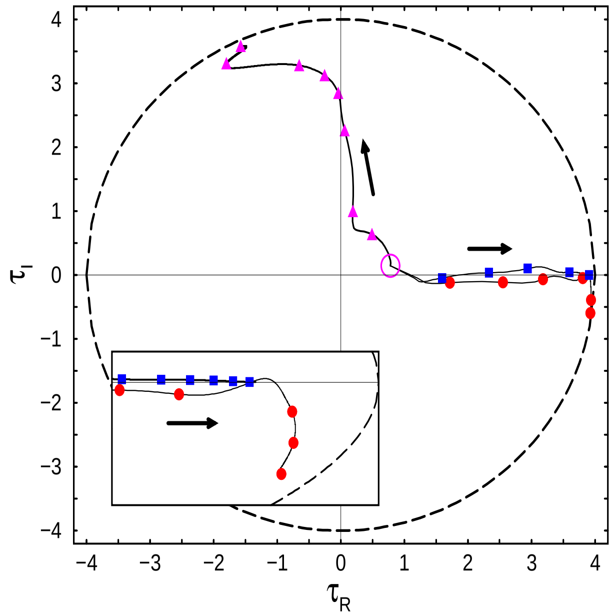
propagation
from initial time

where a_k is different for different objectives.

Convergence of the methods





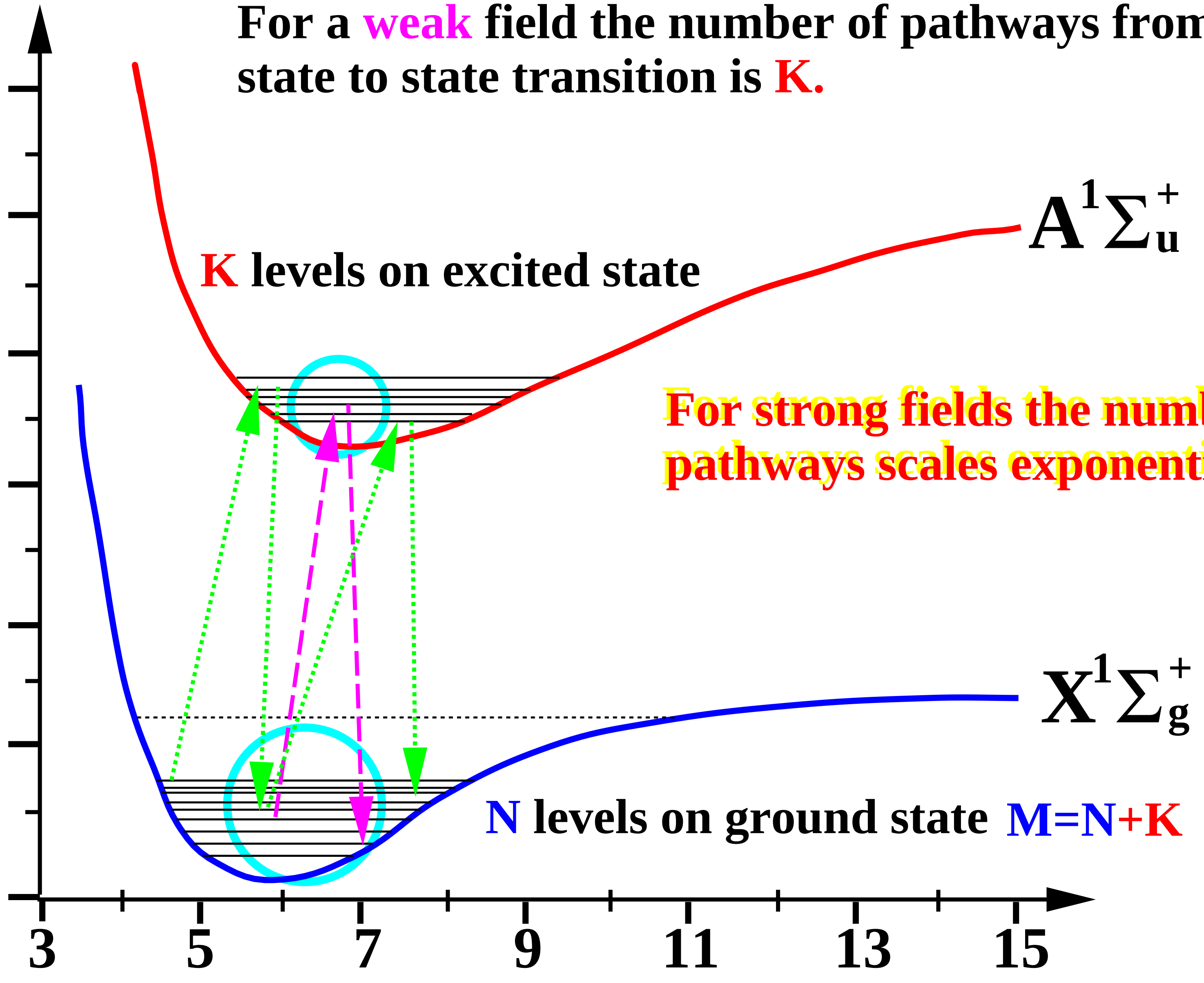


$$\text{Fidelity} = \log_{10}(1-|\tau|^2/N^2)$$

$$\tau = \mathrm{tr}\{O^\dagger \bullet U\} = \sum_{k=1}^{N} \langle \phi_k | O^\dagger U(\varepsilon, T) | \phi_k \rangle$$

Scaling of resources: control resources=interference pathways

For a weak field the number of pathways from a particular state to state transition is K.



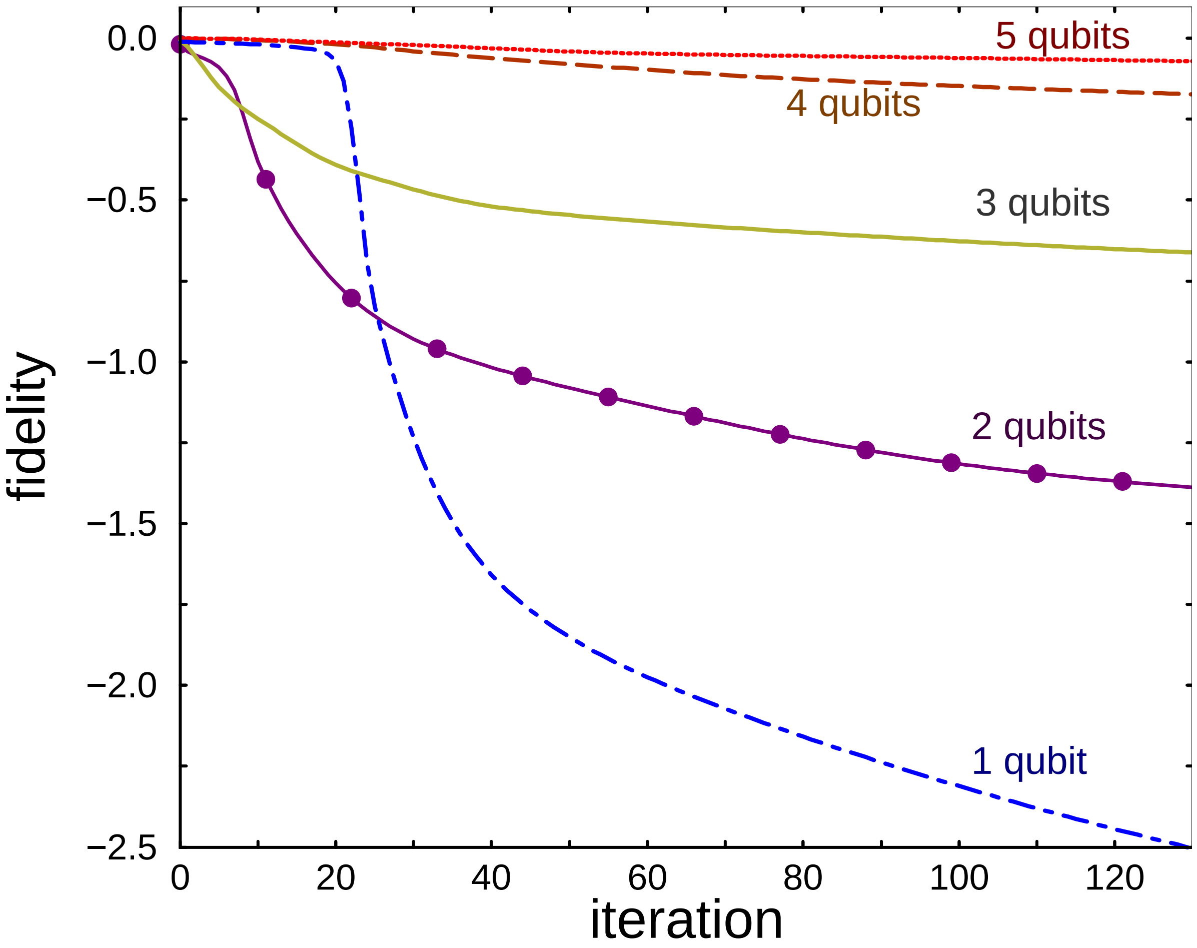
For strong fields the number of interference pathways scales exponentially with intensity

$O(M^{I})$

A moderate increase in intensity with the number of q bits

Scaling of Convergence: finding the field

Simulating a quantum system with a classical computer:



$$\text{Cost} \approx O(2^{Q} M^{2} T \Delta E)$$

Q the number of qubits
M the size of Hilbert space
T simulation time
ΔE energy range

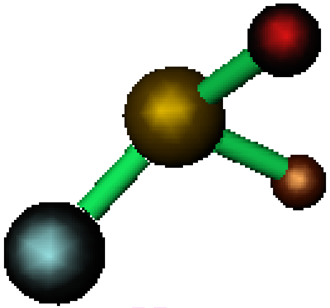
Scaling of the number of iterations required to reach a specific fidelity

$$N_{it} \approx b e^{2^{Q} |\text{fidelity}|/a}$$

The convergence of fidelity vs the number of iterations.

José P. Palao and Ronnie Kosloff, *Optimal control theory for unitary transformations* Phys. Rev. A, 68 062308 (2003).

The quantum Compiler



Scaling of resources

The number of interference pathways scales exponentially with the power of the field the band width ΔE and time scale Δt.

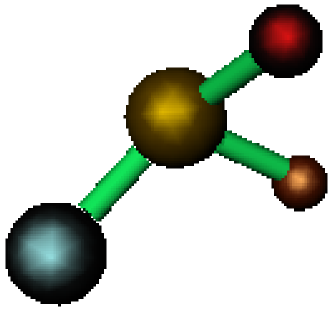
Scaling of convergence.

The convergence of OCT for finding an optimal field for **U** is determined by N simultaneous state to state optimizations. It seems to scale as N! .

Scaling of the computation effort

Simulating a quantum system by a classical computer which is needed for a numerical solution to OCT is exponentially bad.

The inversion: obtaining ε that executes **U** is hard !



Can we teach a molecule (or any other quantum system) to compute?

work of:
J.P. Palao
Z. Amitay

1) Factorizing the computation task.

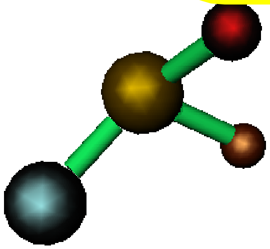
If $\mathbf{U}$ represents the unitary transformation

we want $\mathbf{U} = \prod_i \mathrm{U_i}$ where $\mathrm{U_i}$ is an elementary step.

2) We will build a vocabulary of such $\mathrm{O}=\mathrm{U_i}$, and find the driving field that executes this step.

3) In finding the field that executes O we will rely on state to state optimization.

What is the minimum number of state to state transformations we need to control in order to determine completely the unitary transformation O ?



$$\mathbf{O} = \begin{pmatrix} e^{i\alpha_1} & 0 & \dots & 0 \\ 0 & e^{i\alpha_2} & \dots & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & e^{i\alpha_N} \end{pmatrix}$$

If we diagonalize O we get:

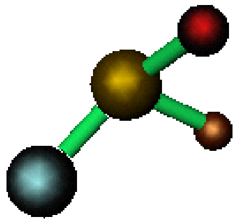
where: $\mathbf{O}\,|\phi_k\rangle = e^{i\phi} e^{i\alpha_k} |\phi_k\rangle$

Now we use the basis $|\phi_k\rangle$ to define **N** simultaneous state to state transformations. Optimizing the final population on each state $|\langle\phi_k|\phi_k\rangle|^2$ when starting from the initial state $|\phi_k\rangle$. This procedure will define the unitary transformation up to the relative phases $e^{i\alpha_k}$.

But the optimization of the last state $|\phi_N\rangle$ can be omitted!

We then omit the last state and replace it with $|\Psi\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} |\phi_j\rangle$

Then: $|\Psi_i\rangle \Rightarrow |\Psi_f\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \mathbf{e}^{\mathbf{i}\alpha_J} |\phi_j\rangle$



The optimization criteria becomes:

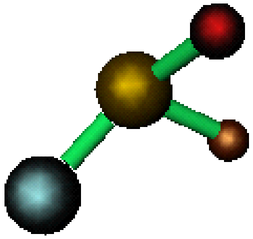
$$\sum_{k=1}^{N-1} |\langle\phi_k|\mathbf{O}^{\dagger}\mathbf{U}(\varepsilon)|\phi_k\rangle|^2 + |\langle\Psi|\mathbf{O}^{\dagger}\mathbf{U}(\varepsilon)|\Psi\rangle|^2$$

final state

Where: $\mathbf{U}(\varepsilon)$ is the actual evolution operator which is a function of the external field ε

Conclusion: optimizing N states simultaneously with respect to the field ε is sufficient to dermine O (up to a phase)

Examples:



$$\mathbf{O} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|\,\mathbf{0}\,\rangle \rightarrow |\,\mathbf{0}\,\rangle$$
$$|\,\mathbf{1}\,\rangle \rightarrow -|\,\mathbf{1}\,\rangle$$

Optimizing $|\langle 0|\mathbf{O}^{\dagger}\mathbf{U}(\varepsilon)|0\rangle|^2 + |\langle 1|\mathbf{O}^{\dagger}\mathbf{U}(\varepsilon)|1\rangle|^2$

will lead to:

$$|\,\mathbf{0}\,\rangle \rightarrow e^{i\beta_0}\,|\,\mathbf{0}\,\rangle$$
$$|\,\mathbf{1}\,\rangle \rightarrow e^{i\beta_1}\,|\,\mathbf{1}\,\rangle$$

but β_1 and β_2 are arbitrary

Chosing the states: $|\,\mathbf{0}\,\rangle \rightarrow |\,\mathbf{0}\,\rangle$

$$|\Psi\rangle = \mathbf{1}/\sqrt{2}(|\,\mathbf{0}\,\rangle + |\,\mathbf{1}\,\rangle)$$

$$\mathbf{1}/\sqrt{2}(|\,\mathbf{0}\,\rangle + |\,\mathbf{1}\,\rangle) \rightarrow \mathbf{1}/\sqrt{2}(|\,\mathbf{0}\,\rangle - |\,\mathbf{1}\,\rangle)$$

Optimizing $|\langle 0|\mathbf{O}^{\dagger}\mathbf{U}(\varepsilon)|0\rangle|^2 + |\langle \Psi|\mathbf{O}^{\dagger}\mathbf{U}(\varepsilon)|\Psi\rangle|^2$

will lead to:

$$|\,\mathbf{0}\,\rangle \rightarrow e^{i\phi}\,|\,\mathbf{0}\,\rangle$$
$$|\,\mathbf{1}\,\rangle \rightarrow -e^{i\phi}\,|\,\mathbf{1}\,\rangle$$

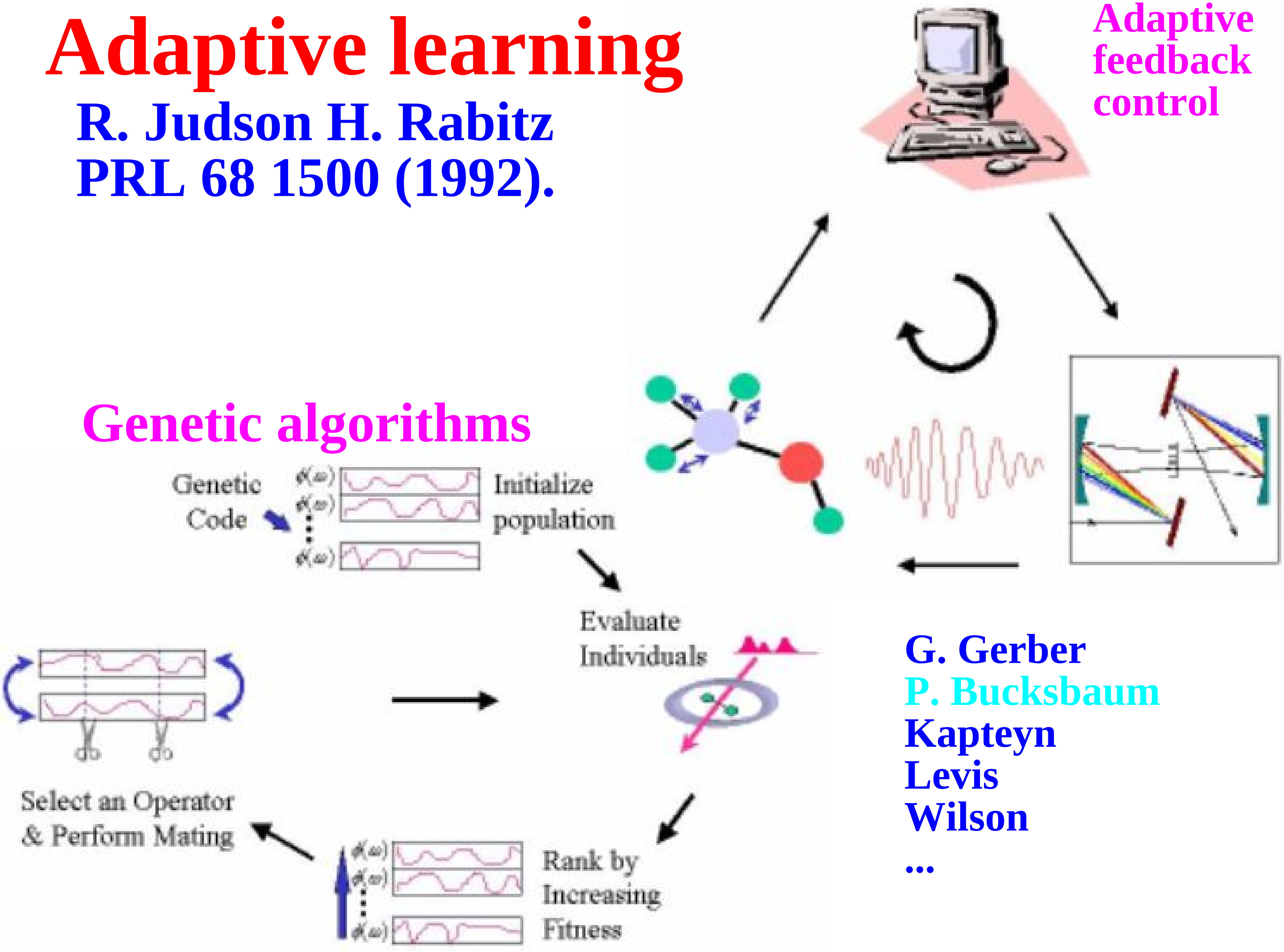
and ϕ is a global phase

Adaptive learning

R. Judson H. Rabitz
PRL 68 1500 (1992).

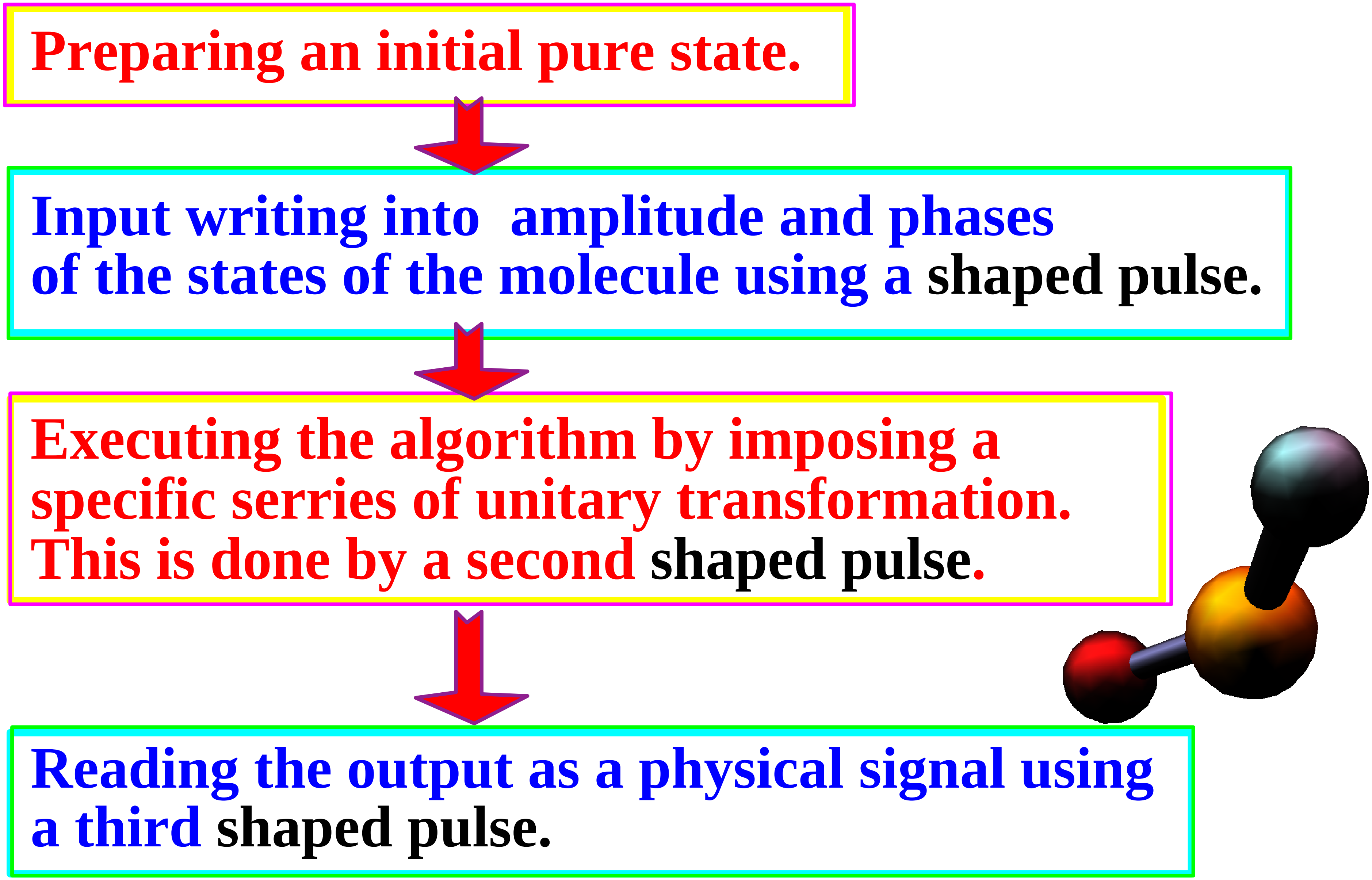
Adaptive
feedback
control

Genetic algorithms



G. Gerber
P. Bucksbaum
Kapteyn
Levis
Wilson
...

Flowchart of a molecular computer



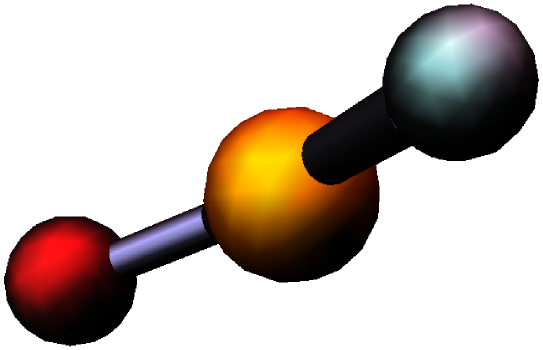
Preparing an initial pure state.

Input writing into amplitude and phases of the states of the molecule using a shaped pulse.

Executing the algorithm by imposing a specific serries of unitary transformation. This is done by a second shaped pulse.

Reading the output as a physical signal using a third shaped pulse.

Conclusions



A molecule can serve as a quantum computer.
The molecular states are addressed by light using 3 pulse shapers. Execution times are ~ 1 psec
Decoherence time scale in the gas phase is > 10 nsec

The quantum Compiler

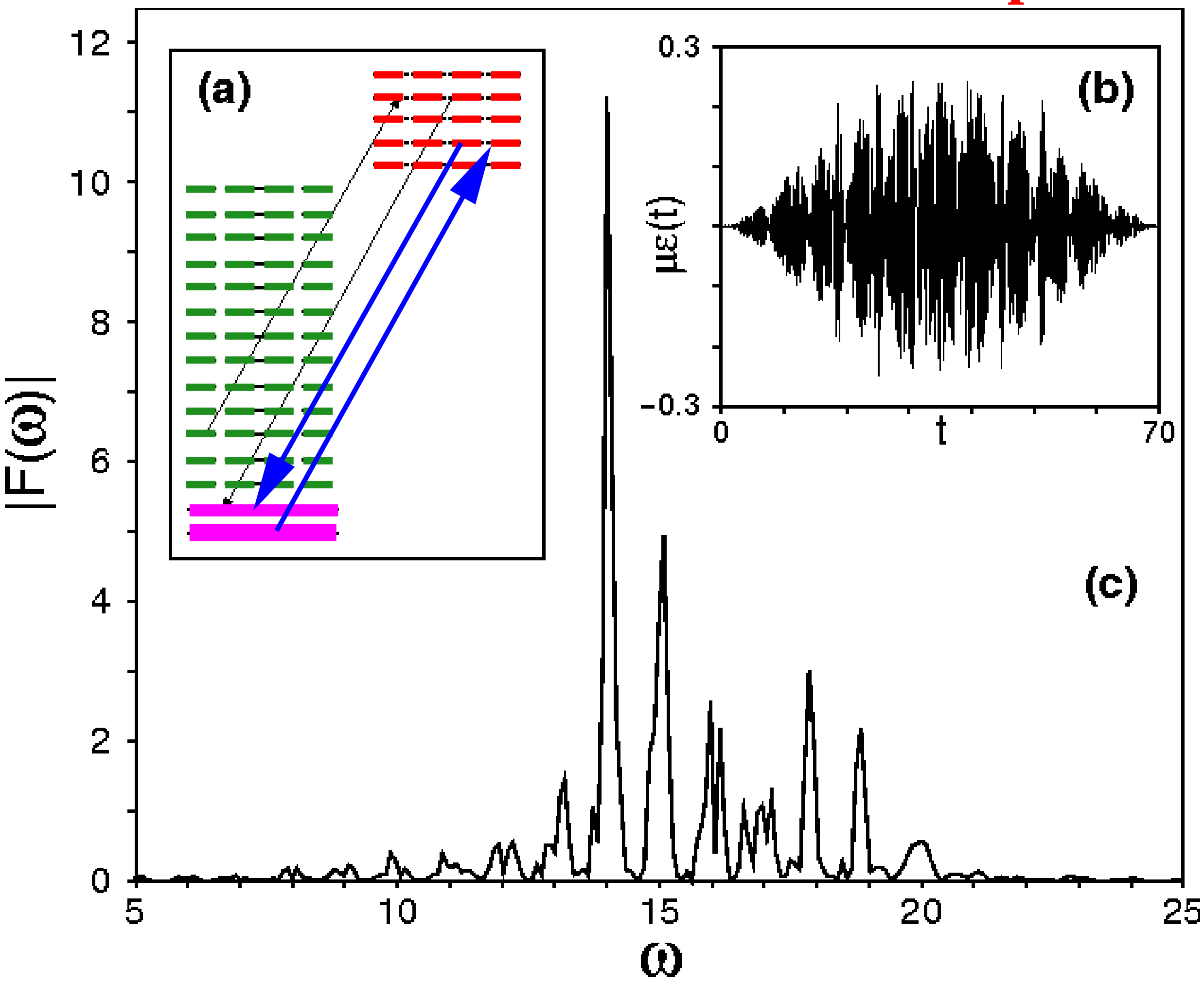
With strong fields the scaling of resources is moderate
Replacing one hard problem, executed by U with another one, inversion to ε

Quantum computer for the Quantum compiler

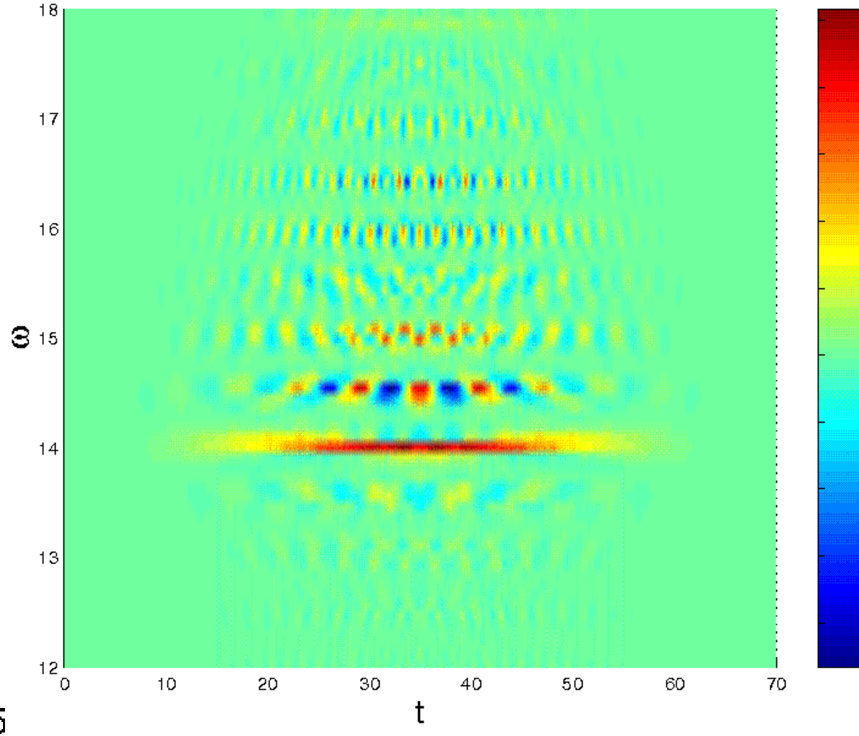
Example: executing the Hadamard rotation: $\mathbf{U} = 1/\sqrt{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

Energy level diagram

Optimal field spectrum



Wigner time frequency plot

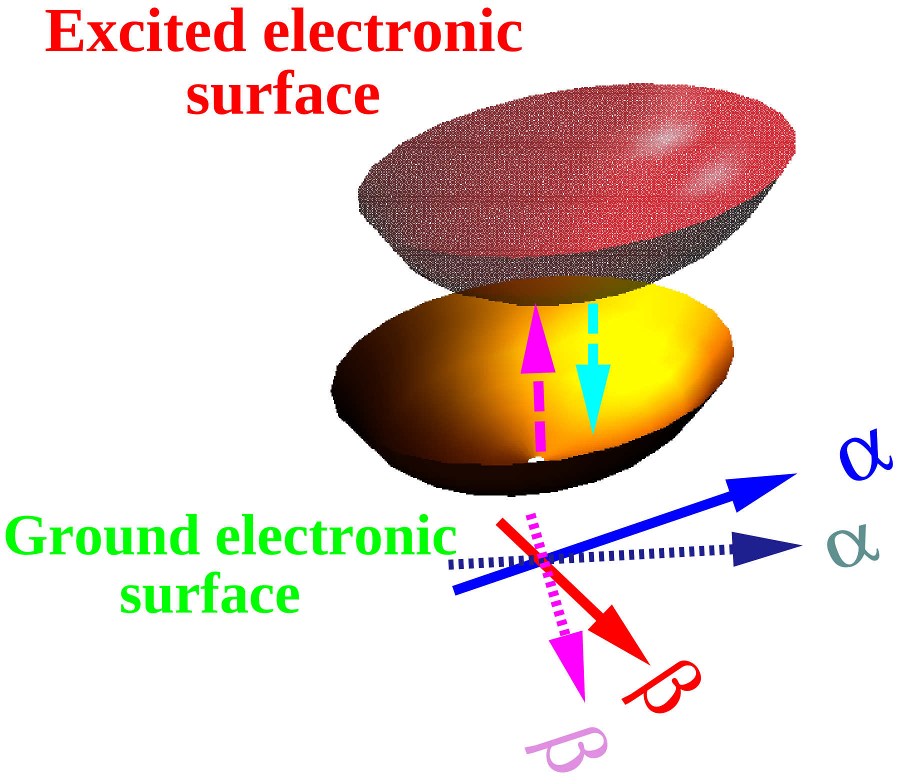


The Fourier transform:

$$U_{FT} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}$$

$$H = \begin{pmatrix} H_e & -\mu\varepsilon \\ -\mu\varepsilon^* & H_g \end{pmatrix}$$

μ the transition dipole ε the field



$$Hg = \omega_\alpha a^+a + \omega_\beta b^+b$$

$$He = \omega_\alpha a^+a + \omega_\beta b^+b + \delta_{\alpha\beta}(a^+b + b^+a)$$

Entanglement!

Duschinsky rotation of normal modes

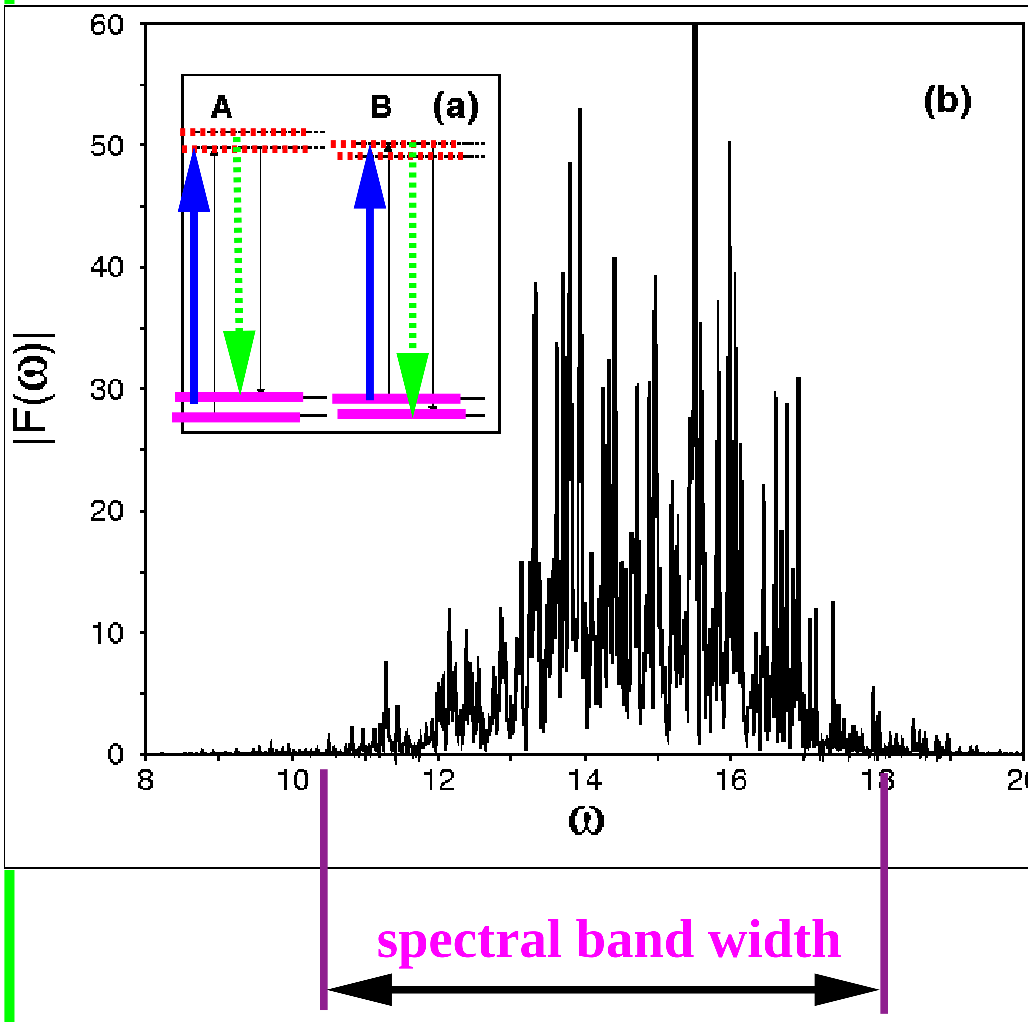
José P. Palao and Ronnie Kosloff

Quantum Computing by an Optimal Control Algorithm for Unitary Transformations

Phys. Rev. Lett. 89, 188501 (2002).

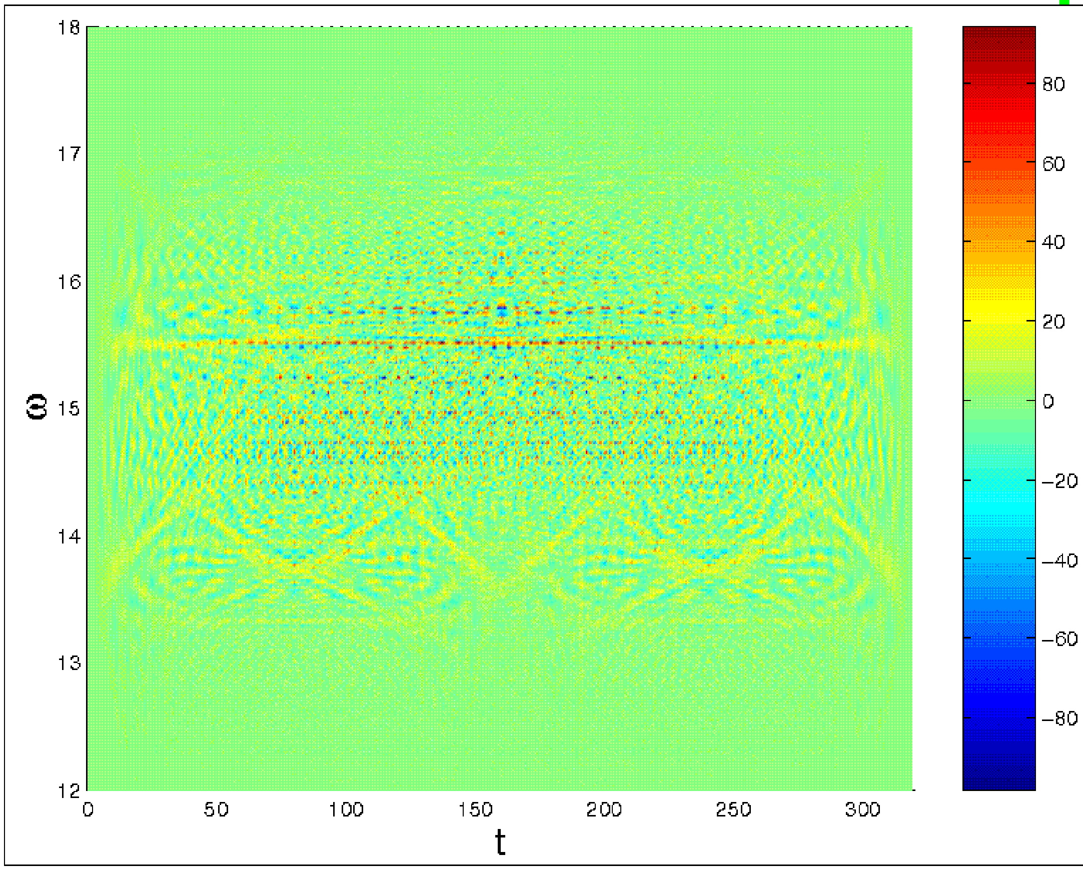
The Fourier transform:

The optimal field $\mathcal{E}(t)$



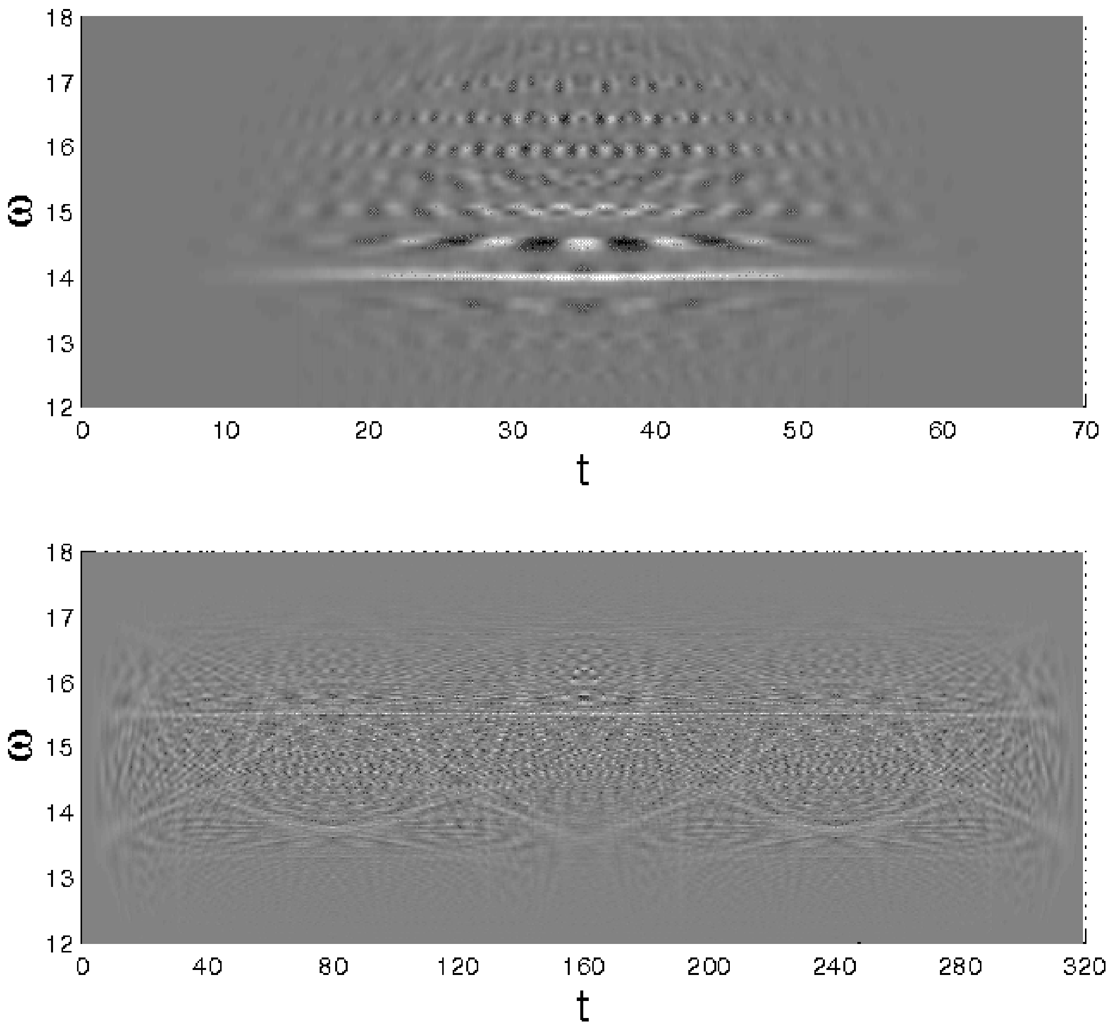
spectral band width

Wigner time−energy spectrum

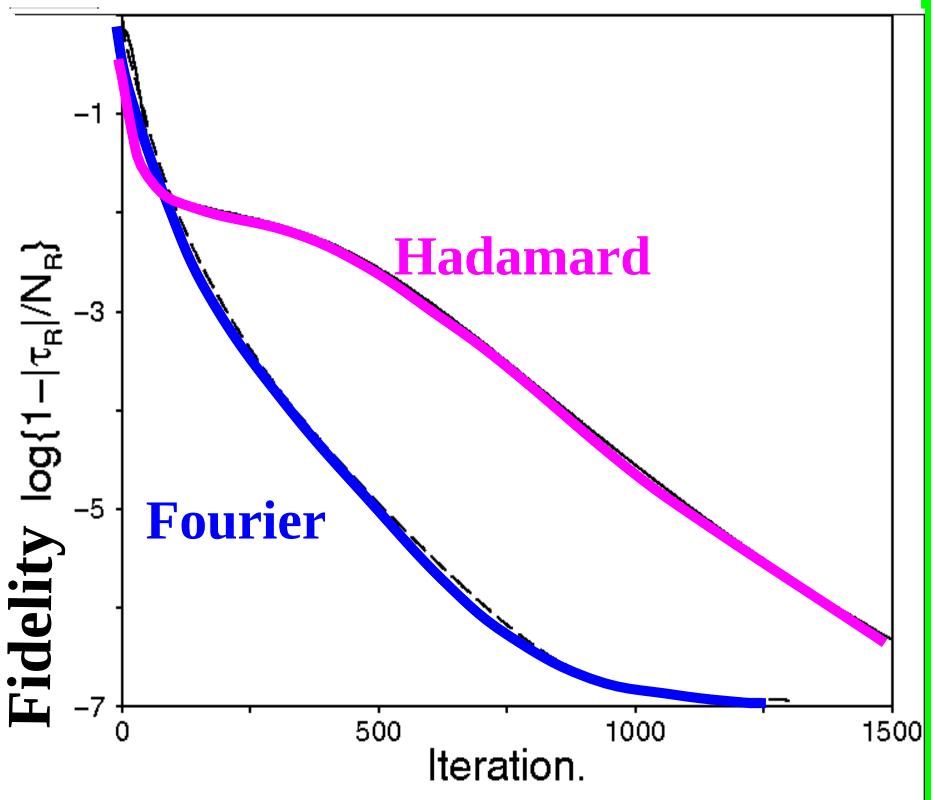


Comparison between the two algorithms:

Time−energy Wigner plots of the field $\mathcal{E}$



Convergence rate



Optimal Control theory

Objective: $$\boxed{J = \mathrm{tr}\{O^{+}U(t_f)\}}$$

O trarget observable
ε control field

$\langle O \rangle$ is optimized with minimum energy investment:

$$\boxed{\int |\varepsilon|^{2} dt} \qquad \boxed{H = H_0 + \mu\varepsilon(t)}$$

Constraints: $$\boxed{\frac{dU}{dt} = -iHU \qquad U(t_i)=I}$$

Modified objective:

$$J' = \mathrm{tr}\{O^{+}U(t_f)\} - \int_{0}^{t_f} (\mathrm{tr}\{(\frac{dU}{dt}+HU)B\} - \lambda|\varepsilon|^{2})dt$$

λ Lagrange multiplier

B operator Lagrange multiplier

Variation of J’ ,δJ’ leads to

$$\frac{\partial U(t)}{\partial t} = -iH(t)U(t) \qquad U(o)=I$$

$$\xrightarrow{\hspace{8em}} \text{time}$$

$$\frac{\partial B(t)}{\partial t} = iH(t)B(t) \qquad B(t_f)=O^{+}$$

$$\text{time} \xleftarrow{\hspace{8em}}$$

$$\varepsilon(t) = -\frac{s(t)}{2\lambda}\mathrm{Im}[\,\mathrm{Tr}\{B(t)\mu U(t)\}]$$