Probing coherence aspects of adiabatic quantum computation

Debabrata Goswami
Department of Chemistry &
Center for Laser Technology
Indian Institute of Technology
Kanpur

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Students: A. Nag, A.K. De, I. Bhattacharyya, S.K.K. Kumar, T. Goswami, S. Maurya, A. Kumar, D.K. Das, D. Roy, N. Mutiyal, B. Saha, S. Ashtekar, A. Basu, P. Samineni, D. Tewari, M. Bera, S. Chakraborty, S. Mukherjee, S. Priyadarshi, S. Chapekar, A. Basu

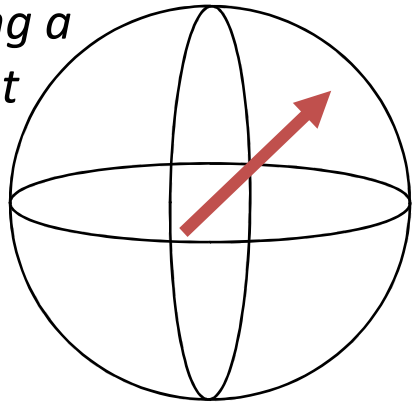
Quantum Aspects

Quantum: Atomic scale & "Confined" by "boundary conditions"

- **Measurement**
  - Observing (**measuring**) quantum system alter its state
  - Example: the **Qubit**

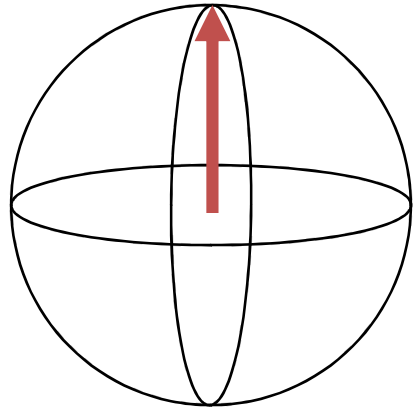
$$|\psi\rangle = a\cdot|0\rangle + b\cdot|1\rangle$$

Before making a measurement

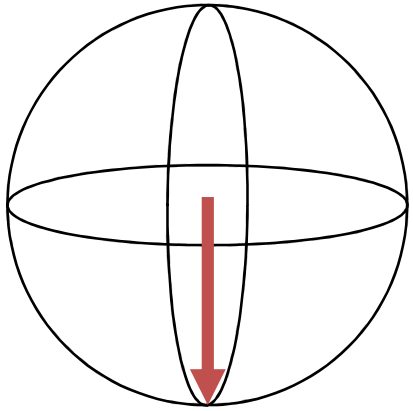


Coherent superposition

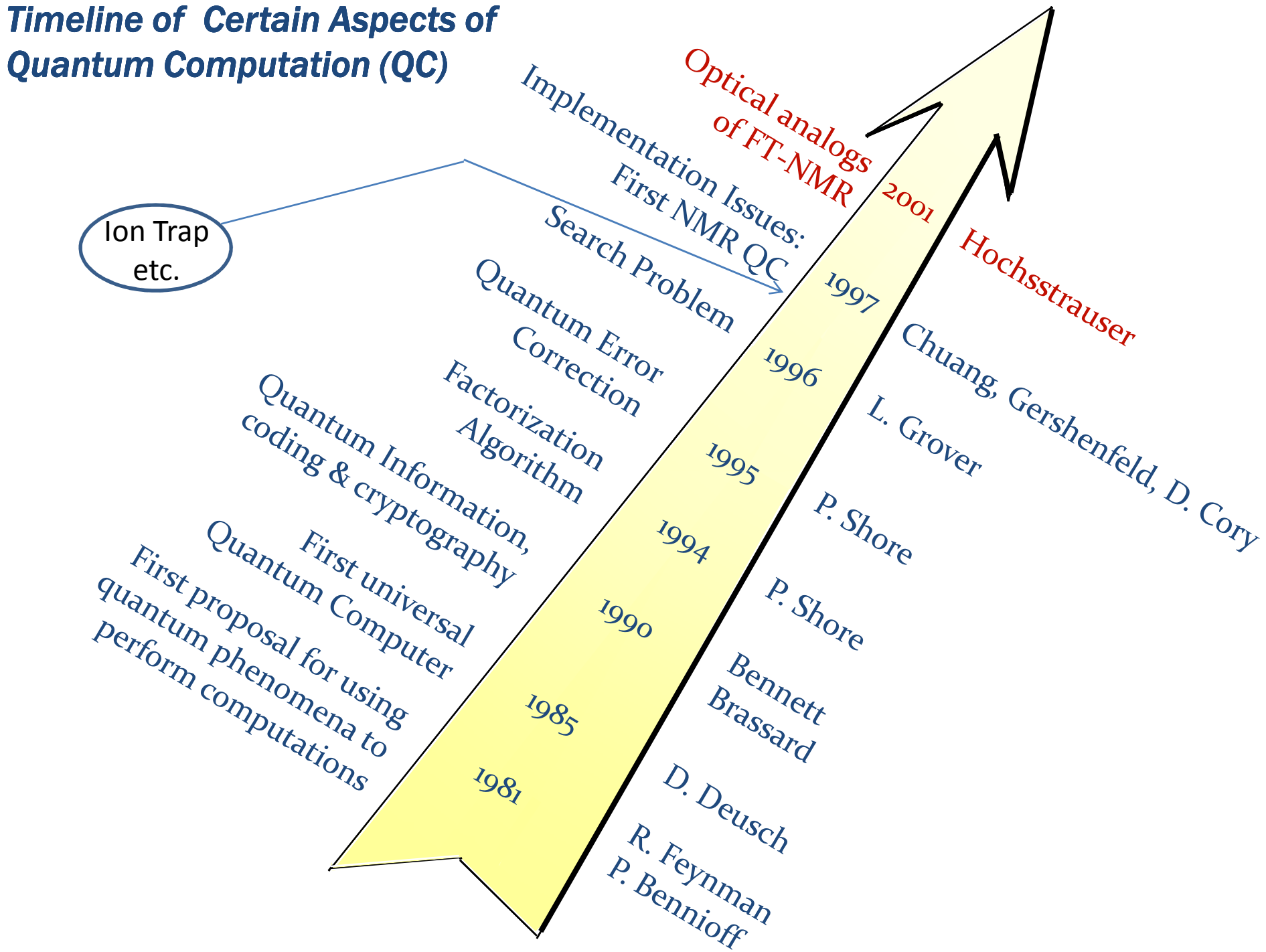
When observed, the state of a qubit will **collapse** to



either *b=0*



or *a=0*


Timeline of Certain Aspects of Quantum Computation (QC)
Ion Trap etc.
Implementation Issues: First NMR QC
Search Problem
Quantum Error Correction
Factorization Algorithm
Quantum Information, coding & cryptography
First universal Quantum Computer
First proposal for using quantum phenomena to perform computations
Optical analogs of FT-NMR
2001
Hochsstrauser
1997
Chuang, Gershenfeld, D. Cory
1996
L. Grover
1995
P. Shore
1994
P. Shore
1990
Bennett Brassard
1985
D. Deusch
1981
R. Feynman
P. Bennioff

Realism in the Quest for QC & QI

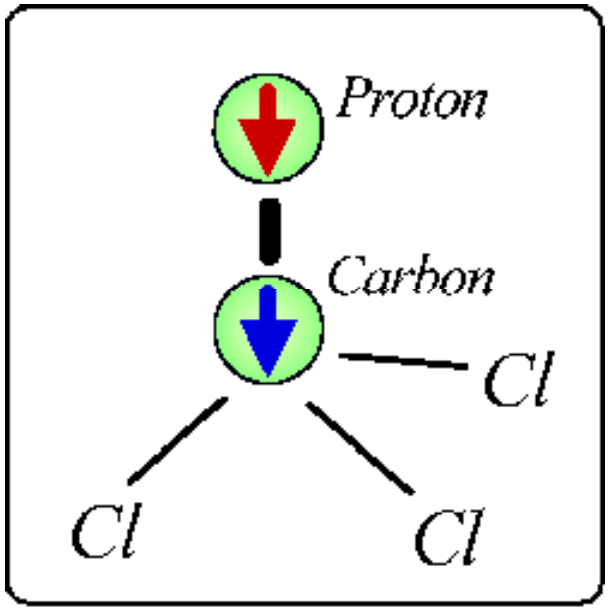
- Quantum Security

  (e.g. DARPA supports QC in the National Labs)

  Why are Companies like HP, Microsoft interested in QC ?
- Only one time use software!
  - Neilson talked about it while he was in Microsoft
- Speed
- Future Market

Basic Principle of NMR Quantum Computer (NMR-QC)

- A nearly ideal physical system that can be used as a QC is a single molecule
  - Nuclear spins of individual atoms in the molecule represent qubits
- The quantum behavior of the spins can be exploited to perform QC
  - e.g., the carbon and hydrogen nuclei in a chloroform molecule represent two qubits
- Application of a RF pulse to the hydrogen nucleus addresses that qubit, and rotates it from |0> state (say) to a superposition state
- Interactions through chemical bonds allow multiple-qubit logic to be performed



$|0\rangle\,|0\rangle$

Solution NMR

Major Drawbacks of NMR-QC

- Solution NMR-QC is not scalable to useful number of spins
- Ideal signal from N-bit QC scales as $N.2^{-N}$ at room temp. Even quantum noise overwhelms quantum signal for moderate N at room temperature
- Even 10 bits (requires a totally asymmetric spin system) will be very hard and the computer will be very slow. 10-100 Hz clock frequency

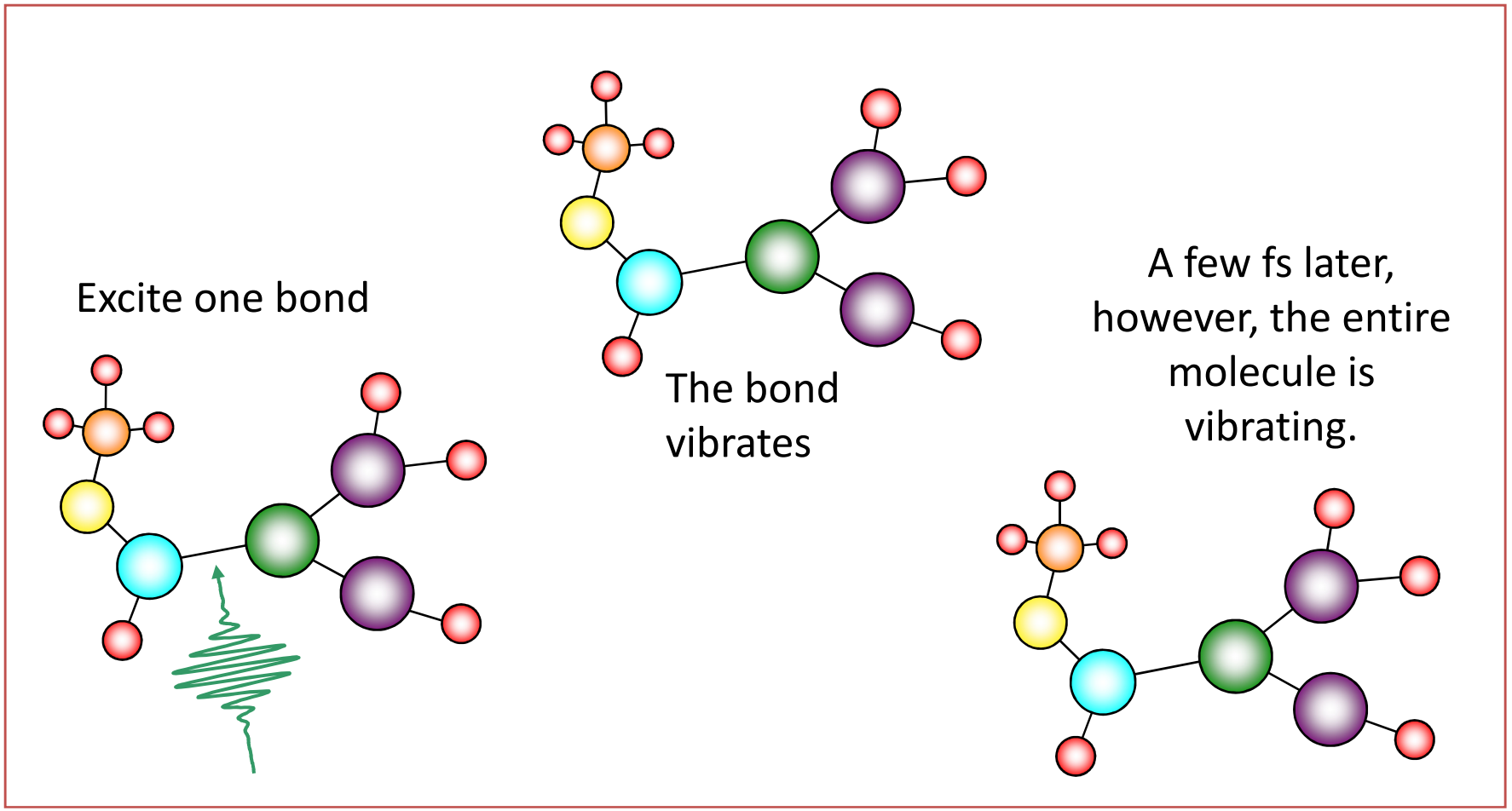
Quest for other schemes necessary

- Optical schemes ?
  - Example: Control of molecular system with lasers
  - Light Polarization state, just like, the "spin"

What is Adiabatic QC ?

- Molecule is the computer as in NMR case
  - Bring in all the goodness in NMR approach
- Logical implementation of quantum gates using
    - ground states, spectral gaps & Hamiltonian language
  - Resulting quantum gate represents a device that performs a unitary transformation on selected qubits in a fixed period of time
- Computational procedure in the adiabatic QC model is described by
  - Continuous time evolution of a time-dependent Hamiltonian with limited energetic resources
    - an aspect often neglected in the unitary gate language

Problem of molecular control: Intramolecular Vibrational redistribution (IVR)



IVR occurs on a few-fs time scale, so long pulses excite entire molecule, and the weakest bond breaks, no matter which bond was excited. We need the pulse in femtosecond regime.

Control: Laser Molecule Interaction

- Intermolecular—Diffusion & Mobility

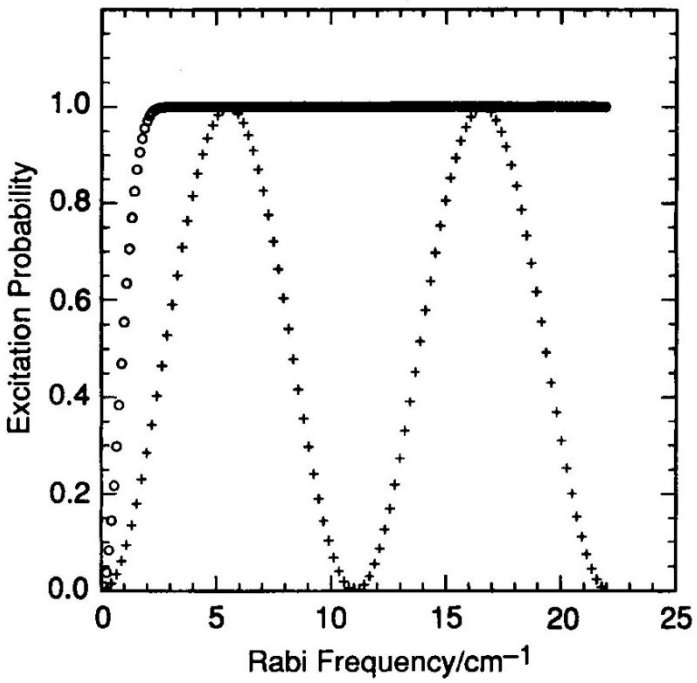
  Timescales Depend on environmental conditions

- Intramolecular—Intrinsic to Molecular States

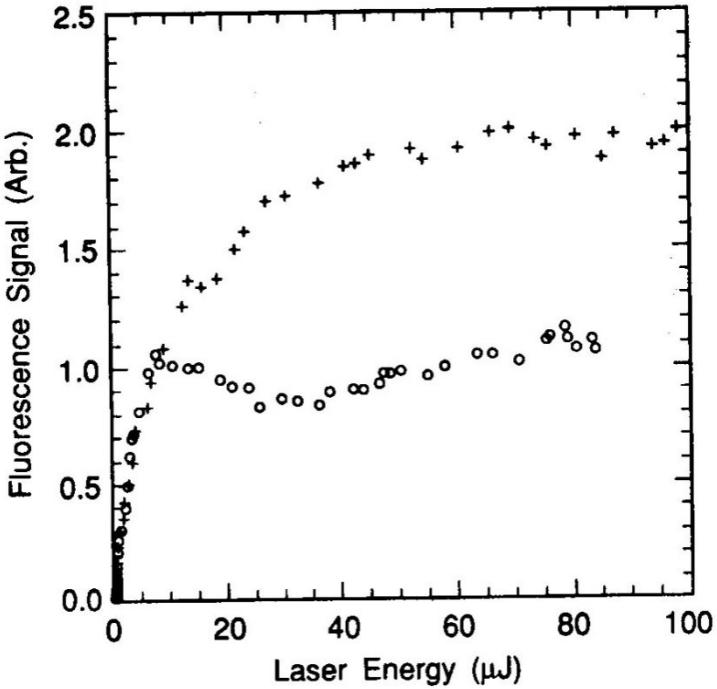
  Timescales typically vary from ns or below depending on whether electronic, vibrational or Rotational States are involved

DECOHERENCE

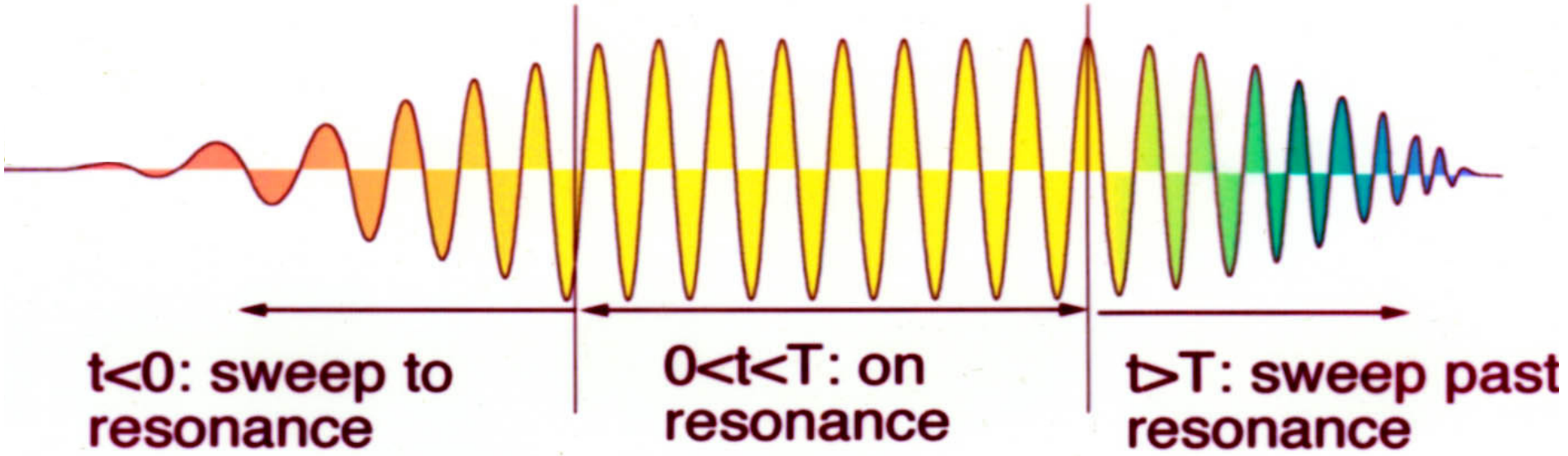
THEORY

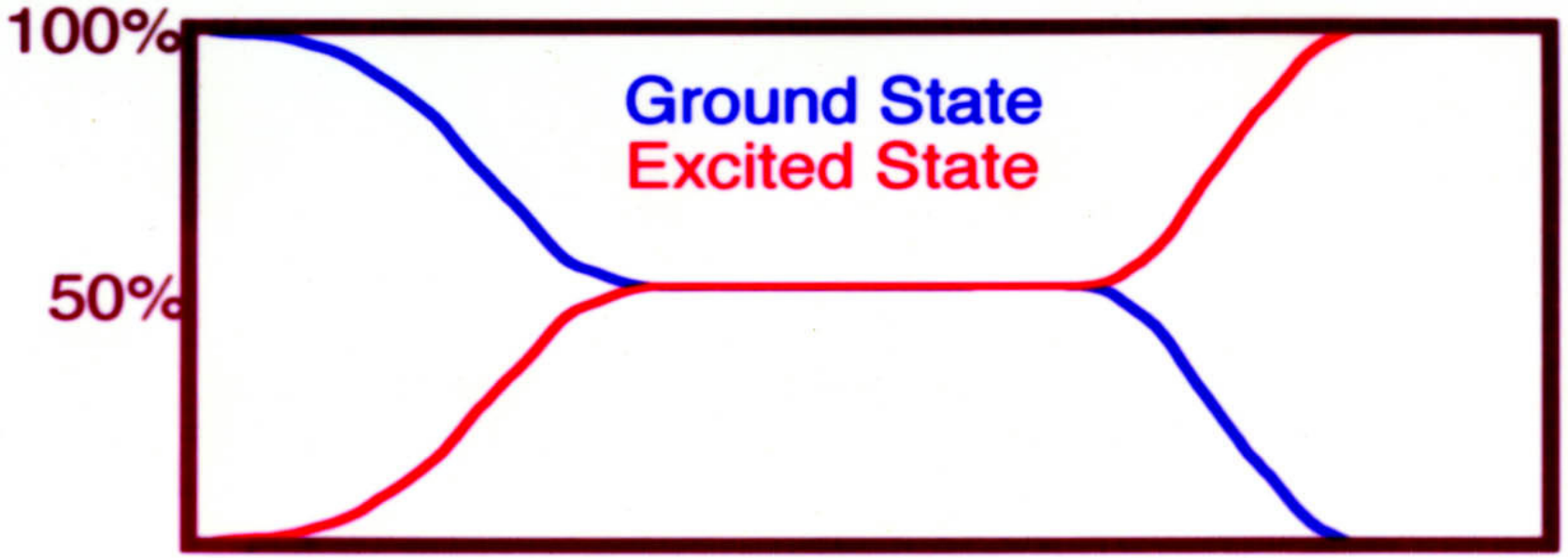


EXPERIMENT



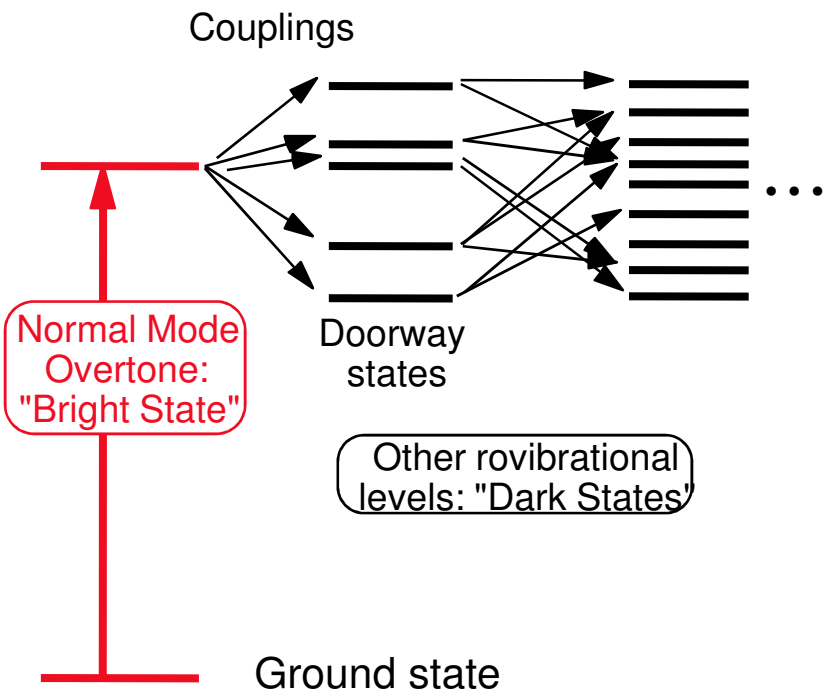
Adiabatic passage in two-level system



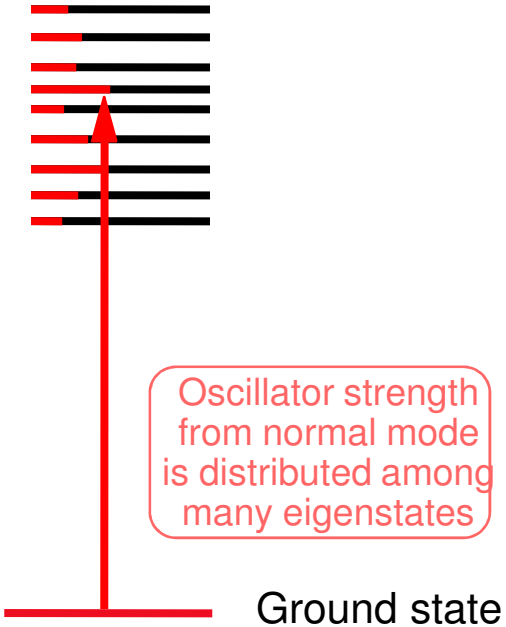


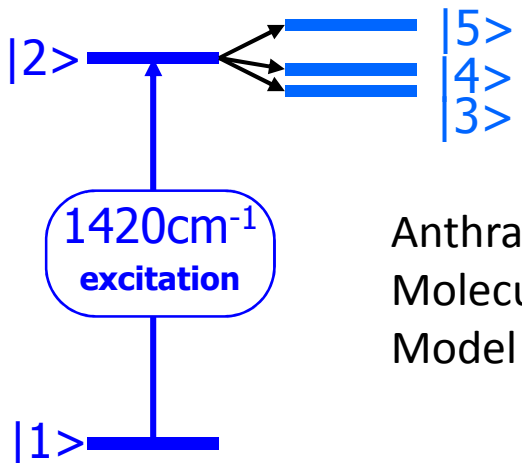
Molecular Decoherence: IVR

Normal Mode Picture

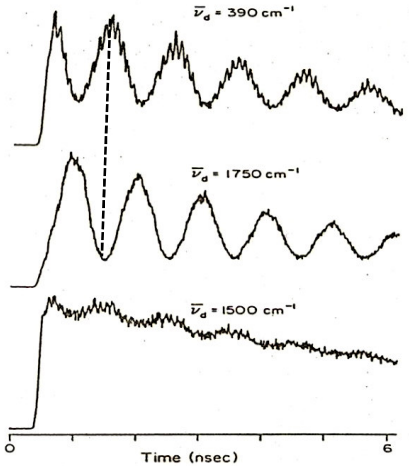


Eigenstate Picture



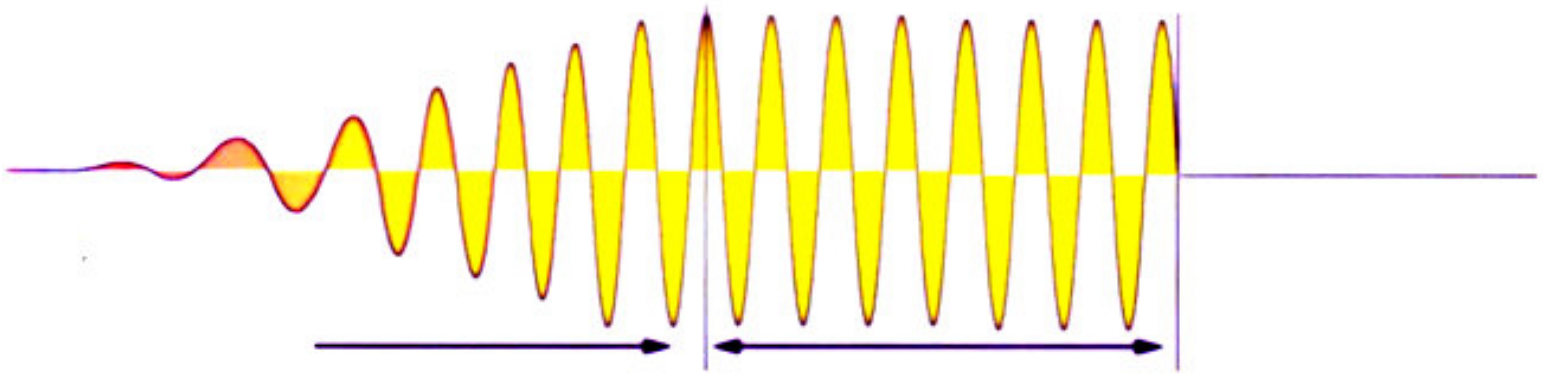


Anthracene Molecule Model System



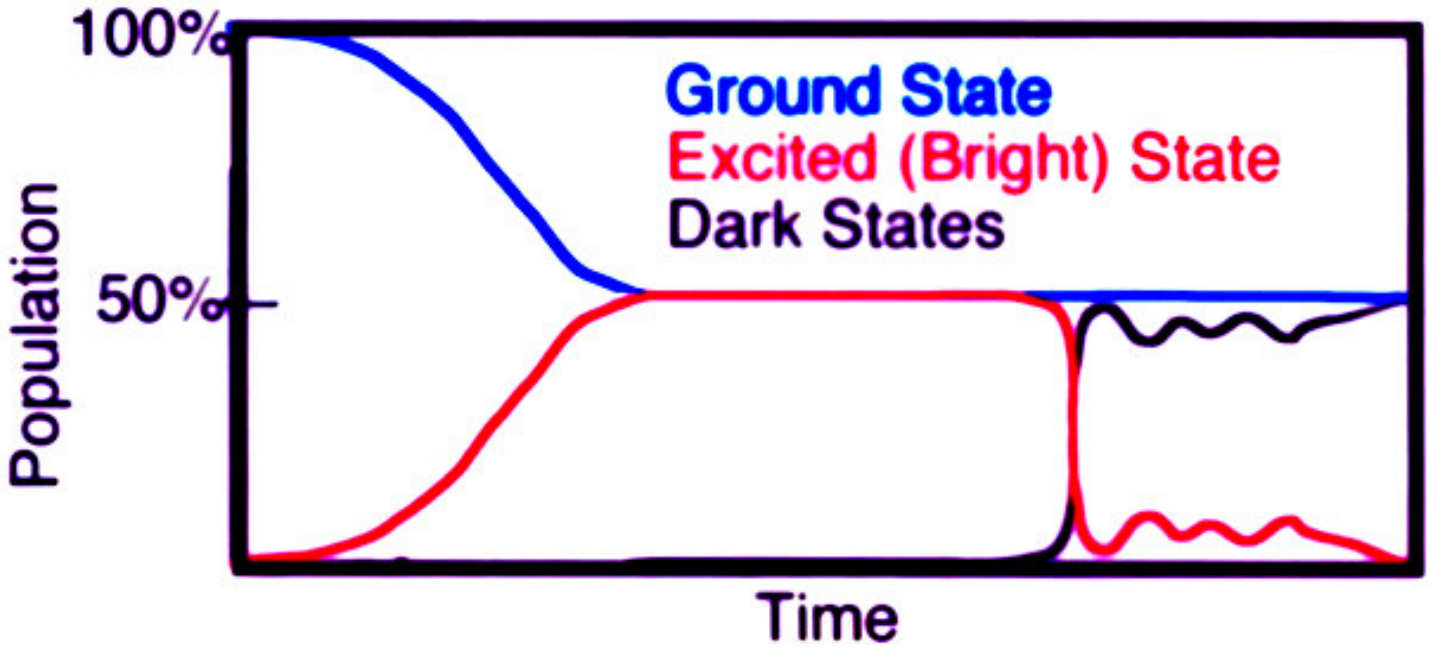
EXPERIMENTAL RESULTS

Adiabatic half passage in coupled systems:



t<0: sweep to resonance

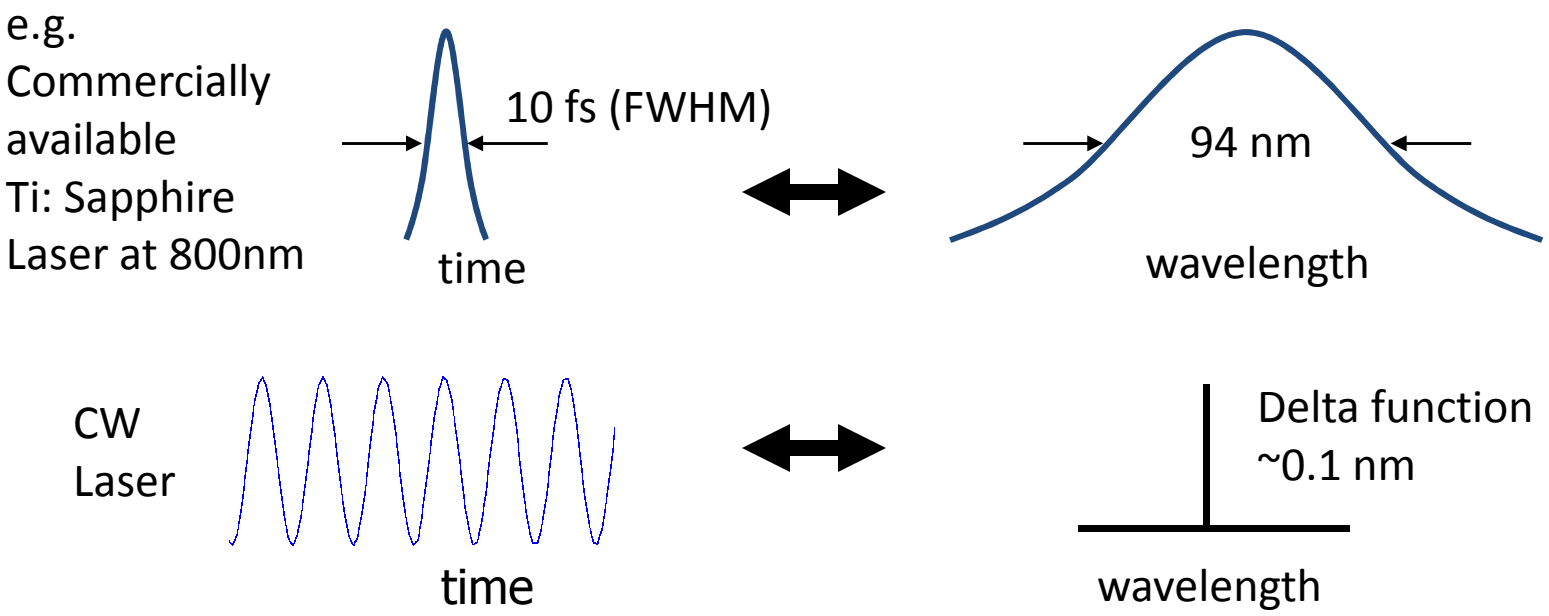
0<t<T: constant amplitude, $\mu \cdot E/\hbar >>$ couplings to dark states



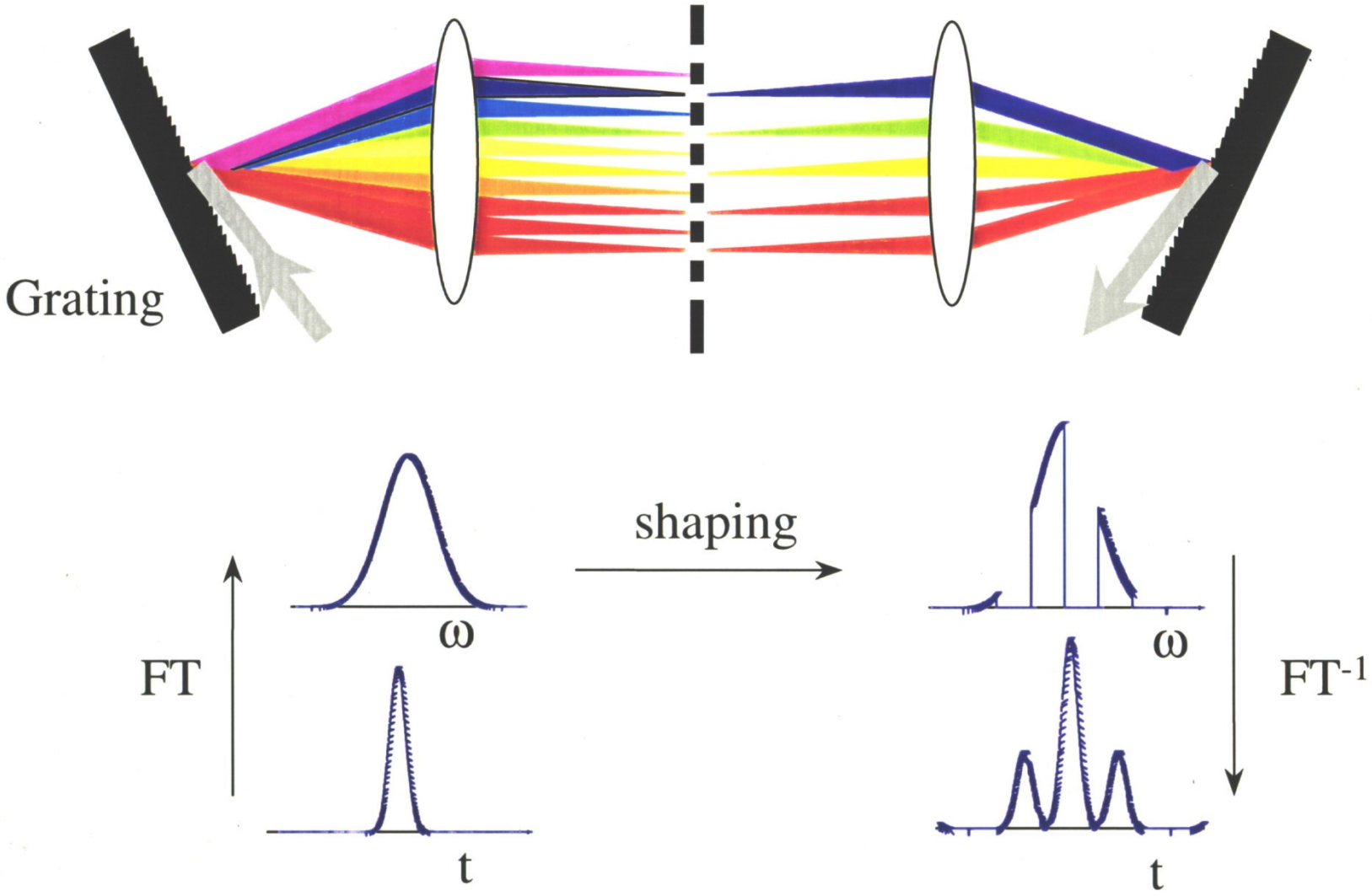
An Ultrafast Laser Pulse

- **Coherent superposition of many monochromatic light waves within a range of frequencies that is inversely proportional to the duration of the pulse**

  Short temporal duration of the ultrafast pulses results in a very broad spectrum quite unlike the notion of monochromatic wavelength property of CW lasers.



Pulse-shaping: Spatial Mask



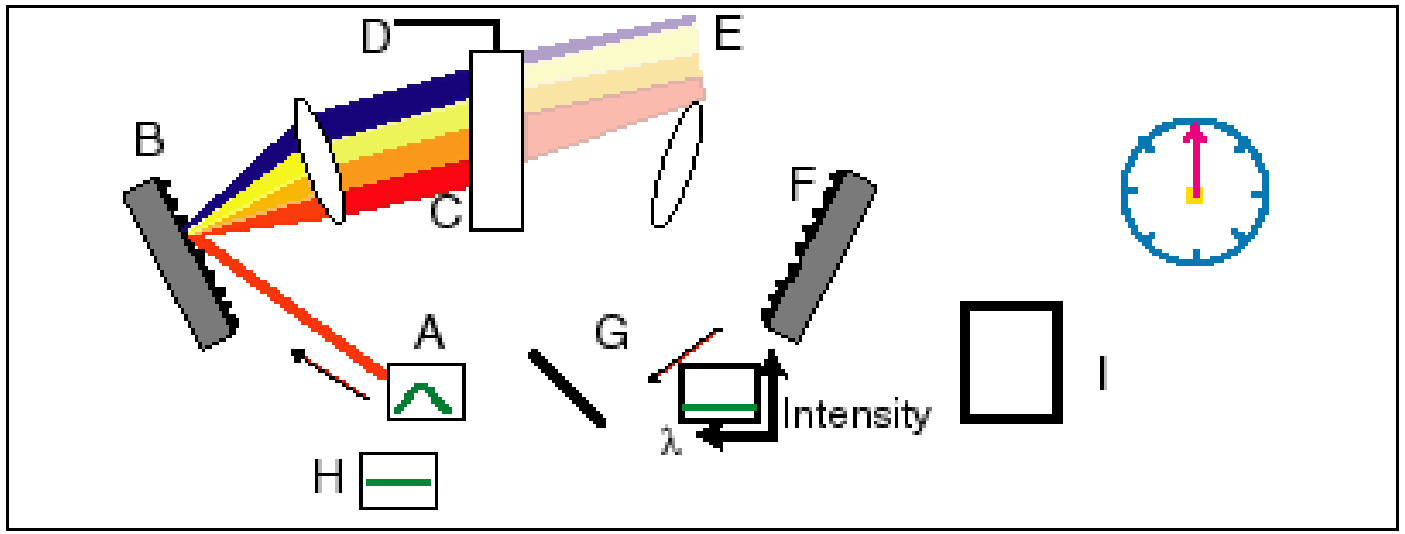
Pulse Shaping

- Control over the amplitude, phase, frequency and/or inter-pulse separation
- Complex pulse shaping aims to control one or more of the above-mentioned parameters in a programmable manner.

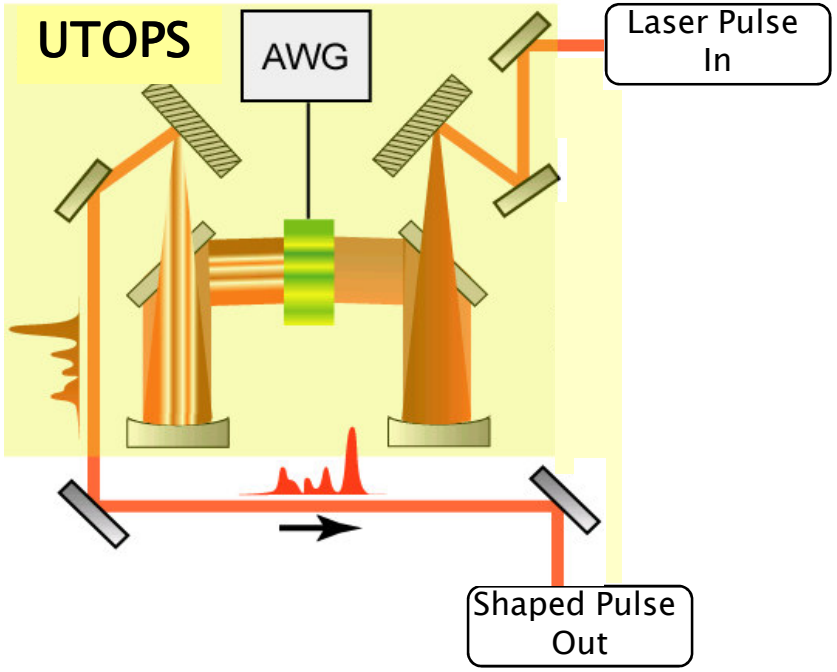
Can be represented by Linear Filtering Scheme:

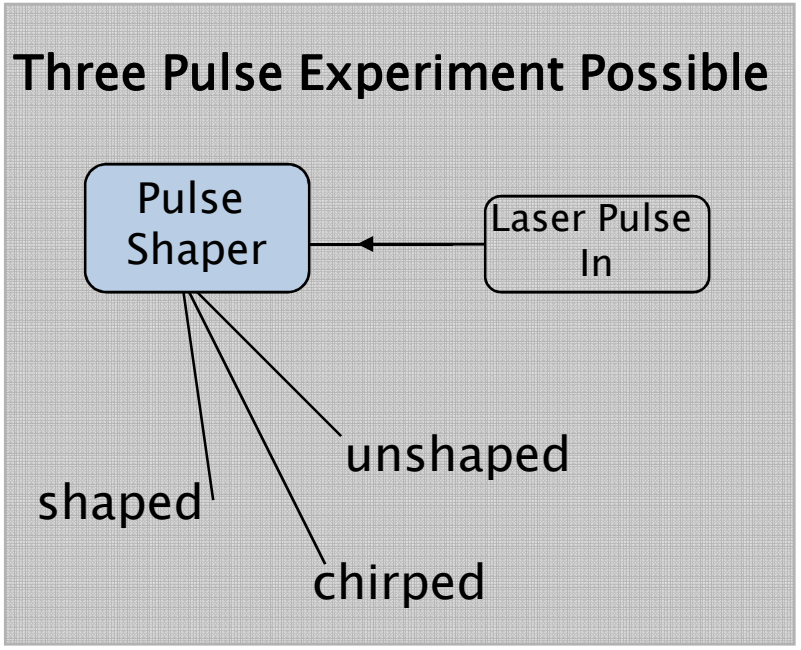
- Time Domain: $E_{out}(t) = E_{in}(t) \otimes g(t)$, where ⊗=>convolution
- Timescales not quite accessible with conventional electronics (typically ns)!
- Frequency Domain $E_{out}(\omega) = E_{in}(\omega) \times G(\omega)$

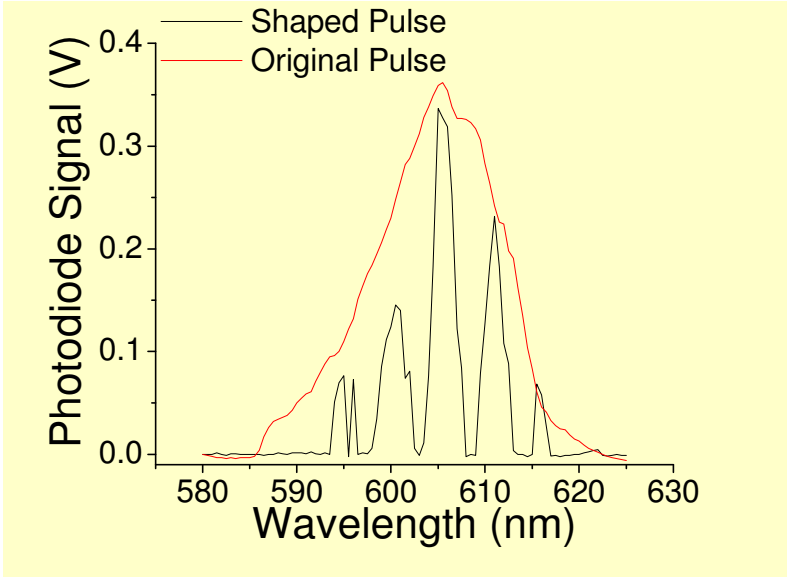
$$G(\omega) = \int dt.g(t).e^{i\omega t} \quad and \quad g(t) = \frac{1}{2\pi}\int dt.g(t).e^{i\omega t}$$

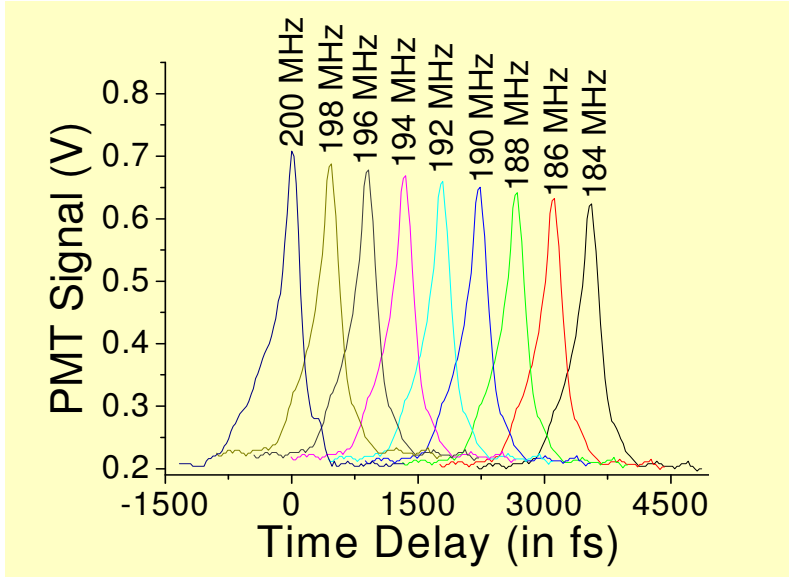


EXPERIMENTS



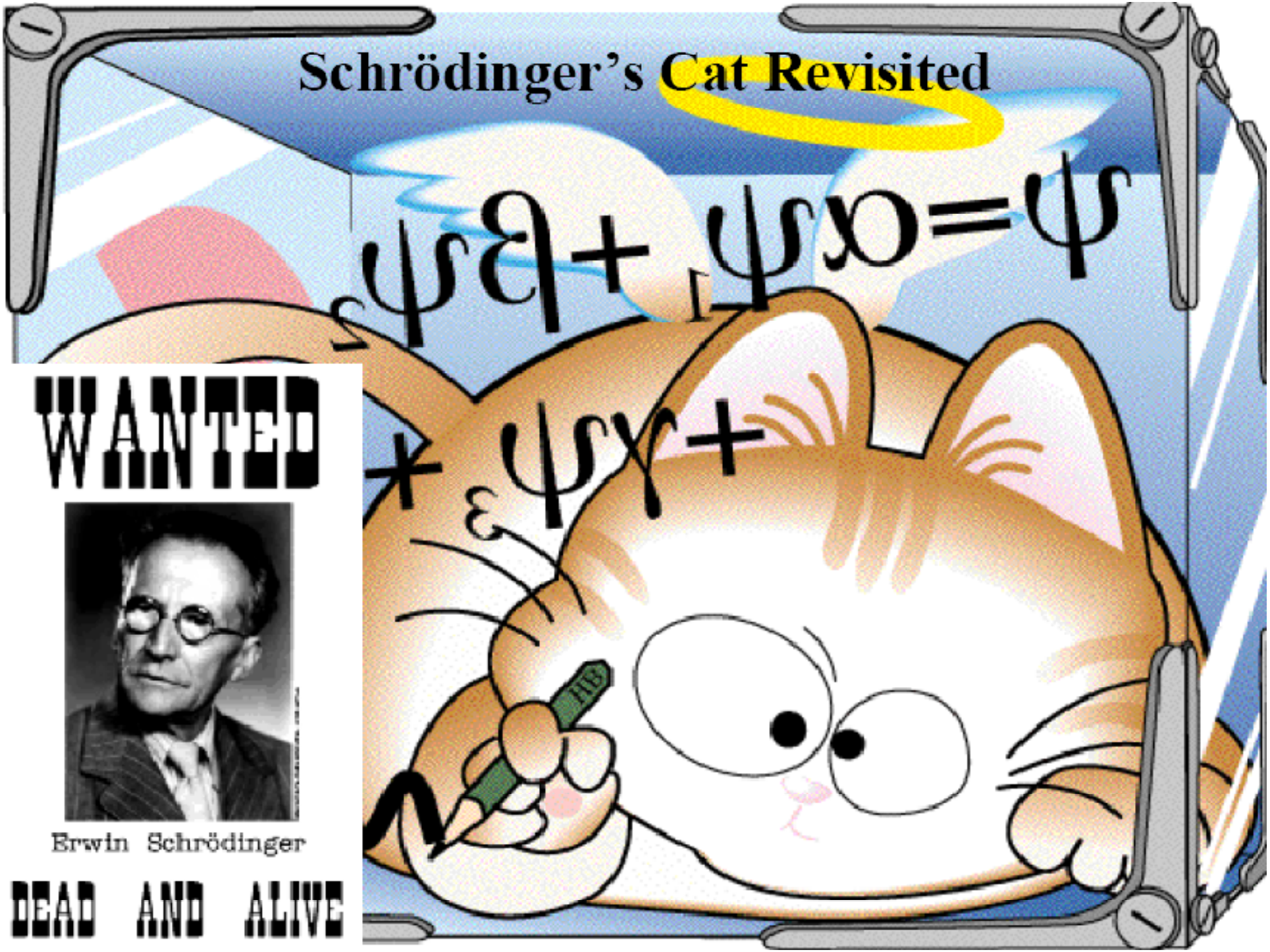




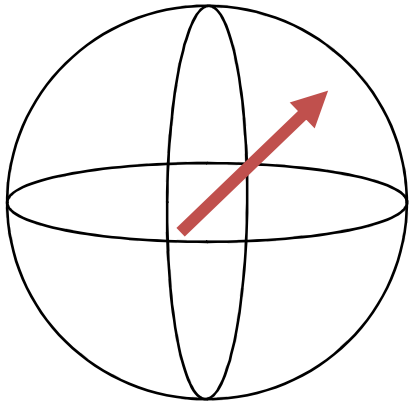


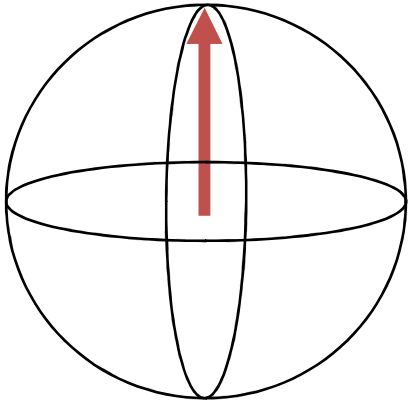
A couple of representative graphs of the pulse shaping capability is shown in the data that are collected in the wavelength and time-domain respectively.

Schrödinger's Cat Revisited



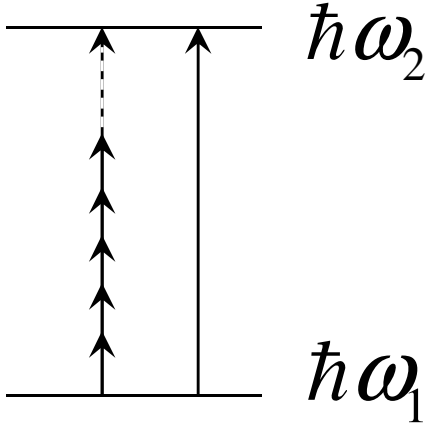
Coherence: Simple Two-Level System





$$H^{FM} = \hbar \begin{bmatrix} \Delta + N\dot{\phi}(t)) & \frac{\Omega_1}{2} \\ \frac{\Omega_1^*}{2} & 0 \end{bmatrix}$$

$$\Delta = \omega_R - N\omega$$

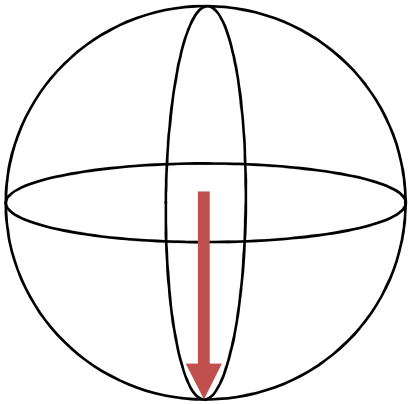


$$\Omega_1(t) = k(\mu_{eff}.\varepsilon(t))^N/\hbar$$

$$\mu_{eff}^N = \prod_n^N \mu_n$$

$$\omega_R = \omega_2 - \omega_1$$

$$\frac{d\rho(t)}{dt} = \frac{i}{\hbar}[\rho(t), H^{FM}(t)]$$



Taylor Series Expansion of Instantaneous Phase

$$\vec{E}(t) = \boldsymbol{\mathcal{E}}_0(t)e^{i\omega.t+i\phi(t)}$$

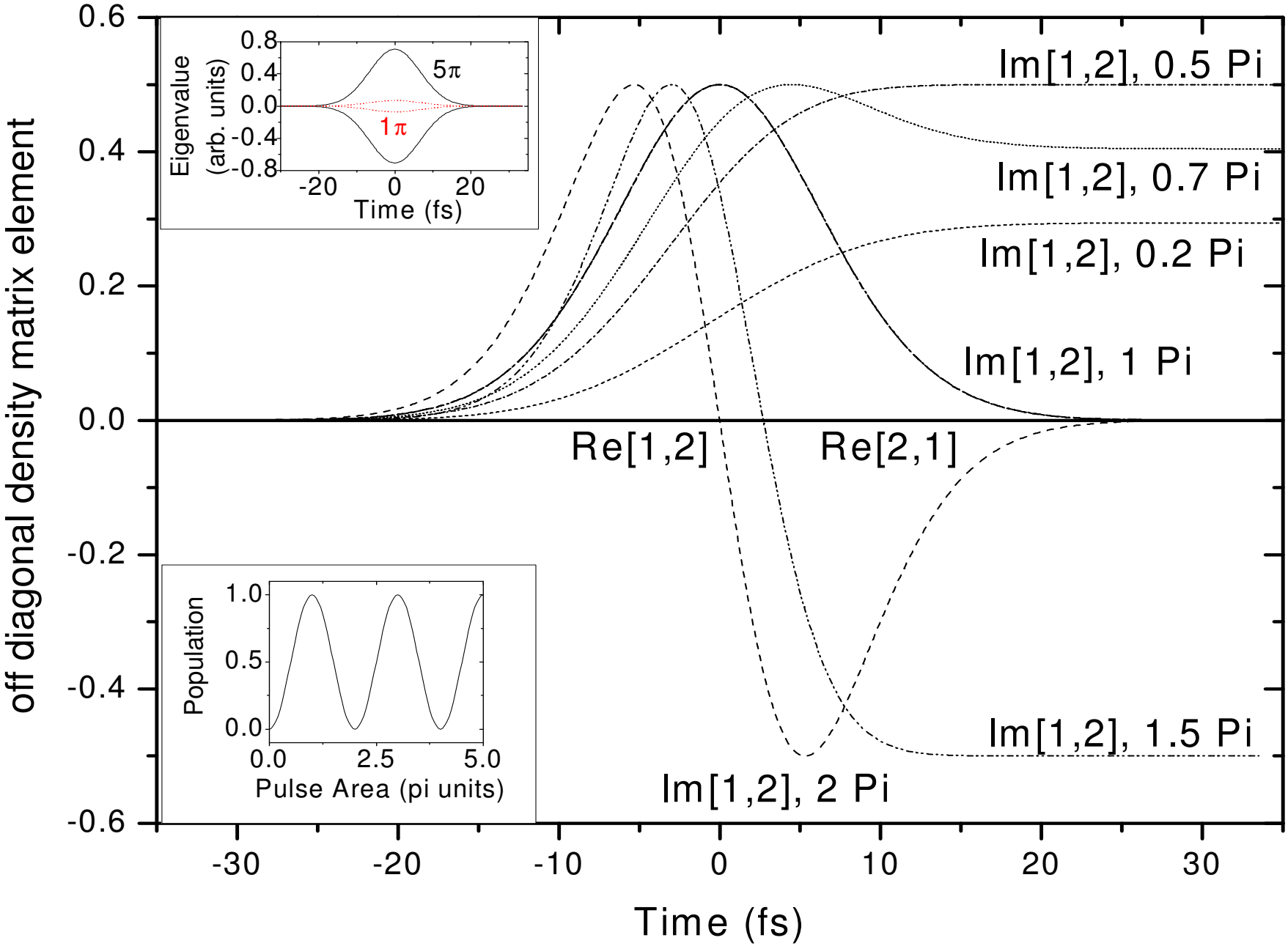
Phase

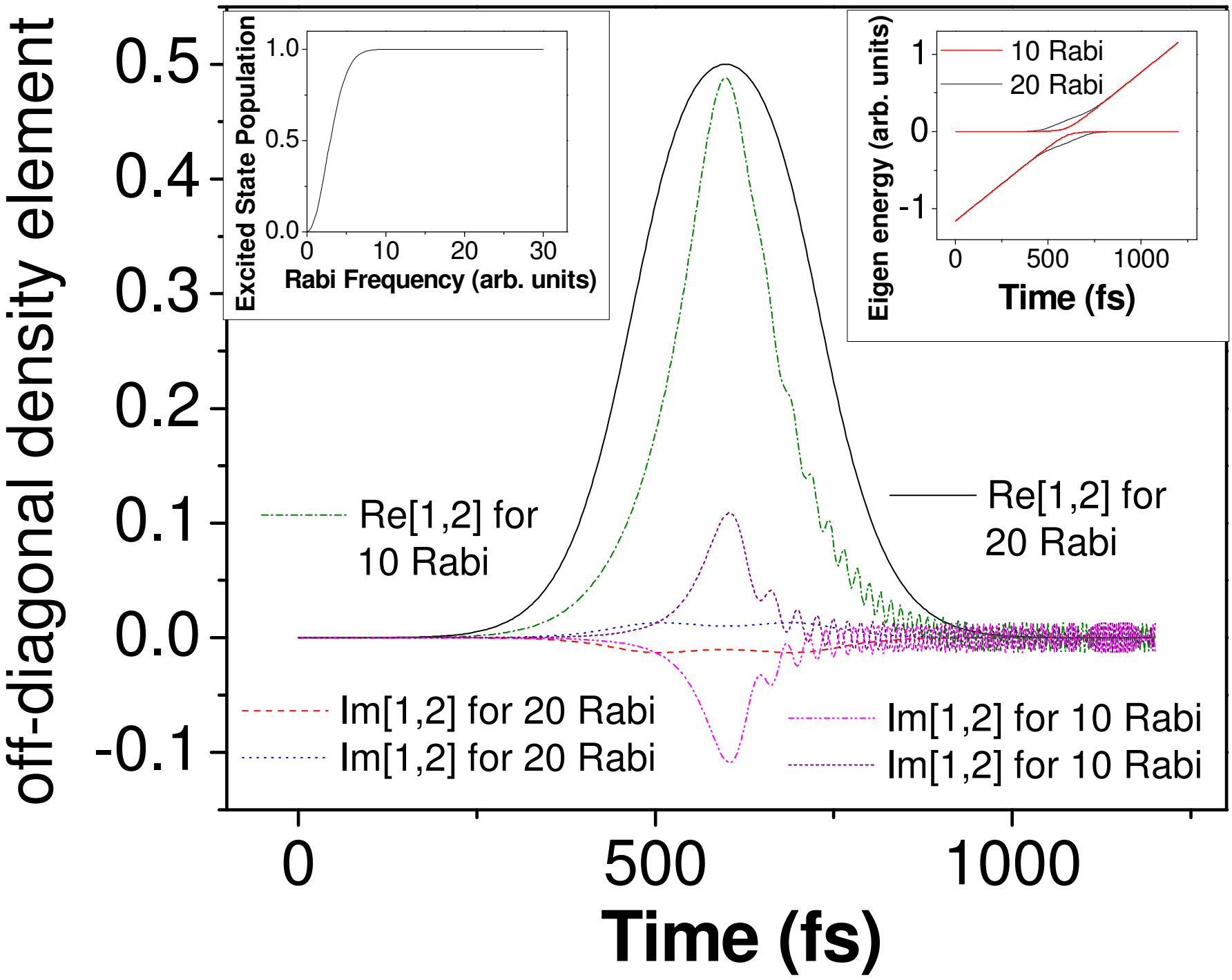
$$\phi(t) = b_0 + b_1 t + b_2 t^2 + b_3 t^3 + b_4 t^4 + b_5 t^5 + \ldots.$$

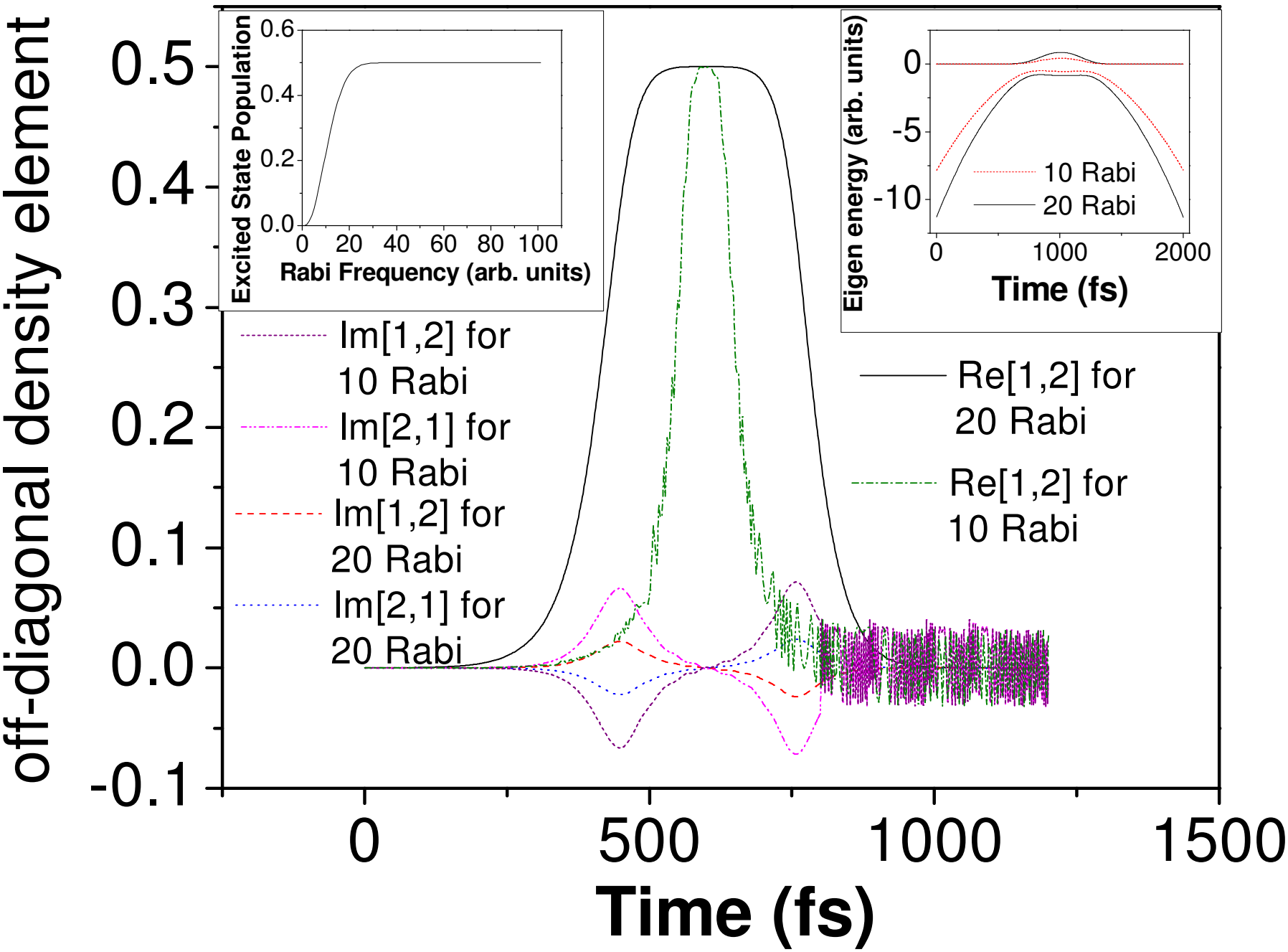
$$\dot{\phi}(t) = \quad b_1 + 2b_2 t + 3b_3 t^2 + 4b_4 t^3 + 5b_5 t^4 + \ldots.$$

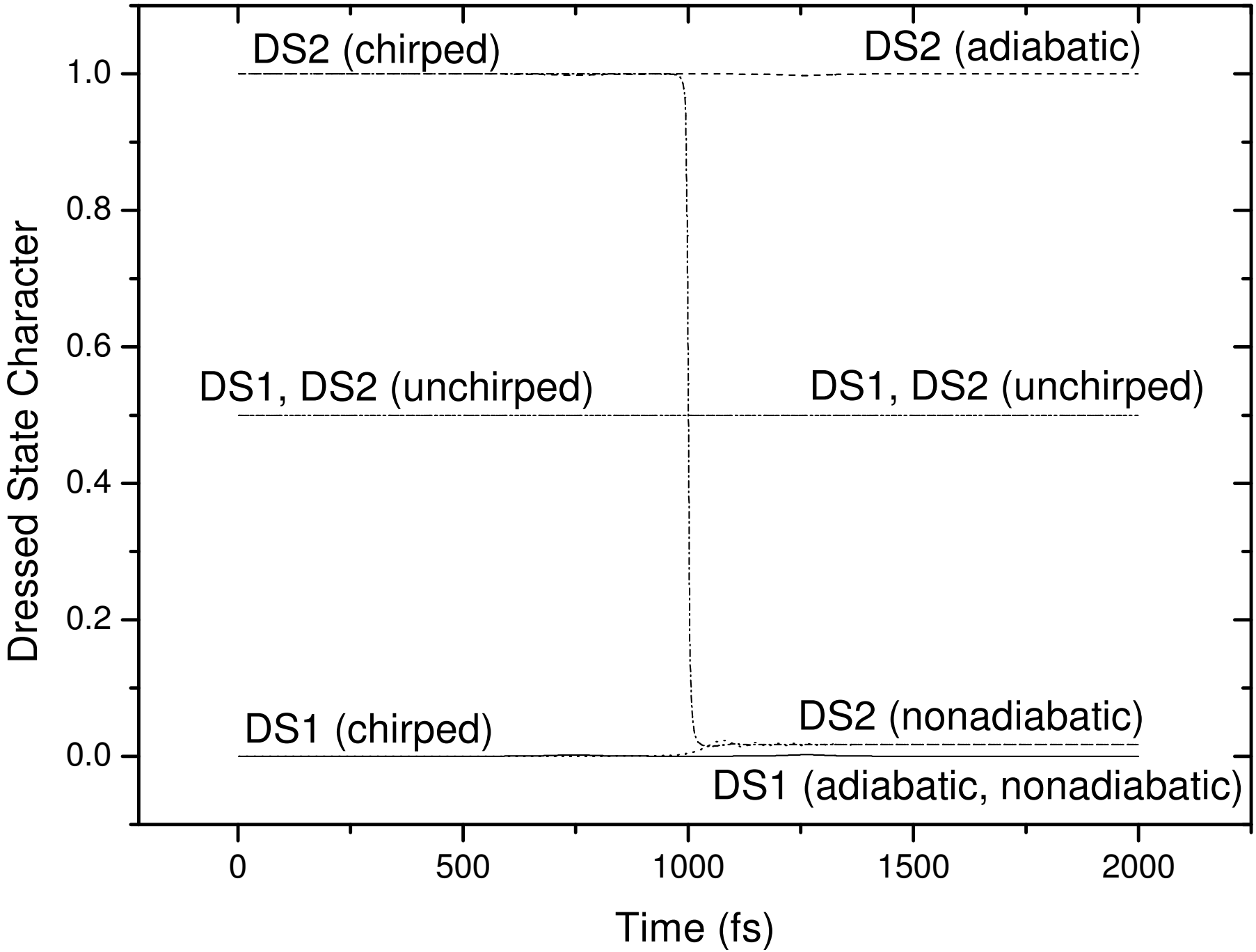
Frequency Sweep

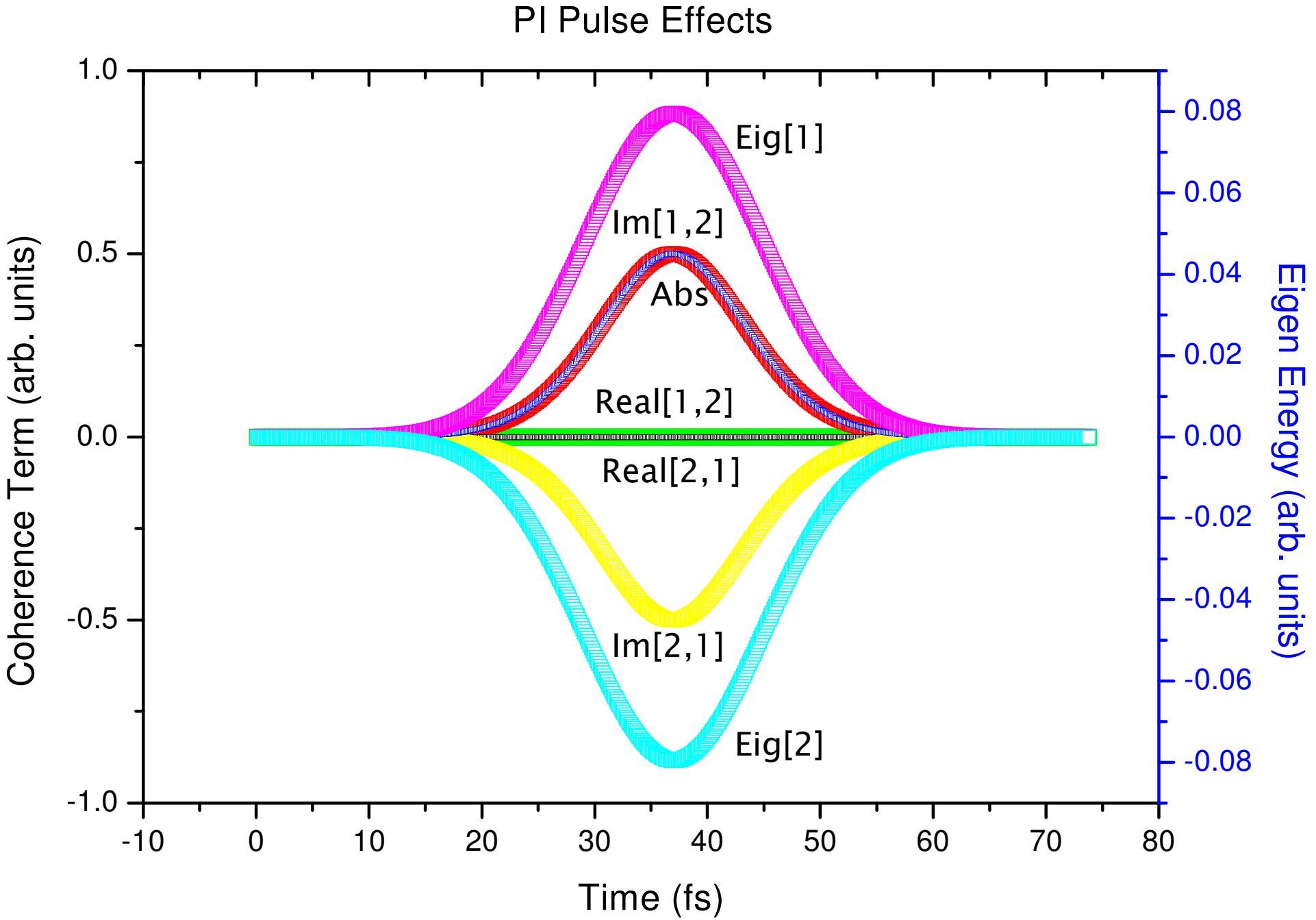
$$\frac{d\rho(t)}{dt} = \frac{i}{\hbar}[\rho(t), H^{FM}(t)]$$

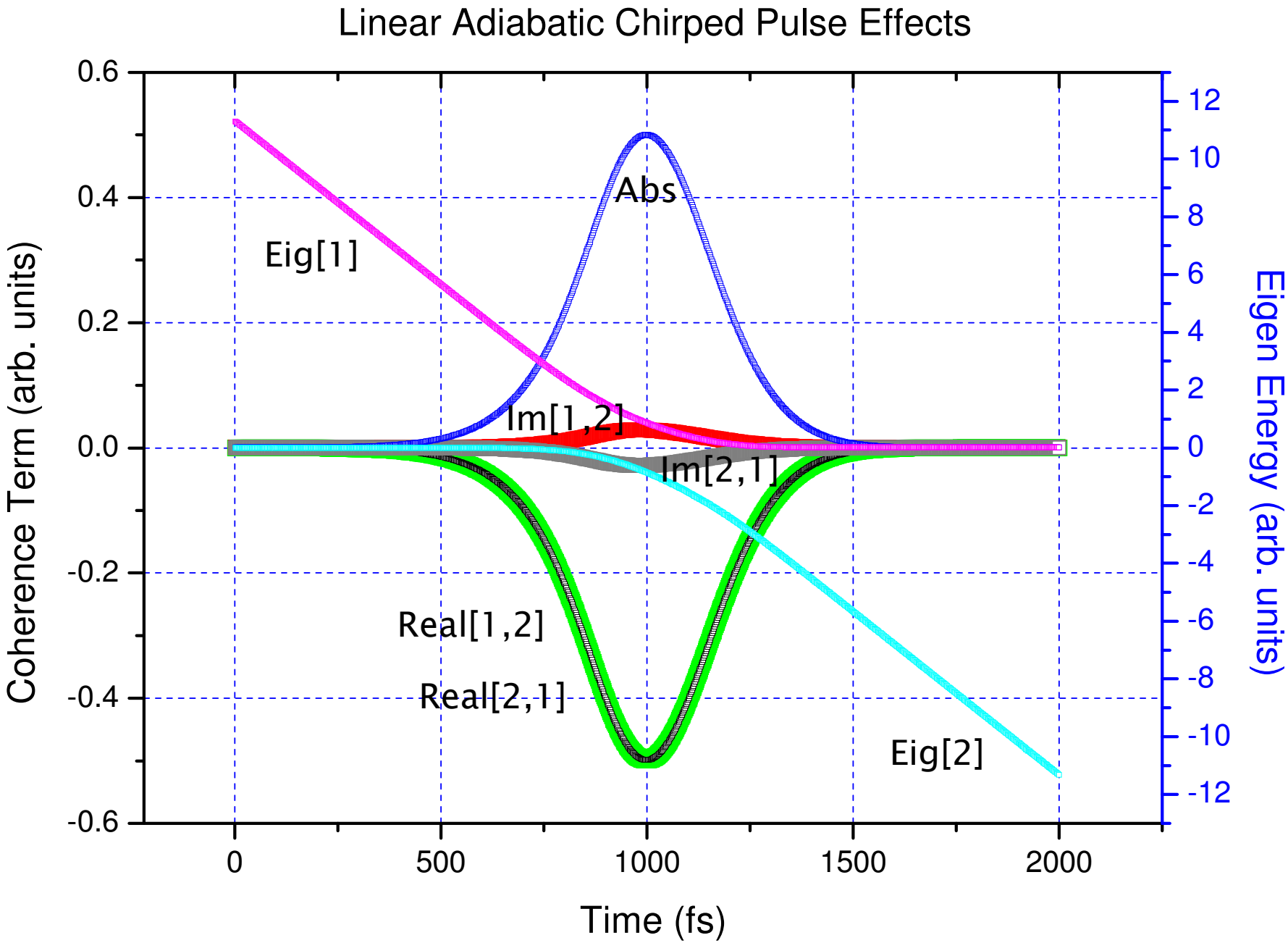

off diagonal density matrix element
Time (fs)
Im[1,2], 0.5 Pi
Im[1,2], 0.7 Pi
Im[1,2], 0.2 Pi
Im[1,2], 1 Pi
Re[1,2]
Re[2,1]
Im[1,2], 1.5 Pi
Im[1,2], 2 Pi
Eigenvalue (arb. units)
5π
1π
Time (fs)
Population
Pulse Area (pi units)


off-diagonal density element
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
0
500
1000
Time (fs)
Re[1,2] for 10 Rabi
Re[1,2] for 20 Rabi
Im[1,2] for 20 Rabi
Im[1,2] for 20 Rabi
Im[1,2] for 10 Rabi
Im[1,2] for 10 Rabi
Excited State Population
1.0
0.5
0.0
0
10
20
30
Rabi Frequency (arb. units)
Eigen energy (arb. units)
1
0
-1
10 Rabi
20 Rabi
0
500
1000
Time (fs)

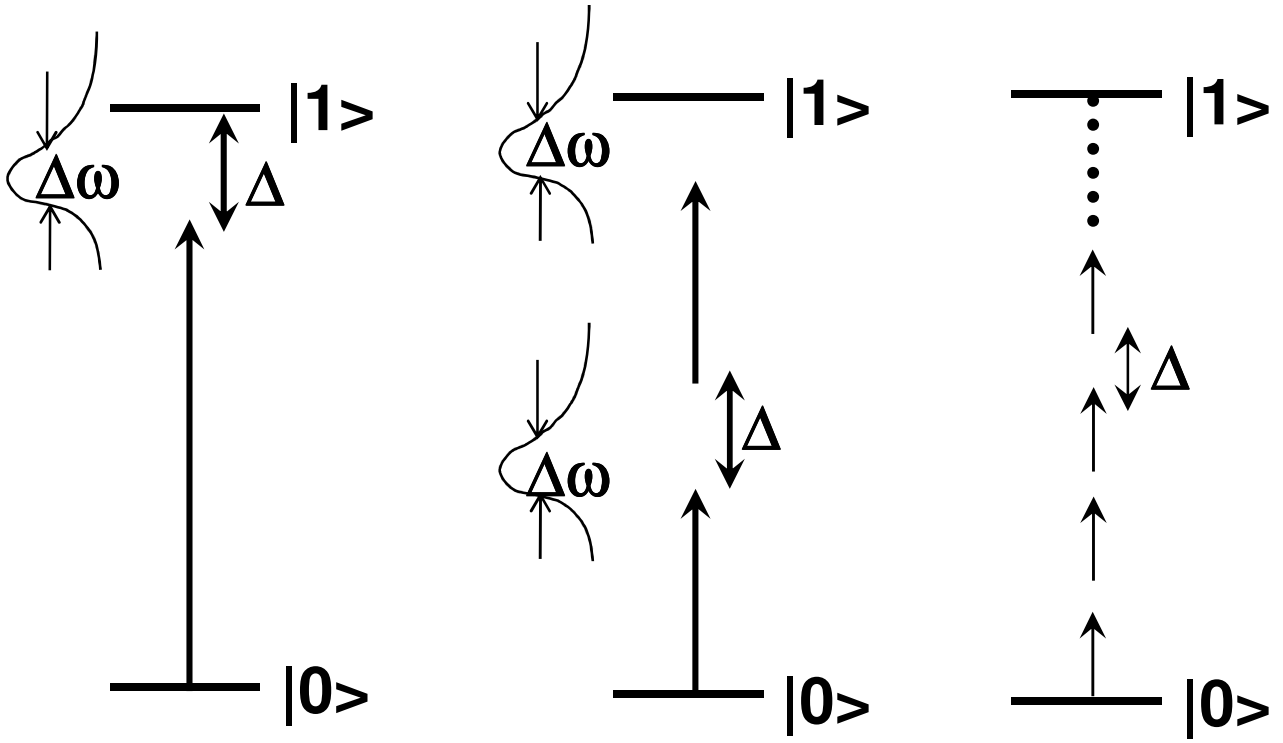

off-diagonal density element
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
0
500
1000
1500
Time (fs)
Im[1,2] for 10 Rabi
Im[2,1] for 10 Rabi
Im[1,2] for 20 Rabi
Im[2,1] for 20 Rabi
Re[1,2] for 20 Rabi
Re[1,2] for 10 Rabi
Excited State Population
0.6
0.4
0.2
0.0
0
20
40
60
80
100
Rabi Frequency (arb. units)
Eigen energy (arb. units)
0
-5
-10
10 Rabi
20 Rabi
0
1000
2000
Time (fs)


DS2 (chirped)
DS2 (adiabatic)
DS1, DS2 (unchirped)
DS1, DS2 (unchirped)
DS1 (chirped)
DS2 (nonadiabatic)
DS1 (adiabatic, nonadiabatic)
Dressed State Character
1.0
0.8
0.6
0.4
0.2
0.0
0
500
1000
1500
2000
Time (fs)

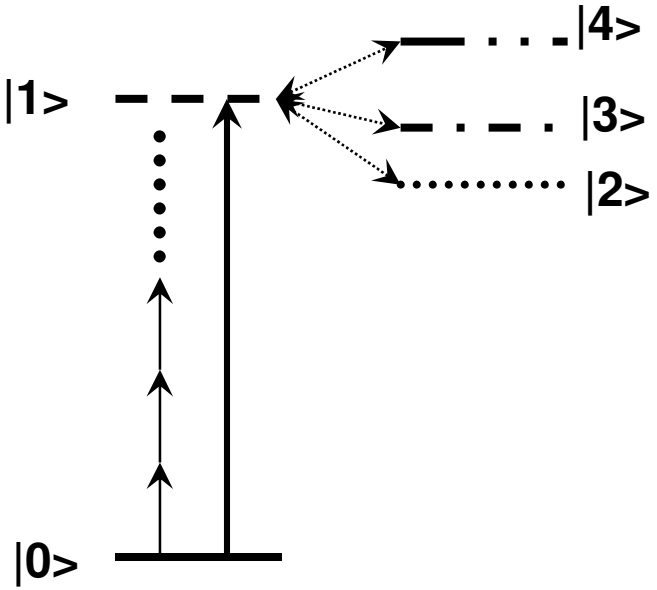

PI Pulse Effects
Coherence Term (arb. units)
Eigen Energy (arb. units)
Time (fs)
1.0
0.5
0.0
-0.5
-1.0
0.08
0.06
0.04
0.02
0.00
-0.02
-0.04
-0.06
-0.08
-10
0
10
20
30
40
50
60
70
80
Eig[1]
Im[1,2]
Abs
Real[1,2]
Real[2,1]
Im[2,1]
Eig[2]

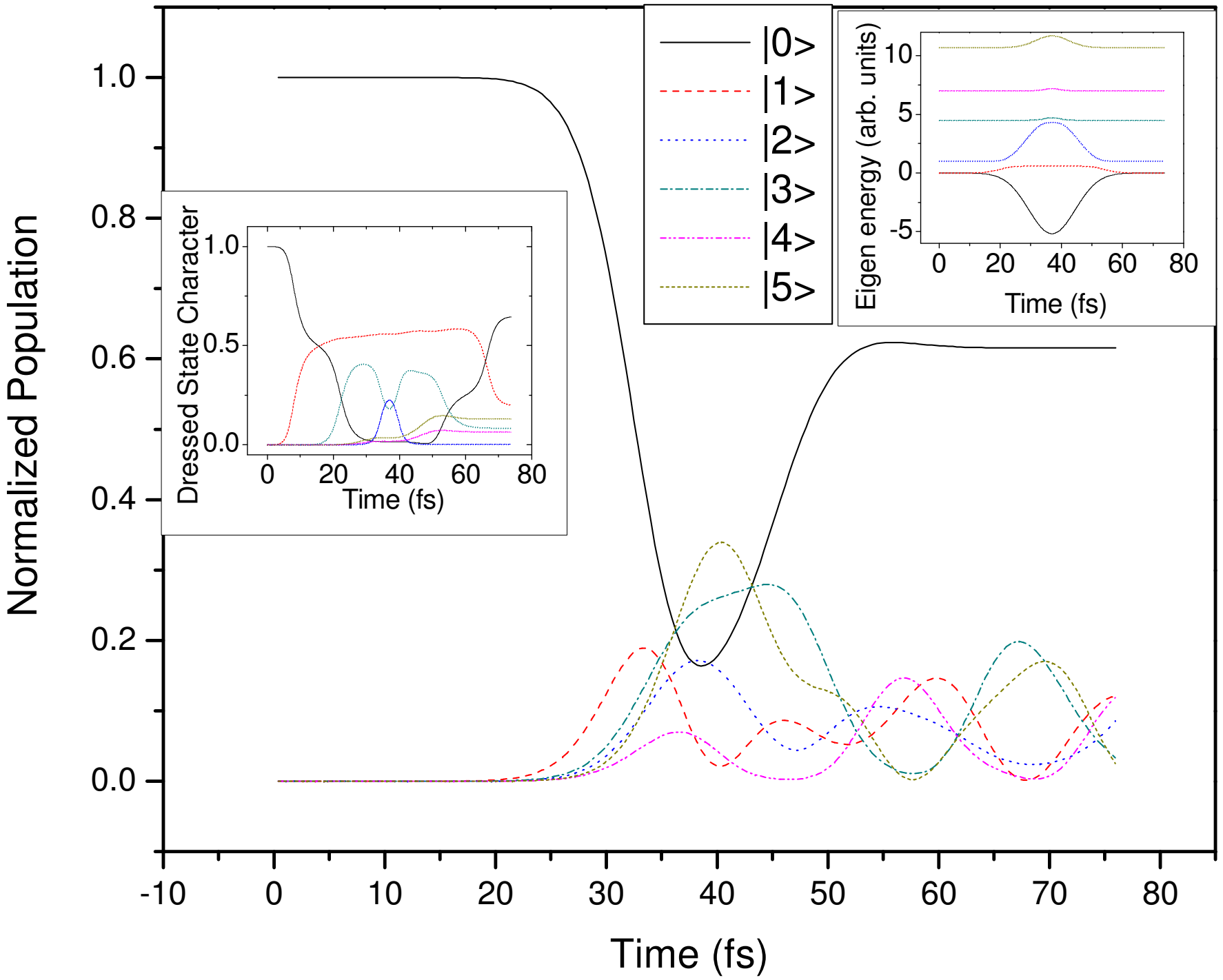

Linear Adiabatic Chirped Pulse Effects
Coherence Term (arb. units)
Eigen Energy (arb. units)
Time (fs)
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
12
10
8
6
4
2
0
-2
-4
-6
-8
-10
-12
0
500
1000
1500
2000
Abs
Eig[1]
Im[1,2]
Im[2,1]
Real[1,2]
Real[2,1]
Eig[2]

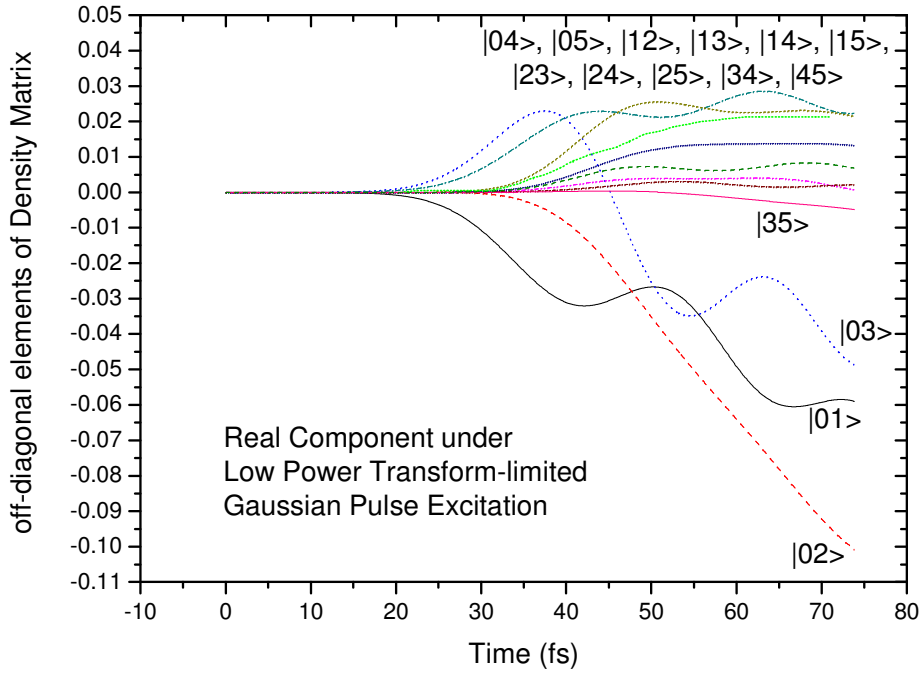
Single & Multiphoton: Model Evolving from Two-Level to Multilevel & IVR

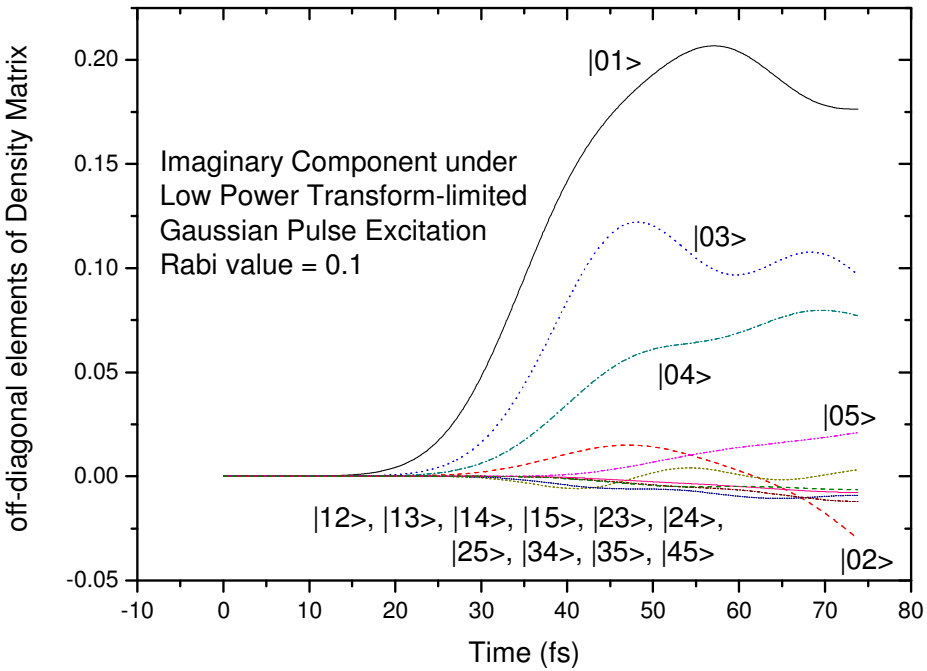


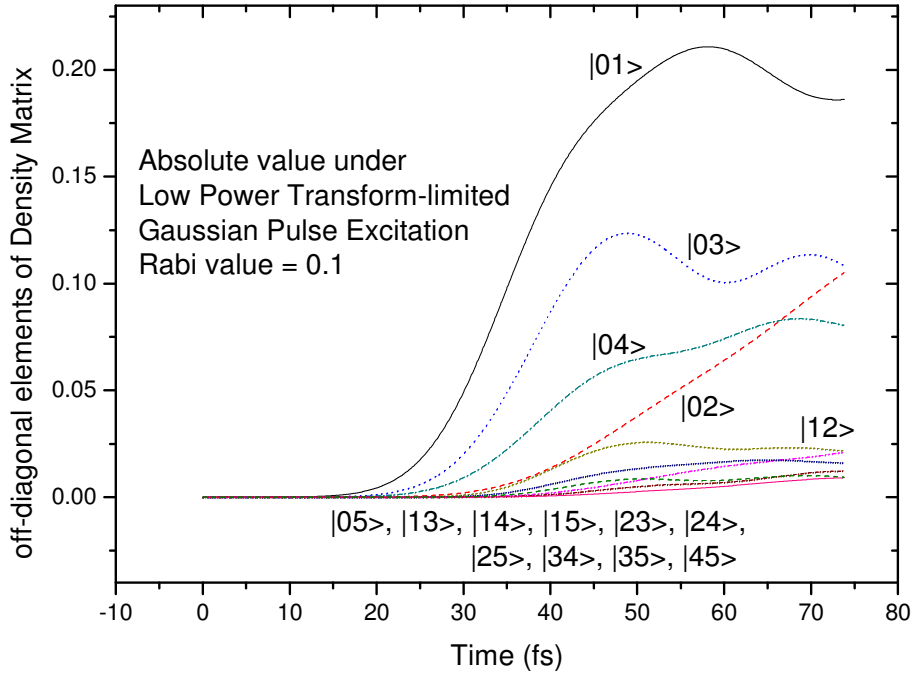
$$\hbar \begin{pmatrix} |0\rangle & |1\rangle & |2\rangle & |3\rangle & |4\rangle & \cdots \\ 0 & \Omega_1(t) & 0 & 0 & 0 & \cdots \\ \Omega_1(t) & \delta_1(t) & V_{12} & V_{12} & V_{12} & \cdots \\ 0 & V_{12} & \delta_2(t) & V_{12} & V_{12} & \cdots \\ 0 & V_{12} & V_{12} & \delta_3(t) & V_{12} & \cdots \\ 0 & V_{12} & V_{12} & V_{12} & \delta_4(t) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

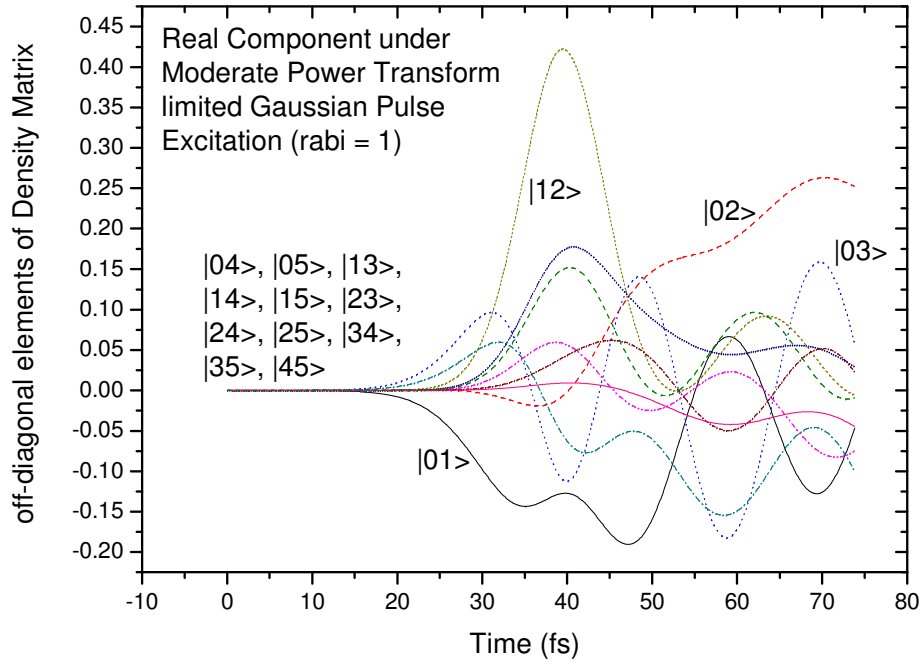


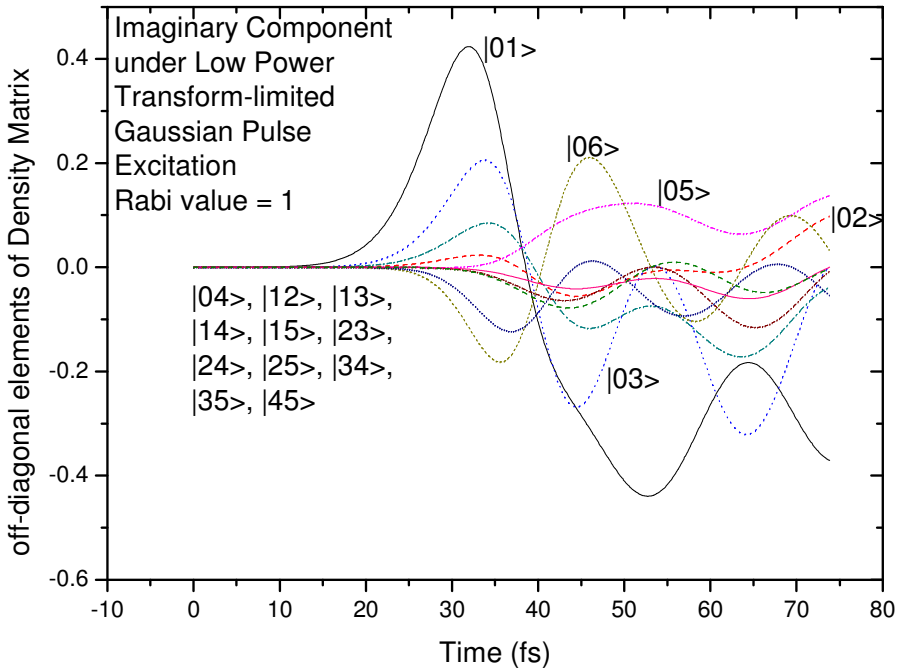

Normalized Population
1.0
0.8
0.6
0.4
0.2
0.0
-10
0
10
20
30
40
50
60
70
80
Time (fs)
|0>
|1>
|2>
|3>
|4>
|5>
Dressed State Character
1.0
0.5
0.0
0
20
40
60
80
Time (fs)
Eigen energy (arb. units)
10
5
0
-5
0
20
40
60
80
Time (fs)

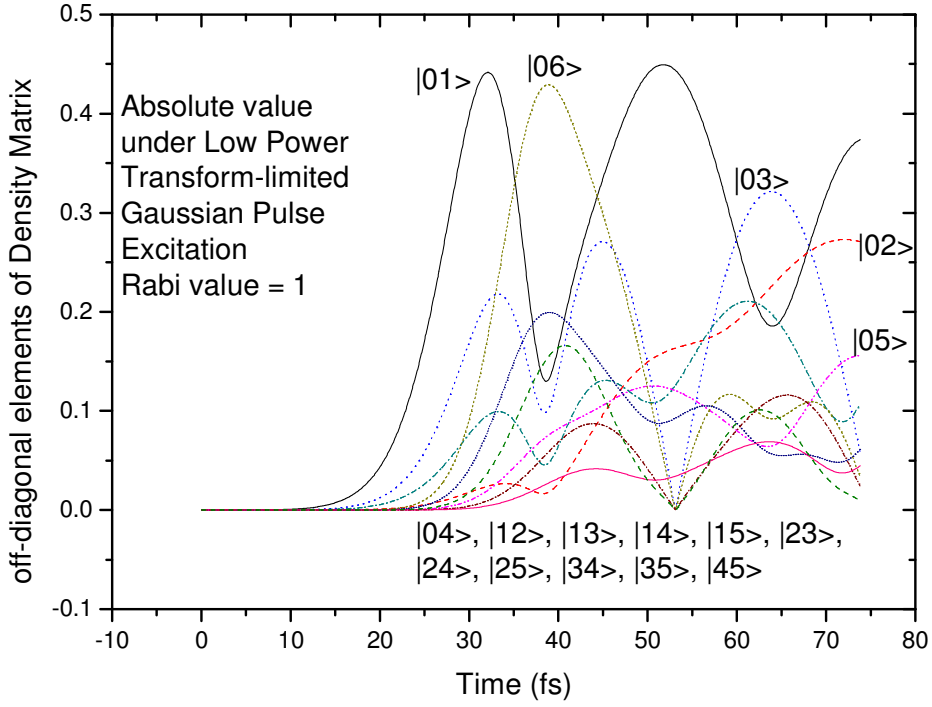

off-diagonal elements of Density Matrix
Time (fs)
|04>, |05>, |12>, |13>, |14>, |15>,
|23>, |24>, |25>, |34>, |45>
|35>
|03>
|01>
|02>
Real Component under
Low Power Transform-limited
Gaussian Pulse Excitation

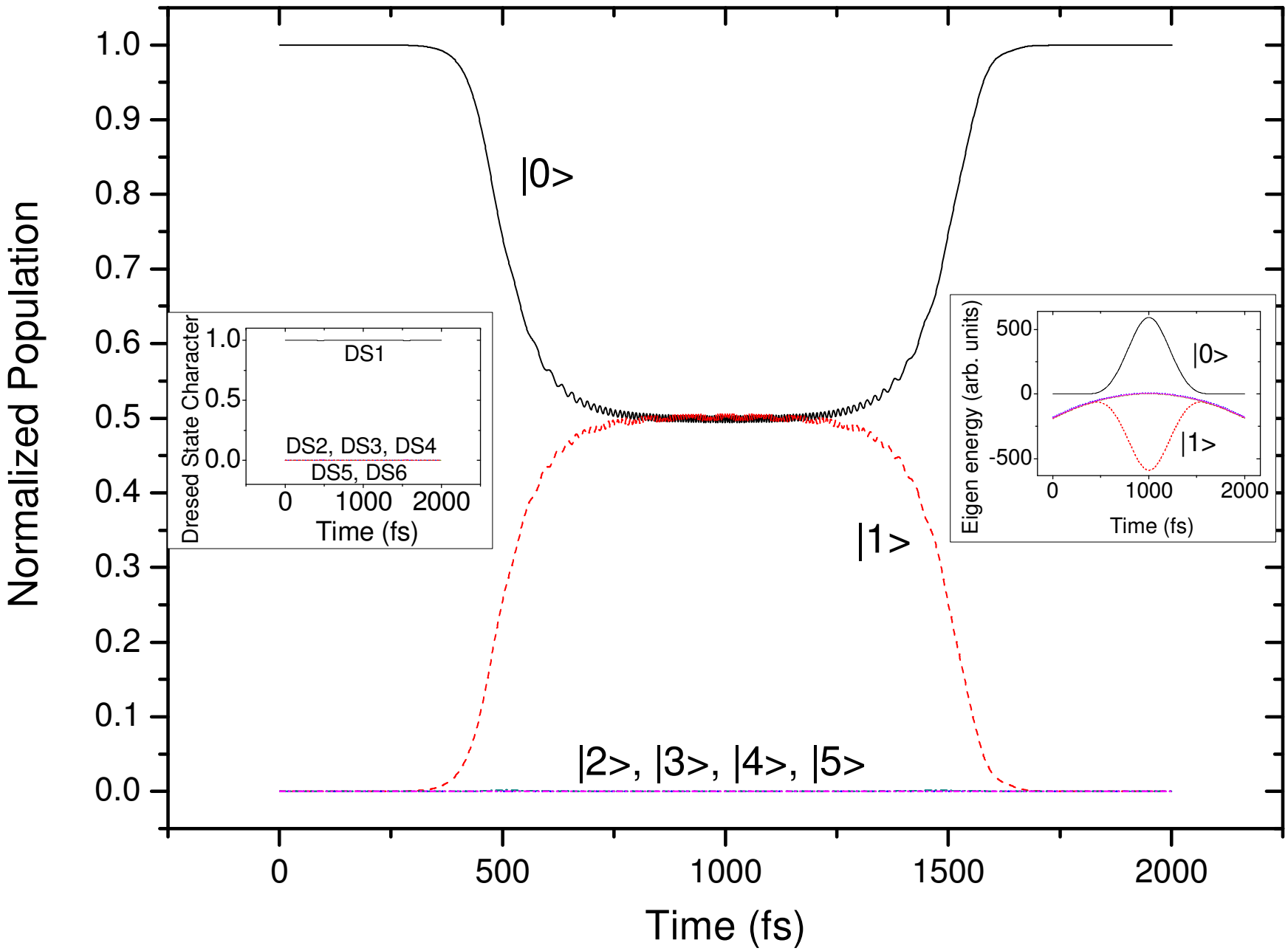

off-diagonal elements of Density Matrix
Time (fs)
|01>
|03>
|04>
|05>
|12>, |13>, |14>, |15>, |23>, |24>,
|25>, |34>, |35>, |45>
|02>
Imaginary Component under
Low Power Transform-limited
Gaussian Pulse Excitation
Rabi value = 0.1

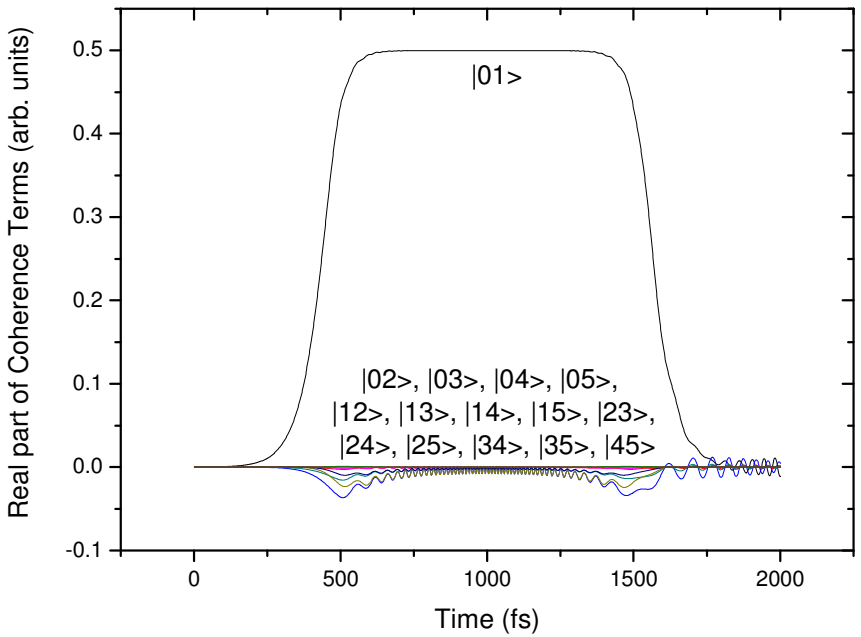

off-diagonal elements of Density Matrix
Time (fs)
|01>
|03>
|04>
|02>
|12>
|05>, |13>, |14>, |15>, |23>, |24>,
|25>, |34>, |35>, |45>
Absolute value under
Low Power Transform-limited
Gaussian Pulse Excitation
Rabi value = 0.1

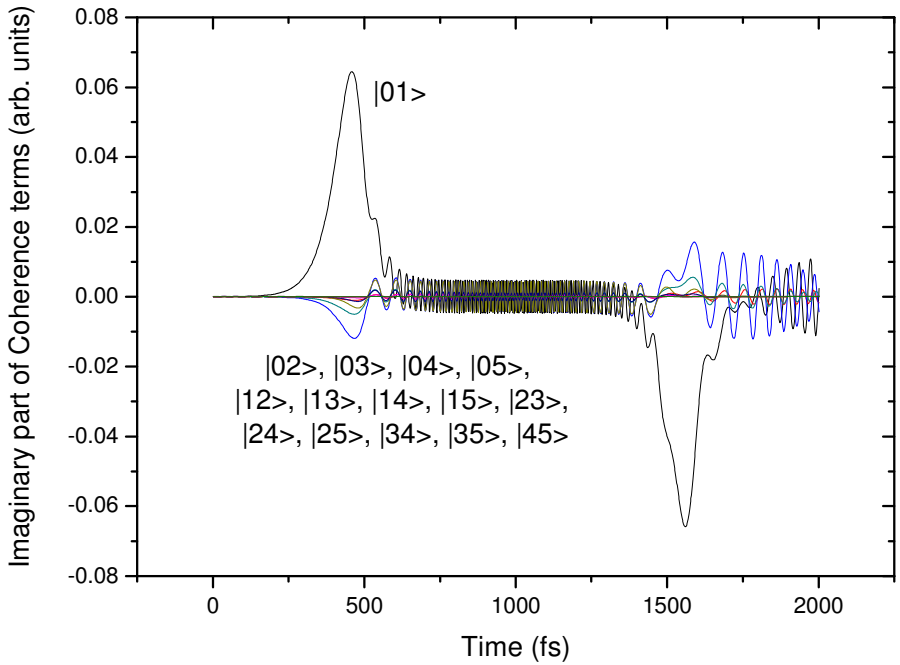

Real Component under
Moderate Power Transform
limited Gaussian Pulse
Excitation (rabi = 1)
|12>
|02>
|03>
|04>, |05>, |13>,
|14>, |15>, |23>,
|24>, |25>, |34>,
|35>, |45>
|01>
off-diagonal elements of Density Matrix
Time (fs)

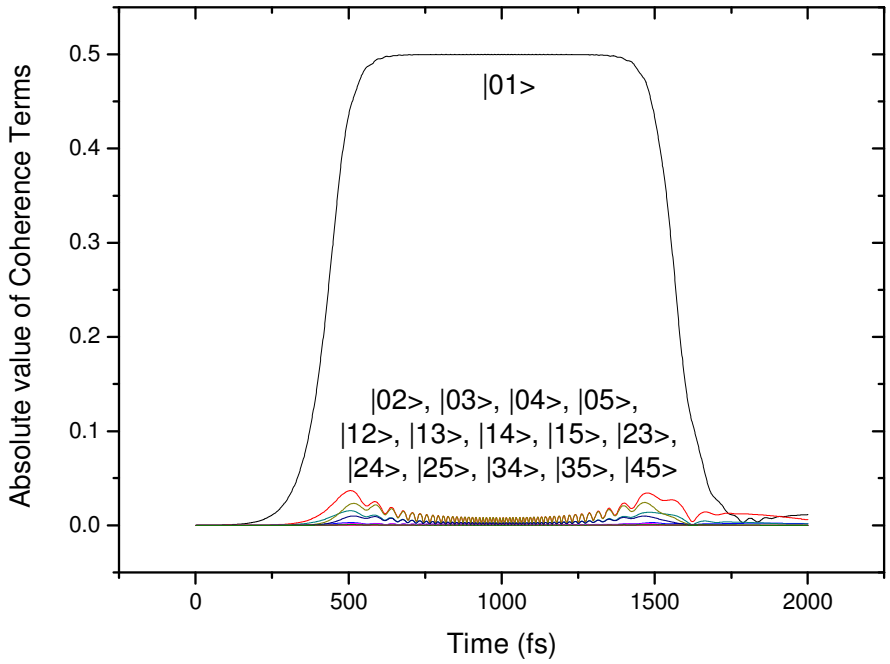

Imaginary Component
under Low Power
Transform-limited
Gaussian Pulse
Excitation
Rabi value = 1
|01>
|06>
|05>
|02>
|04>, |12>, |13>,
|14>, |15>, |23>,
|24>, |25>, |34>,
|35>, |45>
|03>
off-diagonal elements of Density Matrix
Time (fs)


Absolute value
under Low Power
Transform-limited
Gaussian Pulse
Excitation
Rabi value = 1
|01>
|06>
|03>
|02>
|05>
|04>, |12>, |13>, |14>, |15>, |23>,
|24>, |25>, |34>, |35>, |45>
off-diagonal elements of Density Matrix
Time (fs)


Normalized Population
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
500
1000
1500
2000
Time (fs)
|0>
|1>
|2>, |3>, |4>, |5>
Dresed State Character
1.0
0.5
0.0
DS1
DS2, DS3, DS4
DS5, DS6
0
1000
2000
Time (fs)
Eigen energy (arb. units)
500
0
-500
|0>
|1>
0
1000
2000
Time (fs)

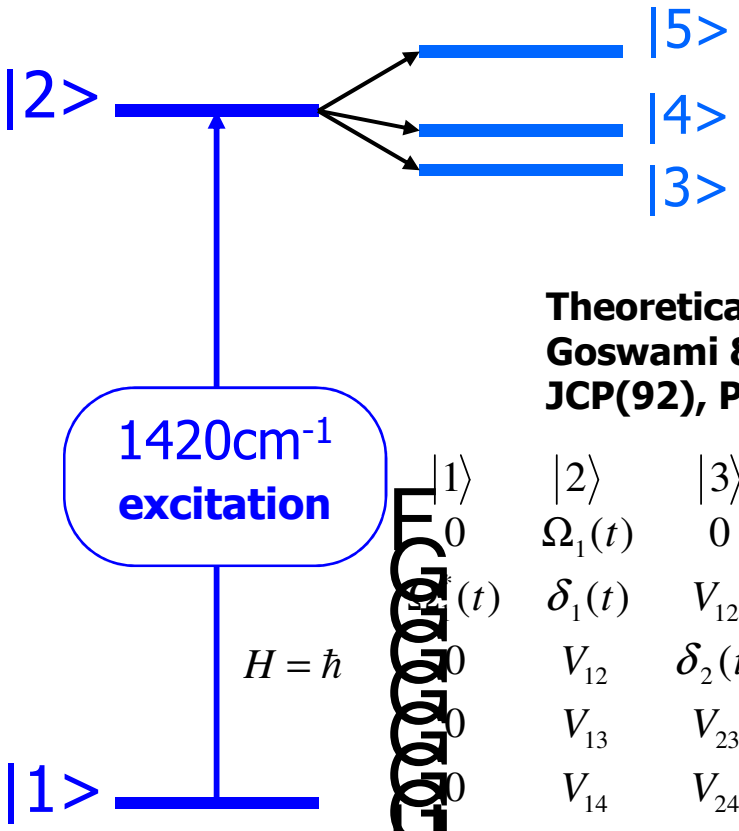

Real part of Coherence Terms (arb. units)
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
0
500
1000
1500
2000
Time (fs)
|01>
|02>, |03>, |04>, |05>,
|12>, |13>, |14>, |15>, |23>,
|24>, |25>, |34>, |35>, |45>


Imaginary part of Coherence terms (arb. units)
0.08
0.06
0.04
0.02
0.00
-0.02
-0.04
-0.06
-0.08
0
500
1000
1500
2000
Time (fs)
|01>
|02>, |03>, |04>, |05>,
|12>, |13>, |14>, |15>, |23>,
|24>, |25>, |34>, |35>, |45>


Absolute value of Coherence Terms
0.5
0.4
0.3
0.2
0.1
0.0
0
500
1000
1500
2000
Time (fs)
|01>
|02>, |03>, |04>, |05>,
|12>, |13>, |14>, |15>, |23>,
|24>, |25>, |34>, |35>, |45>

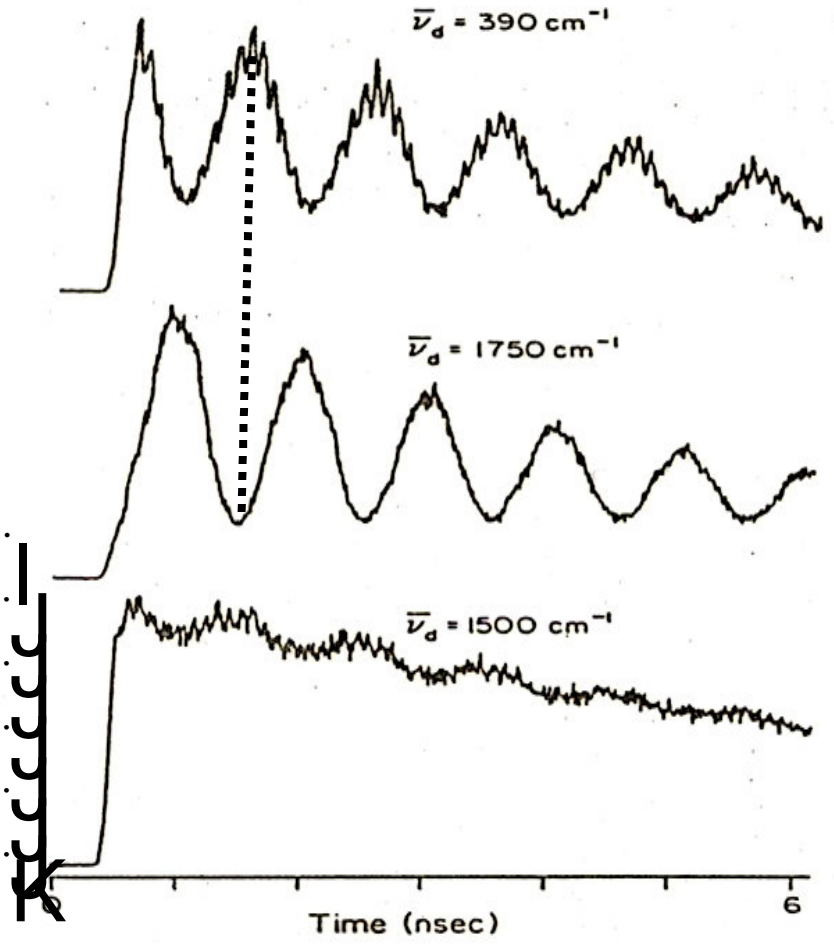
Manifestation of IVR in Anthracene

Effect of Gaussian Pulse



Theoretical Hamiltonian
Goswami & Warren,
JCP(92), PRA(94))

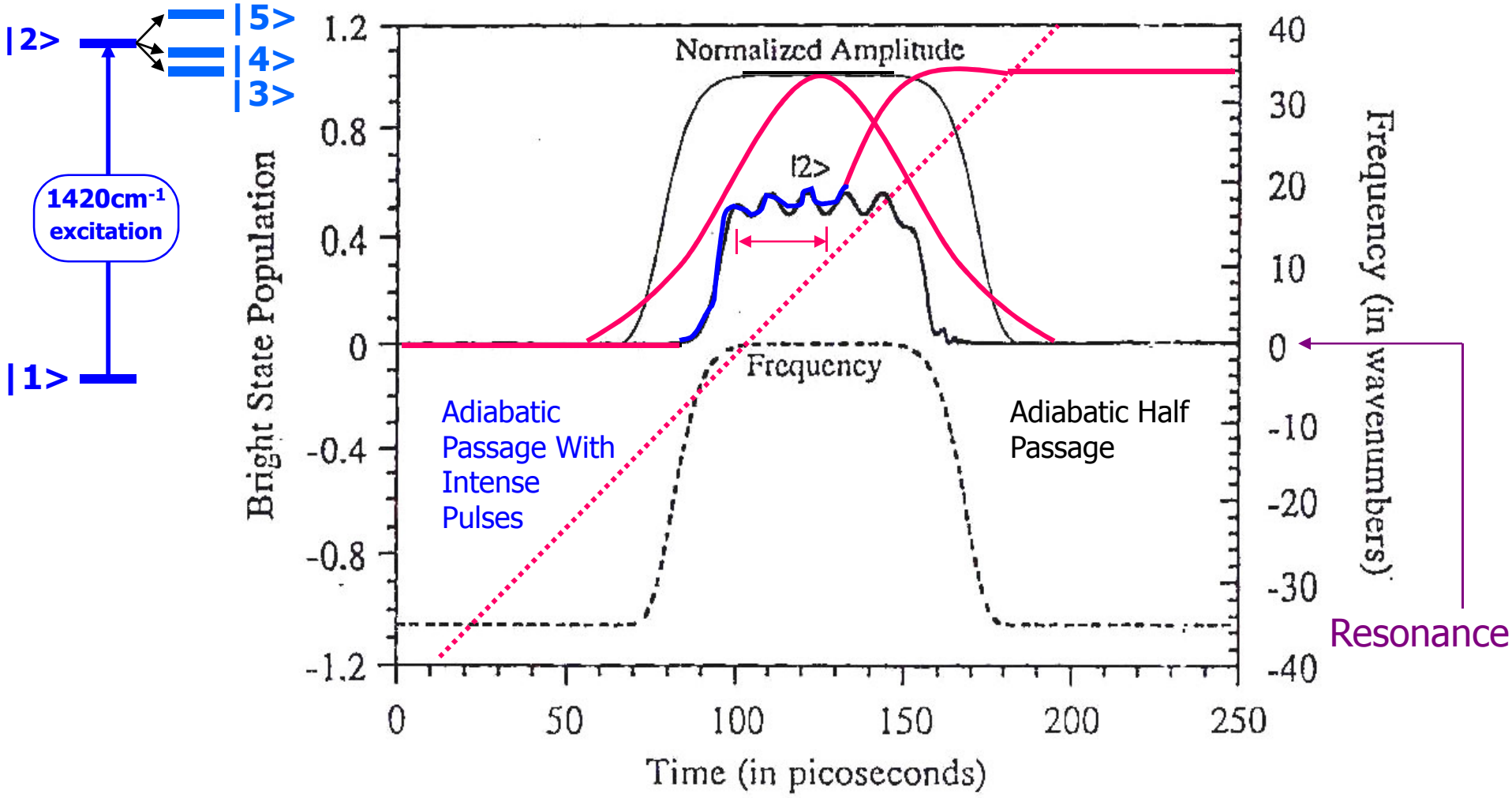
$$H(t) = \begin{array}{c} \\ |1\rangle \\ |2\rangle \\ |3\rangle \\ |4\rangle \\ |5\rangle \\ \vdots \end{array} \begin{array}{c} \begin{array}{ccccc} |1\rangle & |2\rangle & |3\rangle & |4\rangle & |5\rangle & \cdots \end{array} \\ \begin{pmatrix} 0 & \Omega_1(t) & 0 & 0 & 0 & \cdots \\ \Omega_1(t) & \delta_1(t) & V_{12} & V_{13} & V_{14} & \cdots \\ 0 & V_{12} & \delta_2(t) & V_{23} & V_{24} & \cdots \\ 0 & V_{13} & V_{23} & \delta_3(t) & V_{34} & \cdots \\ 0 & V_{14} & V_{24} & V_{34} & \delta_4(t) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \end{array}$$



Experimental Results: Felkar & Zewail, 82, 2961-3010 (1985)

Model Calculations with Shaped Pulses

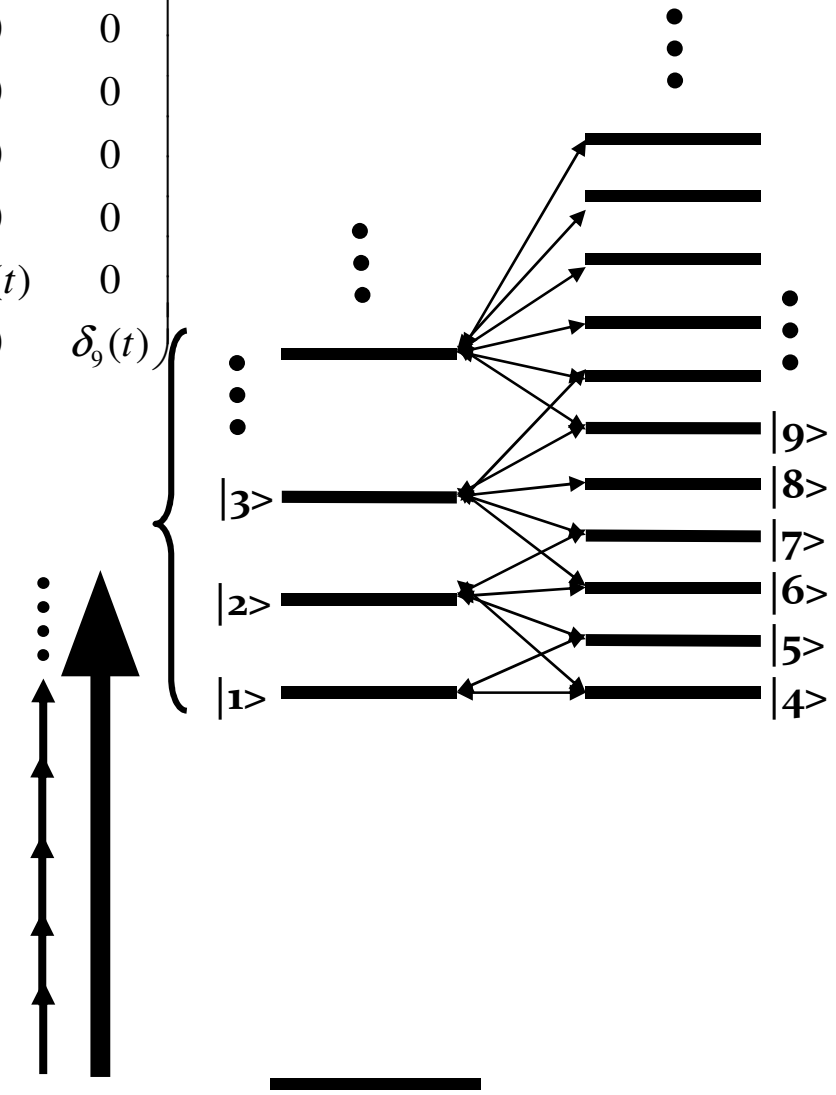
Anthracene



Phys. Rev. Lett. 88, 177901 (2002); J. Chem. Phys. 127, 124305 (2007)

$$
\begin{array}{c}
\begin{array}{ccccccccccc}
 & |0\rangle & |1\rangle & |2\rangle & |3\rangle & |4\rangle & |5\rangle & |6\rangle & |7\rangle & |8\rangle & |9\rangle
\end{array} \\
\hbar \begin{pmatrix}
0 & \Omega_1(t) & \Omega_2(t) & \Omega_3(t) & 0 & 0 & 0 & 0 & 0 & 0 \\
\Omega_1^*(t) & \delta_1(t) & V_{12} & V_{13} & V_{14} & V_{15} & 0 & 0 & 0 & 0 \\
\Omega_2^*(t) & V_{12} & \delta_2(t) & V_{23} & V_{24} & V_{25} & V_{26} & V_{27} & 0 & 0 \\
\Omega_3^*(t) & V_{13} & V_{23} & \delta_3(t) & 0 & 0 & V_{36} & V_{37} & V_{38} & V_{39} \\
0 & V_{14} & V_{24} & 0 & \delta_4(t) & 0 & 0 & 0 & 0 & 0 \\
0 & V_{15} & V_{25} & 0 & 0 & \delta_5(t) & 0 & 0 & 0 & 0 \\
0 & 0 & V_{26} & V_{36} & 0 & 0 & \delta_6(t) & 0 & 0 & 0 \\
0 & 0 & V_{27} & V_{37} & 0 & 0 & 0 & \delta_7(t) & 0 & 0 \\
0 & 0 & 0 & V_{38} & 0 & 0 & 0 & 0 & \delta_8(t) & 0 \\
0 & 0 & 0 & V_{39} & 0 & 0 & 0 & 0 & 0 & \delta_9(t)
\end{pmatrix}
\end{array}
$$

Tier Model of IVR



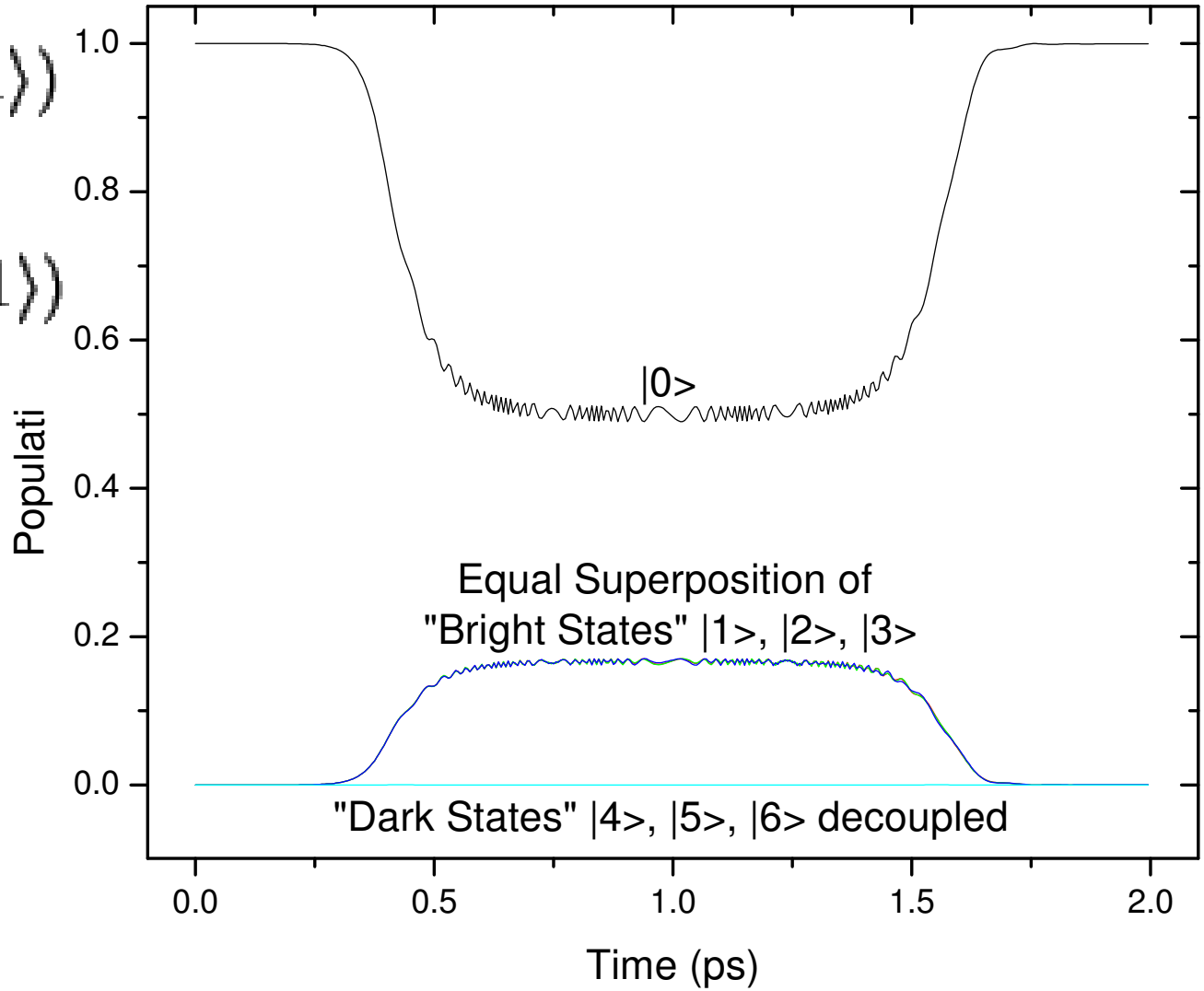
Example of Hadamard Gate in Molecules

Equal superposition between quantum states

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$|1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

More than two states: "Qudits"



Probe Coherence ⇒ Off-Diagonal Elements

From Spectroscopy: All absorptions associated with dispersion

Kramer-Kronig relationship

⇒ All absorptions composed of Real part + Imaginary part

where Real part ⇒ Dispersive part

Imaginary part ⇒ Absorption

Rabi Flopping ⇒ Coupling through absorption

Adiabatic Process ⇒ Coupling through the Dispersive part—no absorption process

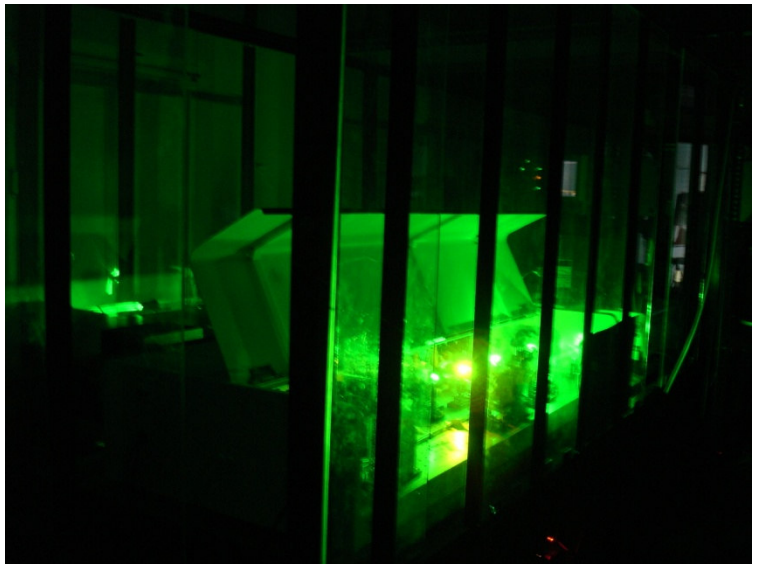
⇒ No population flopping

Benefits of such study:

- **Quantification of 2-level character in a multilevel system**
- **Off-diagonal density matrix elements switch from real to imaginary**
  - **Excitation process changes from being resonant to completely adiabatic**

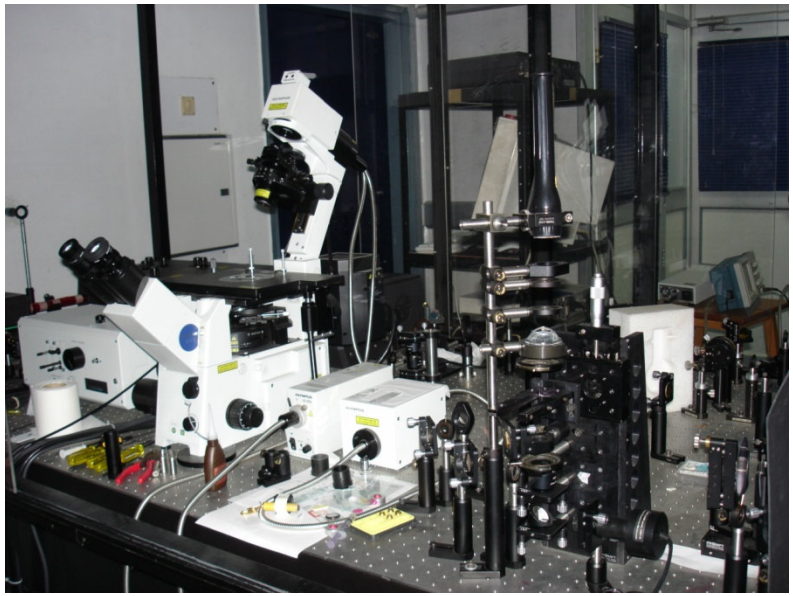
J. Chem. Phys. 127, 124305 (2007)

1 mJ/pulse @ 40fs with 1 kHz rep rate

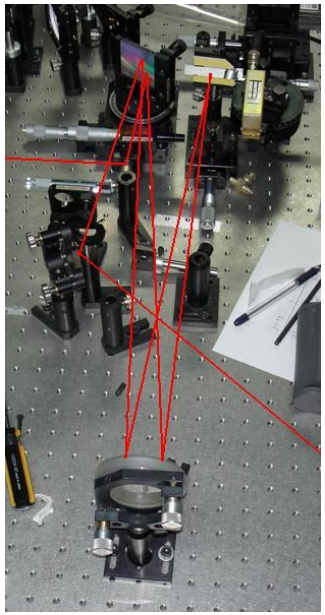


Home Built Femtosecond Oscillator with Commercial Amplifier

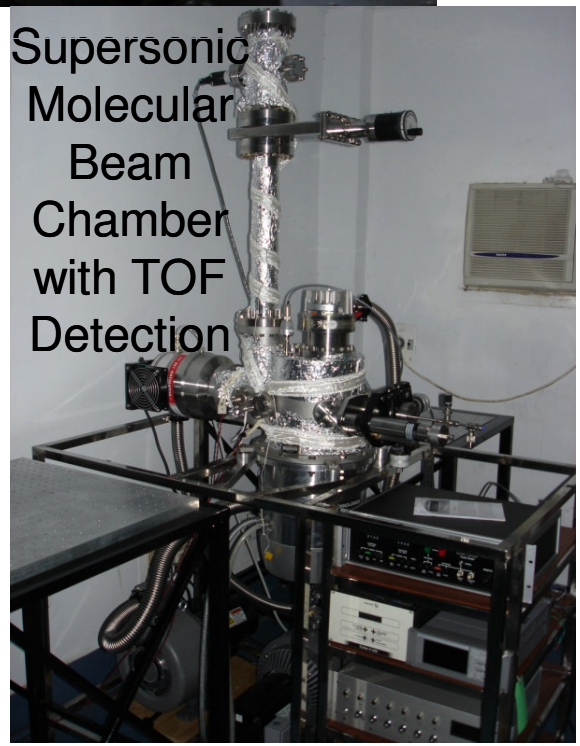
Technology



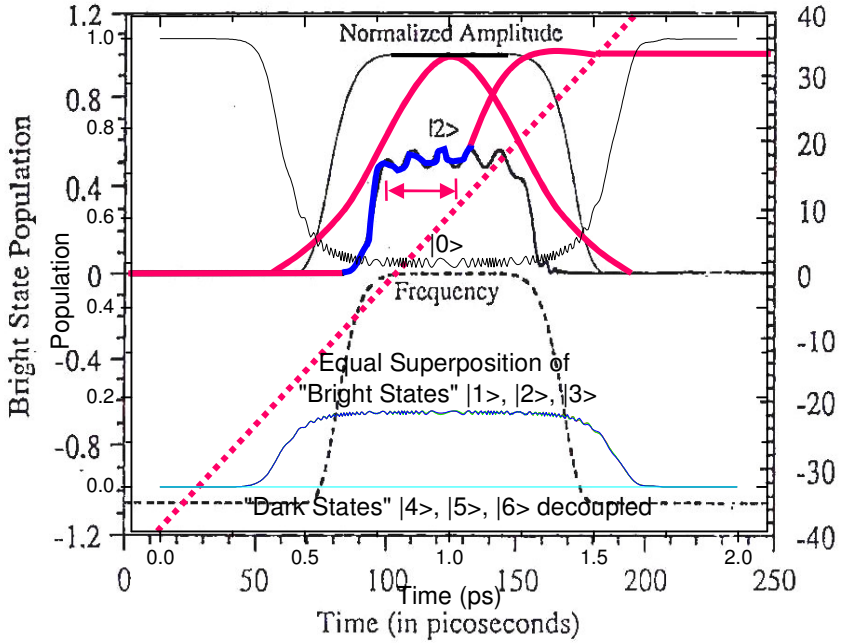
Confocal Microscope & Tweezer



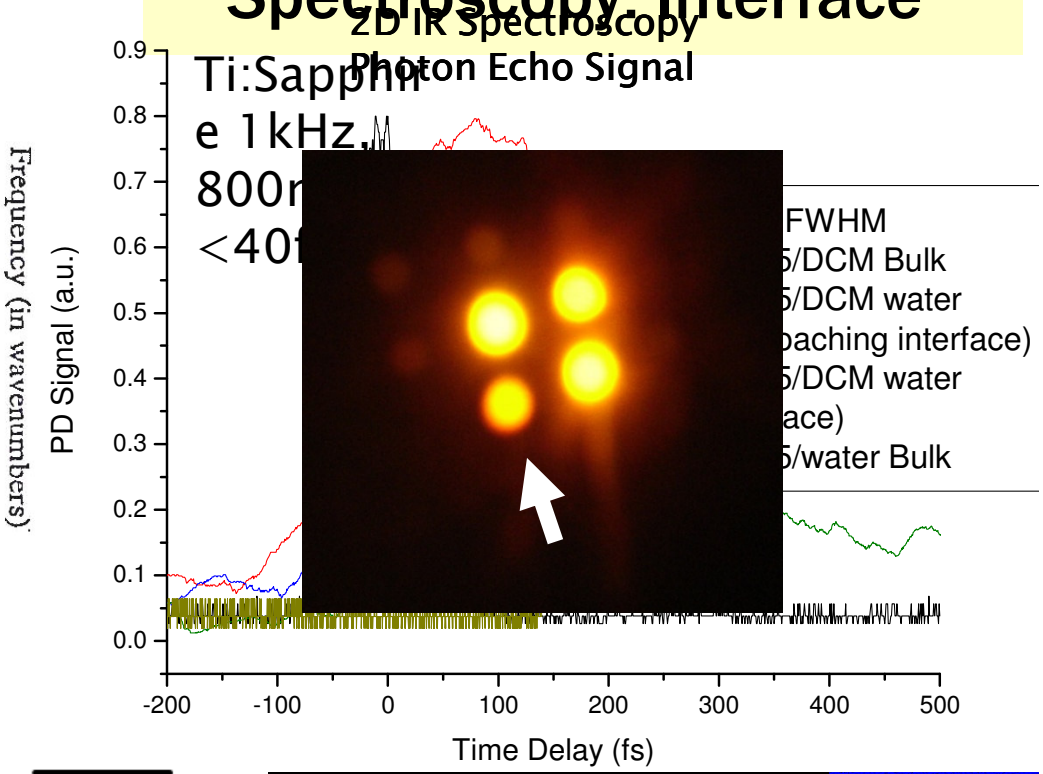
4-F Pulse Shaper



Model Calculations with Shaped Pulses: Quantum Computing

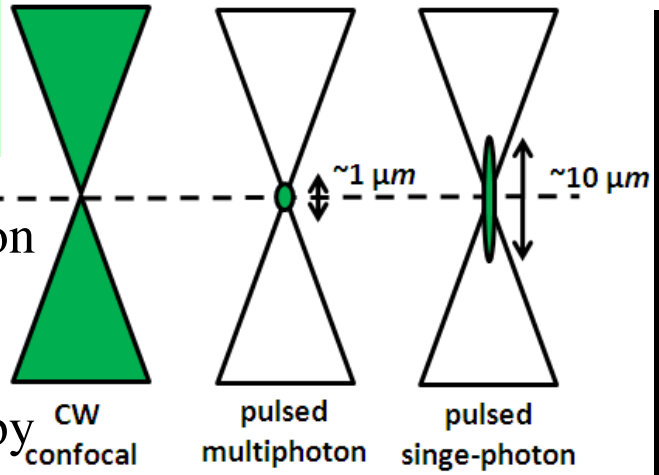


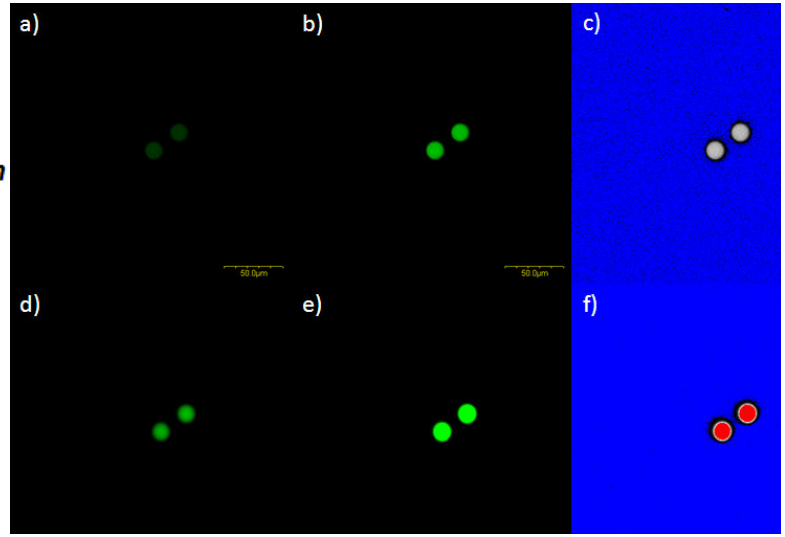
Femtosecond Pump-Probe Spectroscopy: Interface



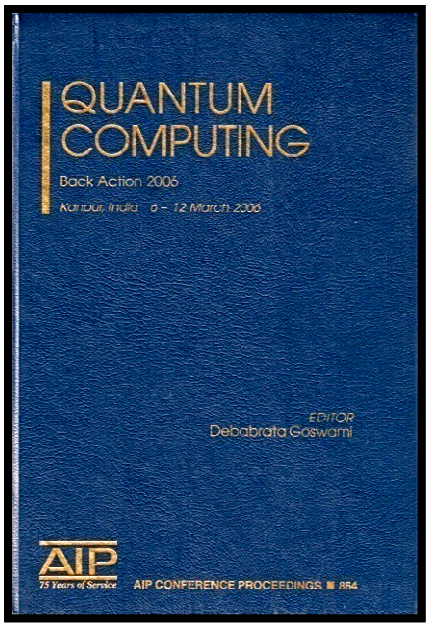
Multiphoton Imaging & Optical Tweezer

Fluorescence generation (shown as green) in confocal, multiphoton and the new microscopy method presented here.





References & Announcement



Watch out for the Back-Action-II early next year!!

- Int. J. Quant. Info. **5**, 179 -188 (2007)
- J. Chem. Phys. **127**, 124305 (2007).