Control and Decoherence:
Weak Field Control of Excited State Objective

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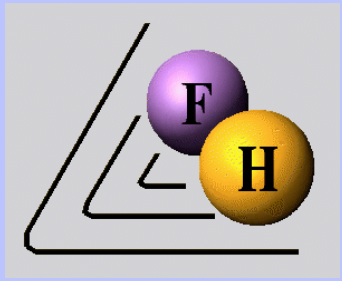


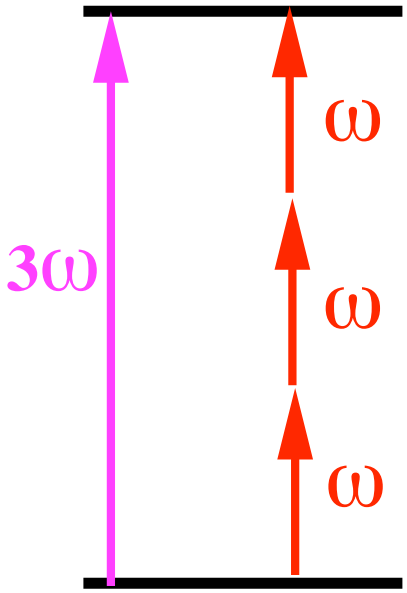
Decoherence in Quantum Dynamical Systems: April 26–30 2010

1) Embed an open system in a larger wavefunction

2) Embed a unitary evolution in an open system

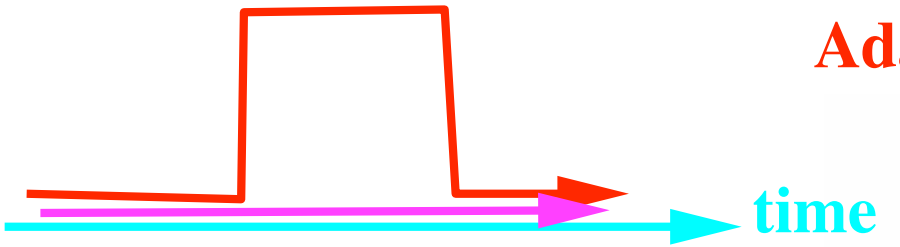
Principles of coherent control

Constructive interference in the desired channel
and destructive interference in all other channels



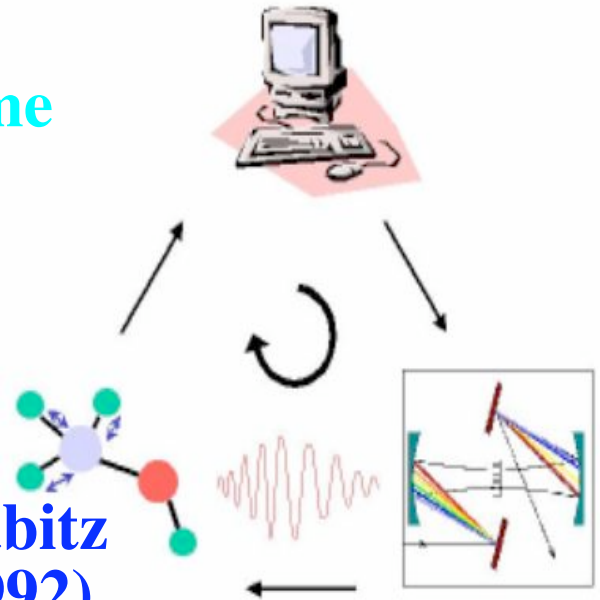
Brumer Shapiro

Pump dump



Tannor Rice Kosloff

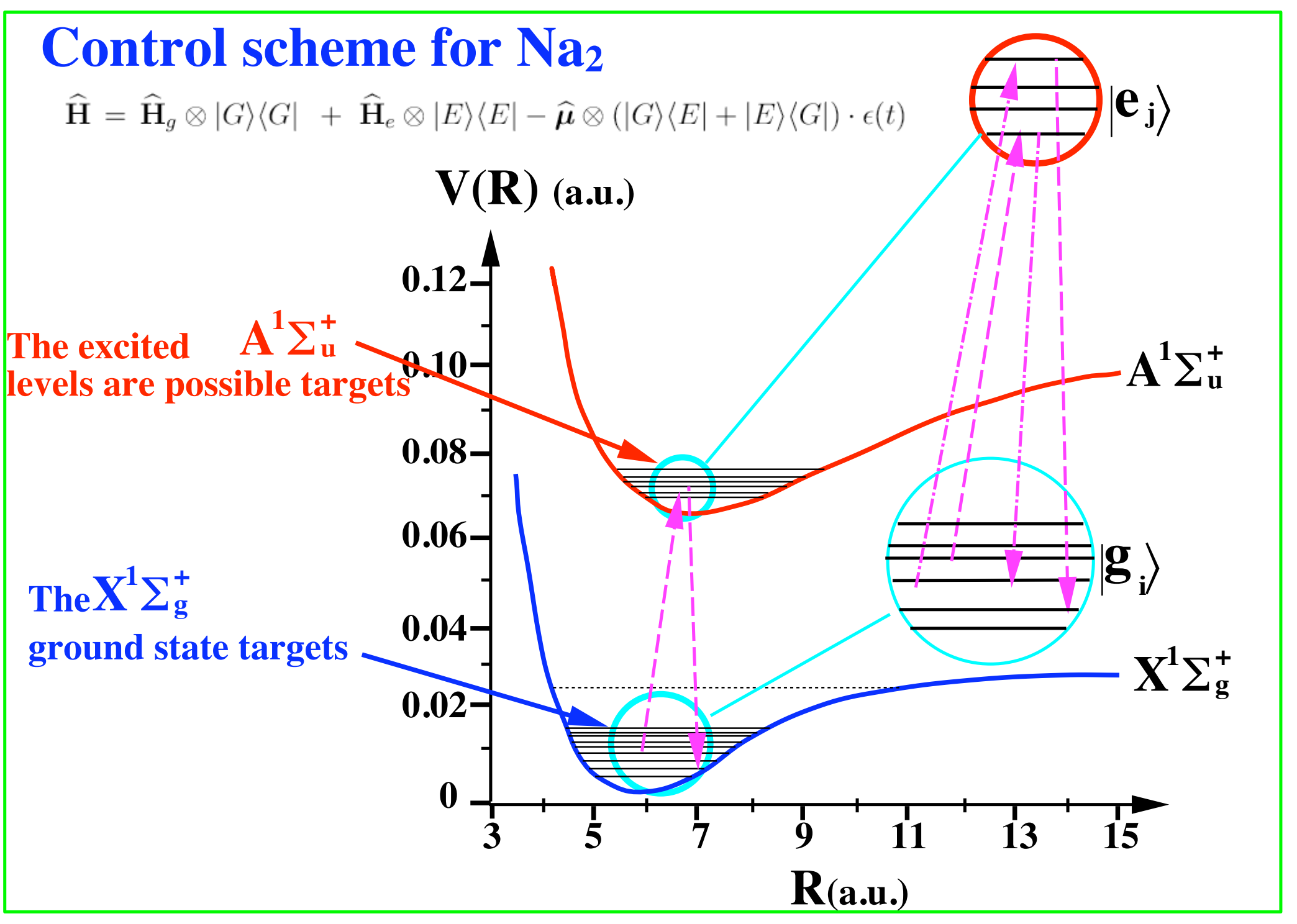
Adaptive learning



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

Control scheme for Na_2

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



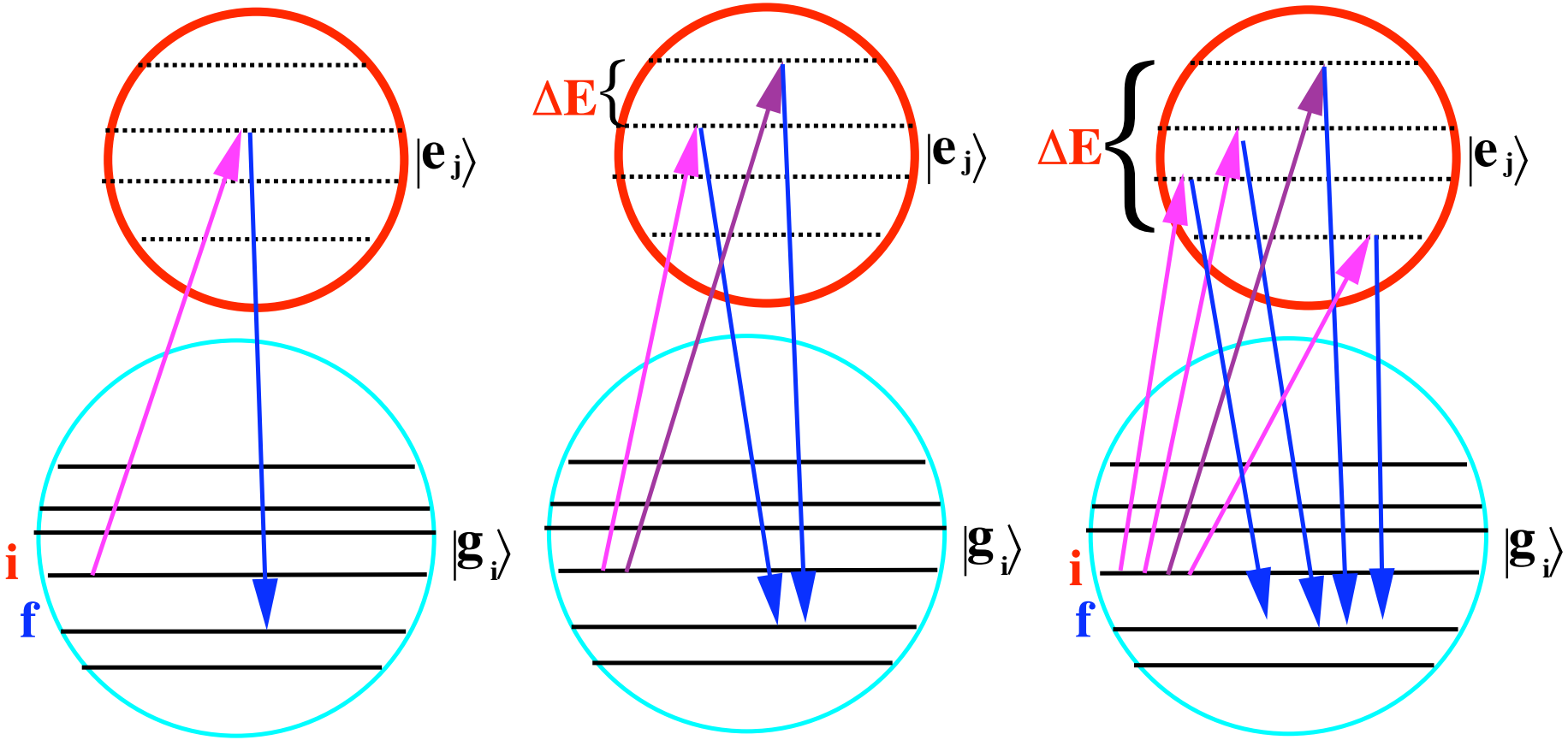
Principles of coherent control: ground state

i → f

I
State–to–State Weak field

II
State–to–State Weak field
Coherent Control

III
State–to–State Weak field
More Coherent Control



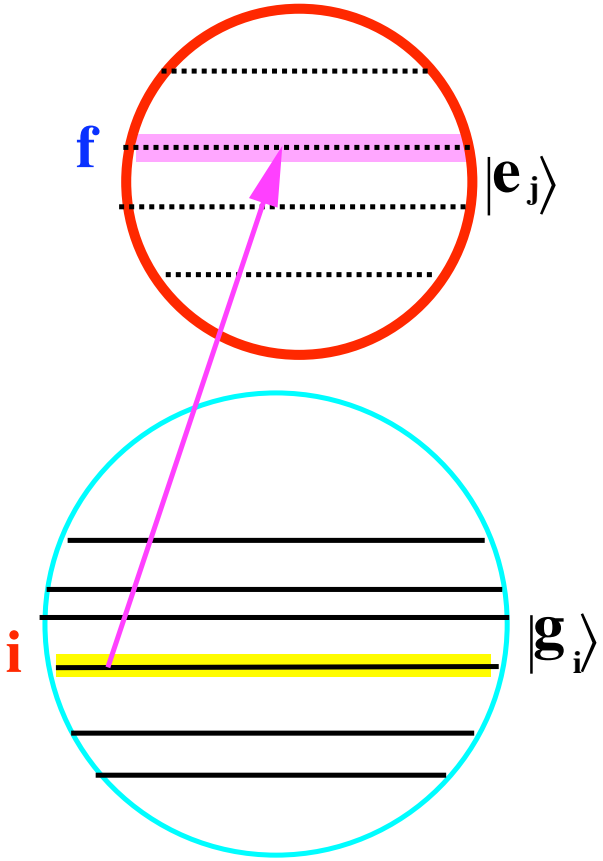
		I	II	III
Band width	ΔE	very small	vibratioanl spacing	N vibratioanl spacings
Time scale	Δt	adiabatic	vibrational period	vibrational period
# of paths		1	2	N

Principles of coherent control: Excited state

$i \rightarrow f$

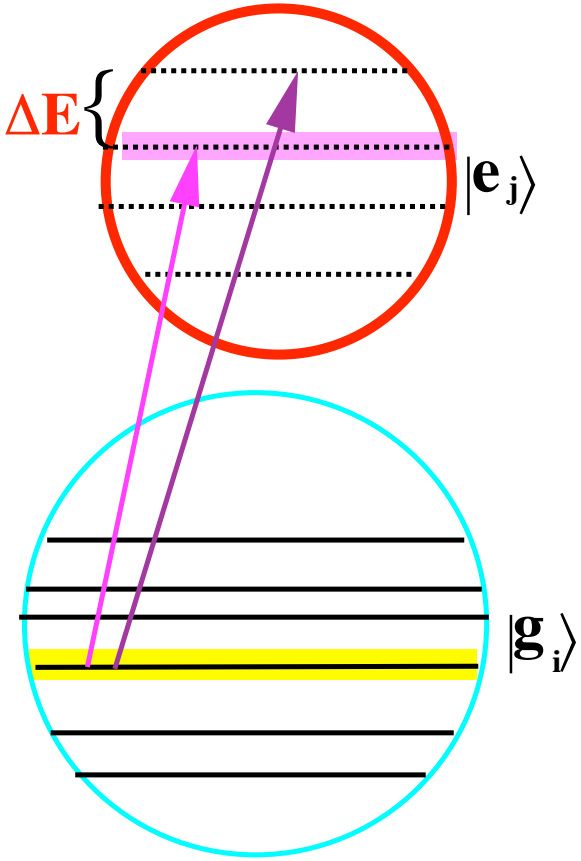
I

State–to–State Weak field



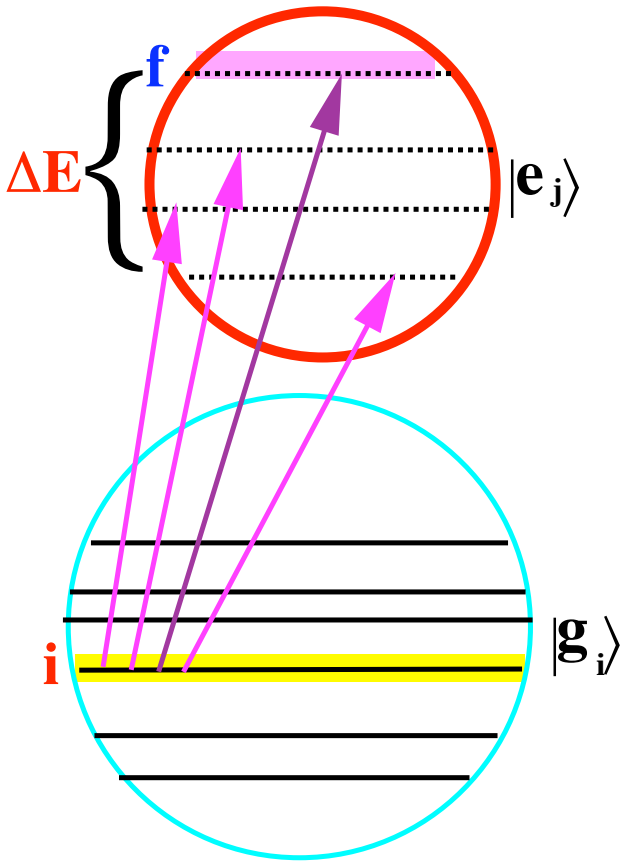
II

State–to–State Weak field
Coherent Control ?



III

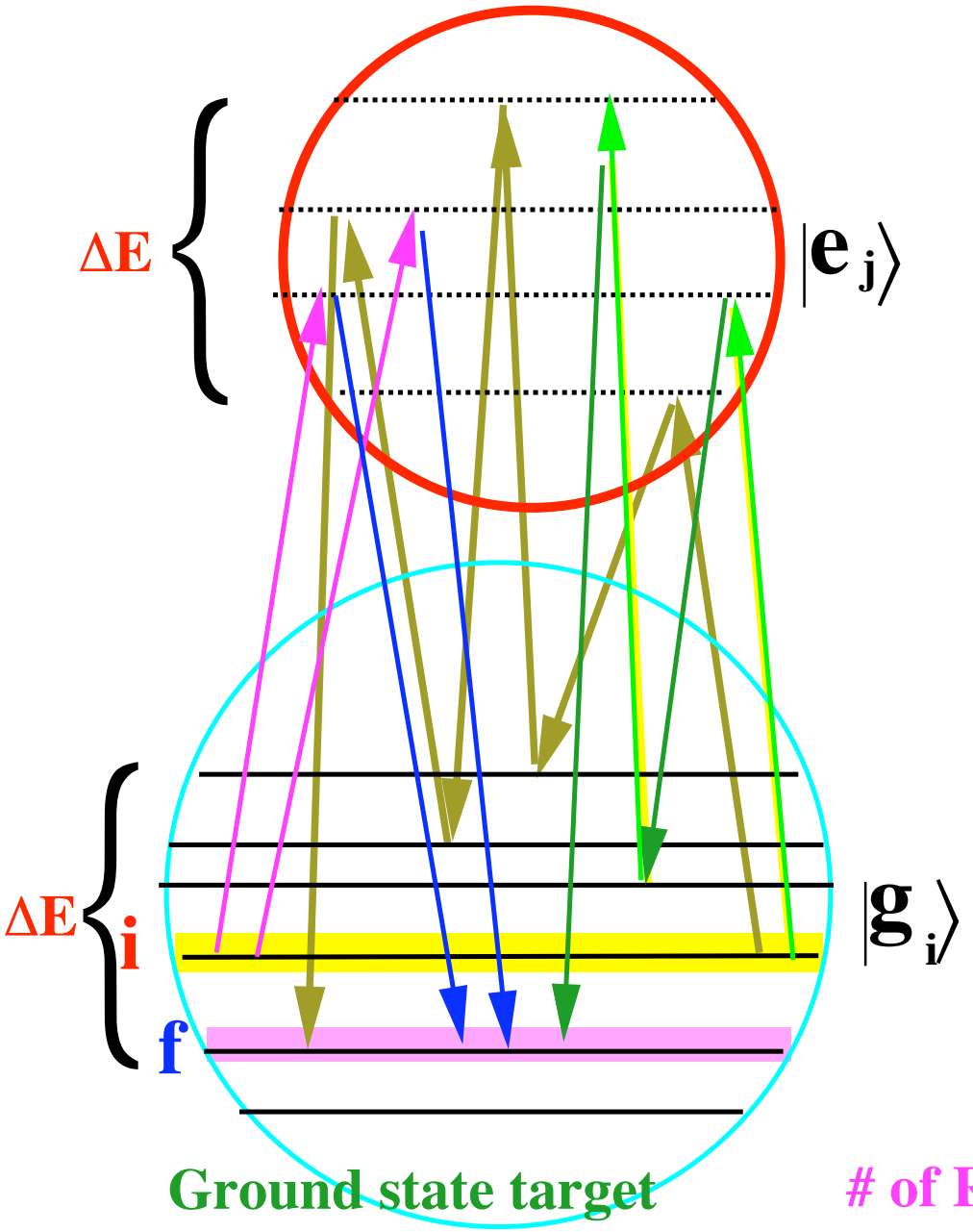
State–to–State Weak field
More Coherent Control ?



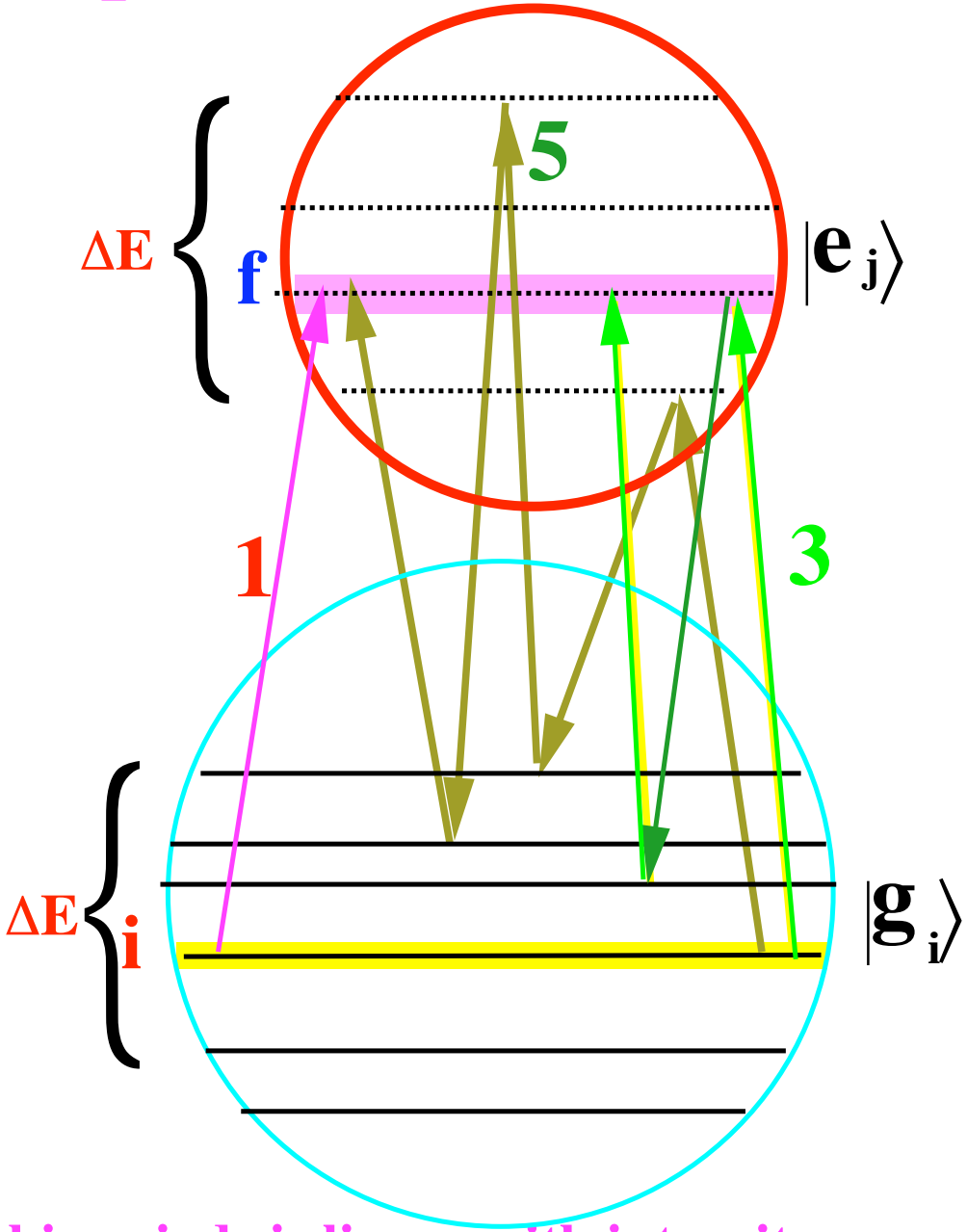
		I	II	III
Band width	ΔE	very small	vibratioanl spacing	N vibratioanl spacings
Time scale	Δt	adiabatic	vibrational period	vibrational period
# of paths		1	2	N

State–to–State strong field
More Coherent Control

$i \rightarrow f$

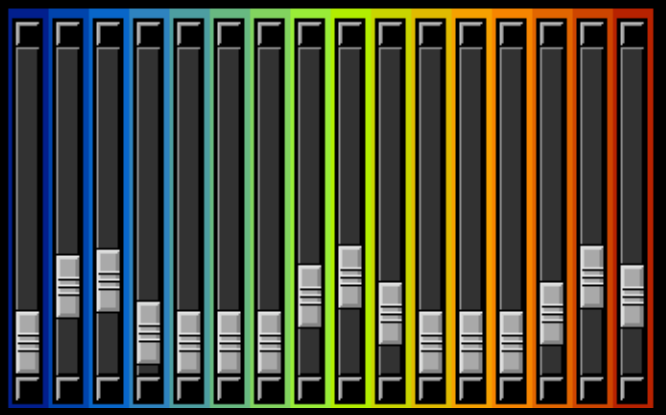


Excited state target

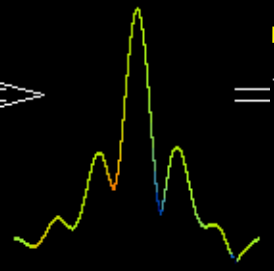


# of Rabi periods is linear with intensity

Spatial light modulator

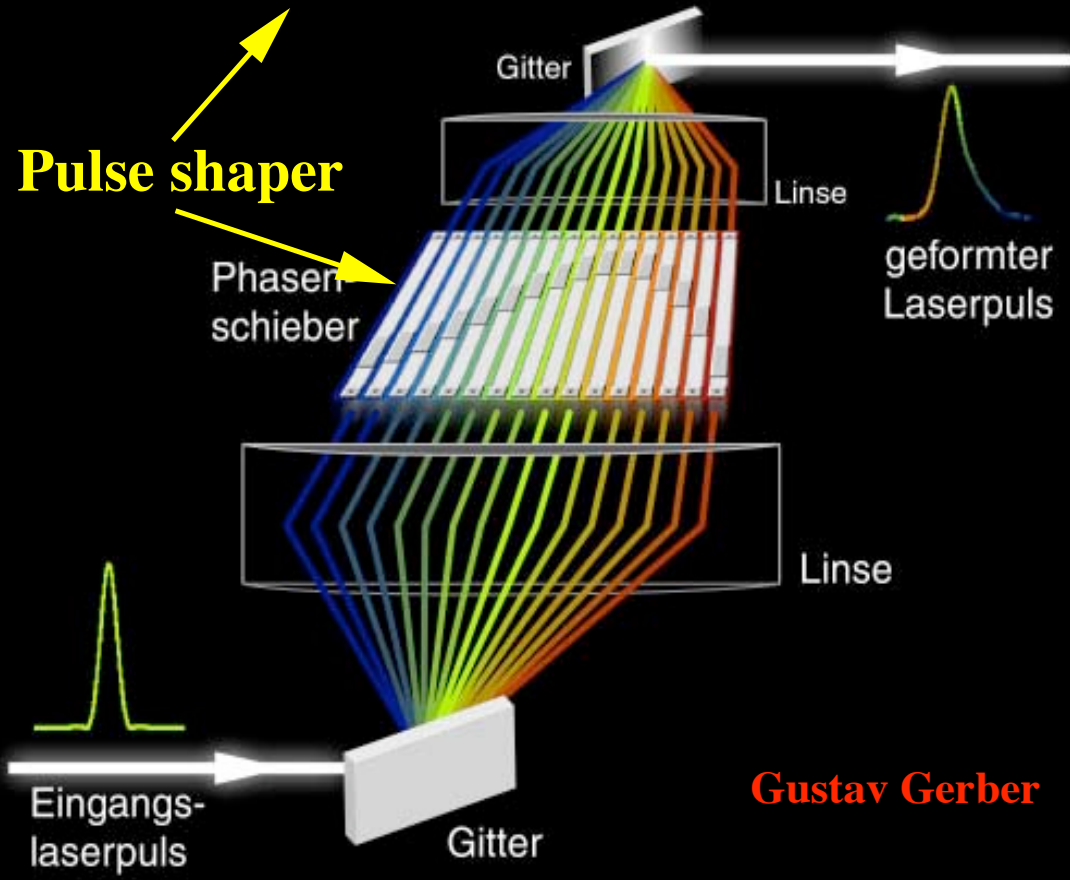


The shaped pulse in time

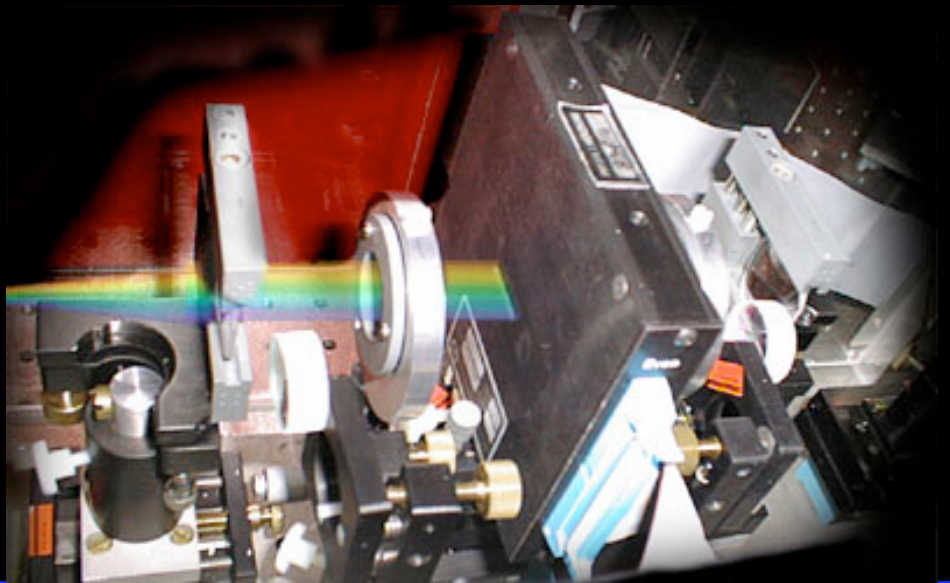


The molecules

Pulse shaper



Spatial light Modulator



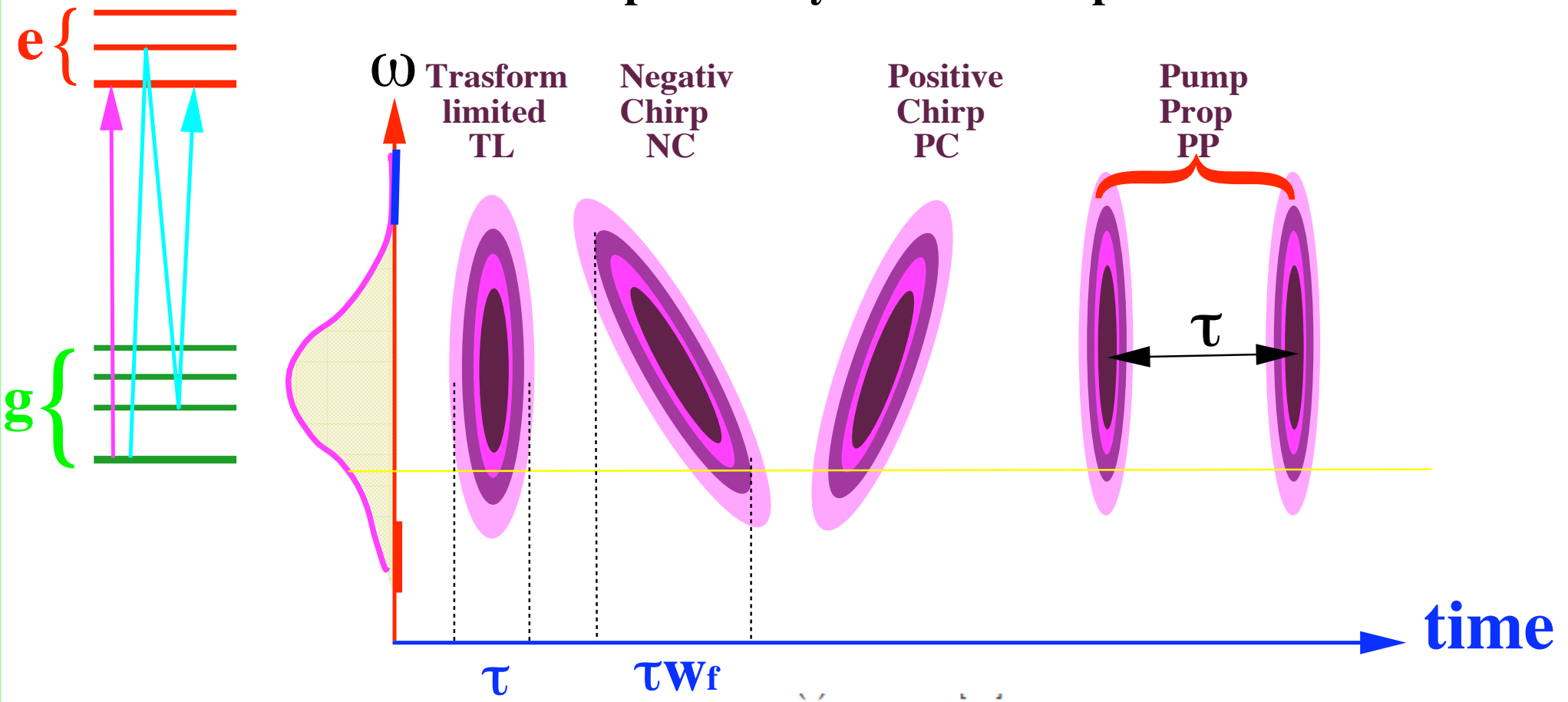
Gustav Gerber

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

The problem of weak field coherent control

A necessary condition is at least two indistinguishable pathways

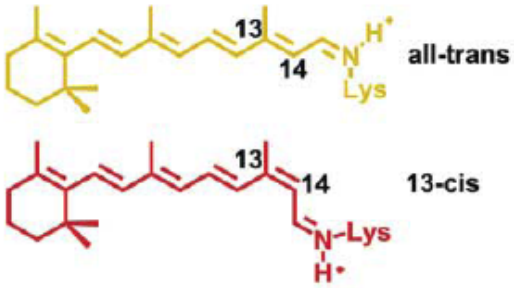
If the target operator P commutes with H , [P,H]=0
then weak field phase only control is impossible

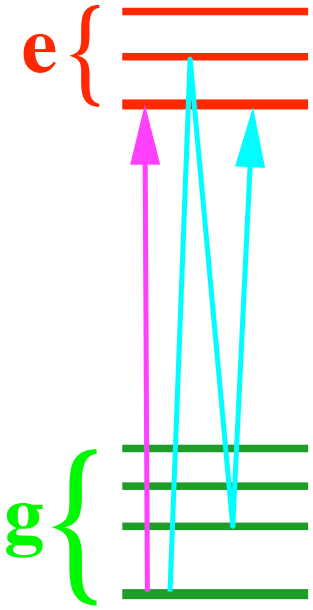


$$\epsilon(t) = \tilde{\Omega}_0 \exp\left[-\frac{t^2}{\tau_0^2 + 2i\phi''} + i\omega_0 t\right] = \frac{\Omega_0}{w_F} \exp\left[-\frac{t^2}{w_F^2 \tau_0^2} + i\frac{1}{2}\chi t^2 + i\omega_0 t\right]$$

The problem of weak field coherent control

Experimental evidence for weak field phase only control

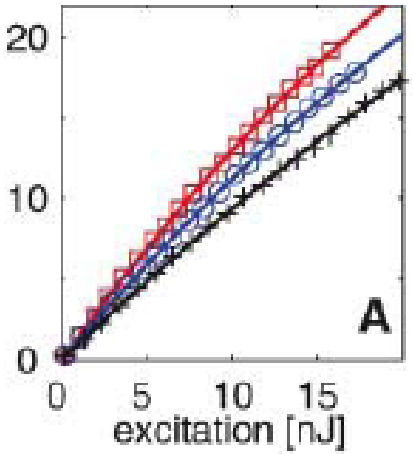


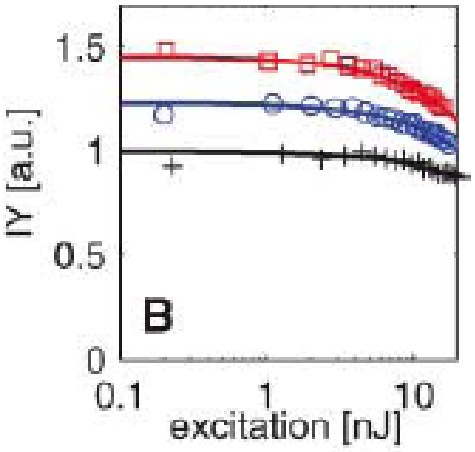


Coherent Control of Retinal Isomerization in Bacteriorhodopsin

Valentyn I. Prokhorenko,[1] Andrea M. Nagy,[1] Stephen A. Waschuk,[2] Leonid S. Brown,[2] Robert R. Birge,[3] R. J. Dwayne Miller[1]*

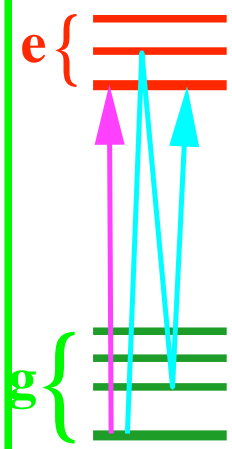
Fig. 6. Energy dependence of (**A**) the ΔA signal, measured at 630 nm 20 ps after excitation, and (**B**) the corresponding isomerization yields. Both plots show results for the optimal (red), anti-optimal (black), and transform-limited (blue) pulses. A quadratic fit (solid lines) shows the energy dependence to be essentially linear at low energies, with a small deviation (due to saturation of the absorbance) of less than 18% at the





The problem of weak field coherent control

Experimental evidence



Comment on "Coherent Control of Retinal Isomerization in Bacteriorhodopsin"

Manuel Joffre[1,2]

Prokhorenko *et al*. (Research Articles, 1 September 2006, p. 1257) reported that, in the weak-field regime, the efficiency of retinal isomerization in bacteriorhodopsin can be controlled by modulating the spectral phase of the photoexcitation pulse. However, in the linear excitation regime, the signal measured in an experiment involving a time-invariant, stationary process can be shown to be independent of the pulse spectral phase.

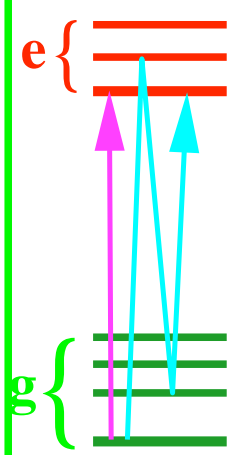
Response to Comment on "Coherent Control of Retinal Isomerization in Bacteriorhodopsin"

Valentyn I. Prokhorenko,[1] Andrea M. Nagy,[1] Stephen A. Waschuk,[2] Leonid S. Brown,[2] Robert R. Birge,[3] R. J. Dwayne Miller[1*]

Joffre attempts to show that the linear response of any quantum system to an external perturbation is phase insensitive, but he uses incorrect mathematical assumptions, misinterprets the time invariance principle, and ignores causality. We argue that the opposite case—an explicit phase dependence for a signal measured in the linear excitation regime—can equally be shown using Joffre's approach and assumptions.

The problem of weak field coherent control

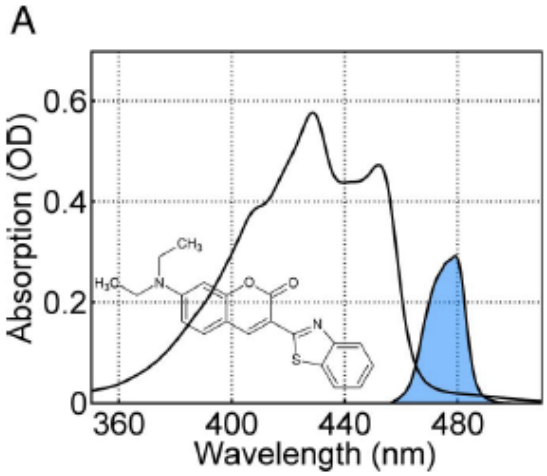
Experimental evidence



Quantum control experiment reveals solvation-induced decoherence

P. van der Walle[a,1], M. T. W. Milder[a], L. Kuipers[a,b], and J. L. Herek[a,b,1]

7714–7717 | PNAS | May 12, 2009 | vol. 106 | no. 19



Optimal pulse shape

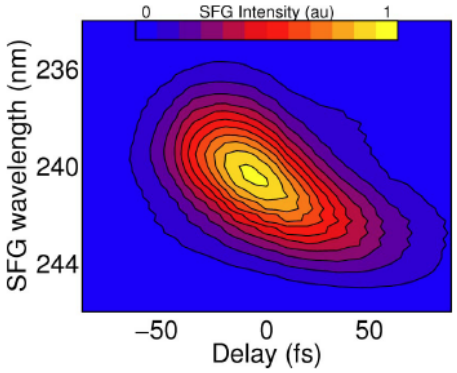
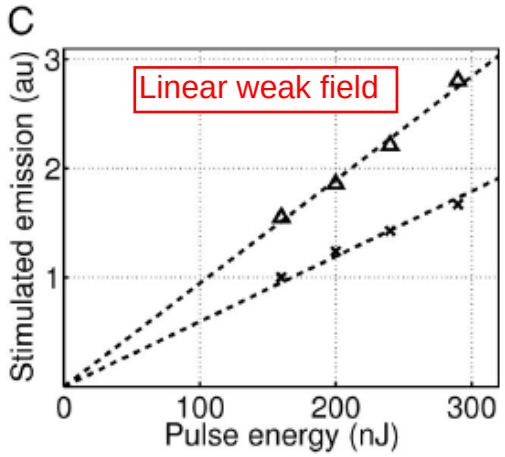
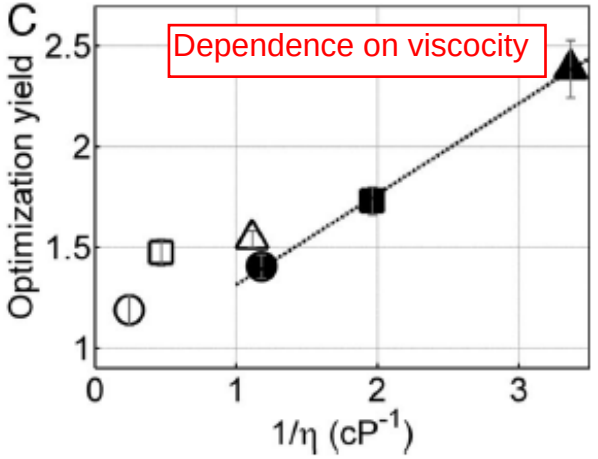


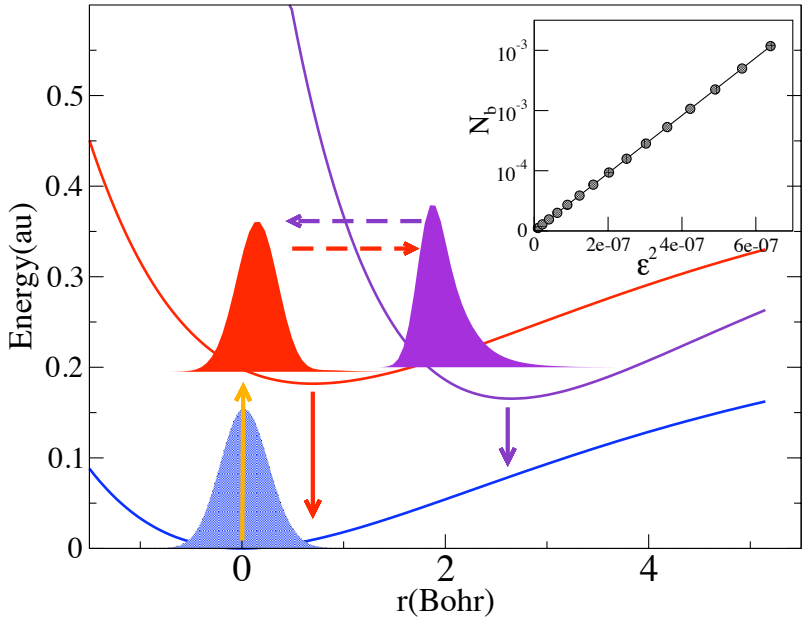
Fig. 3. Two-dimensional representation (X-FROG) of the optimal pulse shape found by the algorithm, showing a nonlinear down-chirp.





Model system

$$\hat{\mathbf{H}}_S = \begin{pmatrix} \hat{\mathbf{H}}_g & \hat{\boldsymbol{\mu}}_{gb}\epsilon(t) & 0 \\ \hat{\boldsymbol{\mu}}_{bg}\epsilon^*(t) & \hat{\mathbf{H}}_b & \hat{\mathbf{V}}_{bd} \\ 0 & \hat{\mathbf{V}}_{db} & \hat{\mathbf{H}}_d \end{pmatrix}$$



$\hat{\mathbf{H}}_k = \frac{\hat{\mathbf{P}}^2}{2\mu} + \hat{\mathbf{V}}_k$ is the surface Hamiltonian $k = \{g, b, d\}$

$\hat{\boldsymbol{\mu}}_{gb}(r)$ represents the transition dipole operator

$\epsilon(t)$ represents the time dependent electromagnetic field

$\hat{\mathbf{V}}_{bd}(r)$ represents the non-adiabatic potential

System bath coupling

$$\hat{\mathbf{H}}_T = \hat{\mathbf{H}}_S + \hat{\mathbf{H}}_B + \hat{\mathbf{H}}_{B^{\text{“}}} + \hat{\mathbf{H}}_{SB} + \hat{\mathbf{H}}_{BB^{\text{“}}},$$

$$\hat{\mathbf{H}}_B = \sum_j \omega_j \hat{\boldsymbol{\sigma}}_j^+ \hat{\boldsymbol{\sigma}}_j \qquad \hat{\mathbf{H}}_{SB} = \hat{\mathbf{A}}_S \otimes \sum_j^N \lambda_j (\hat{\boldsymbol{\sigma}}_j^\dagger + \hat{\boldsymbol{\sigma}}_j)$$

Reduced dynamics

$$H = H_S + H_B + H_{SB}$$

System

Bath

How to describe the bath?

1) Correlated system bath initial state $\rho \neq \rho_S \otimes \rho_B$

2) Non Markovian description $\dot{\rho} \neq L(\rho)$

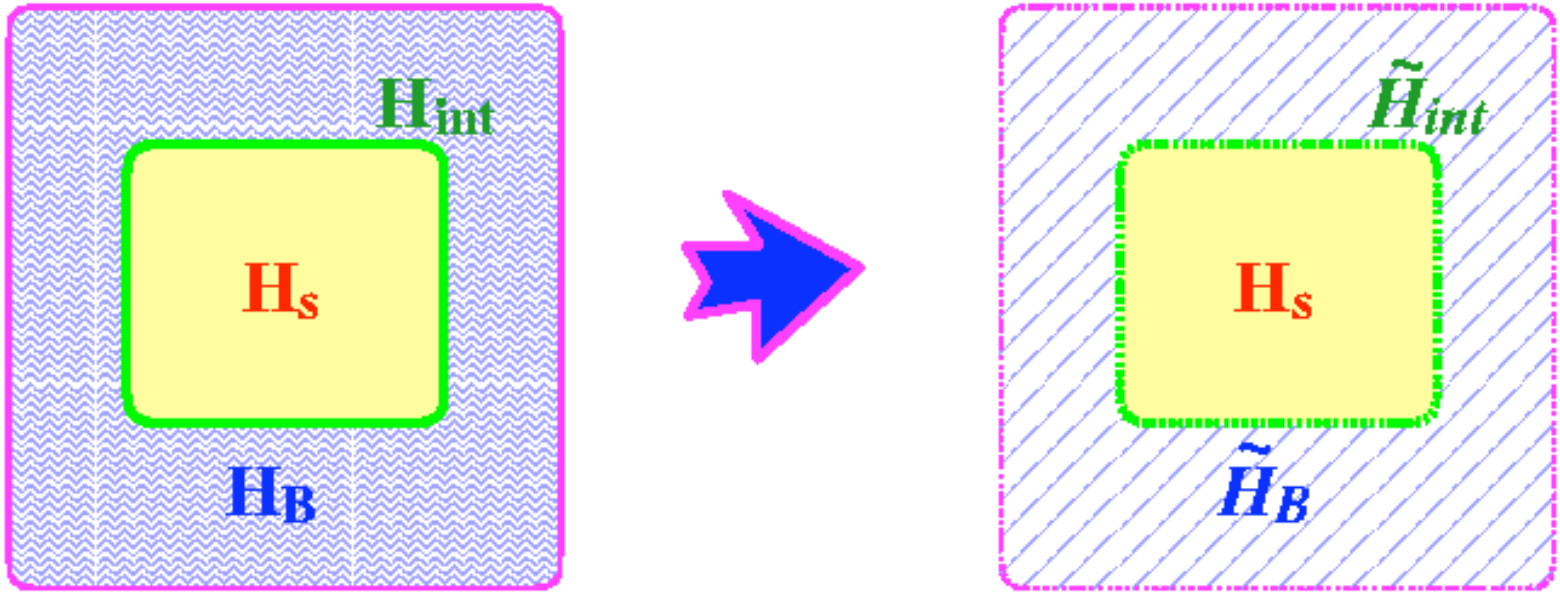
3) System bath coupling is influenced by the external field.

Solution: Surrogate Dynamics

embedding the system in a larger Hilbert space

The surrogate Hamiltonian approach

$$H = H_S + H_{int} + H_B \quad \Rightarrow \quad H = H_S + \tilde{H}_{int} + \tilde{H}_B$$



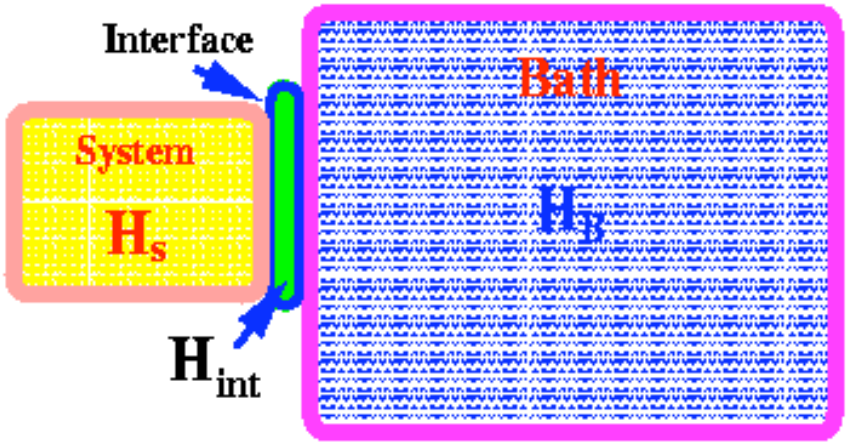
If our measurements apply
to system operators $A = A_S \otimes I_B$

$\langle A \rangle = tr\{\rho_S \cdot A\}$ where $\rho_S = tr\{\rho_{SB}\}$

For sufficiently short times we can dilute the sepctrum of the bath Hamiltonain

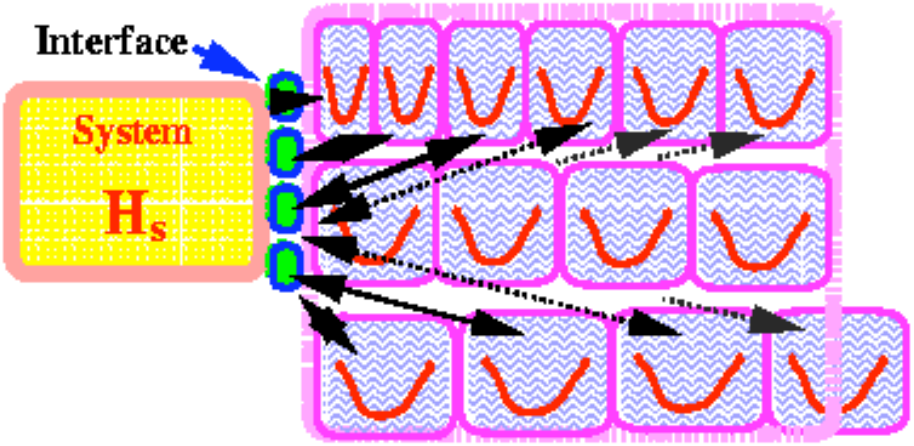
Then we look for a compact bath Hamiltonain
which generates an equivalent system dynamics

I The surrogate Hamiltonian approach



$$H = H_s + H_{int} + H_B$$

II Weak coupling limit



Normal mode analysis

$$H_s = T + V_s(R)$$

$$H_B = \sum \varepsilon_j b_j^* b_j$$

$$H_{int} = f(R) \sum \kappa_j (b_j + b_j^*)$$

III Discrete bath approximation

$$H_{int} = f(R)\sum U_m(B_m + B_m^*)$$

$$H_B = \sum \varepsilon_m B_m^* B_m$$

Renormalizing the interaction

$$U_m = \sqrt{J(\epsilon_m)/\rho(\epsilon_m)}$$

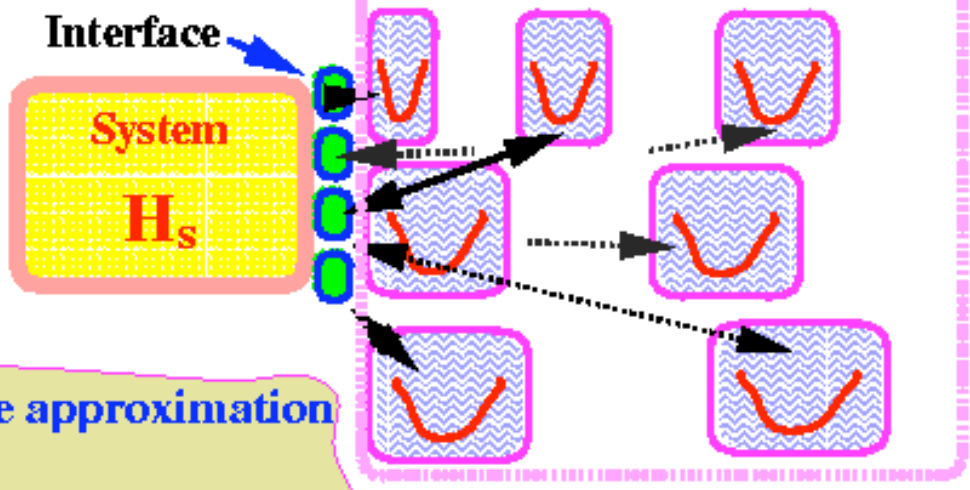
Spectral density

$$J(\epsilon) = \sum_j |V_j|^2 \delta(\epsilon_j - \epsilon)$$

Density of states

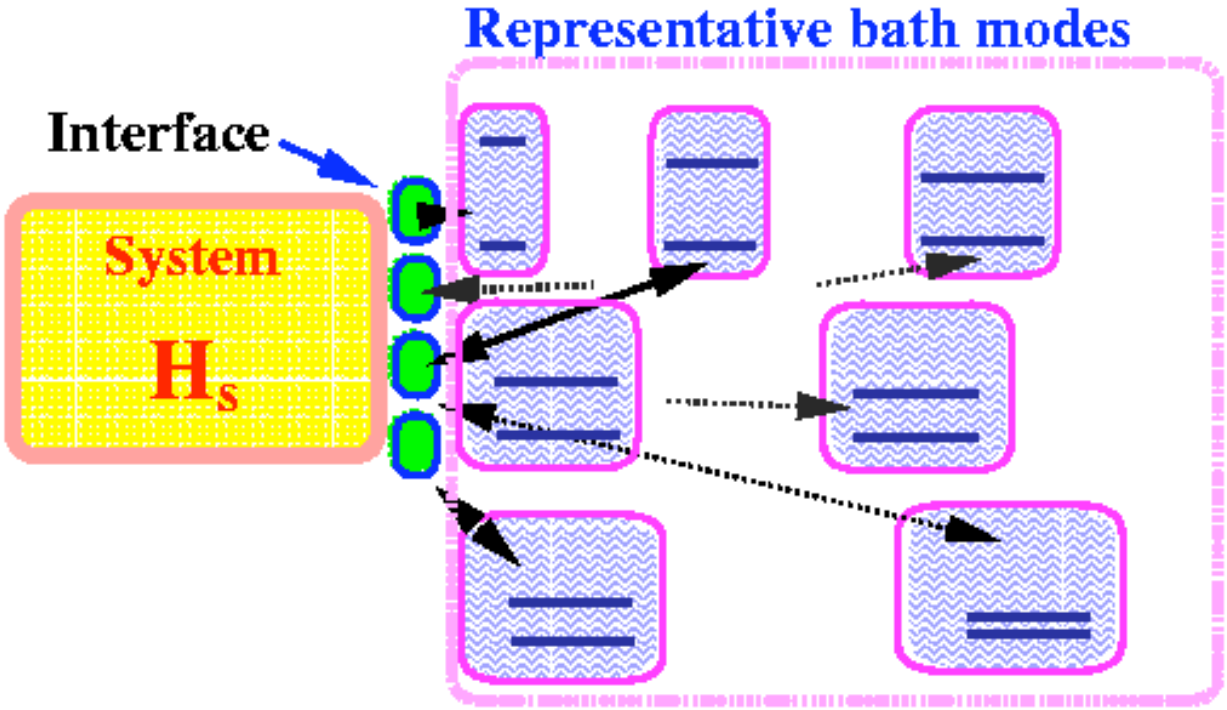
$$\rho(\epsilon_m) \approx (\epsilon_{m+1} - \epsilon_m)^{-1}$$

Representative bath modes



Short time approximation

IV Alternative spin bath representation

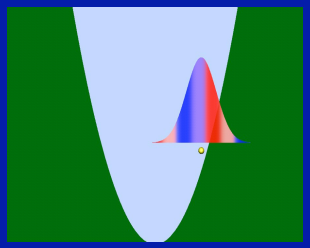


$$H_s = T + V_s(R)$$

$$H_B = \sum \varepsilon_j \sigma_j^+ \sigma_j^- + \sum \Delta_{jk} \sigma_j^+ \sigma_k^-$$

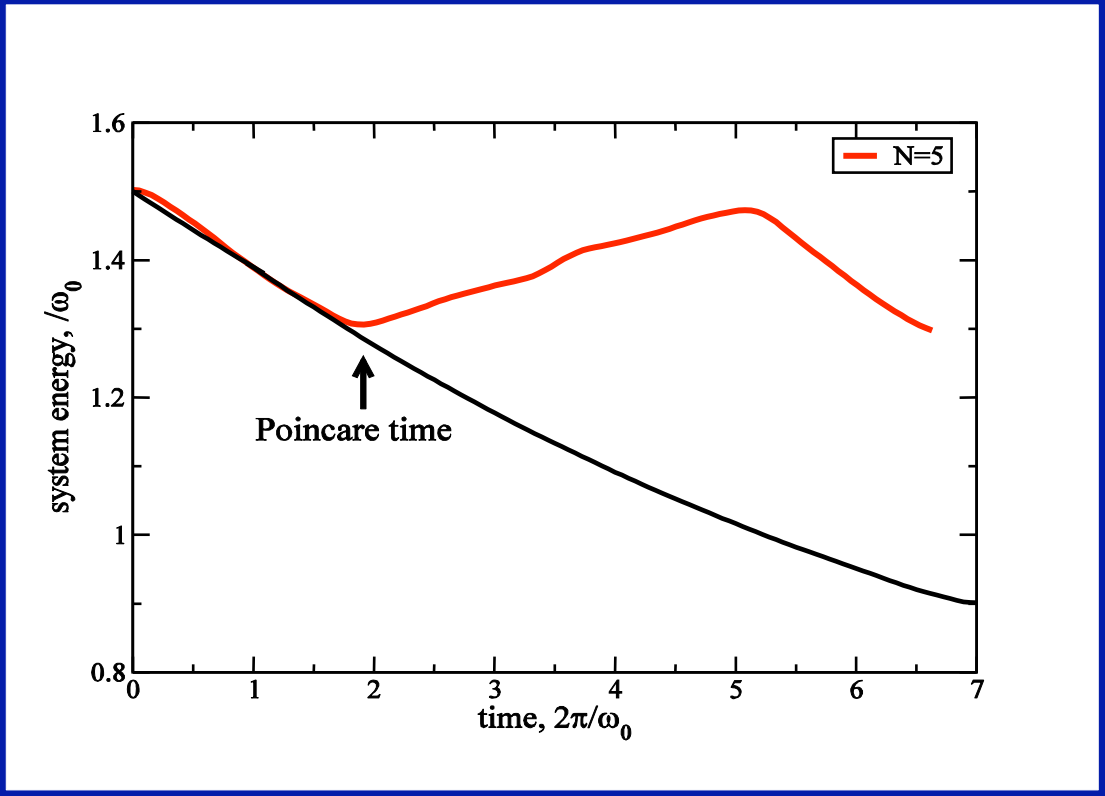
$$H_{int} = f(R) \sum \kappa_j (\sigma_j^+ + \sigma_j^-)$$

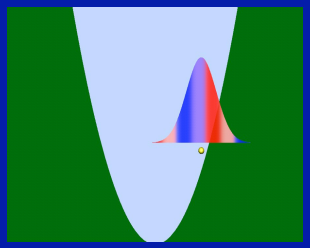
Baer, Zeiri & kosloff PRB 55 10952 (1997)
Baer & Kosloff JCP 106 8862 (1997)



Vibrational relaxation

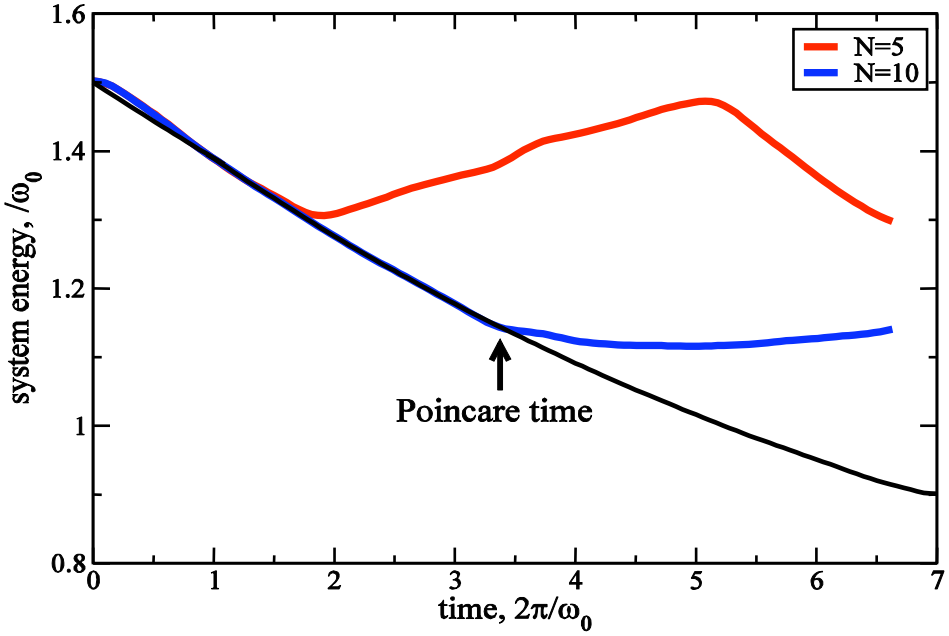
energy relaxation

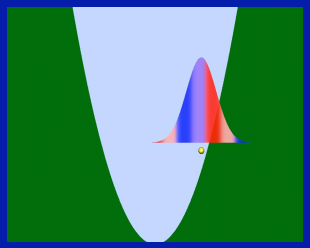




Vibrational relaxation

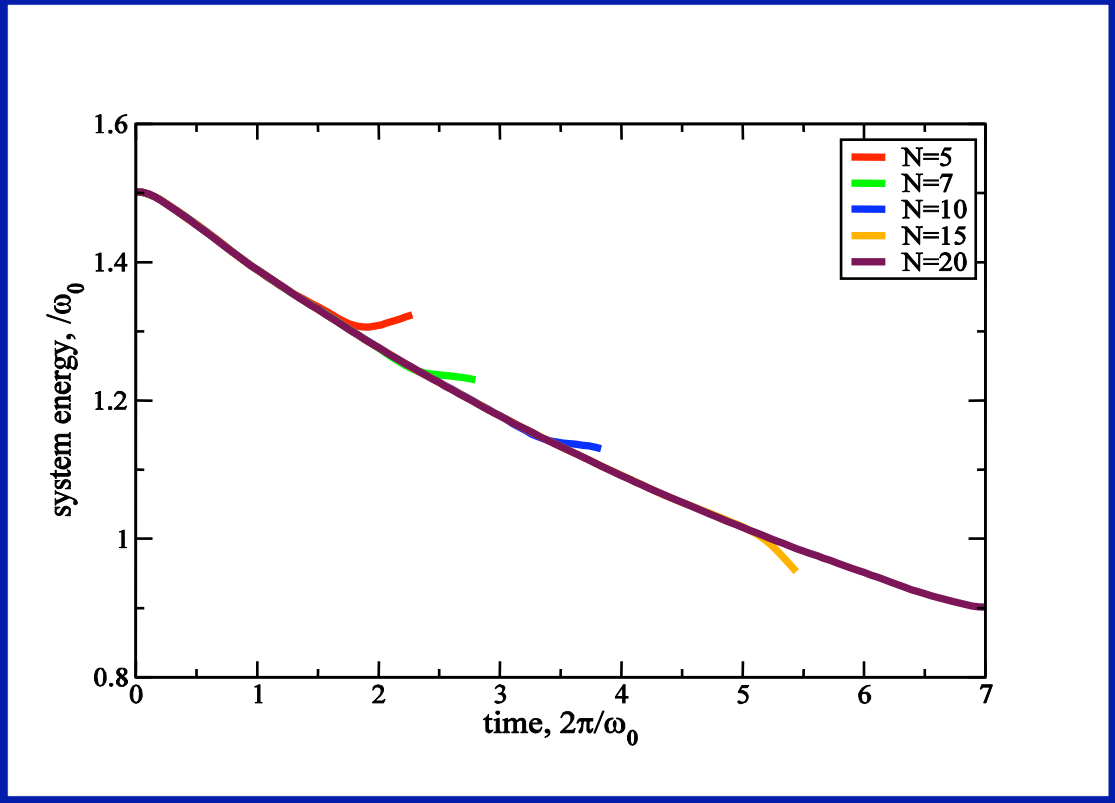
energy relaxation





Vibrational relaxation

energy relaxation



The problem with the Surrogate Hamiltonian method

The simulation cost grows exponentially with the time scale

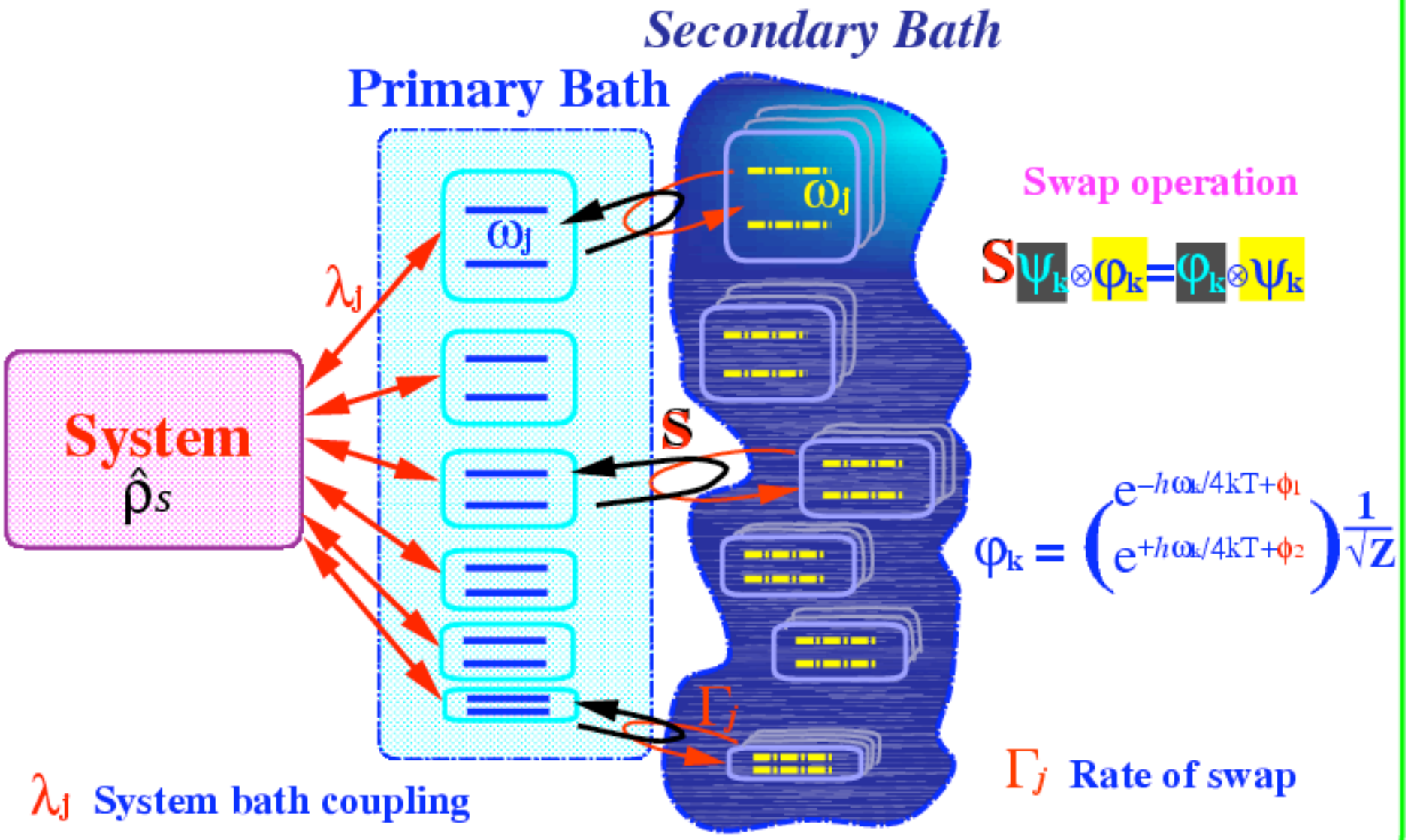
System bath entanglement and bath–bath entanglement grow without bounds

Solution: Extending the time scale to equilibrium

adding a stochastic layer = secondary bath

Gil Katz, David Gelman, Mark A. Ratner, and Ronnie Kosloff
Stochastic surrogate Hamiltonian J. Chem.Phys. 129 034108 (2008).

V Replacing the bath modes $H_T = H_S + H_B + H_{B'} + H_{SB} + H_{BB'}$



Homogenizer

$$\rho_{s(1)} = Tr\{U\rho_{s(0)}\otimes\sigma_B U^\dagger\}$$

$$\rho_{s(N)} = Tr\{U_N \ldots U_1\rho_{s(0)}\otimes\sigma_B U_1^\dagger \ldots U_N^\dagger\}$$

Swap operation: $S|\psi\rangle\otimes|\phi\rangle = |\phi\rangle\otimes|\psi\rangle$

Partial swap operation: $P(\eta) = \cos(\eta)I + i\sin(\eta)S$

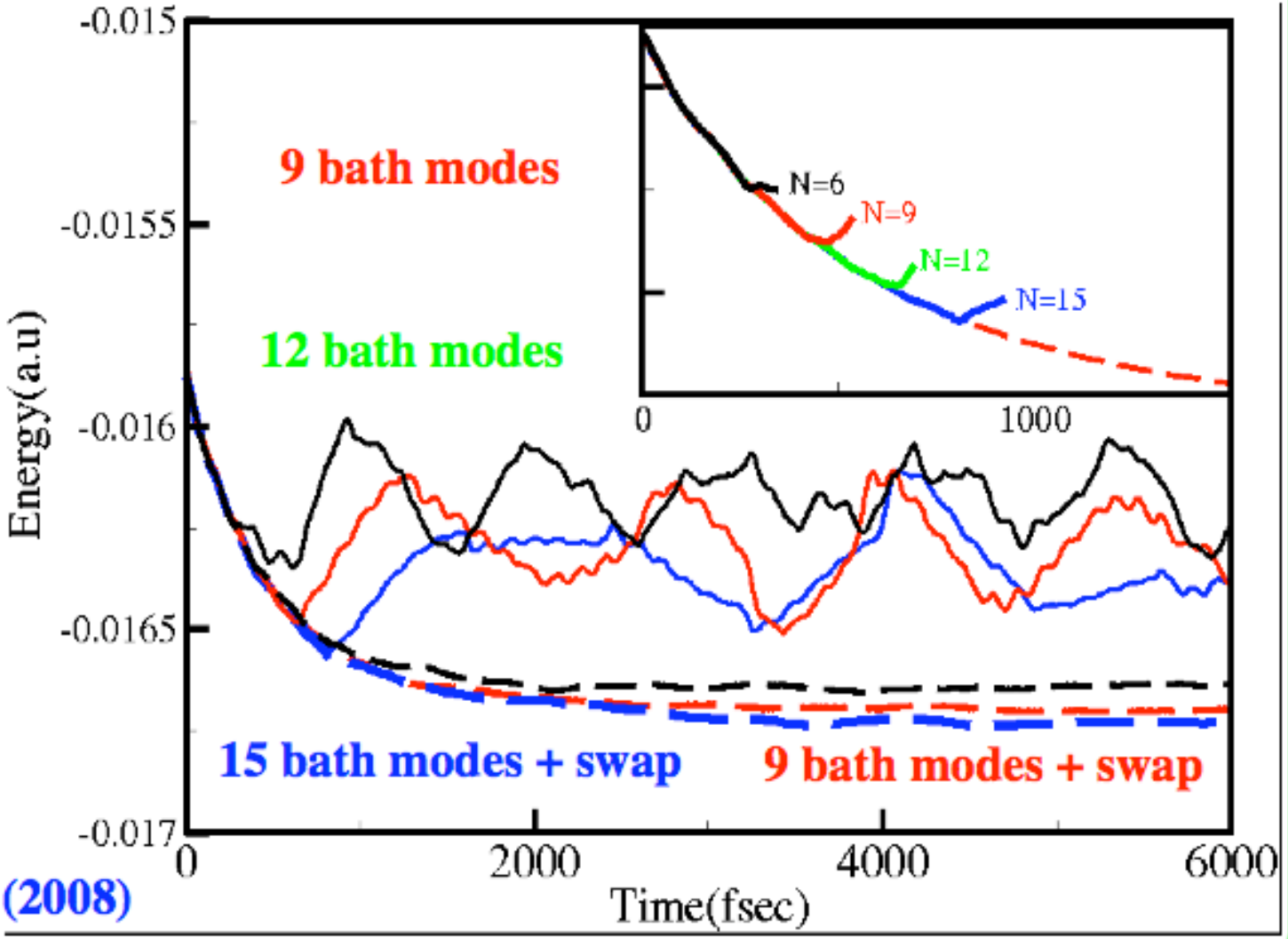
Zinan M, Stelmachovic P, Buzek V, Hillery M, Scarani V, Gisin N , Phys. Rev. A 65, 042105 (2002)

Decay of an oscillator to a bath

$$\hat{\mathbf{H}}_S = \frac{\hat{\mathbf{P}}^2}{2M} + D\left(e^{-2\alpha\hat{\mathbf{R}}} - 2e^{-\alpha\hat{\mathbf{R}}}\right) \quad \hat{\mathbf{H}}_{SB} = \hat{\mathbf{A}}_S \otimes \sum_j^N \lambda_j(\hat{\sigma}_j^\dagger + \hat{\sigma}_j) \quad \hat{\mathbf{H}}_B = \sum_j \omega_j \hat{\sigma}_j^\dagger \hat{\sigma}_j$$

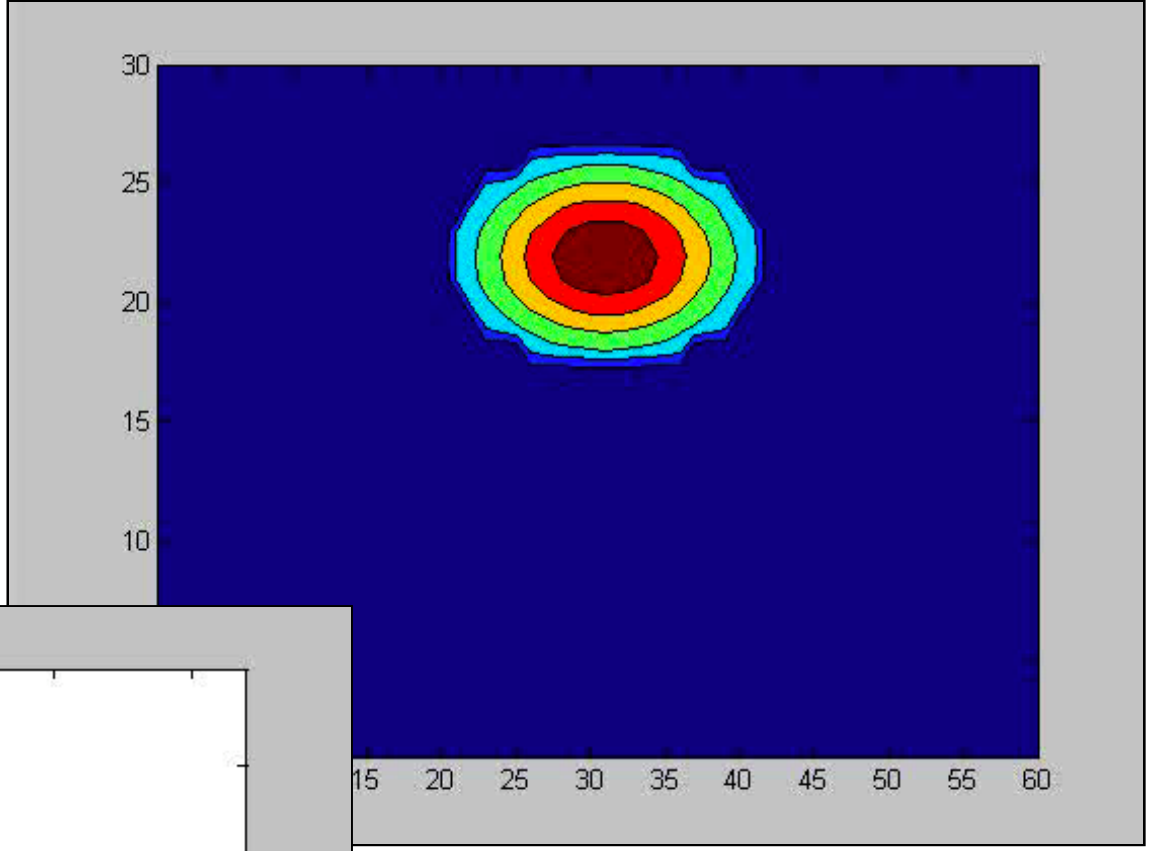
$$f(\hat{\mathbf{R}}) = \frac{1 - e^{-\alpha\hat{\mathbf{R}}}}{\alpha}.$$

$$J(\omega) = M\gamma\omega$$



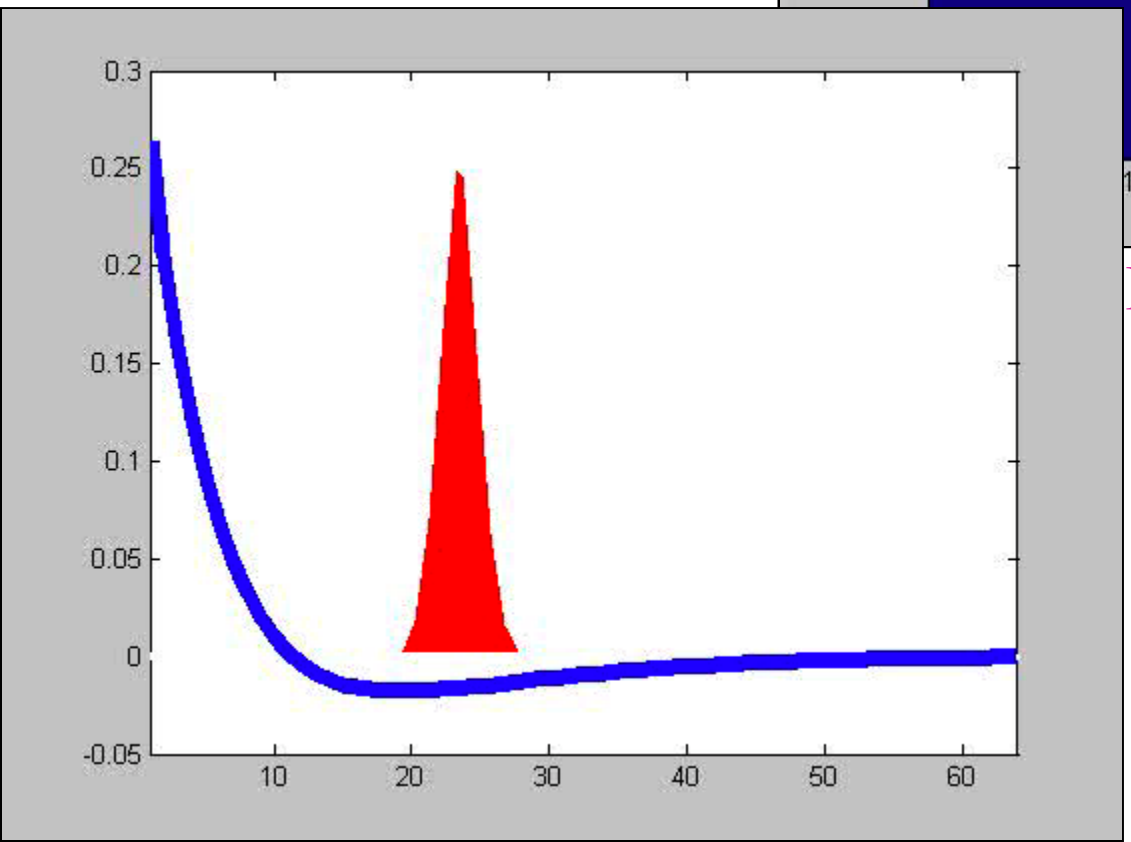
JCP 129, 034108 (2008)

Cooling to thermal equilibrium



Phase space Wigner function

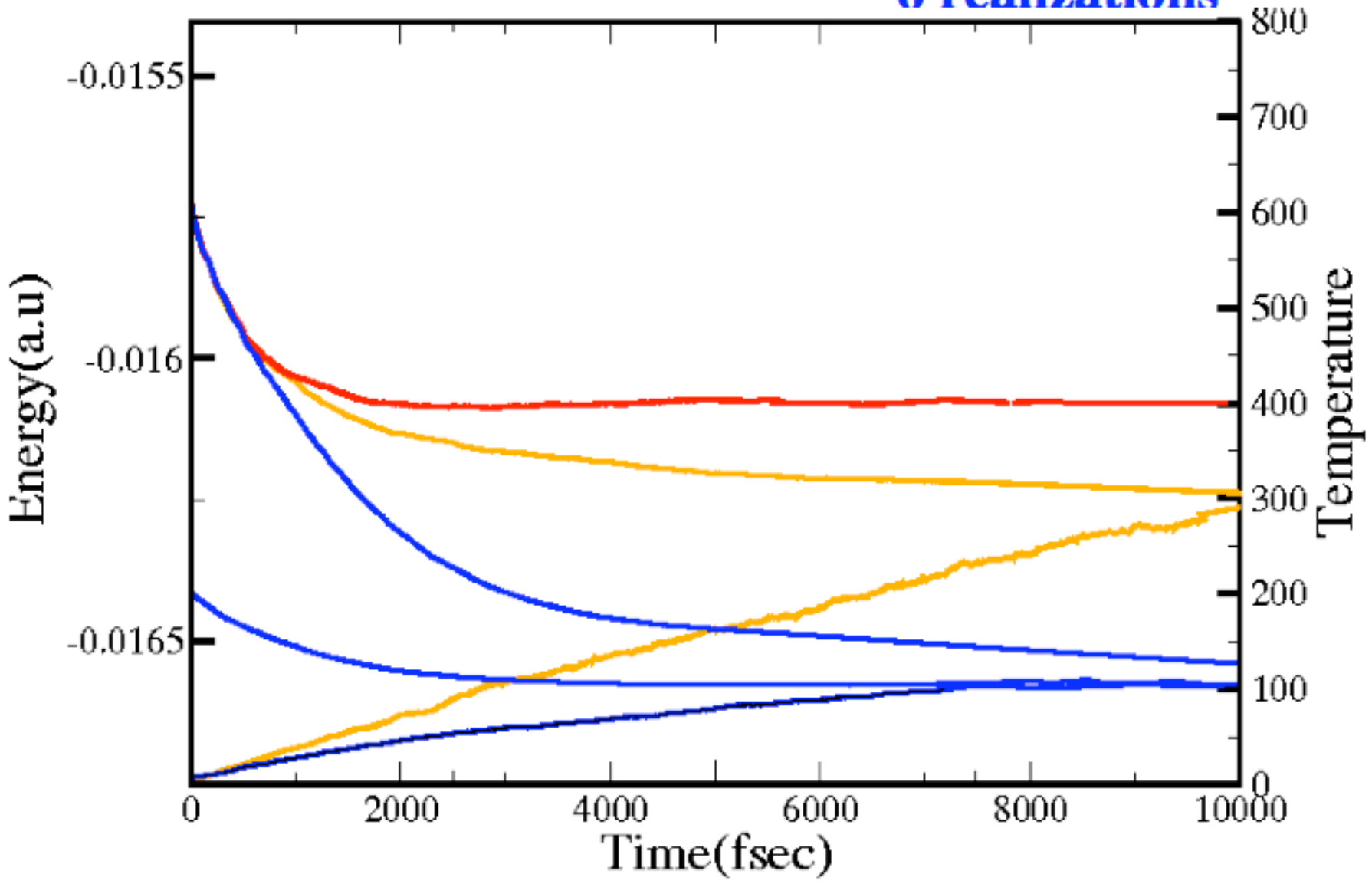
Coordinate representation



Approaching thermal equilibrium

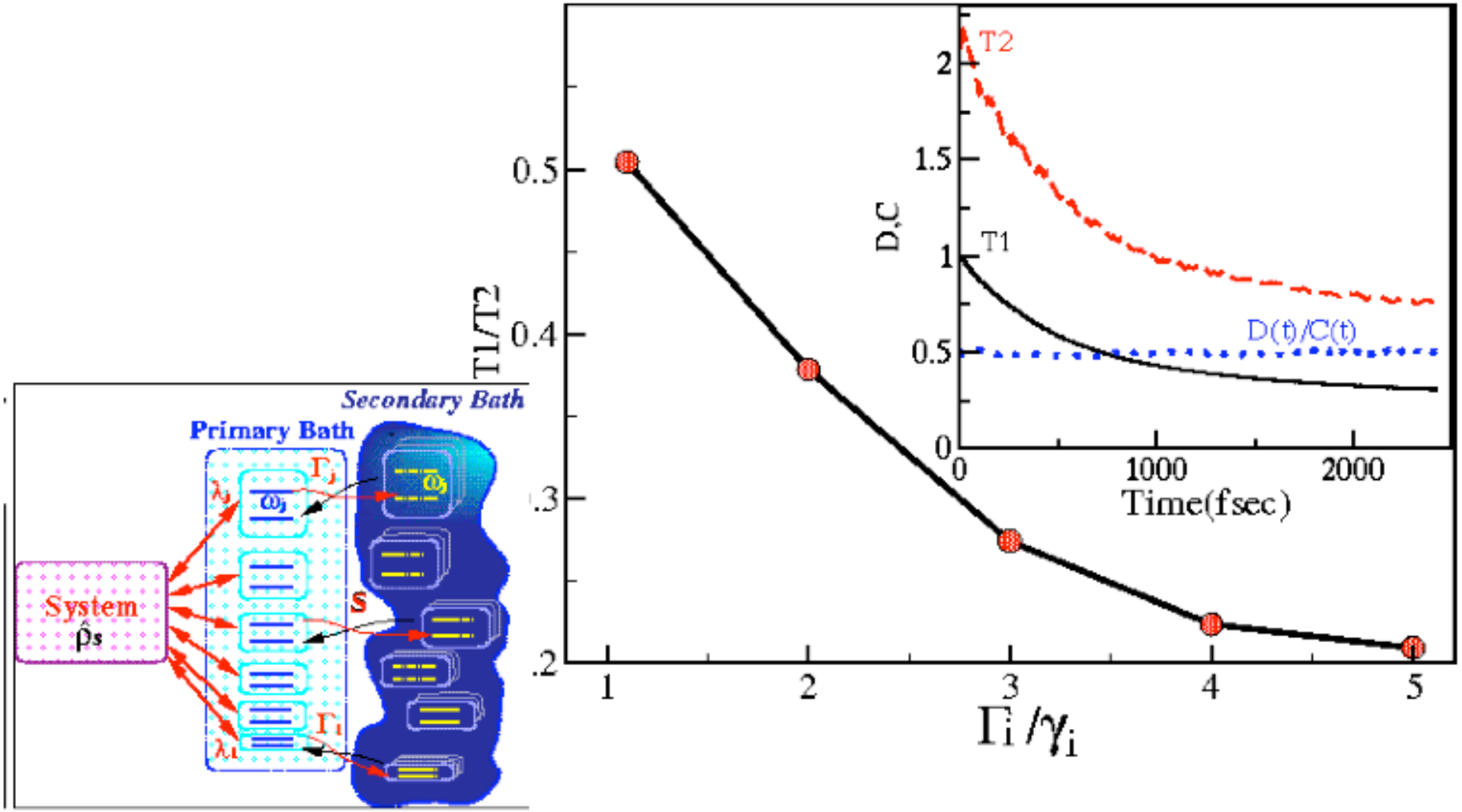
9 bath modes+swap

6 realizations

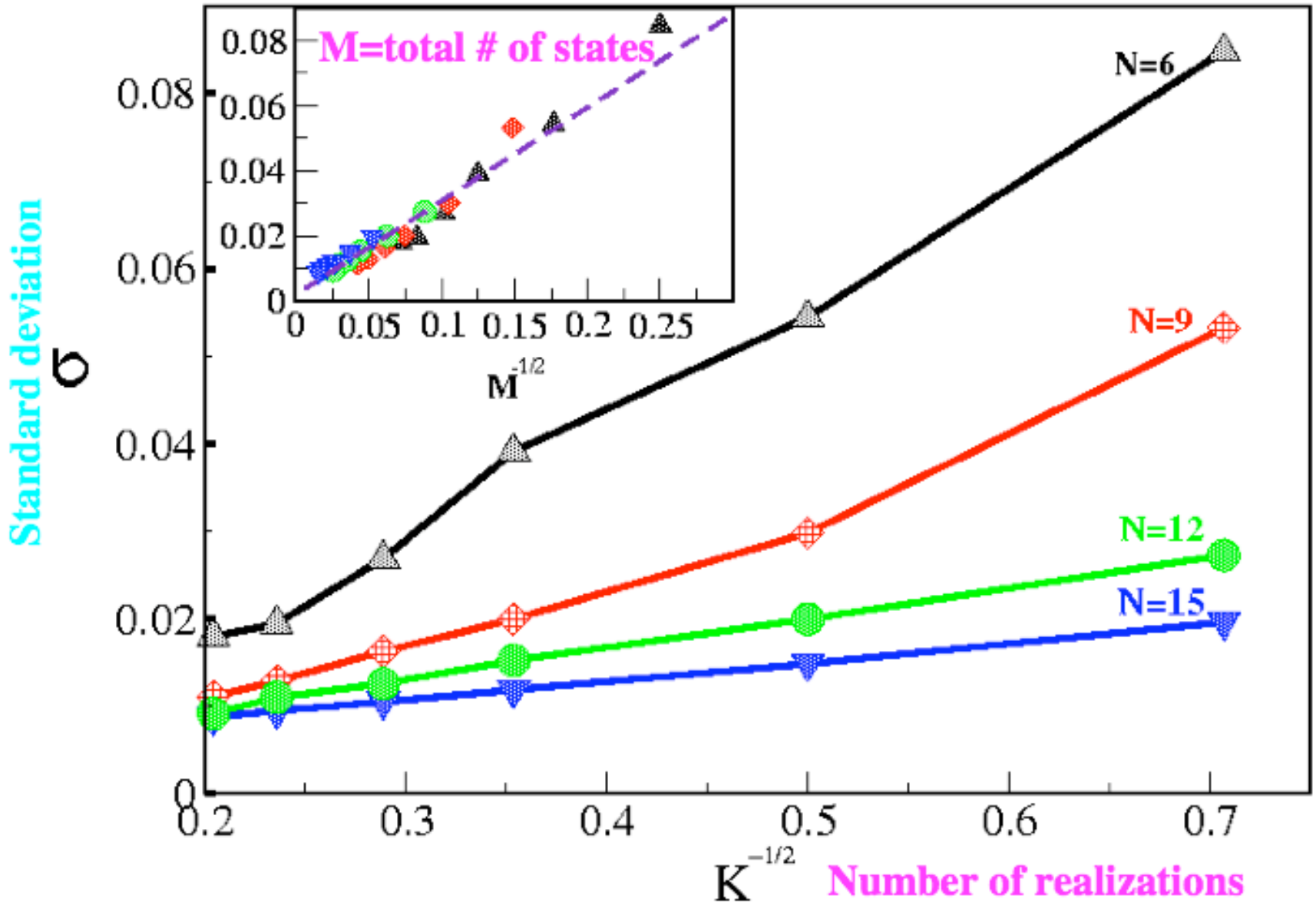


The ratio between energy and phase relaxation T1/T2

The ratio between the primary and secondary rates of energy transfer



Convergence properties of the stochastic surrogate Hamiltonain



Wavefunction description

1) The Surrogate Hamiltonian method is a consistent non-Markovian system-bath reduction.

It can deal with

Time dependent Hamiltonians such as coherent control

Finite temperature bath.

Problem: good for only short time dynamics.

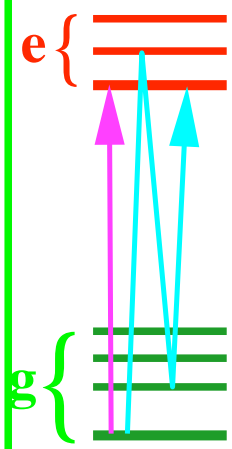
2) The stochastic secondary bath extends the timescale up to equilibrium.

If the Hilbert space is large the # of realizations n be very small.

The swap operation limits the growth of entanglement.
Classical limit induced by noise.

The problem of weak field coherent control

Phase only control



The bath introduces a new time scale

Energy dissipation time scale T_1

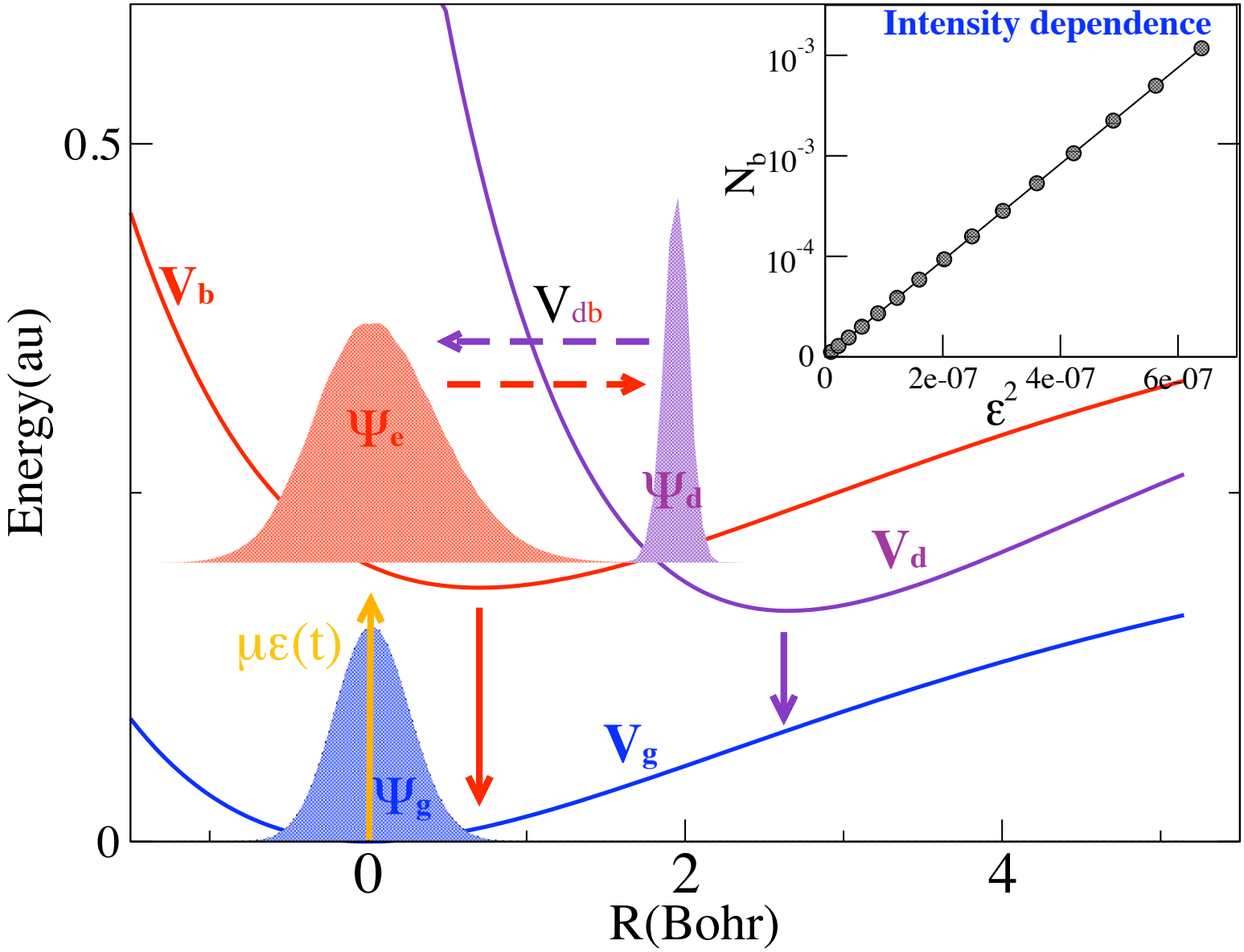
Phase loss time scale T_2

This time scale should be compared to the nonadiabatic time scale $\hbar/V_{12}$

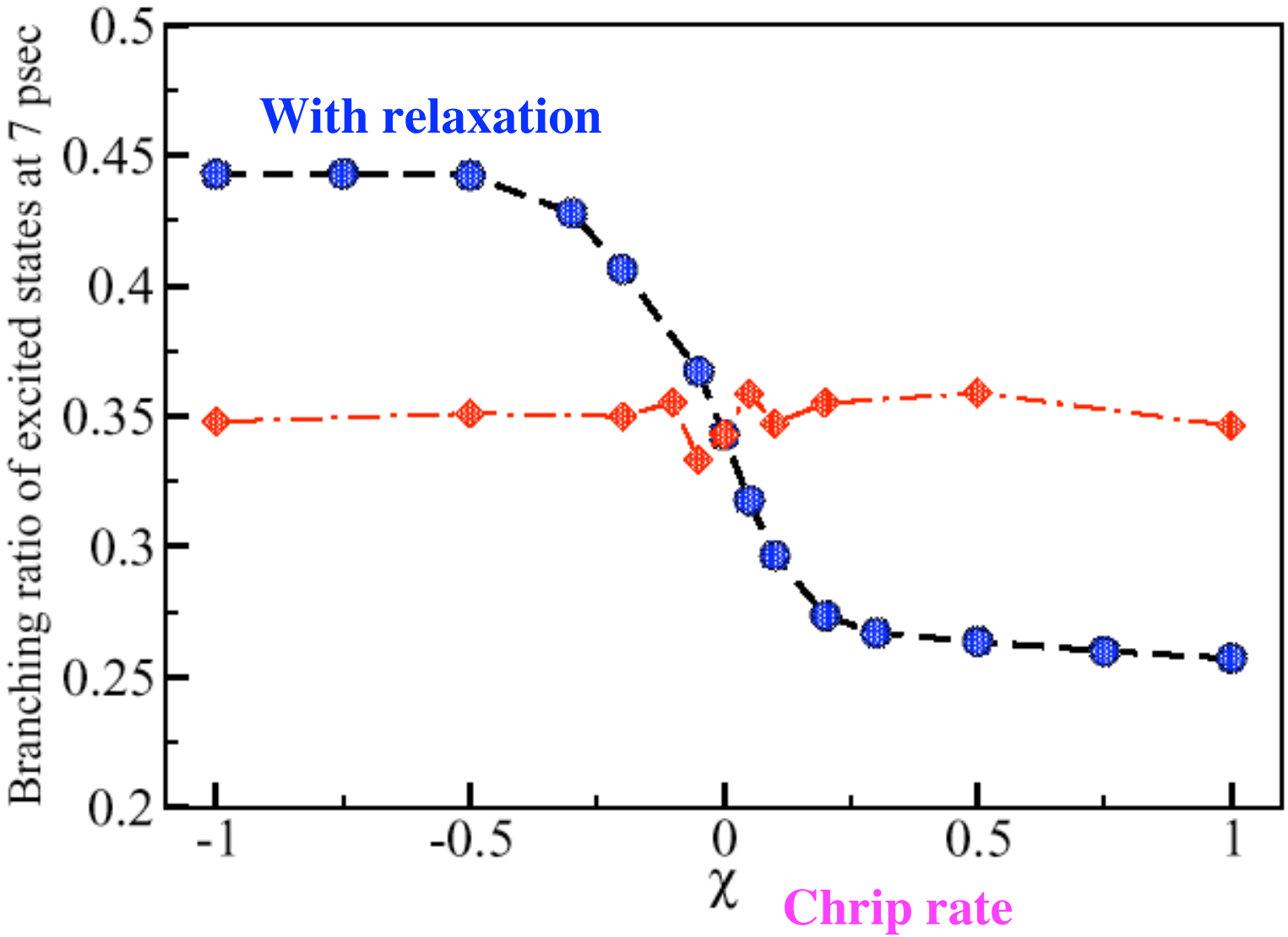
Model system for weak field control

phase only control

Target: change the branching ratio on the excited state

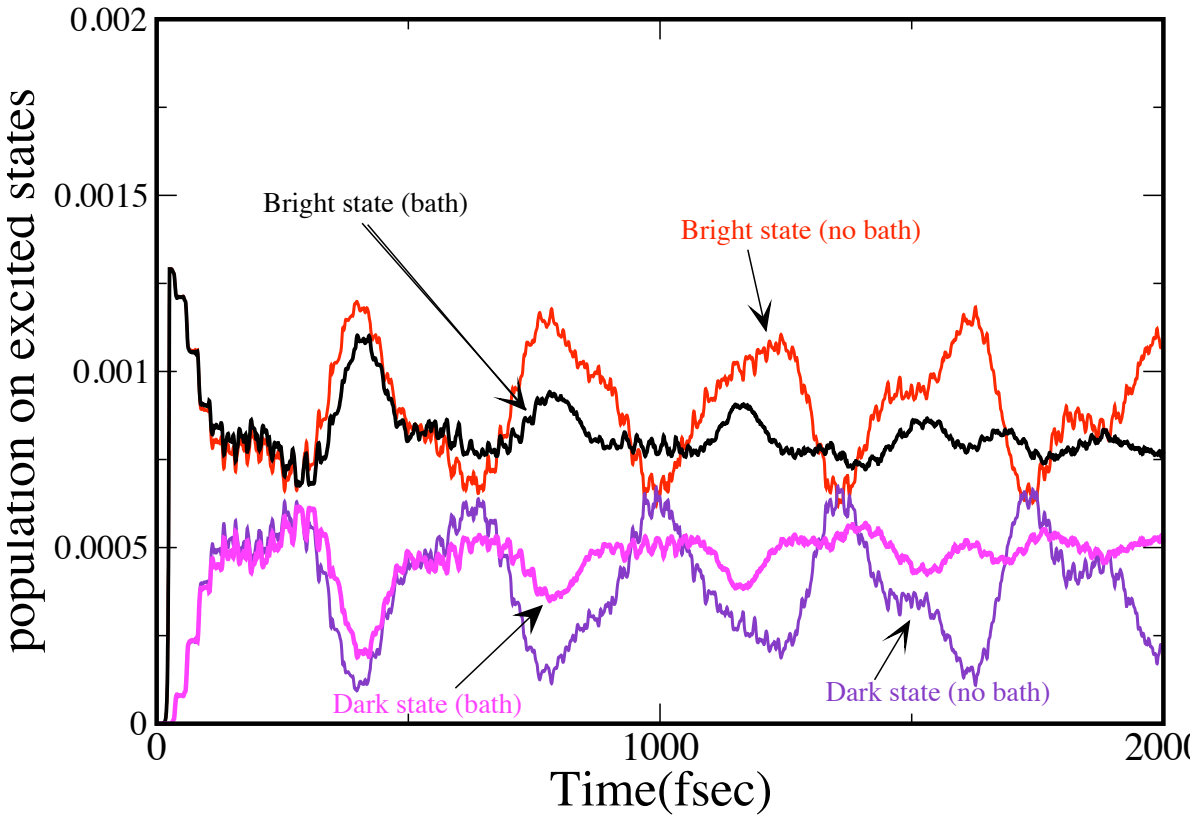


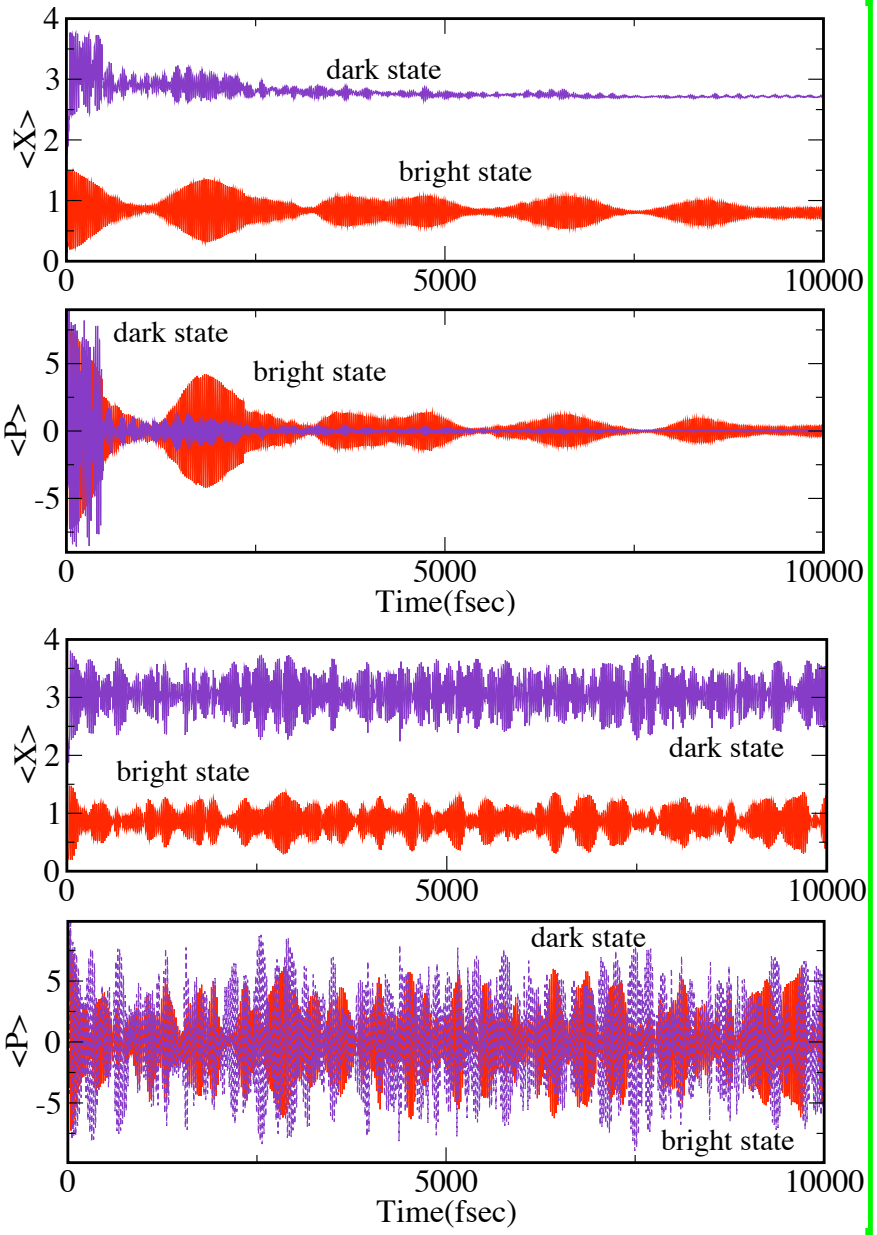
Phase only control with relaxation compared to free propagation

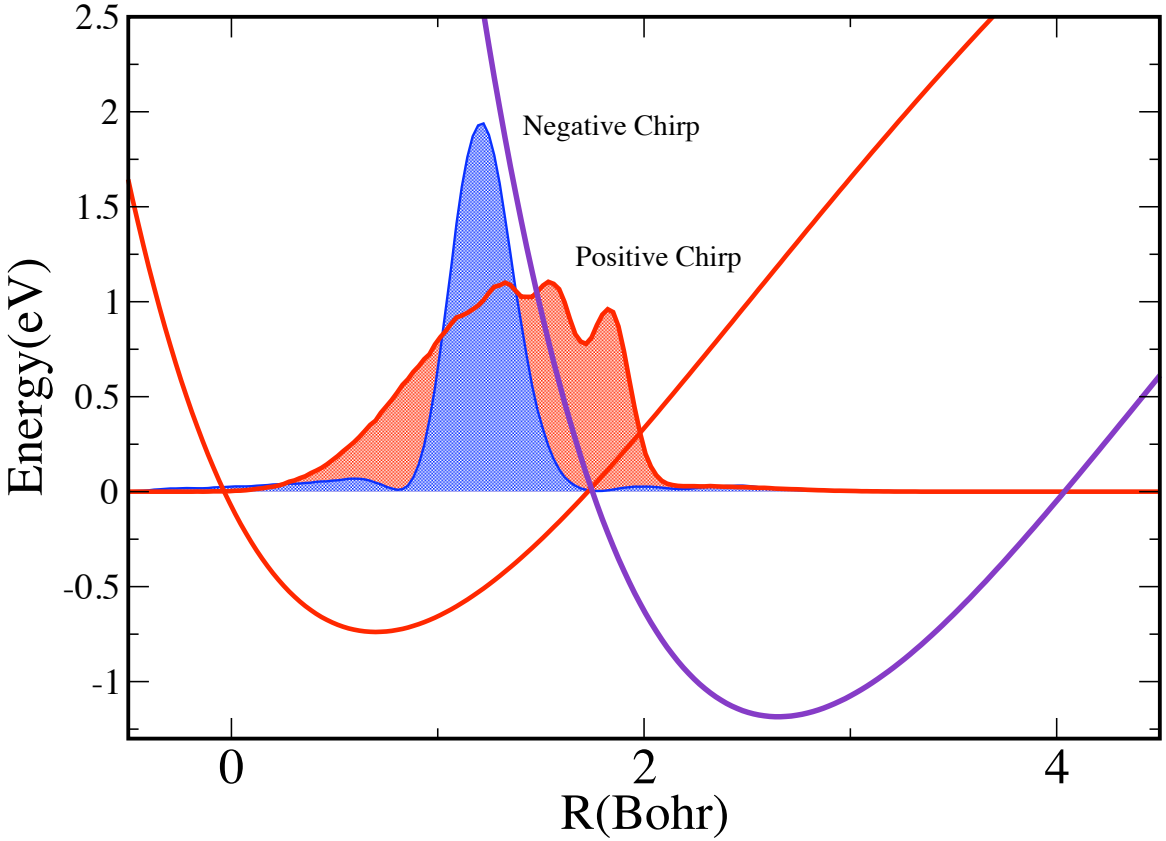


Position/momentum expectations

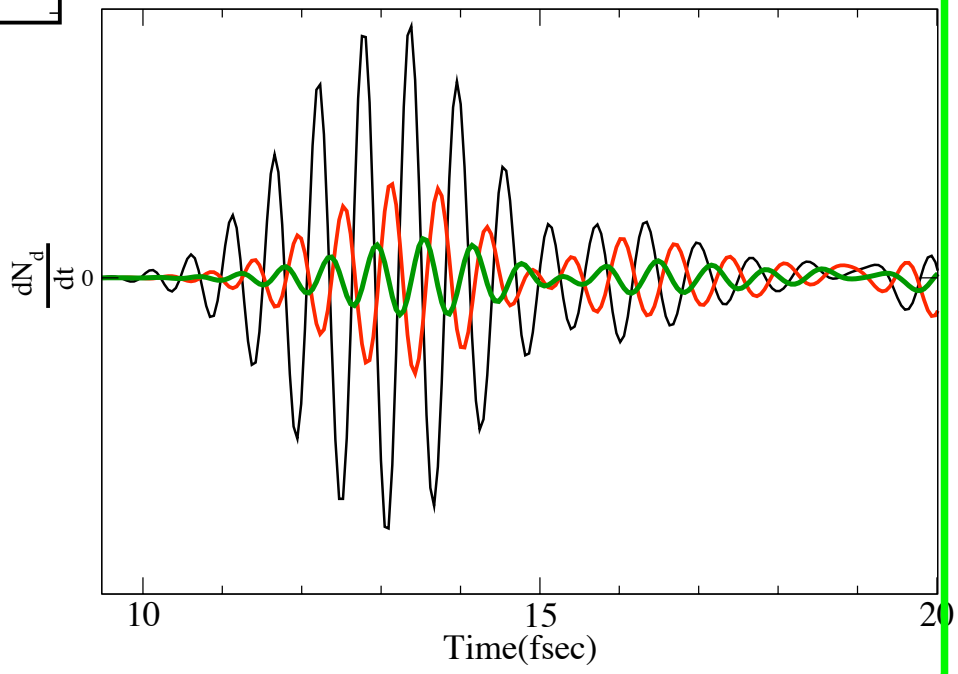
Population dynamics





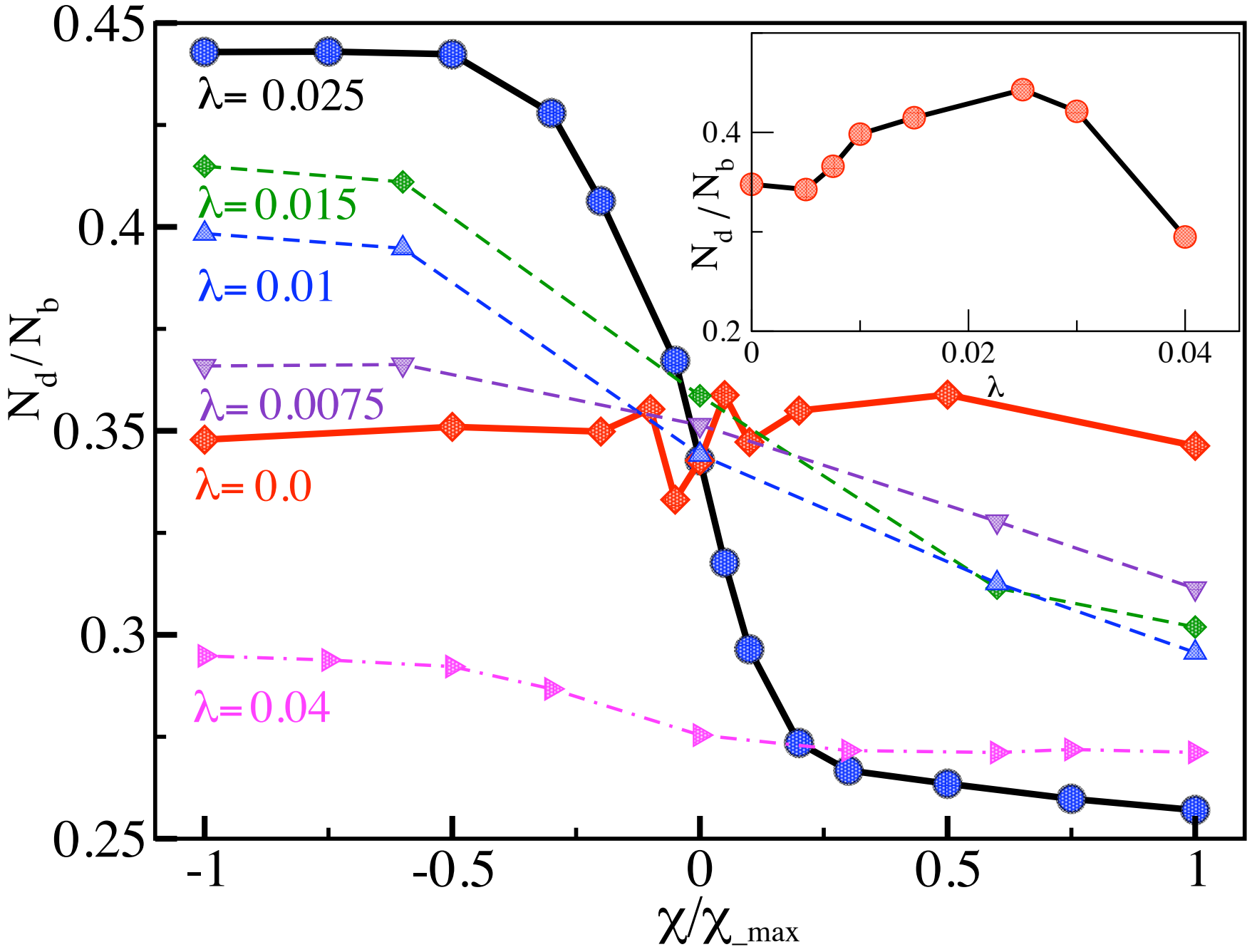


$$\frac{dN}{dt} = \frac{2}{h}\mathrm{Im}\langle \psi_d | V_{db} | \psi_b \rangle$$

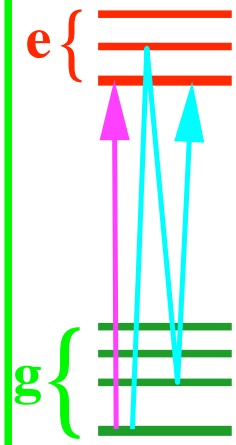


Focusing the wavefunction

The influence of the bath: different system–bath coupling



Weak field coherent control
Phase only control is possible!



The bath introduces a new time scale $T_1 \approx 500$fsec

vibrational frequency $\nu = 940\ cm^{-1}$, $V_{bd}/h = 40 cm^{-1}$

Negative chirp is optimal: $\tau = 12$ fsec, $w_f = 1.38$

A turnover: optimum system–bath coupling

We have more control in an open system

Efficient simulation of quantum many particle dynamics

Basic facts:

1) The computational effort of a complete quantum simulation scales with the size of Hilbert space.

2) The size of Hilbert space scales exponentially with the number of degrees of freedom.

Quantum computing

Exploiting the inherent parallellyism in quantum interference

The best example (Feynman):

Simulate one quantum system by another

reduction of exponential complexity

All or nothing approach:

If we know the wavefunction $\Psi(r_1,r_2,r_3,\ldots,\ldots,r_N,t)$ at all times we can calculate the evolution of any observable $\langle B\rangle = \langle\Psi|B|\Psi\rangle$

Now Ψ obeys the time dependent Shrodinger equation $i\hbar\,\dot{\Psi} = H\Psi$

with solution $\Psi(t) = e^{-i/\hbar Ht}\ \Psi(0)$

The computation resources scale as D^{δ}

where D is the size of Hilbert space

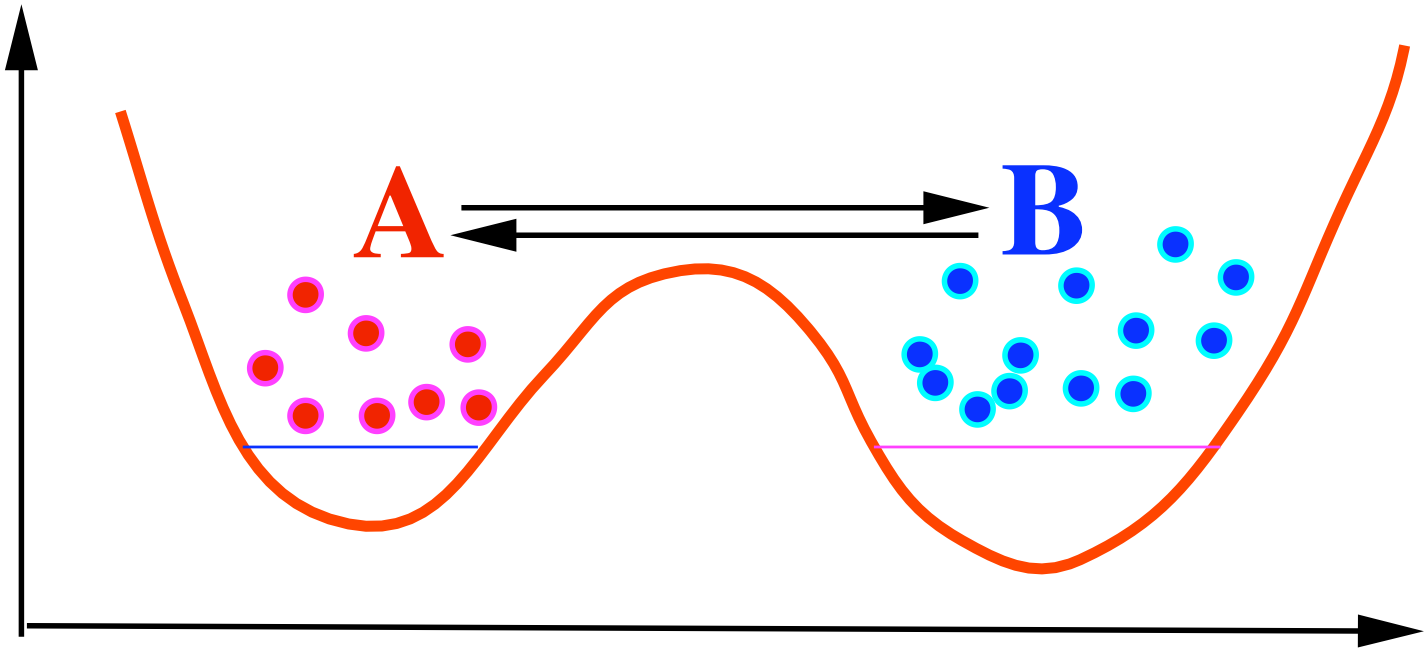
$$D = d^N$$

and δ is larger then 1.

N number of particles

Direct solutions become prohibitively expensive!

The Problem: Tunneling Hamiltonian for N



bosons

$$H = \omega_a N_a + \omega_b N_b + \Delta(a^\dagger b + b^\dagger a) + U(N_a^2 + N_b^2)$$

single particle tunneling term

inter–particle interaction

What is the # of states?

We define

$$J_x = \frac{1}{2}\left(a^\dagger b + b^\dagger a\right)$$
$$J_y = \frac{1}{2i}\left(a^\dagger b - b^\dagger a\right)$$
$$J_z = \frac{1}{2}\left(a^\dagger a - b^\dagger b\right)$$

and the total number of particles is conserved

$$N = N_a + N_b$$

Then:

$$H = -\omega J_x + \frac{U}{N} J_z^2$$

The # of states
= size of Hilbert space
D=N+1

is the effective many body non linear Hamiltonain

Definition: Zero order scaling

The simulation of dynamics of a Lie subalgebra of observables is efficient if and only if the necessary memory and the CPU resources do not depend on the Hilbert space representation D.

A dynamical simulation may be possible if we limit our scope

We will be interested only in a limited set of *dynamical* observables.

Example: for the Hamiltonian $H = \omega J_x$

we can solve Heisenberg equations $\dot{X} = i[H,X]$ for the the set J_x, J_y, J_z

$$\begin{cases} \dot{J}_x = i/h\,[H,J_x] = 0 \\ \dot{J}_y = i/h\,[H,J_y] = -\omega J_z \\ \dot{J}_z = i/h\,[H,J_z] = \omega J_y \end{cases}$$

We get a closed set of 3 coupled linear equations independent of the size of the Hilbert space

What can be done with a non linear Hamiltonain?

$$H = -\omega J_x + \frac{U}{N} J_z^2$$

The Heisenberg equations of motion include all powers of operators $J_x, J_x^2, J_x^3 \ldots$ and combinations $J_x J_y, J_x J_y^2, \ldots$
and we obtain **D(D−1) coupled** equations of motion.

If we start with the state (all particles in the left well)
$\Psi(0) = |-j\rangle$ after a short time:

$$\Psi(t) = \exp\{-i/h\, \mathbf{H}t\}\, \Psi(0) = \sum_{k=-j}^{+j} C_k\, |k\rangle$$

and C_k has amplitude for all k

In general for $H=H_0+H_1$, if the commutators:
$A_1=[H_0, H_1]$, $A_2=[H_0. [H_0,H_1]$, $A_3=\ldots$ generate the full Hilbert space
The computational problem becomes prohibitively expensive!

If we limit ourselves to the dynamics of $\langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle$? **then ...**

Surrogate Dynamics

An equivalent dynamics which preserve the original dynamics of $\langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle$ but are easier to solve.

Information on other expectation values may be lost!

Embedding the unitary dynamics in a non unitary open system dynamics.

Replacing Schrödingers equation:

$$i\hbar \frac{\partial \psi}{\partial t} = \mathbf{H}\,\psi$$

by the Liouville von Neumann equation

$$\frac{d\rho}{dt} = -i\,[\mathbf{H},\rho] + L_D(\rho)$$

but replacing the wavefunction by a density operator makes the computational problem more difficult?

Surrogate Dynamics

We need to solve three problems:

1)What is the open system dynamics that preserves the dynamics of the expectations $\langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle$?

2) Can the open system dynamics limit the growth of the representation?

3) Ho to solve the Liouville von Neumann equation without using a density operator?

Surrogate Dynamics

We start with problem 3

Ho to solve the Liouville von Neumann equation without using a density operator?

$$\frac{d\rho}{dt} = -i\,[H,\rho] + L_D(\rho)$$

where $L_D(\rho)$ is Lindblad form $V\rho V^\dagger - 1/2\{V^\dagger V,\rho\}$

Gisin,(PRL 1984) Percival, Diosi .. developed a Stochastic Non Linear Schrodinger Equation (sNLSE) where:

$$d\psi = \{-i\,H dt + (f(\langle V\rangle)d\xi_j\}\psi$$

where $\langle\xi_j\rangle = 0$ and $\langle\xi_j\,\xi_k\rangle = \delta_{jk}\,\gamma\,dt$

and the density operator ρ is the average of stochastic realizations

$$\rho(t) = 1/N\sum|\psi_l\rangle\langle\psi_l|\ ,\ \text{when } N\to\infty$$

This realization is not unique !

Surrogate Dynamics

moving to problem 2

2) Can the open system dynamics limit the growth of the representation?

Idea: ***Aplying a measurement of the operator A collapses the state of the system to an eigenfunction of A***

We employ the theory of weak continuous measurement, (Diosi) causing partial collapse.
This process can be described by the Lindblad semigrop generator:

$$L_D(\rho) = -\gamma\,[\,\mathbf{A},[\mathbf{A},\rho]]$$

Specifically collapsing on to the submanifold

$$L_D(\rho) = -\gamma(\,[\,J_x,[J_x,\rho]]+[\,J_y,[J_y,\rho]]+[\,J_y,[J_y,\rho]]\,)$$

This is realized by the **sNLSE**

$$d\psi = \{-i\,H dt - \gamma\sum_{i=1}^{3}(J_i - \langle J_i\rangle_\psi)^2 dt + \sum_{i=1}^{3}(J_i - \langle J_i\rangle_\psi)d\xi_j\}\psi$$

Surrogate Dynamics

lets solve problem 1:

1) What is the open system dynamics that preserves the dynamics of the expectations $\langle J_x \rangle$, $\langle J_y \rangle$, $\langle J_z \rangle$?

Analogy with pure dephasing $\mathcal{L}(\rho) = -i[H,\rho] - \gamma [H, [H,\rho]]$

The dissipator does not change energy

The Heisenberg equation of motion:

$$\dot{X} = i[H,X] - \gamma \sum_{i=1}^{3} [J_i, [J_i, X]] \qquad H = -\omega J_x + \frac{U}{N} J_z^2$$

The eigenvalue of the linear part: $Y(t) = \exp((-i\omega - c\gamma)\tau)$

Therefore when $\gamma c \ll \omega$ **the dynamics of** J_i **is not affected**

We have a competition between localization caused by the dissipator and dispersion on all states caused by the non linear term J_z^2

How can we exploit this property?

Generalized Coherent states (GCS)

Choice of time dependent basis functions χ_n

Looking for the states with minimum uncertainty with respect to the operators of the algebra: $\Delta(\Psi) = \langle \Delta J_x^2 \rangle + \langle \Delta J_y^2 \rangle + \langle \Delta J_z^2 \rangle$

$$= \langle J_x^2 + J_y^2 + J_z^2 \rangle - (\langle J_x \rangle^2 + \langle J_y \rangle^2 + \langle J_z \rangle^2)$$

Generalized purity: $P(\psi) = (\langle J_x \rangle_\psi^2 + \langle J_y \rangle_\psi^2 + \langle J_z \rangle_\psi^2)$

Casimir $C = J_x^2 + J_y^2 + J_z^2 \quad \langle C \rangle = j(j+1)$

Maximum purity = Minimum uncertainty

The purity is invariant to a unitary transformation U (rotation) generated by the group $U = \exp(-i (\alpha J_x + \beta J_y + \chi J_z))$

$P(\psi) = P(U\psi)$

Generalized Coherent states (GCS)

Choice of time dependent basis functions χ_n

$\chi_n = \mathbf{U_n}\,\psi_0$ $\quad n=1, 2 \ldots N$ N non−orthogonal basis states

Any matrix element can be calculated within the algebra.

for example: $\langle\chi_n|\mathbf{J_y}\,|\chi_\mathbf{m}\rangle = \langle\psi_0\mathbf{U}_n^\dagger|\mathbf{J_y}\,|\mathbf{U_m}\psi_0\rangle$

The computation complexity is independent of the size of the Hilbert space.

We start by creating a uniform distribution of GCS: χ_n

We find the overlap matrix $S_{nm} = \langle\chi_n\,|\chi_\mathbf{m}\rangle$ and invert it $\mathbf{S^{-1}}$

We can either move the basis functions χ_n or the operators by a global time dependent unitary operator

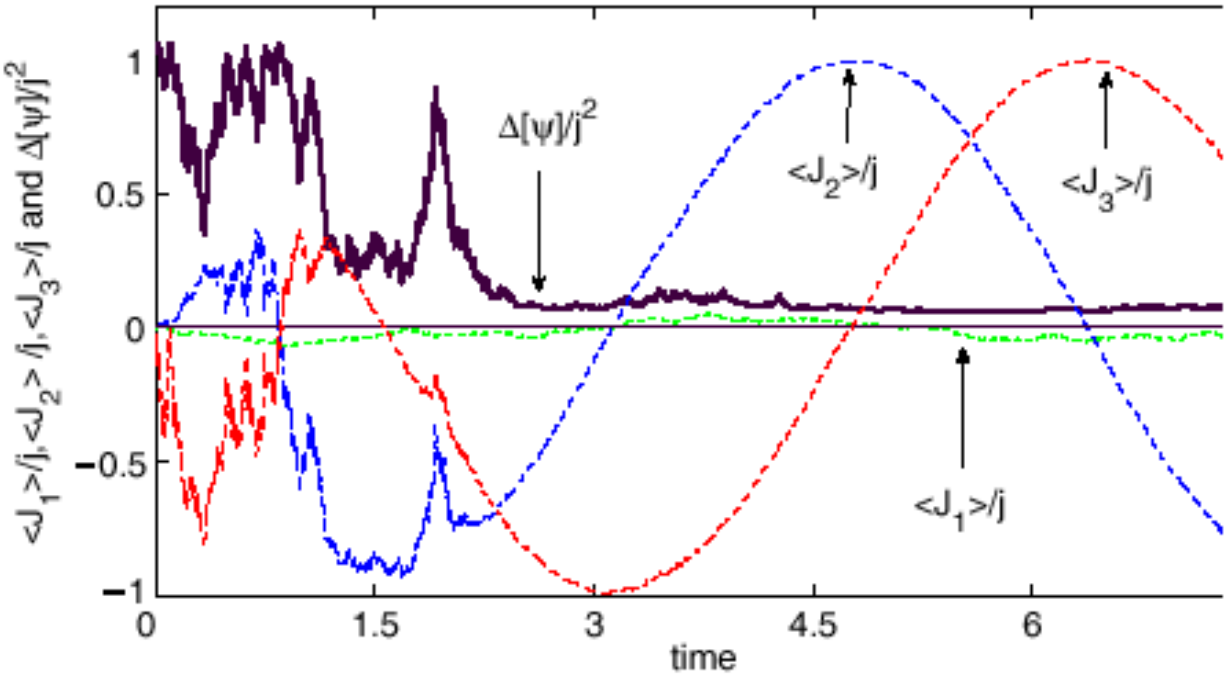
$\mathbf{U(t)} = \exp(-i\,(\alpha(t)J_x + \beta(t)J_y + \gamma(t)J_z))$

Generalized Coherent states (GCS)

The global stable solution of the Stochastic Schrodinger equation

Khasin &Kosloff, JPA 41 (2008) 365203

$$\dot{\mathbf{x}} = i\omega[J_x,X]-\gamma\sum_{i=1}^{3}[\,J_i,\,[J_i,X]]$$



Superposition initial state

$\psi_0=(|-j\rangle+|\,j\rangle)/\sqrt{2}$

Minimal uncertainty

$\Delta(\Psi)=1/16$

$$d\psi = \{-i\omega J_x dt - \gamma\sum_{i=1}^{3}(J_i-\langle J_i\rangle_\psi)^2 dt + \sum_{i=1}^{3}(J_i-\langle J_i\rangle_\psi)d\xi_j\}\psi$$

Under this dynamics
any superposition initial state will collapse to a single GCS

Surrogate Dynamics

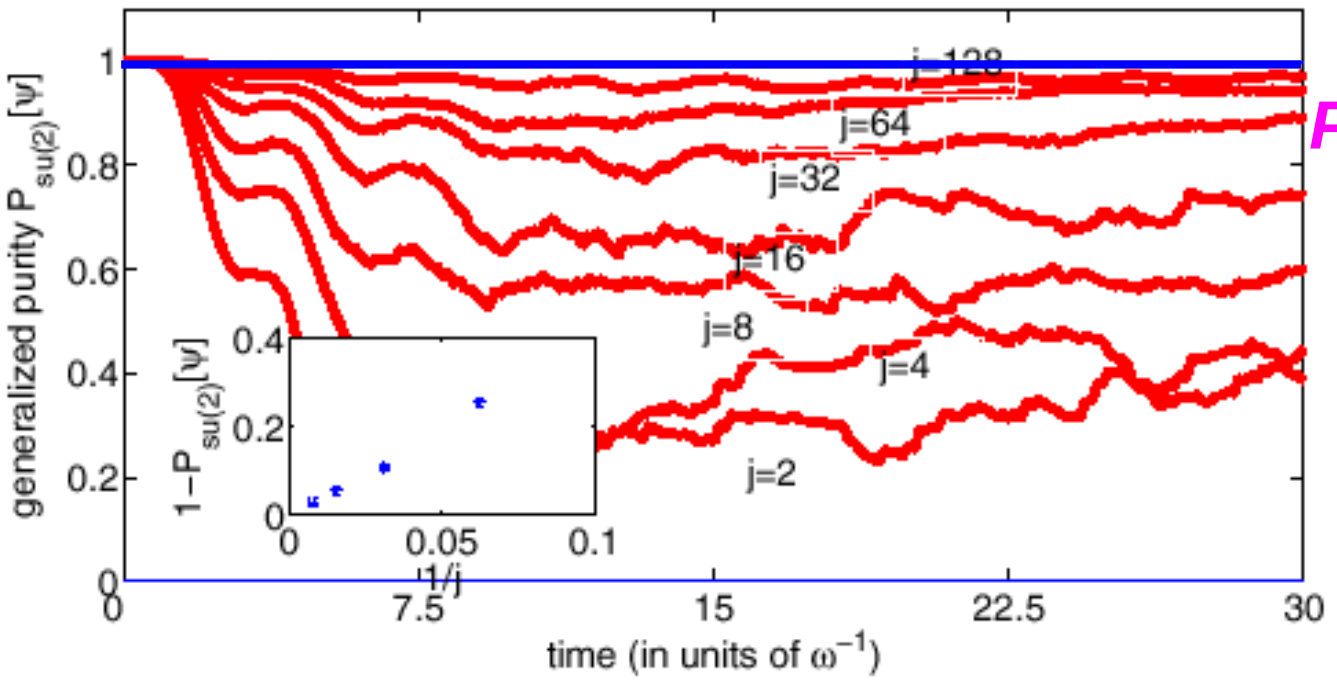
Efficient simulation of quantum evolution using dynamical coarse graining

Khasin & Kosloff PRA 78 (2008) 012321

Expanding the wavefunction with time dependent GCS functions:

$$\psi(t)=\sum_{i=1}^{M} c_i(t)\, U(t)\phi_i$$

Efficient simulation is obtained if M does not depend on the size of the Hilbert space $\sim j$ we find $M=(2j+1)(1-\sqrt{P}) \approx 3$

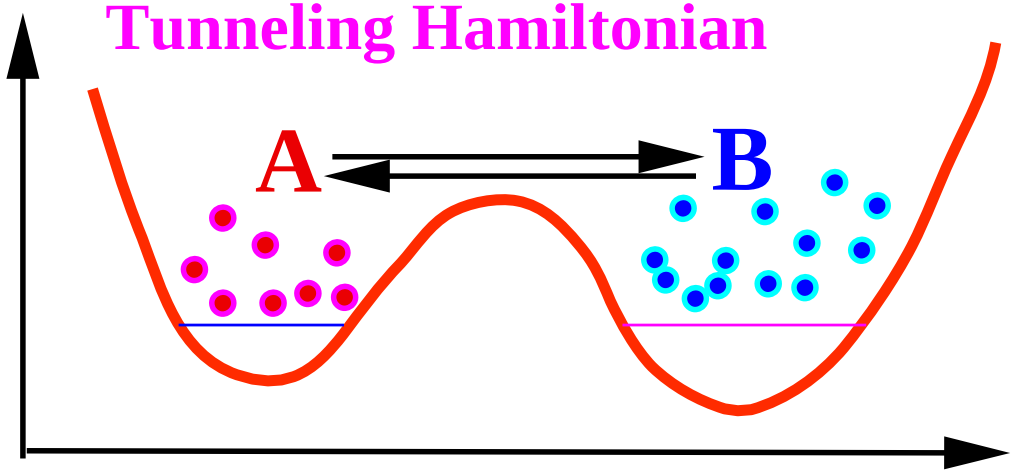


***P* the purity**

$$P=\langle J_x\rangle_\psi^2+\langle J_y\rangle_\psi^2+\langle J_z\rangle_\psi^2$$

When the Hilbert space increases the # of expansion states M decreases

Tunneling Hamiltonian



Surrogate Dynamics

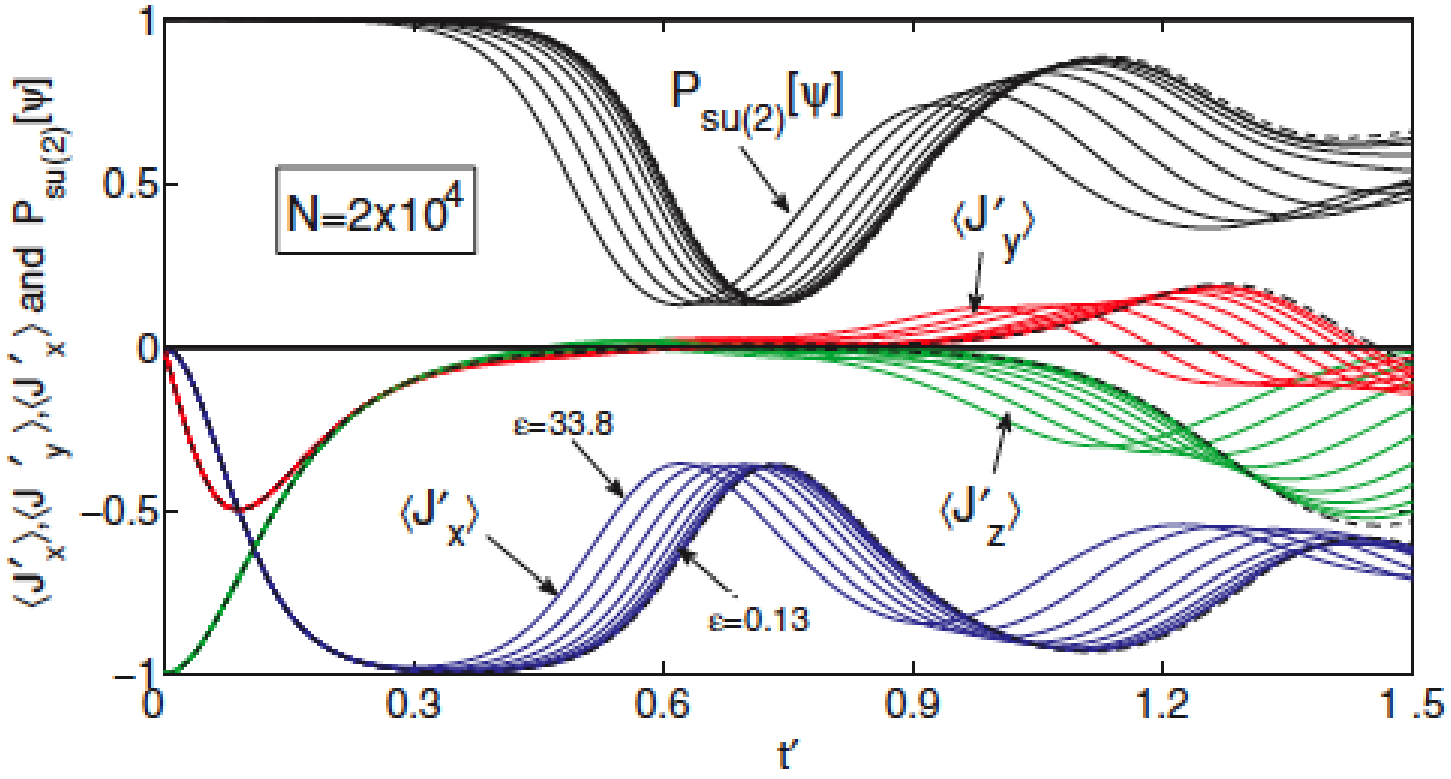
N= 20 000 particles

2000 stochastic realizations

Size of the expansion M=60

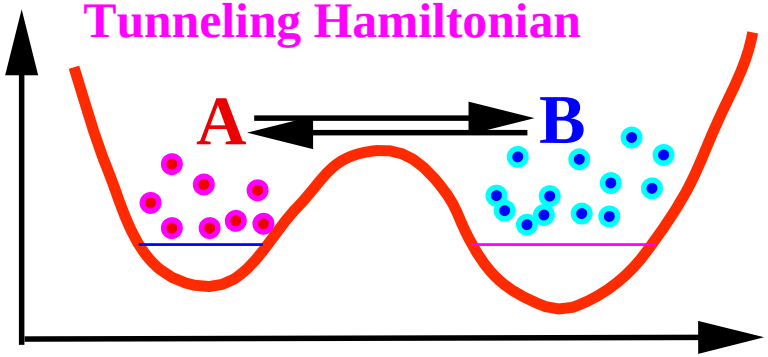
decreasing values of γ

$$H= \omega Na+\omega Nb+\Delta(a^{\dagger}b+b^{\dagger}a)+U(Na+Nb)^2=-\omega\, J_x+\frac{U}{N}J_z^2$$



$U/2\omega=1$

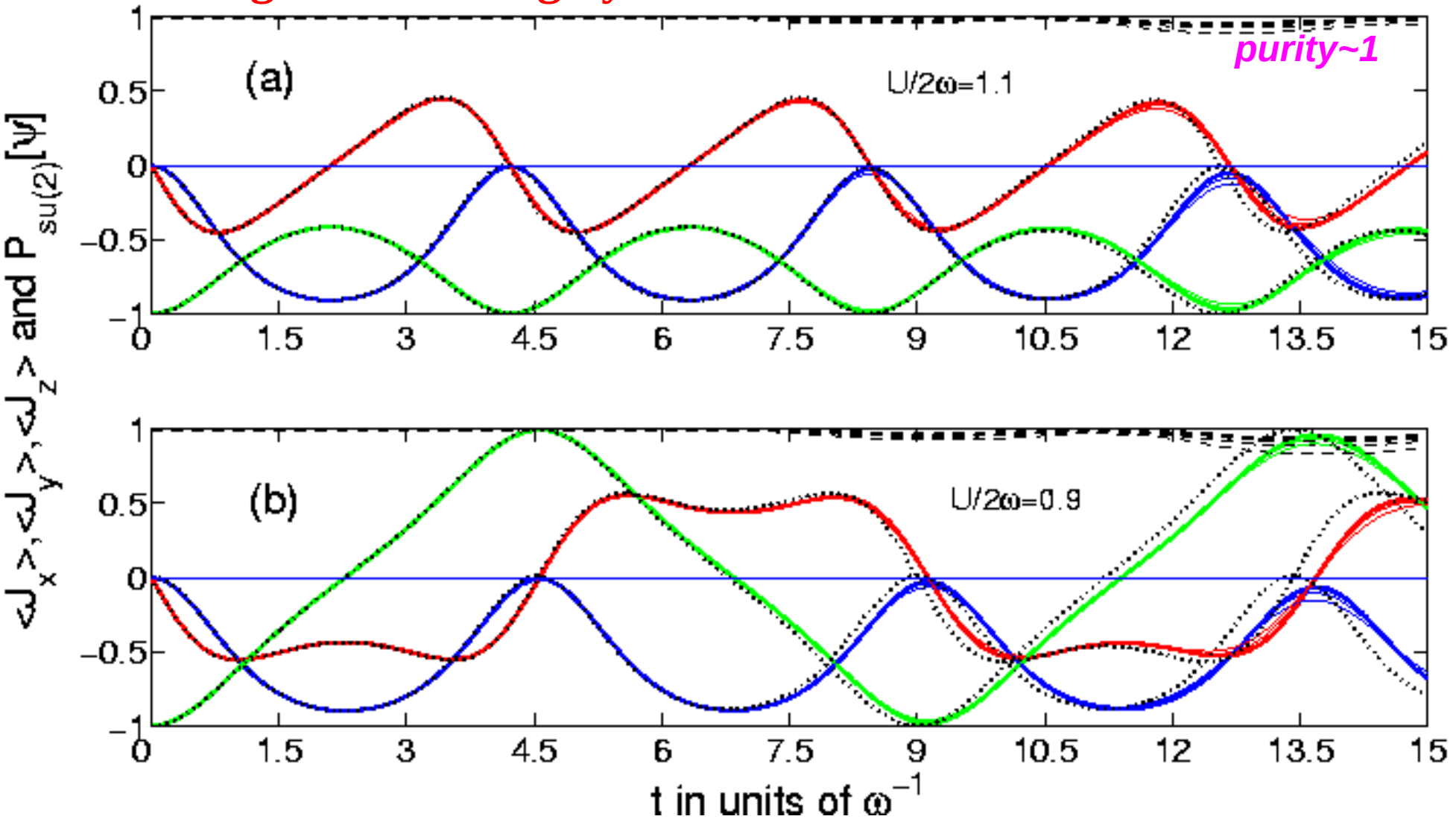
Tunneling Hamiltonian



Different values of the inerparticle coupling

$$H = -\omega J_x + \frac{U}{N} J_z^2$$

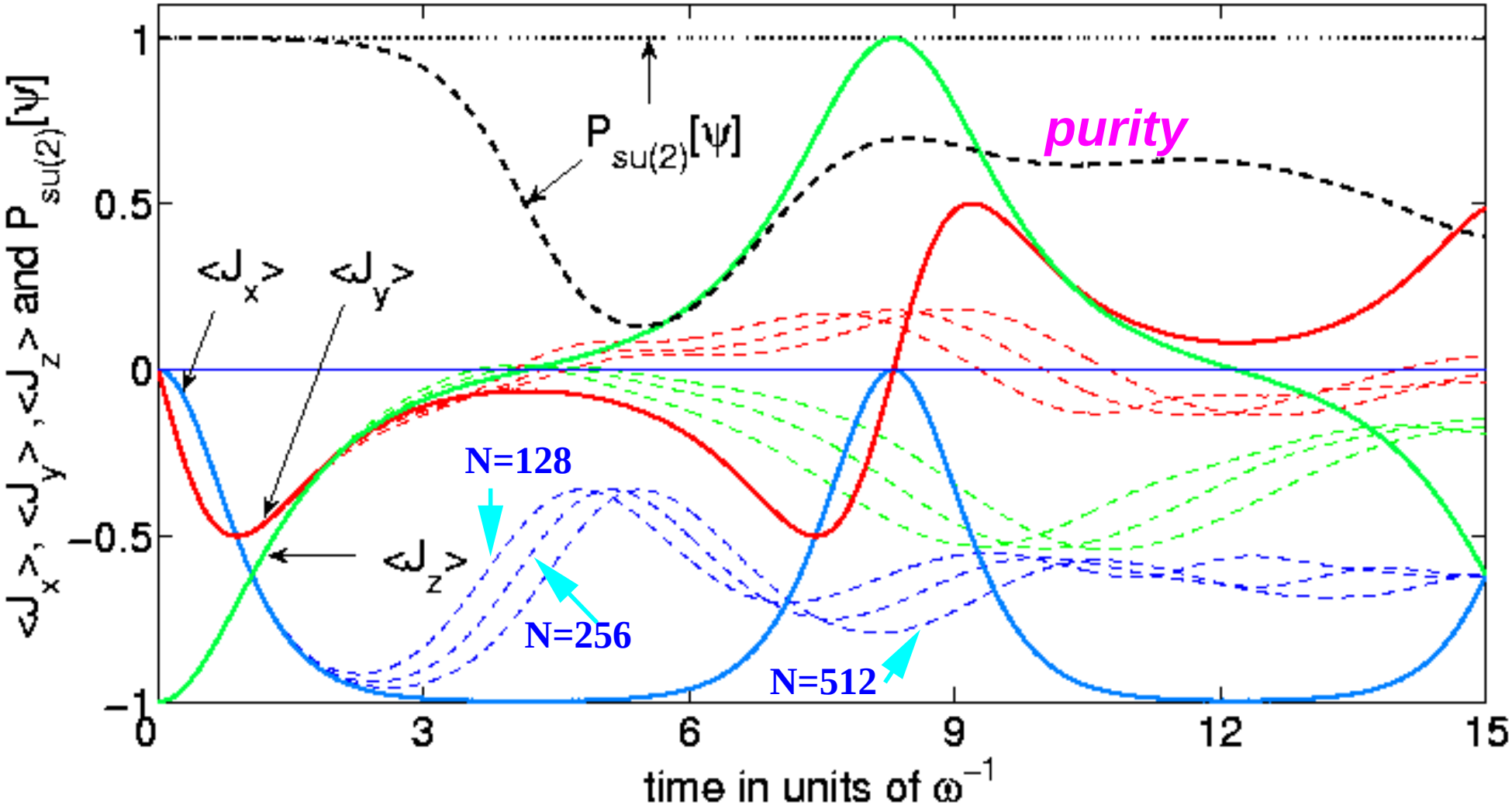
change in tunneling dynamics at $U/2\omega=1$



Surrogate Dynamics

Analysis: Breakup of mean field solutions

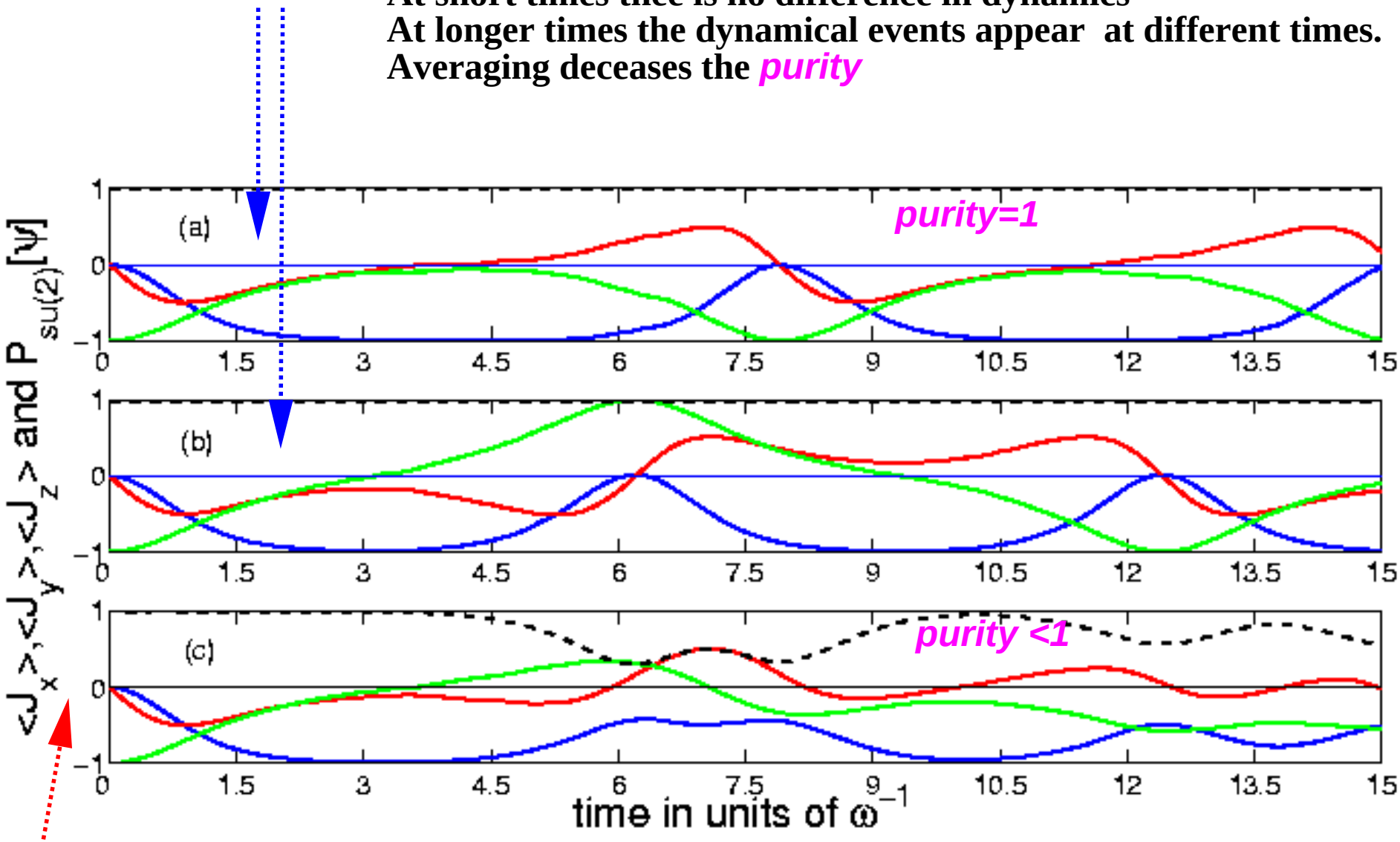
U/2ω=1 **N=512**



Surrogate Dynamics

Analysis: Two individual realizations of the sNLSE

At short times thee is no difference in dynamics
At longer times the dynamical events appear at different times.
Averaging deceases the *purity*



Average of the two realizations

Surrogate Dynamics *Generalization*

1) **The observables $\langle X_i \rangle$ are a member of the set $\{X_i\}$ forming a Lie algebra.**

2) **The Hamiltonain has the form:**

$$H = \sum a_j X_j + \sum b_{jk} X_j X_k + \sum c_{jkl} X_j X_k X_l + \ldots.$$

3) $$\frac{d\rho}{dt} = -i\,[H,\rho] + L_D(\rho) \qquad L_D(\rho) = -\gamma\Big(\sum [\,X_i, [X_i,\rho]]\Big)$$

non unitary dynamics

$$d\psi = \Big\{ -i\,H dt - \gamma \sum_{i=1}^{K} (X_i - \langle X_i \rangle_\psi)^2 dt + \sum_{i=1}^{K} (X_i - \langle X_i \rangle_\psi) d\xi_j \Big\} \psi$$

sNLSE where $\langle \xi_j \rangle = 0$ and $\langle \xi_j \xi_k \rangle = \delta_{jk}\,\gamma\,dt$

4) $$\psi(t) = \sum_{i=1}^{M} c_i(t)\, U(t) \phi_i$$

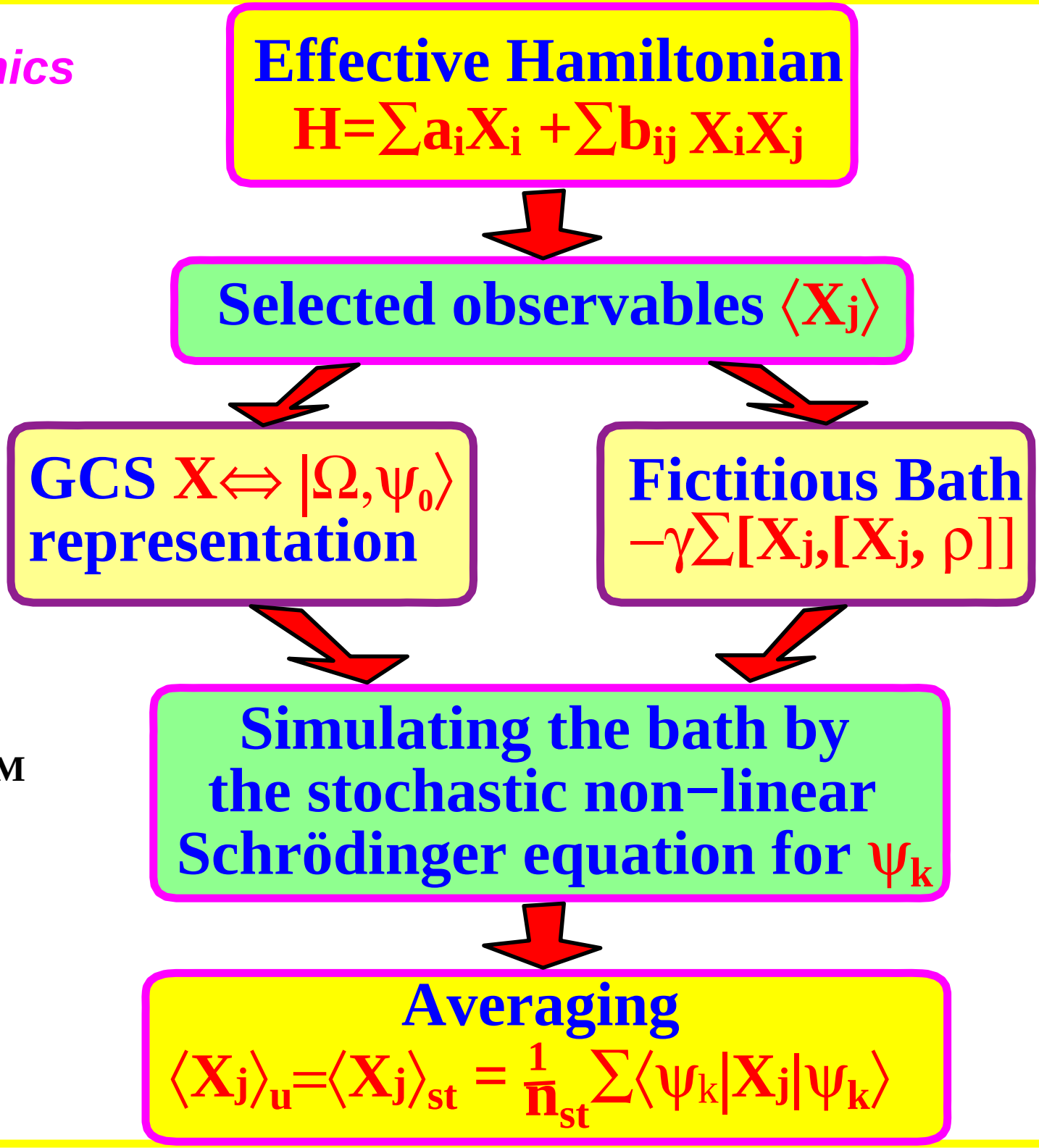
basis set

ϕ **generalized coherent states GCS**

maximizing the *purity*, $P = \Sigma \langle X_i \rangle^2$

Surrogate Dynamics

Flowchart

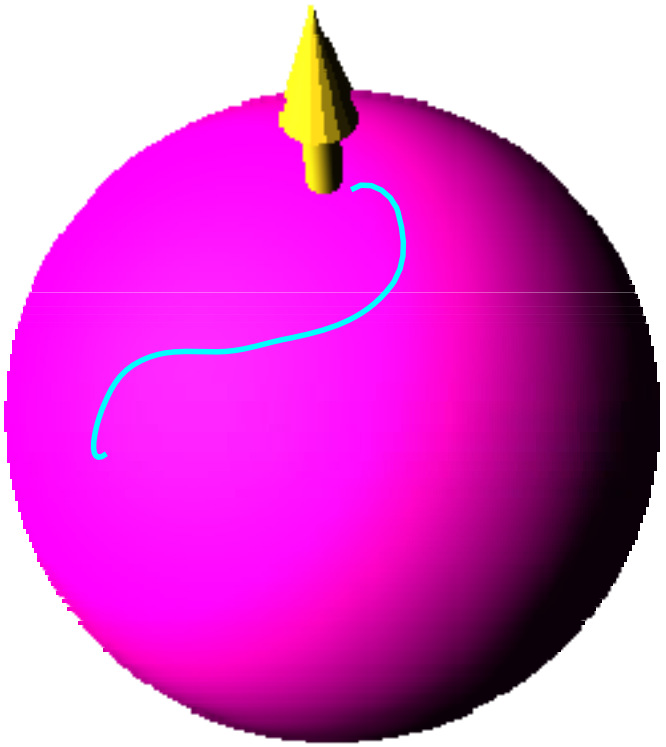


The # of basis functions **M** is much smaller than N
N=20000 **M~60**

The # of realizations is determined by the dispersion or *purity*

The time step still is determined by N

Thank you




END

Coherent control in the context of many body dynamics

$$H = -\omega(t) J_x + \frac{U}{N} J_z^2$$

Mathematically our many body Hamiltonian is compleatly controllable. This means that there exist an external field $\omega(t)$ that will lead the system from any initial state to any final state.

Moreover the control can generate any unitary transformation U

We found that when the size of the Hilbert space increases the only possible state to state control is between GCS states.

Control between states that are not GCS become extremaly sensative any noise in the control $\omega(t)$ will collapse the system to a GCS!

This fact could severely restrict the possibility of quantum computing.

Semiclassical viewpoint

$\Psi = c(\tau,\tau^*)e^{-\tau J_+}|-j\rangle$ $\quad\quad$ $\tau = \cos\theta/2\, e^{-i\phi}$

$$\mathcal{H}(\tau,\tau^*) \equiv \left\langle \psi|\hat{\mathrm{H}}|\psi \right\rangle = -\omega j \frac{\tau+\tau^*}{|\tau|^2+1} + \frac{2j-1}{4} U \left(\frac{|\tau|^2-1}{|\tau|^2+1}\right)^2$$

$$-i\dot{\tau} = -\frac{\omega}{2}(1-\tau^2) + \frac{2j-1}{2j} U\tau \frac{|\tau|^2-1}{|\tau|^2+1}$$

The unstable fixed point $\mathcal{H}(-1,-1) = \omega j.$

The initial state chosen is τ=0 $\mathcal{H}(0,0) = \frac{2j-1}{4}U.$

The initial state is unstable if: $\mathcal{H}(-1,-1) = \mathcal{H}(0,0),$

Then: $\frac{U}{2\omega} = \frac{2j}{2j-1} = 1 + \frac{1}{2j} + O(j^{-2}),$ **~1**

Stochastic version of the mean field solution:

$$d\tau = i\left\{-\frac{\omega}{2}(1-\tau^2)+\frac{2j-1}{2j}U\tau\frac{|\tau|^2-1}{|\tau|^2+1}\right\}dt + \frac{1}{2}(1-\tau^2)d\xi_x+\frac{1}{2i}(1+\tau^2)d\xi_y+\tau d\xi_z,$$

$$< d\xi_i >= 0, \quad d\xi_i d\xi_j = 2\gamma\delta_{ij}dt.$$

U/2j=1