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
Control scheme for Na$_2$

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

The excited $A^1\Sigma_u^+$ levels are possible targets.

The $X^1\Sigma_g^+$ ground state targets.
Principles of coherent control: ground state

I

State-to-State Weak field

$|e_i\rangle$

$|g_i\rangle$

$\mathbf{i} \rightarrow \mathbf{f}$

Band width $\Delta E$

Time scale $\Delta t$

$\#$ of paths

very small

adiabatic

II

State-to-State Weak field

Coherent Control

$\Delta E$

$|e_i\rangle$

$|g_i\rangle$

vibrational spacing

vibrational period

III

State-to-State Weak field

More Coherent Control

$\Delta E$

$|e_i\rangle$

$|g_i\rangle$

N vibrational spacings

vibrational period
Principles of coherent control: **Excited state**

I. State-to-State Weak field

- \( i \rightarrow f \)
- \( |e_i\rangle \)
- \( |e_f\rangle \)
- Band width: \( \Delta E \)
- Time scale: \( \Delta t \)
- \# of paths: adiabatic 1

II. State-to-State Weak field

- Coherent Control?
- \( |e_i\rangle \)
- \( |e_f\rangle \)
- \( \Delta E \)
- Vibrational spacing: vibrational period 2

III. State-to-State Weak field

- More Coherent Control?
- \( |e_i\rangle \)
- \( |e_f\rangle \)
- \( \Delta E \)
- N vibrational spacings: vibrational period N
State-to-State strong field control

More Coherent Control

\[ i \rightarrow f \]

Ground state target

\[ g_i \]

\[ \Delta E \]

Excited state target

\[ e_j \]

\[ \Delta E \]

# of Rabi periods is linear with intensity
Spatial light modulator

The shaped pulse in time

The molecules

Pulse shaper

Spatial light Modulator

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.

$$\epsilon(t) = \tilde{\Omega}_0 \exp\left[-\frac{t^2}{\tau_0^2} + 2i\phi \right] = \frac{\Omega_0}{w_p} \exp\left[-\frac{t^2}{w_p^2} - 2i\phi t + i\omega_0 t \right]$$

Diagram:

- e\{0, 1, 2\}
- g\{0, 1, 2\}

$\omega$ Trasform limited TL
Negativ Chirp NC
Positive Chirp PC
Pump Prop PP

$\tau$, $\tau W_f$
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 Miller1*

Fig. 6. Energy dependence of (A) the ∆A 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

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, Andrea M. Nagy, Stephen A. Waschuk, Leonid S. Brown, Robert R. Birge, R. J. Dwayne Miller

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, M. T. W. Milder, L. Kuipers, and J. L. Herek

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

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**A**

Absorption (OD)

---

**B**

Optimal pulse shape

---

**C**

Dependence on viscosity

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

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

\[ \hat{H}_k = \frac{\hat{P}^2}{2\mu} + \hat{V}_k \] is the surface Hamiltonian \( k = \{g, b, d\} \)

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

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

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

\[ \hat{H}_T = \hat{H}_S + \hat{H}_B + \hat{H}_{B''} + \hat{H}_{SB} + \hat{H}_{BB''} \]

\[ \hat{H}_B = \sum_j \omega_j \hat{\sigma}_j^+ \hat{\sigma}_j \]

\[ \hat{H}_{SB} = \hat{A}_S \otimes \sum_j \lambda_j (\hat{\sigma}_j^+ + \hat{\sigma}_j) \]
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: Surrogates Dynamics
embedding the system in a larger Hilbert space
The surrogate Hamiltonian approach

\[ H = H_S + H_{\text{int}} + H_B \]

Wavefunction description

\[ H = H_S + \tilde{H}_{\text{int}} + \tilde{H}_B \]

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

\[ \langle A \rangle = \text{tr}\{\rho_S \cdot A\} \quad \text{where} \quad \rho_S = \text{tr}\{\rho_{SB}\} \]

For sufficiently short times we can dilute the spectrum of the bath Hamiltonian

Then we look for a compact bath Hamiltonian which generates an equivalent system dynamics
The surrogate Hamiltonian approach

\[ H = H_s + H_{\text{int}} + H_B \]

\[ H_s = T + V_s(R) \]

\[ H_B = \sum \varepsilon_j b_j^* b_j \]

\[ H_{\text{int}} = f(R) \sum \kappa_j (b_j + b_j^*) \]
III Discrete bath approximation

\[ H_{\text{int}} = f(R) \sum U_m (B_m + B^*_m) \]

\[ H_B = \sum \epsilon_m B_m B^*_m \]

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

\[ \rho(\epsilon_m) \approx (\epsilon_{m+1} - \epsilon_m)^{-1} \]
IV Alternative spin bath representation

System $H_S$

Representative bath modes

Interface

$H_S = T + V_s(R)$

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

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

Baer, Zeiri & Kosloff PRB 55 10952 (1997)

Baer & Kosloff JCP 106 8862 (1997)
Vibrational relaxation

energy relaxation

![Graph showing energy relaxation over time](image)
Vibrational relaxation

energy relaxation

![Graph showing system energy over time for different values of N, with a Poincare time indicated on the graph.](image)
Vibrational relaxation

energy relaxation

![Graph showing system energy as a function of time](image)
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
Replacing the bath modes: \[ H_T = H_S + H_B + H_{B'} + H_{SB} + H_{BB'} \]

- **System** \( \hat{\rho}_S \)
- **Primary Bath**
  - \( \lambda_j \) System bath coupling
- **Secondary Bath**
  - Swap operation: \( S \psi_k \otimes \varphi_k = \varphi_k \otimes \psi_k \)
  - \( \varphi_k = \left( \frac{e^{-\frac{\hbar \omega_k}{4kT} + \phi_1} + e^{\frac{\hbar \omega_k}{4kT} + \phi_2}}{\sqrt{Z}} \right) \)
- **Rate of swap** \( \Gamma_j \)

\[ \text{Diagram showing the coupling between system and bath modes.} \]
Homogenizer

\[
\rho_s(1) = \text{Tr} \left\{ U \rho_s(0) \otimes \sigma_B U^\dagger \right\} \\
\rho_s(N) = \text{Tr} \left\{ U_N \cdots U_1 \rho_s(0) \otimes \sigma_B U_1^\dagger \cdots U_N^\dagger \right\}
\]

Swap operation: \( S \left| \psi \right\rangle \otimes \left| \phi \right\rangle = \left| \phi \right\rangle \otimes \left| \psi \right\rangle \)

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

Decay of an oscillator to a bath

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

\[ f(\hat{R}) = \frac{1 - e^{-a\hat{R}}}{\alpha} \]
\[ J(\omega) = M\gamma\omega \]

9 bath modes

12 bath modes

15 bath modes + swap

9 bath modes + swap

JCP 129, 034108 (2008)
Cooling to thermal equilibrium

Coordinate representation

Phase space Wigner function
Approaching thermal equilibrium  9 bath modes + swap  6 realizations
The ratio between energy and phase relaxation $T_1/T_2$

The ratio between the primary and secondary rates of energy transfer
Convergence properties of the stochastic surrogate Hamiltonian

- $M =$ total # of states

- $N =$ number of realizations

- $K^{-1/2}$: Number of realizations

- Standard deviation vs. $M^{-1/2}$
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 $\frac{\hbar}{V_{12}}$
Model system for weak field control  

Target: change the branching ratio on the excited state
Phase only control with relaxation compared to free propagation

![Graph showing branching ratio of excited states at 7 psec vs. chirp rate with relaxation](image)
Population dynamics

Position/momentum expectations
\[
\frac{dN}{dt} = \frac{2}{\hbar} \text{Im} \langle \psi_d | V_{db} | \psi_b \rangle
\]

Focusing the wavefunction
The influence of the bath: different system–bath coupling

\[
\frac{N_d}{N_b} \quad \lambda = 0.025 \\
\frac{N_d}{N_b} \quad \lambda = 0.015 \\
\frac{N_d}{N_b} \quad \lambda = 0.01 \\
\frac{N_d}{N_b} \quad \lambda = 0.0075 \\
\frac{N_d}{N_b} \quad \lambda = 0.0 \\
\frac{N_d}{N_b} \quad \lambda = 0.04
\]

\[
\chi / \chi_{\text{max}}
\]

\[
\text{Inset:} \quad N_d / N_b \quad \lambda
\]

\[
\begin{align*}
\text{Figure:} \quad \frac{N_d}{N_b} & \quad \lambda = 0.025 \\
& \quad \lambda = 0.015 \\
& \quad \lambda = 0.01 \\
& \quad \lambda = 0.0075 \\
& \quad \lambda = 0.0 \\
& \quad \lambda = 0.04
\end{align*}
\]
Weak field coherent control
Phase only control is possible!

The bath introduces a new time scale \( T_1 \approx 500 \text{fsec} \)

Vibrational frequency \( \nu = 940 \text{ cm}^{-1} \), \( V_{bd}/h = 40 \text{ cm}^{-1} \)

Negative chirp is optimal: \( \tau = 12 \text{ fsec}, w_f = 1.38 \)

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

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

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

The computation resources scale as $D^N$ where $D$ is the size of Hilbert space $D = d^\delta$ and $\delta$ is larger then 1.

$N$ number of particles

Direct solutions become prohibitively expensive!
The Problem: Tunneling Hamiltonian for N particle interaction

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

single particle tunneling term

inter-particle interaction
We define

\[ J_x = \frac{1}{2} (a^\dagger b + b^\dagger a) \]
\[ J_y = \frac{1}{2i} (a^\dagger b - b^\dagger a) \]
\[ J_z = \frac{1}{2} (a^\dagger a - b^\dagger b) \]

and the total number of particles is conserved

\[ N = N_a + N_b \]

Then:

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

is the effective many body non linear Hamiltonian

The # of states

\[ D = N + 1 \]

= size of Hilbert space
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 set $J_x, J_y, J_z$

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

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 Hamiltonian?

\[ H = -\omega \mathbf{J}_x + \frac{U}{N} \mathbf{J}_z^2 \]

The Heisenberg equations of motion include all powers of operators \( \mathbf{J}_x, \mathbf{J}_x^2, \mathbf{J}_x^3 \ldots \) and combinations \( \mathbf{J}_x \mathbf{J}_y, \mathbf{J}_x \mathbf{J}_y^2, \ldots \) 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:
\[ \Psi(t) = \exp\{ -i/\hbar \mathbf{H}t \} \Psi(0) = \sum_{k=-j}^{+j} C_k |k\rangle \]
and \( C_k \) has amplitude for all \( k \)

In general for \( \mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1 \), if the commutators:
\( A_1 = [\mathbf{H}_0, \mathbf{H}_1], \ A_2 = [\mathbf{H}_0, [\mathbf{H}_0, \mathbf{H}_1]], \ A_3 = \ldots \) generate the full Hilbert space

The computational problem becomes prohibitively expensive!

If we limit ourselves to the dynamics of \( \langle \mathbf{J}_x \rangle, \langle \mathbf{J}_y \rangle, \langle \mathbf{J}_z \rangle \) 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 Schrödinger's equation:

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

by the Liouville von Neumann equation

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

but replacing the wavefunction by a density operator makes the computational problem more difficult?
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) How to solve the Liouville von Neumann equation without using a density operator?
**Surrogate Dynamics**

**We start with problem 3**

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

\[
\frac{d\rho}{dt} = -i [H, \rho] + \mathcal{L}_D(\rho)
\]

where \( \mathcal{L}_D(\rho) \) is Lindblad form \( \mathbf{V}\rho \mathbf{V}^\dagger - \frac{1}{2}\{\mathbf{V}^\dagger \mathbf{V}, \rho\} \)

Gisin, (PRL 1984) Percival, Diosi .. developed a

**Stochastic Non Linear Schrödinger Equation (sNLSE)** where:

\[
d\psi = \left\{-i H dt + (f(\langle V \rangle) d\xi_j}\right\} \psi
\]

where \( \langle \xi_j \rangle = 0 \) and \( \langle \xi_j \xi_k \rangle = \delta_{jk} \gamma dt \)

and the density operator \( \rho \) is the average of stochastic realizations

\[
\rho(t) = \frac{1}{N} \sum |\psi_1\rangle \langle \psi_1|, \text{ when } N \to \infty
\]

This realization is not unique!
2) Can the open system dynamics limit the growth of the representation?

**Idea:** Applying 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 semigroup generator:

$$\mathcal{L}_D(\rho) = -\gamma [A, [A, \rho]]$$

Specifically collapsing on to the submanifold

$$\mathcal{L}_D(\rho) = -\gamma ( [J_x, [J_x, \rho]] + [J_y, [J_y, \rho]] + [J_y, [J_y, \rho]] )$$

This is realized by the sNLSE

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

$$\dot{X} = i[H, X] - \gamma \sum_{i=1}^{3} [J_i, [J_i, X]]$$

$$H = -\omega J_x + \sum_{\mathbb{N}} J_z^2$$

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 $\chi_n$

Looking for the states with minimum uncertainty with respect to the operators of the algebra:

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

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

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

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** $\chi_n$

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

Any matrix element can be calculated within the algebra.

for example:  
$$\langle \chi_n | J_y | \chi_m \rangle = \langle \psi_0 U_n^\dagger | J_y | U_m \psi_0 \rangle$$

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

We start by creating a uniform distribution of GCS: $\chi_n$

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

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

$$U(t) = \exp(-i (\alpha(t)J_x + \beta(t)J_y + \gamma(t)J_z))$$
Generalized Coherent states (GCS)

The global stable solution of the Stochastic Schrödinger equation
Khasin & Kosloff, JPA 41 (2008) 365203

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

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
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 \( M = (2j+1)(1-\sqrt{P}) \approx 3 \)

\[ P = \langle J_x \rangle^2 \psi + \langle J_y \rangle^2 \psi + \langle J_z \rangle^2 \psi \]

When the Hilbert space increases the # of expansion states \( M \) decreases
Tunneling Hamiltonian

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

Surrogate Dynamics

$N = 20,000$ particles
2000 stochastic realizations
Size of the expansion $M = 60$

decreasing values of $\gamma$

$\frac{U}{2\omega} = 1$
Tunneling Hamiltonian

Different values of the inerparticle coupling

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

Change in tunneling dynamics at \( U/2\omega = 1 \)

(a) Purity \( \approx 1 \)

(b)
Surrogate Dynamics

Analysis: Breakup of mean field solutions

$U/2\omega = 1 \quad N = 512$
**Surrogate Dynamics**

**Analysis:** Two individual realizations of the sNLSE

At short times there is no difference in dynamics.
At longer times the dynamical events appear at different times.
Averaging decreases 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 Hamiltonian 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) \[
\frac{d\rho}{dt} = -i [H, \rho] + \mathcal{L}_D(\rho) \quad \mathcal{L}_D(\rho) = -\gamma \left( \sum \left[ X_i, [X_i, \rho] \right] \right) \\
\text{non unitary dynamics}
\]

4) \[
\psi(t) = \sum_{i=1}^M c_i(t) U(t) \phi_i \quad \phi \text{ generalized coherent states GCS}
\]

basis set

maximizing the purity, $P = \sum \langle X_i \rangle^2$
Effective Hamiltonian
\[ H = \sum a_i X_i + \sum b_{ij} X_i X_j \]

Selected observables \( \langle X_j \rangle \)

GCS \( X \leftrightarrow |\Omega, \psi_0\rangle \) representation

Fictitious Bath
\[ -\gamma \sum [X_j, [X_j, \rho]] \]

Simulating the bath by the stochastic non-linear Schrödinger equation for \( \psi_k \)

Averaging
\[ \langle X_j \rangle_u = \langle X_j \rangle_{st} = \frac{1}{n_{st}} \sum \langle \psi_k | X_j | \psi_k \rangle \]

Surrogate Dynamics

Flowchart

The number of basis functions \( M \) is much smaller than \( N \)
\( N = 20000 \quad M \sim 60 \)

The number of realizations is determined by the dispersion or purity

The time step still is determined by \( N \)
Thank you
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 completely 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 sensitive 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

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

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

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

The unstable fixed point

$$\mathcal{H}(-1, -1) = \omega j.$$

The initial state chosen is $\tau = 0$

$$\mathcal{H}(0, 0) = \frac{2j - 1}{4} U.$$

The initial state is unstable if:

$$\mathcal{H}(-1, -1) = \mathcal{H}(0, 0),$$

Then:

$$\frac{U}{2\omega} = \frac{2j}{2j - 1} = 1 + \frac{1}{2j} + O(j^{-2}), \sim 1$$
Stochastic version of the mean field solution:

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

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