THE FRITZ HABER RESEARCH CENTER
FOR MOLECULAR DYNAMICS

Surrogate Dynamics

Efficient simulation of quantum many particle dynamics

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Noise and control: good and bad noise

Control Hamiltonian

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \hat{\mathrm{H}}_1(\omega)$$

Controls

$$\hat{\mathrm{H}}_1(\omega) = \sum_j \omega_j(t)\hat{\mathrm{A}}_j$$

Complete controllability if:

$$\hat{\mathrm{B}}_1 = [\hat{\mathrm{H}}_0, \hat{\mathrm{H}}_1]$$
$$\hat{\mathrm{B}}_2 = [\hat{\mathrm{H}}_0, [\hat{\mathrm{H}}_0, \hat{\mathrm{H}}_1]]$$
$$\hat{\mathrm{B}}_3 = [\hat{\mathrm{H}} - 0, [\hat{\mathrm{H}}_0, [\hat{\mathrm{H}}_0, \hat{\mathrm{H}}_1]]]$$
$$\hat{\mathrm{B}}_n = [\hat{\mathrm{H}} - 0, [\hat{\mathrm{H}}_0, [\hat{\mathrm{H}}_0, [....[....[\hat{\mathrm{H}}_0, \hat{\mathrm{H}}_1]]..]...]$$

the set $\hat{\mathrm{B}}$ generates the full Hilbert space.

Tarn, Clark, Rabitz, Ramakrishna

Example 1: adiabatic following

Maintaining the density operator diagonal in the energy representation

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_{int} + \hat{\mathrm{H}}_{ext}(\omega)$$

$$\hat{\mathrm{H}}_{int} = \frac{1}{2}\hbar J\left(\hat{\boldsymbol{\sigma}}_x^1 \otimes \hat{\boldsymbol{\sigma}}_x^2 - \hat{\boldsymbol{\sigma}}_y^1 \otimes \hat{\boldsymbol{\sigma}}_y^2\right) \equiv \hbar J \hat{\mathrm{B}}_2$$

$$\hat{\mathrm{H}}_{ext} = \frac{1}{2}\hbar\omega(t)\left(\hat{\boldsymbol{\sigma}}_z^1 \otimes \hat{\mathbf{I}}^2 + \hat{\mathbf{I}}^1 \otimes \boldsymbol{\sigma}_z^2\right) \equiv \omega(t)\hat{\mathrm{B}}_1$$

The $\mathbf{SU(2)}$ is closed with $\hat{\mathrm{B}}_3 = \frac{1}{2}\left(\hat{\boldsymbol{\sigma}}_y^1 \otimes \hat{\boldsymbol{\sigma}}_x^2 + \hat{\boldsymbol{\sigma}}_x^1 \otimes \hat{\boldsymbol{\sigma}}_y^2\right)$ and $[\hat{\mathrm{B}}_1, \hat{\mathrm{B}}_2] \equiv 2i\hat{\mathrm{B}}_3$.

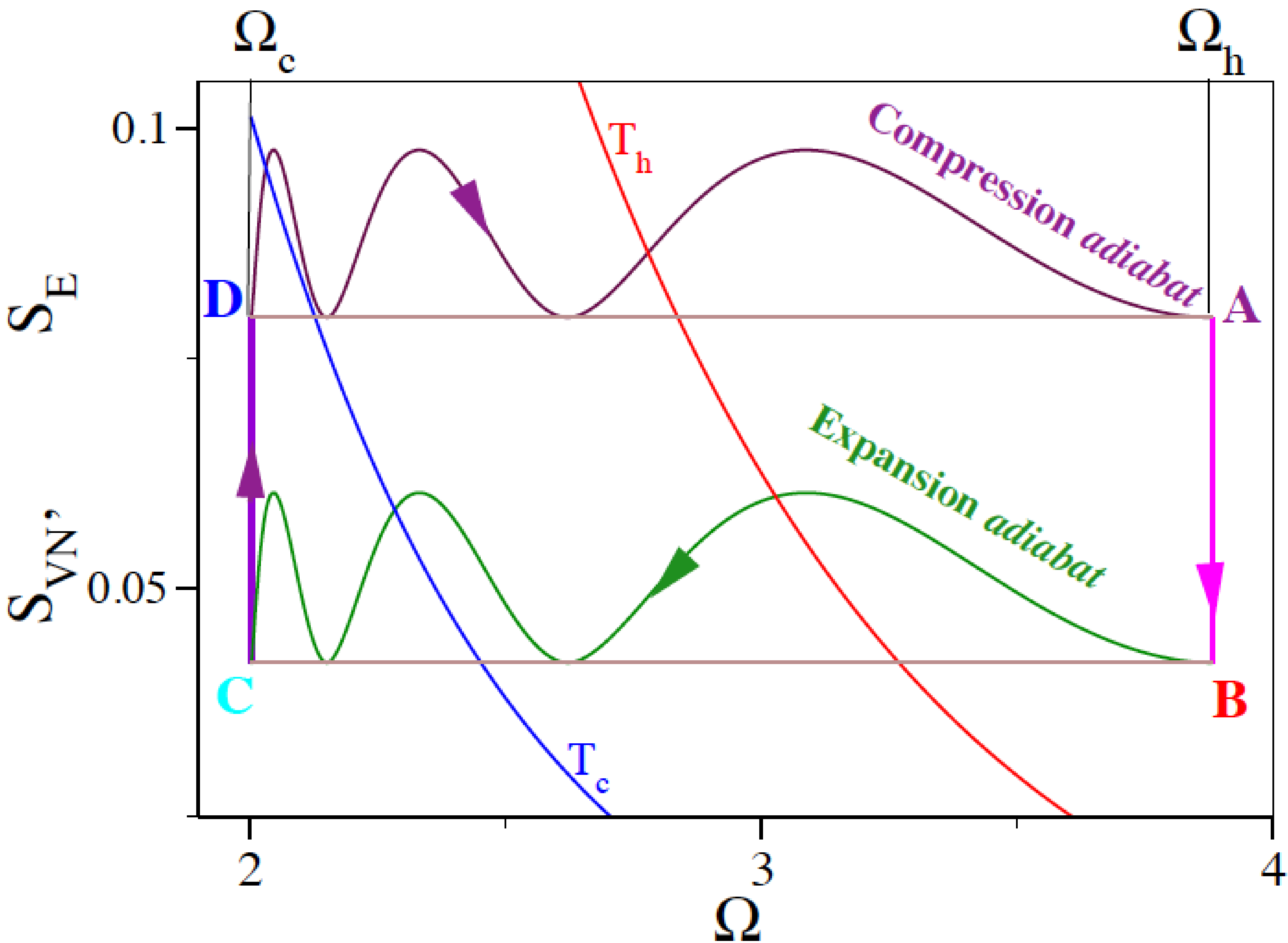
$$\hat{\mathrm{H}} = \hbar\left(\omega(t)\hat{\mathrm{B}}_1 + \mathrm{J}\hat{\mathrm{B}}_2\right)$$

$$\epsilon_1 = -\hbar\Omega,\ \epsilon_{2/3} = 0,\ \epsilon_4 = \hbar\Omega$$

$$\Omega = \sqrt{\omega^2 + J^2}.$$

We want to change the energy scale from Ω_h to Ω_c

Motivation: Quantum refrigerator



State of the system and vector space

$$\hat{\mathrm{H}} = \omega(\mathrm{t})\hat{\mathbf{B}}_1 + \mathrm{J}\hat{\mathbf{B}}_2 \;,\; \hat{\mathrm{L}} = -\mathrm{J}\hat{\mathbf{B}}_1 + \omega(\mathrm{t})\hat{\mathbf{B}}_2 \;,\; \hat{\mathrm{C}} = \Omega(\mathrm{t})\hat{\mathbf{B}}_3$$

$$\hat{\mathrm{V}} = \Omega\hat{\mathrm{B}}_4 = \tfrac{1}{2}\Omega(\hat{\mathrm{I}}^1 \otimes \hat{\boldsymbol{\sigma}}_z^2 - \hat{\mathrm{I}}^2 \otimes \hat{\boldsymbol{\sigma}}_z^1) \text{ and } \hat{\mathrm{D}} = \Omega\hat{\mathrm{B}}_5 = \Omega\hat{\boldsymbol{\sigma}}_z^1 \otimes \hat{\boldsymbol{\sigma}}_z^2$$

$$\hat{\rho} = \frac{1}{4}\hat{\mathrm{I}} + \frac{1}{\Omega}\left(\langle\hat{\mathrm{H}}\rangle\hat{\mathrm{H}} + \langle\hat{\mathrm{L}}\rangle\hat{\mathrm{L}} + \langle\hat{\mathrm{C}}\rangle\hat{\mathrm{C}} + \langle\hat{\mathrm{V}}\rangle\hat{\mathrm{V}} + \langle\hat{\mathrm{D}}\rangle\hat{\mathrm{D}}\right)$$

$$\hat{\rho}_e = \frac{1}{4}\begin{pmatrix} 1+\frac{4}{\Omega}(D-E) & 0 & 0 & \frac{4}{\Omega}(L+iC) \\ 0 & 1-\frac{4}{\Omega}D & 0 & 0 \\ 0 & 0 & 1-\frac{4}{\Omega}D & 0 \\ \frac{4}{\Omega}(L-iC) & 0 & 0 & 1+\frac{4}{\Omega}(D+E) \end{pmatrix}$$

Equation of motion

$$\frac{d\hat{\mathbf{A}}}{dt} = \frac{i}{\hbar}[\hat{\mathbf{H}}, \hat{\mathbf{A}}] + \mathcal{L}_D(\hat{\mathbf{A}}) + \frac{\partial \hat{\mathbf{A}}}{\partial t}$$

$$\frac{d}{dt}\begin{pmatrix} \hat{\mathbf{B}}_1 \\ \hat{\mathbf{B}}_2 \\ \hat{\mathbf{B}}_3 \end{pmatrix}(t) = \begin{pmatrix} 0 & 0 & J \\ 0 & 0 & -\omega \\ -J & \omega & 0 \end{pmatrix}\begin{pmatrix} \hat{\mathbf{B}}_1 \\ \hat{\mathbf{B}}_2 \\ \hat{\mathbf{B}}_3 \end{pmatrix}$$

$$\frac{d}{\Omega dt}\begin{pmatrix} \hat{\mathbf{H}} \\ \hat{\mathbf{L}} \\ \hat{\mathbf{C}} \end{pmatrix}(t) = \begin{pmatrix} \frac{\dot{\Omega}}{\Omega^2} & -\frac{J\dot{\omega}}{\Omega^3} & 0 \\ \frac{J\dot{\omega}}{\Omega^3} & \frac{\dot{\Omega}}{\Omega^2} & -1 \\ 0 & 1 & \frac{\dot{\Omega}}{\Omega^2} \end{pmatrix}\begin{pmatrix} \hat{\mathbf{H}} \\ \hat{\mathbf{L}} \\ \hat{\mathbf{C}} \end{pmatrix}$$

Adiabatic parameter

$$m = \frac{J\dot{\omega}}{\Omega^3}$$

The propagator $\mathcal{U}_{hc} = \mathcal{U}_1 \mathcal{U}_2$

Energy scaling $\mathcal{U}_1 = e^{(\int_0^{\tau_{hc}} \frac{\dot{\Omega}}{\Omega} dt)} \hat{1} = \frac{\Omega_c}{\Omega_h} \hat{1}$

$$\mathcal{U}_2 = \begin{pmatrix} \frac{1+m^2c}{q^2} & -\frac{ms}{q} & \frac{m(1-c)}{q^2} \\ \frac{ms}{q} & c & -\frac{s}{q} \\ \frac{m(1-c)}{q^2} & \frac{s}{q} & \frac{m^2+c}{q^2} \end{pmatrix}$$

$$q = \sqrt{1+m^2};$$

$s = sin(q\Theta)$ and $c = cos(q\Theta)$

$$\Theta_{hc} = \tau_{hc} \frac{1}{K_{hc}} \Phi_{hc}$$

Deviation from adiabatic following $\delta = 1 - \mathcal{U}_2(1,1).$

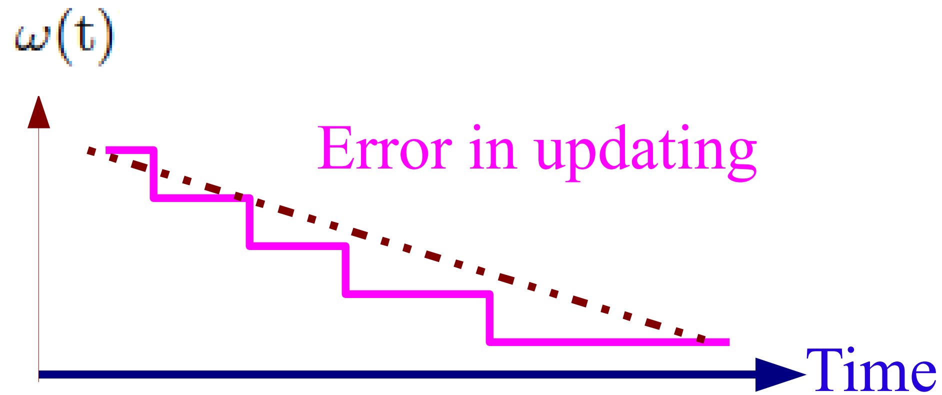
whenever $q\Theta = 2\pi l \quad l = 0, 1, 2...$ $\quad \delta = 0.$

Quantization of the adiabatic parameter $m = \left(\left(\frac{2\pi l}{\Phi_{hc}} \right)^2 - 1 \right)^{-\frac{1}{2}}$

Noise in the controls

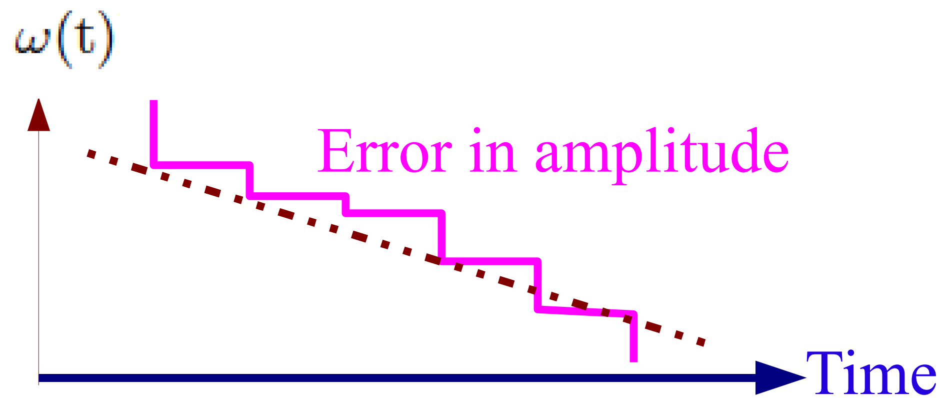
Phase noise

$$\mathcal{L}_{N_a}(\hat{A}) \;=\; -\gamma_a[\hat{H},[\hat{H},\hat{A}]]$$



Amplitude noise

$$\mathcal{L}_{\omega}\hat{X} = -\gamma_b[\hat{B}_1,[\hat{B}_1,\hat{X}]].$$



Dynamics with phase noise

$$\frac{d}{\Omega dt}\begin{pmatrix}\hat{\mathrm{H}}\\ \hat{\mathrm{L}}\\ \hat{\mathrm{C}}\end{pmatrix}(t)=\begin{pmatrix}\frac{\dot\Omega}{\Omega^2} & -\frac{J\dot\omega}{\Omega^3} & 0\\ \frac{J\dot\omega}{\Omega^3} & \frac{\dot\Omega}{\Omega^2}-\gamma_a\Omega & -1\\ 0 & 1 & \frac{\dot\Omega}{\Omega^2}-\gamma_a\Omega\end{pmatrix}\begin{pmatrix}\hat{\mathrm{H}}\\ \hat{\mathrm{L}}\\ \hat{\mathrm{C}}\end{pmatrix}$$

The propagator $\mathcal{U}_a = \mathcal{U}_1\mathcal{U}_2\mathcal{U}_3$

interaction representation:

$$\frac{d}{\Omega dt}\mathcal{U}_3(t) = \mathcal{U}_2(-t)\begin{pmatrix}0 & 0 & 0\\ 0 & -\gamma_a\Omega & 0\\ 0 & 0 & -\gamma_a\Omega\end{pmatrix}\mathcal{U}_2(t)\,\mathcal{U}_3(t) = \mathcal{W}(t)\mathcal{U}_3(t)$$

$$\mathcal{U}_3(\Theta = 2\pi) \approx e^{\mathcal{M}_1+\mathcal{M}_2+\ldots}$$

$$\mathcal{U}_3(\Theta = 2\pi)_{M_2} \approx \begin{pmatrix} C & -S & 0 \\ S & C & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$S = \sin\alpha$ and $C = \cos\alpha$. $\alpha = \gamma_a \pi m \sqrt{9m^2 + 4}$ $m \to 0$ $\alpha = \gamma_a 2\pi m \approx \Phi_{hc}\gamma_a \frac{1}{l}$,

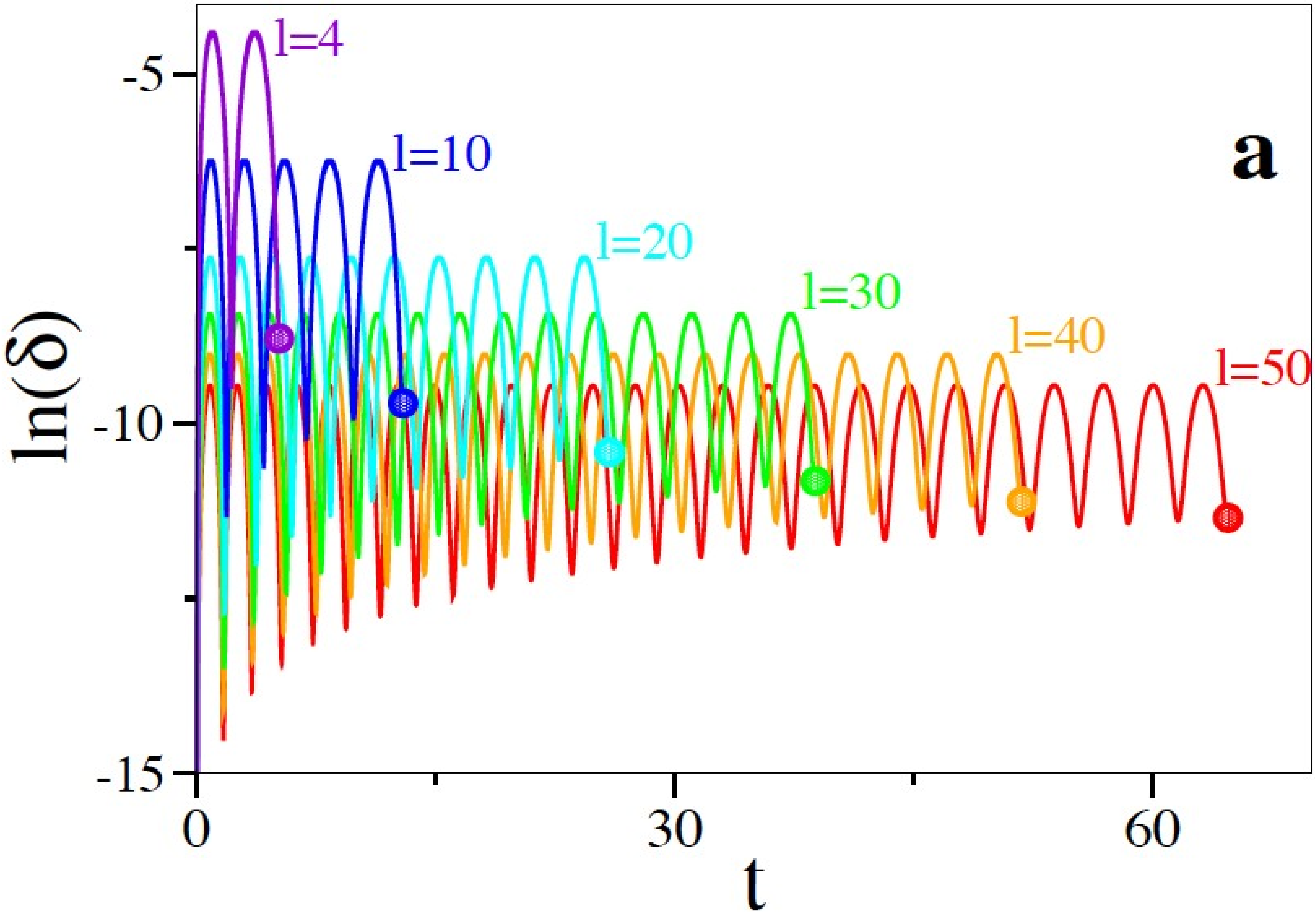
$\mathcal{U}_3(\tau_{hc})$, for l revolutions. $\alpha = \Phi_{hc}\gamma_a$

Asymptotic minimum phase noise

$m \to 0$

$$\delta_{min} = 1 - \cos(\Phi_{hc}\gamma_a) \approx \Phi_{hc}^2\gamma_a^2/2$$

For amplitude noise $\delta = 1 - \mathcal{U}_3(1,1) \approx 1 - e^{-\gamma_b \frac{J^2}{\Omega_c^2}\tau_{hc}}$

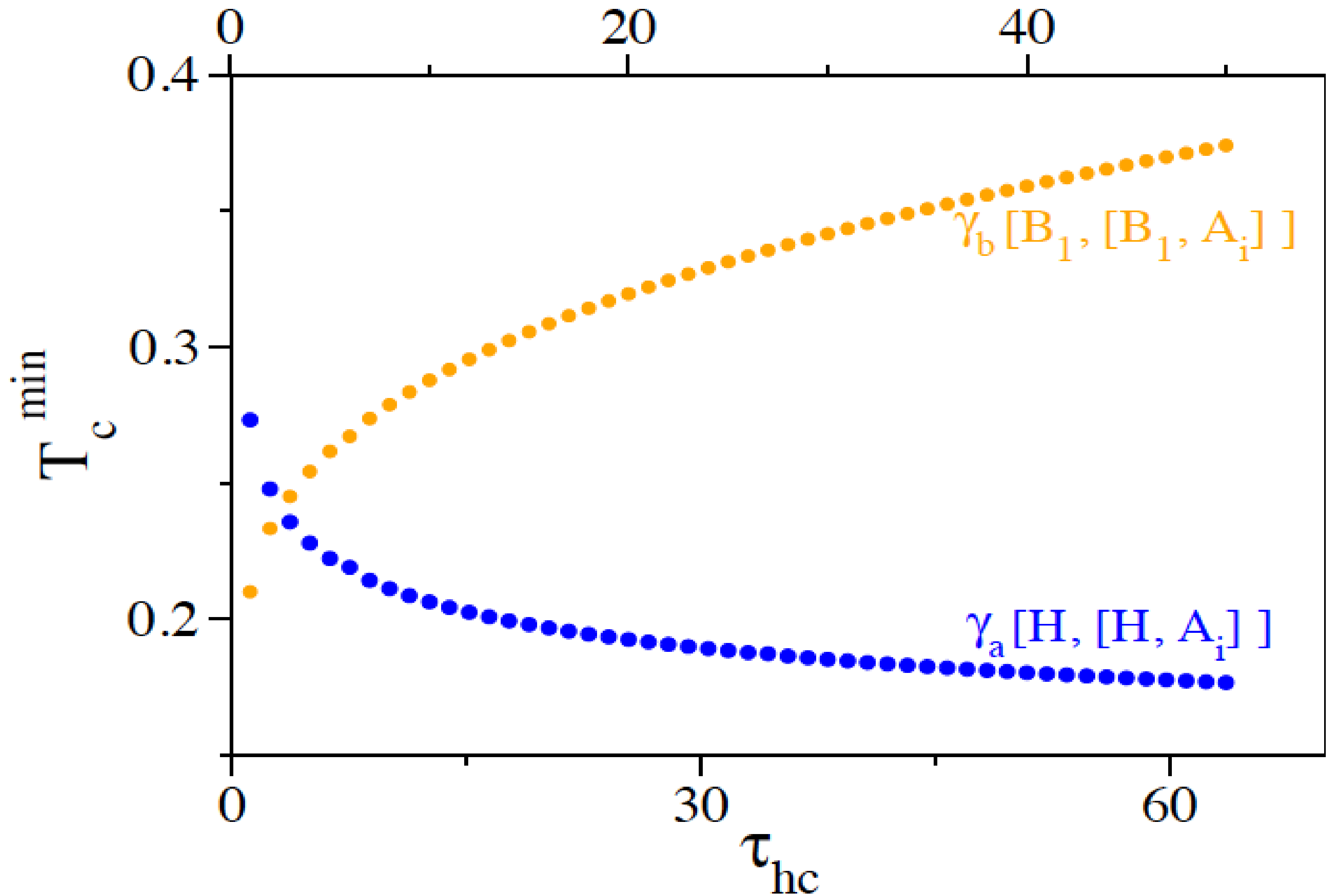


l=4
l=10
l=20
l=30
l=40
l=50
a
-5
-10
-15
ln(δ)
0
30
60
t

The minimum temperature
Quantum refrigerator

$$T_c \geq \frac{\hbar J}{-k_B \log(\delta/2)}$$

1



Good noise

Surrogate dynamics

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

The computation resources scale as D^{δ}

where D is the size of Hilbert space

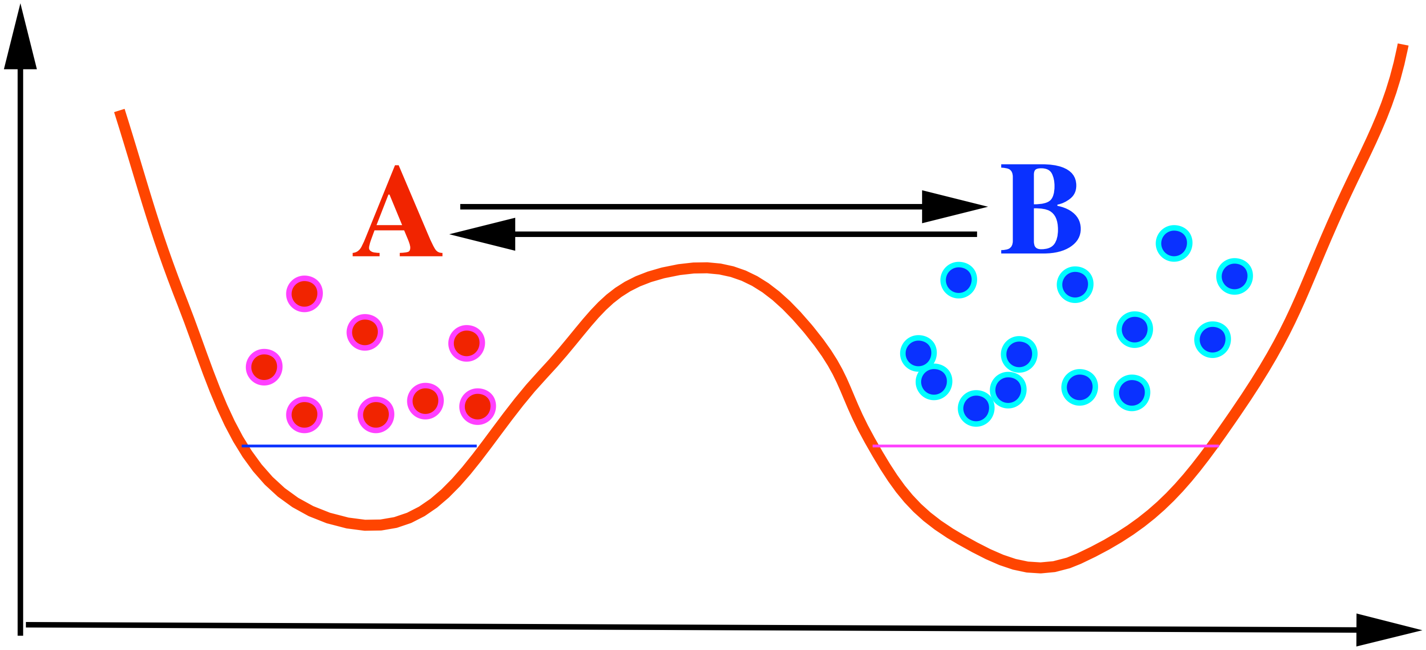
$D = d^{N}$

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 $\mathbf{H} = \omega\, \mathbf{J}_x$

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:

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

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 $\langle \mathbf{J_x} \rangle, \langle \mathbf{J_y} \rangle, \langle \mathbf{J_z} \rangle$ 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:

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

by the Liouville von Neumann equation

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

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

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

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

$$L_D(\rho) = -\gamma([\mathbf{J}_x, [\mathbf{J}_x,\rho]]+[\mathbf{J}_y, [\mathbf{J}_y,\rho]] +[\mathbf{J}_y, [\mathbf{J}_y,\rho]])$$

This is realized by the **sNLSE**

$$\mathbf{d}\psi = \left\{ -i\, \mathrm{H}dt - \gamma \sum_{i=1}^{3} (\mathbf{J}_i - \langle \mathbf{J}_i \rangle_\psi)^2 dt + \sum_{i=1}^{3} (\mathbf{J}_i - \langle \mathbf{J}_i \rangle_\psi) d\xi_j \right\} \psi$$

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 $L(\rho) = -i[H,\rho] - \gamma [H, [H,\rho]]$

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?

For the open system dynamics defined by:

$$\dot{\hat{\rho}} = -i\left[\hat{\mathrm{H}}_0 + \sum_i u_i(t)\hat{\mathrm{X}}_i, \hat{\rho}\right] - \frac{1}{2}\sum_i \gamma_i \left[\hat{\mathrm{X}}_i, \left[\hat{\mathrm{X}}_i, \hat{\rho}\right]\right].$$

And the uncertainty: $\Delta[\psi] \equiv \sum_i \left\langle \left(\hat{\mathrm{X}}_i - \left\langle \hat{\mathrm{X}}_i \right\rangle\right)^2 \right\rangle.$

Then the loss of purity: $$\frac{d}{dt} Tr\{\hat{\rho}^2\} = -4\gamma\Delta(\psi)$$

for $\hat{\rho} = |\psi\rangle\langle\psi|$.

We can estimate: $\Delta(\psi)$

$$\Delta_{min} \leq \Delta[\psi] \leq \Delta[\psi]_{max} = C_{\mathcal{H}},$$

Boxio, Viola, Ortiz EPL 79 40007 (2007).

Then we obtain the condition on γ

$$\gamma \ll \frac{\omega}{\Delta_{min}}$$

or a better estimate for SU(2)

$$\boxed{\gamma \ll \frac{\omega}{j \ln j}}$$

The timescale of the noise has to be much longer than the timescale of the unitary dynamics.

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

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

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

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 χ_n

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

Any matrix element can be calculated within the algebra.

for example: $\langle \chi_n | \mathbf{J_y} | \chi_\mathbf{m} \rangle = \langle \psi_0 \mathbf{U}_n^\dagger | \mathbf{J_y} | \mathbf{U_m} \psi_\mathbf{0} \rangle$

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 $S_{\mathbf{nm}} = \langle \chi_n | \chi_\mathbf{m} \rangle$ and invert it $\mathbf{S}^{-1}$

We can either move the basis functions $\chi_\mathbf{n}$ **or the operators by a global time dependent unitary operator**

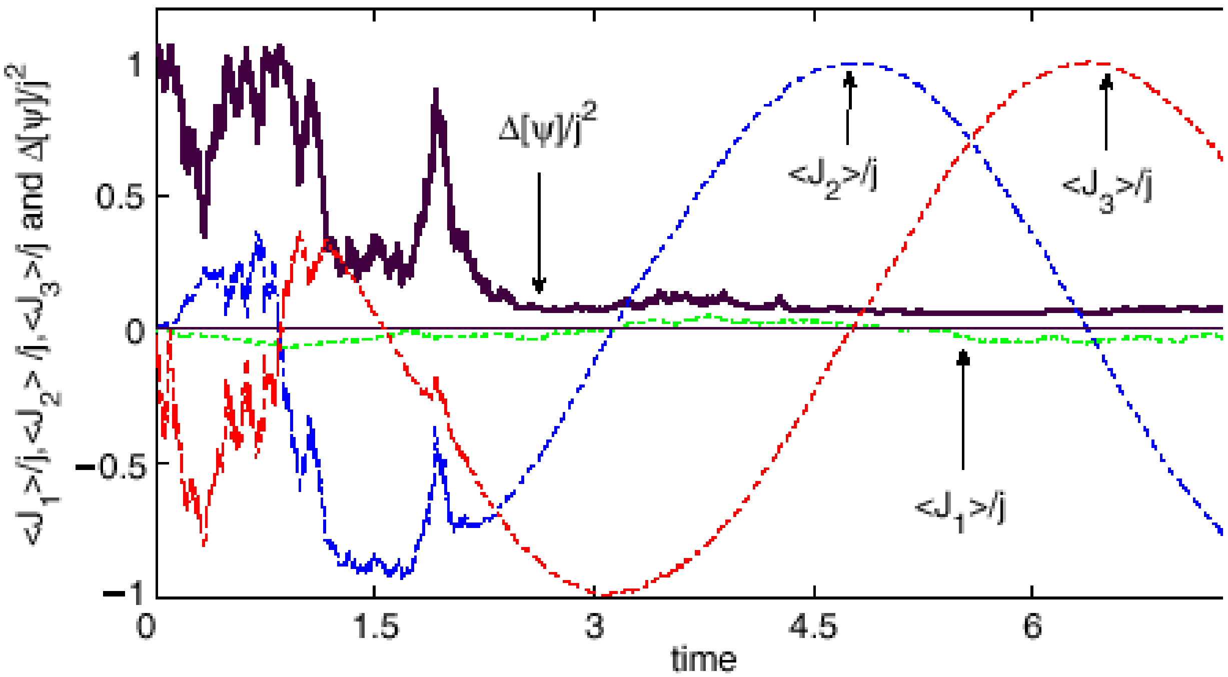
$\mathbf{U(t)} = \mathbf{exp}\left(-\mathbf{i}\,(\, \alpha(t) \mathbf{J_x} + \beta(t) \mathbf{J_y} + \gamma(t) \mathbf{J_z}\,)\right)$

Generalized Coherent states (GCS)

The global stable solution of the Stochastic Schrodinger equation

Khasin &Kosloff, JPA 41 (2008) 365203

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



Superposition initial state

$\Psi_0 = (|-j\rangle + |\,j\rangle)/\sqrt{2}$

Minimal uncertianty

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

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

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

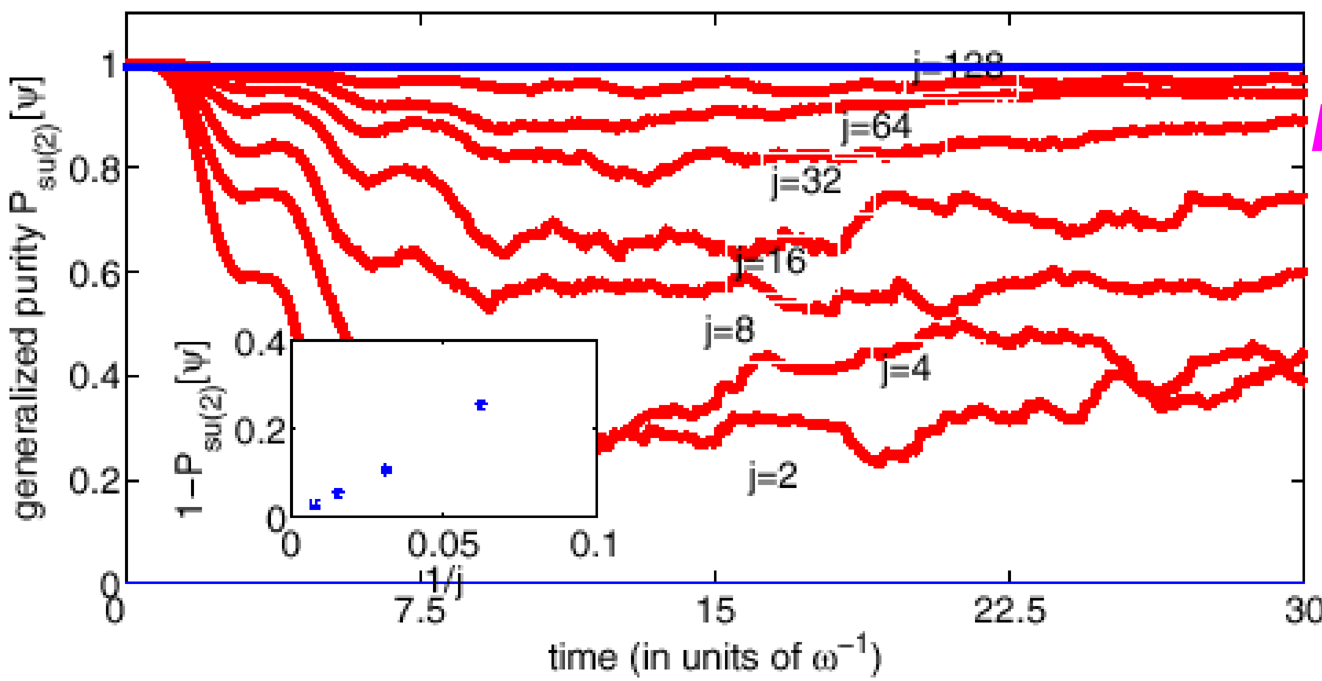
Expanding the wavefunction with time dependent GCS functions:

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

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

***P* the purity**

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

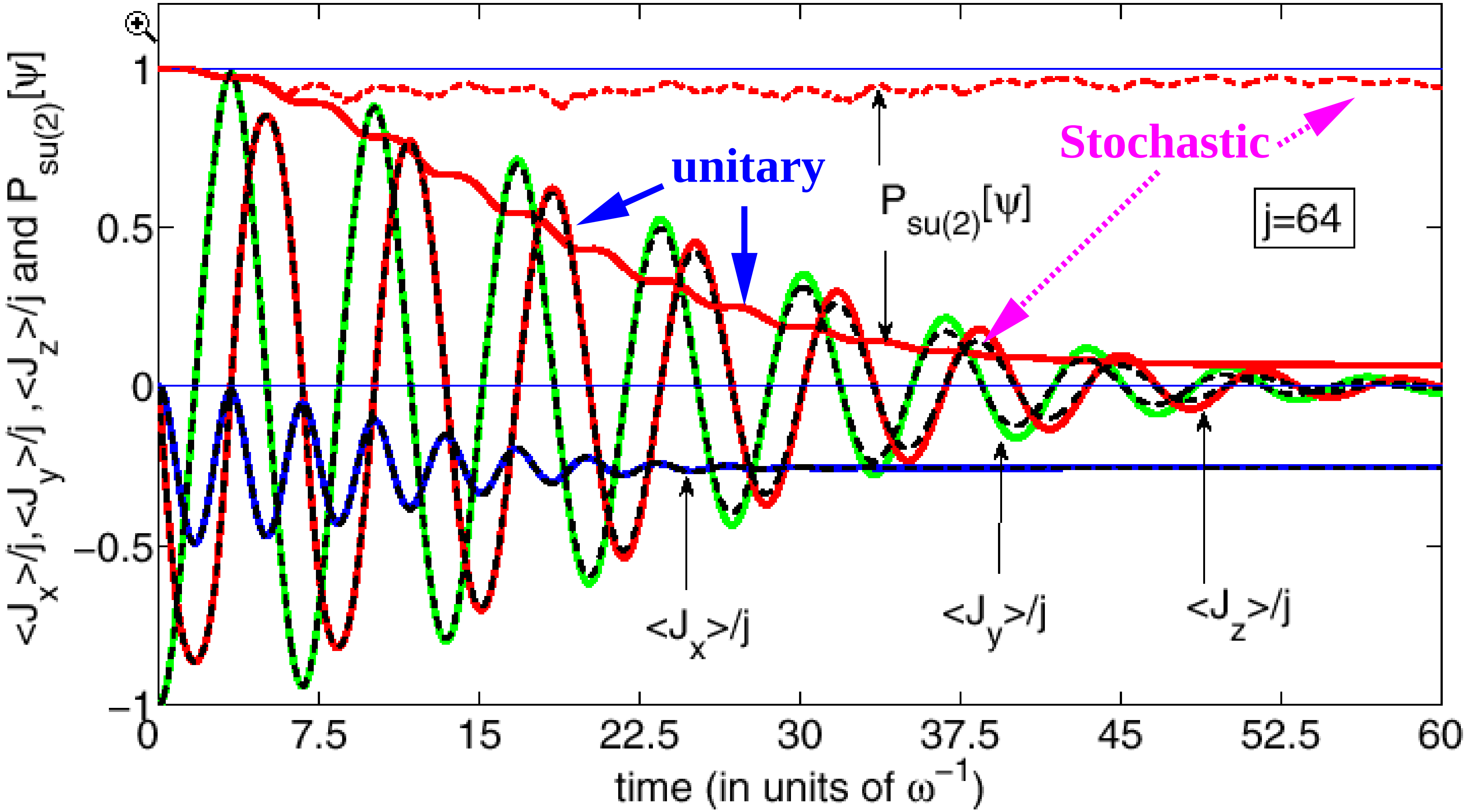


When the Hilbert space increases the # of expansion states M decreases

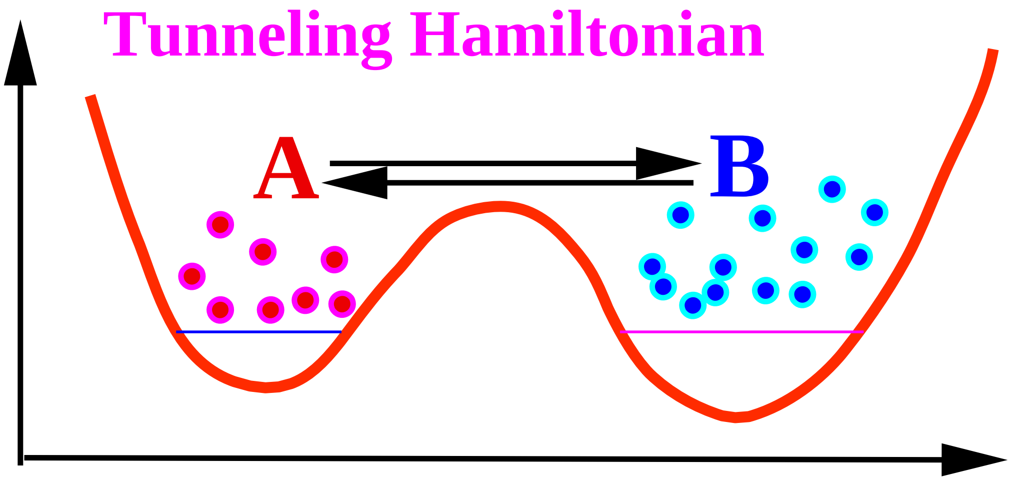
Surrogate Dynamics

Comparing unitary to non unitary dynamics

Unitary obtained by direct propagation (solid) **j=64**



The bath does not affect the dynamics of $\langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle$



Surrogate Dynamics

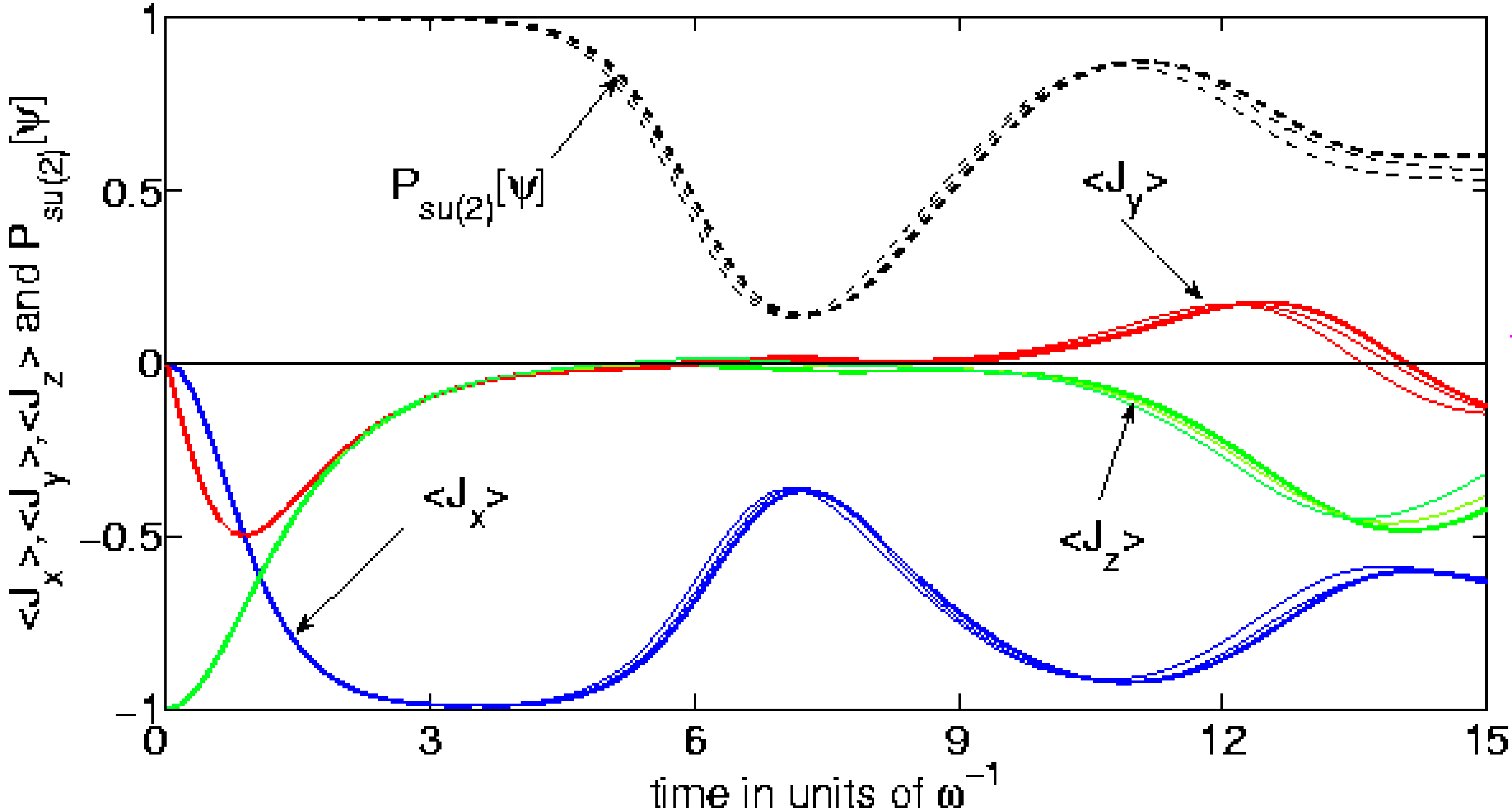
N= 20 000 particles

2000 stochastic realizations

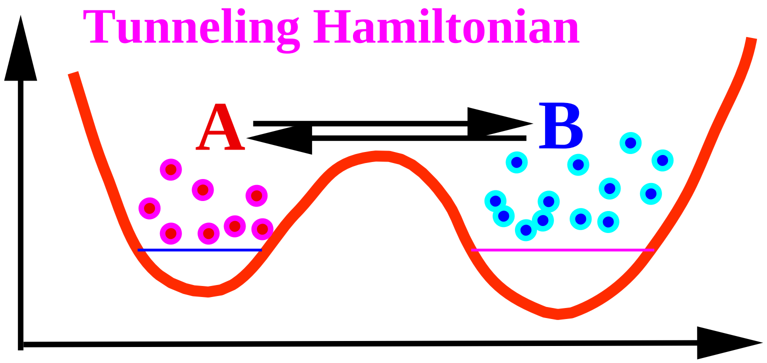
Size of the expansion M=60

decreasing values of γ

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



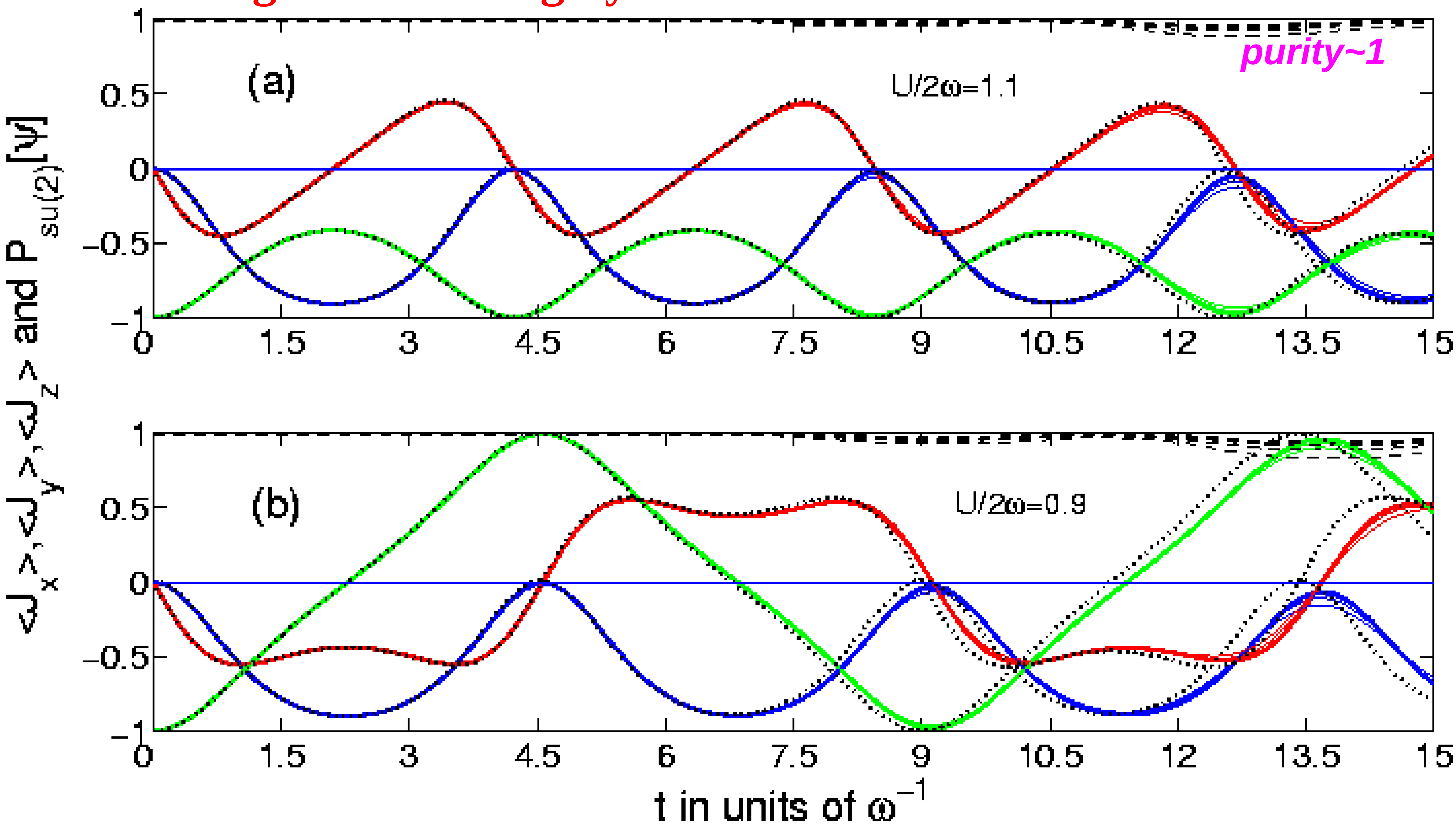
U/2ω=1



Different values of the inerparticle coupling

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

change in tunneling dynamics at U/2ω=1

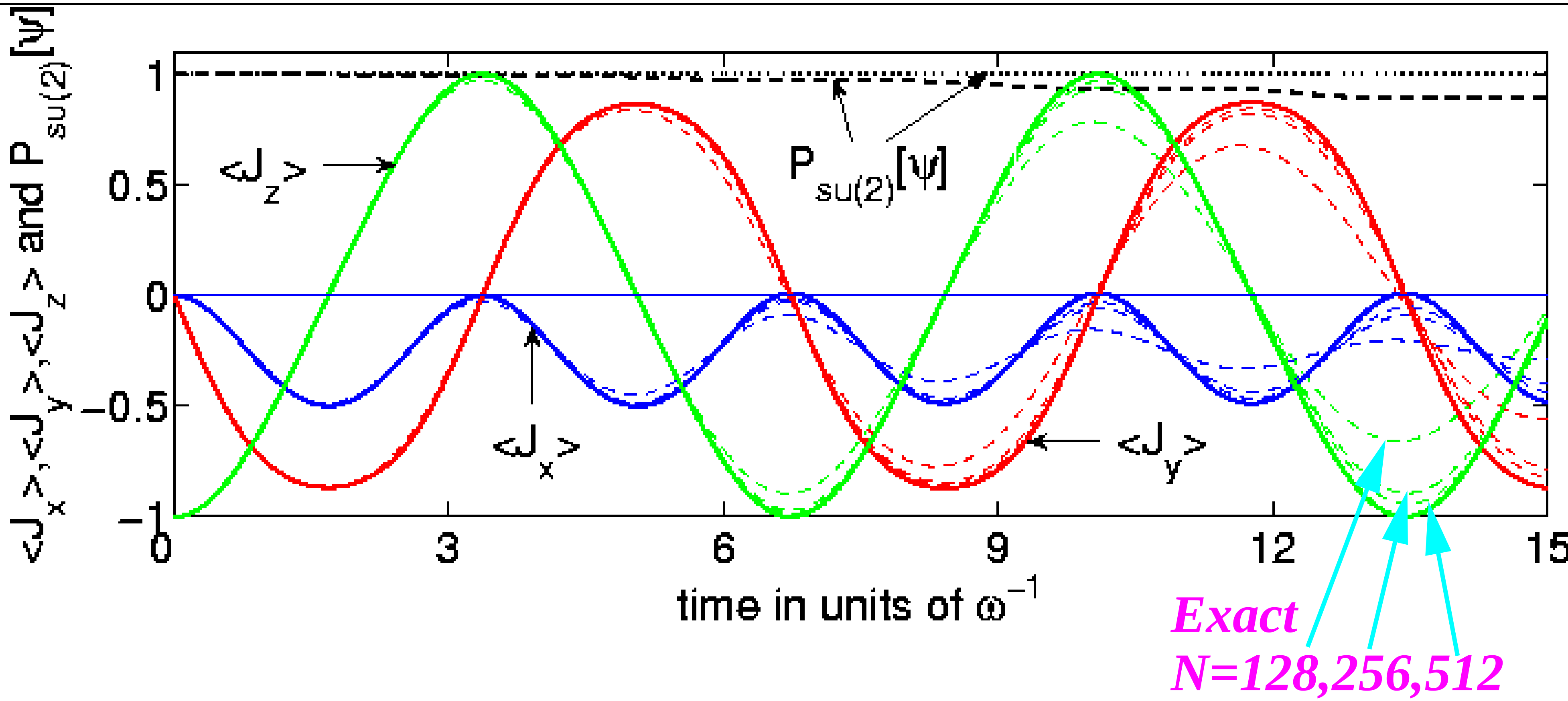


Surrogate Dynamics

Analysis: Comparison to mean field solutions

calculations carried out with a single GCS: $\Psi = \Psi(\langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle)$

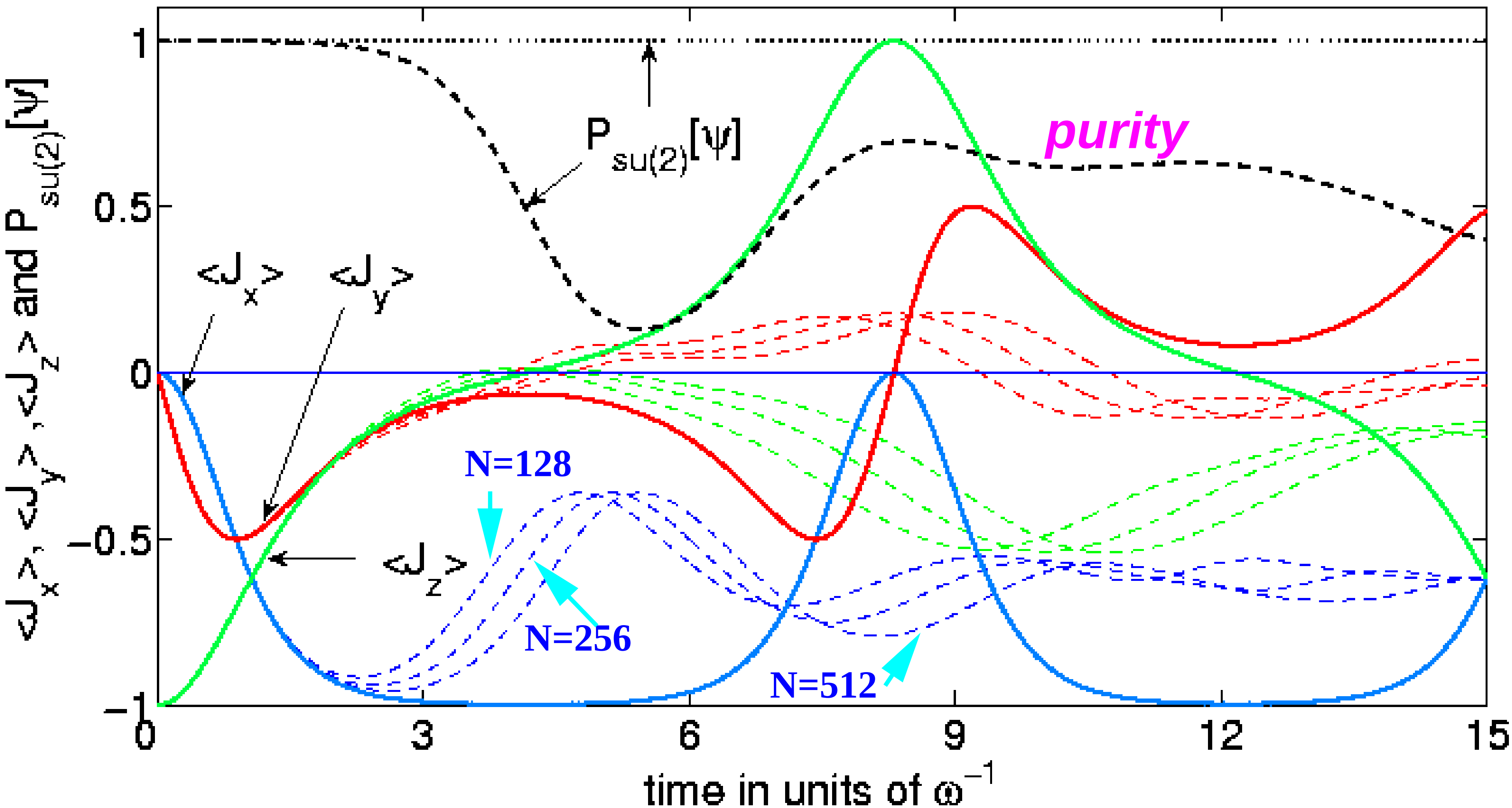
$U/2\omega = 1/2$ N=512



Surrogate Dynamics

Analysis: Breakup of mean field solutions

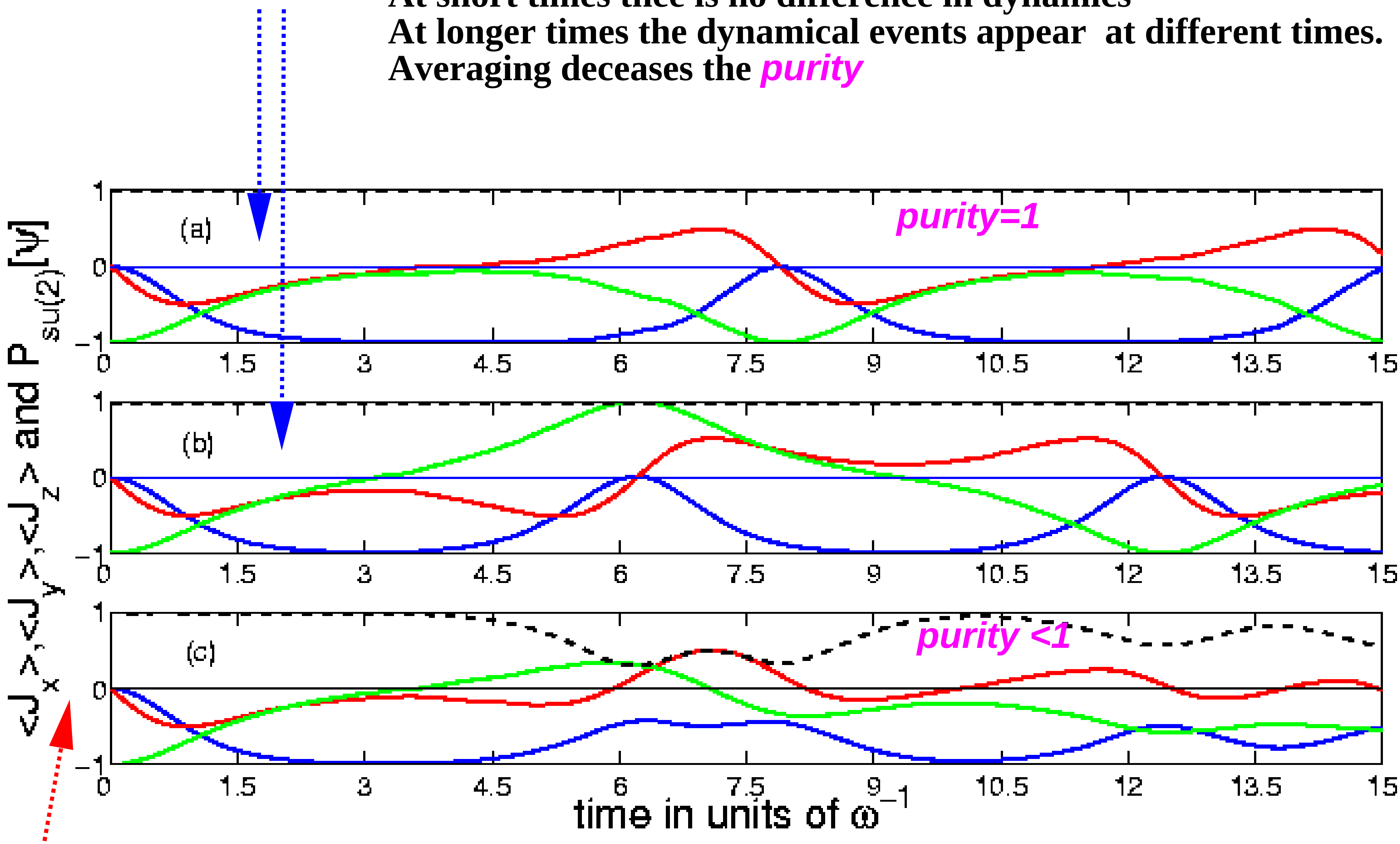
U/2ω=1 N=512



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

non unitary dynamics

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

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*, $P = \sum \langle X_i \rangle^2$

Semiclassical viewpoint

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

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

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

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

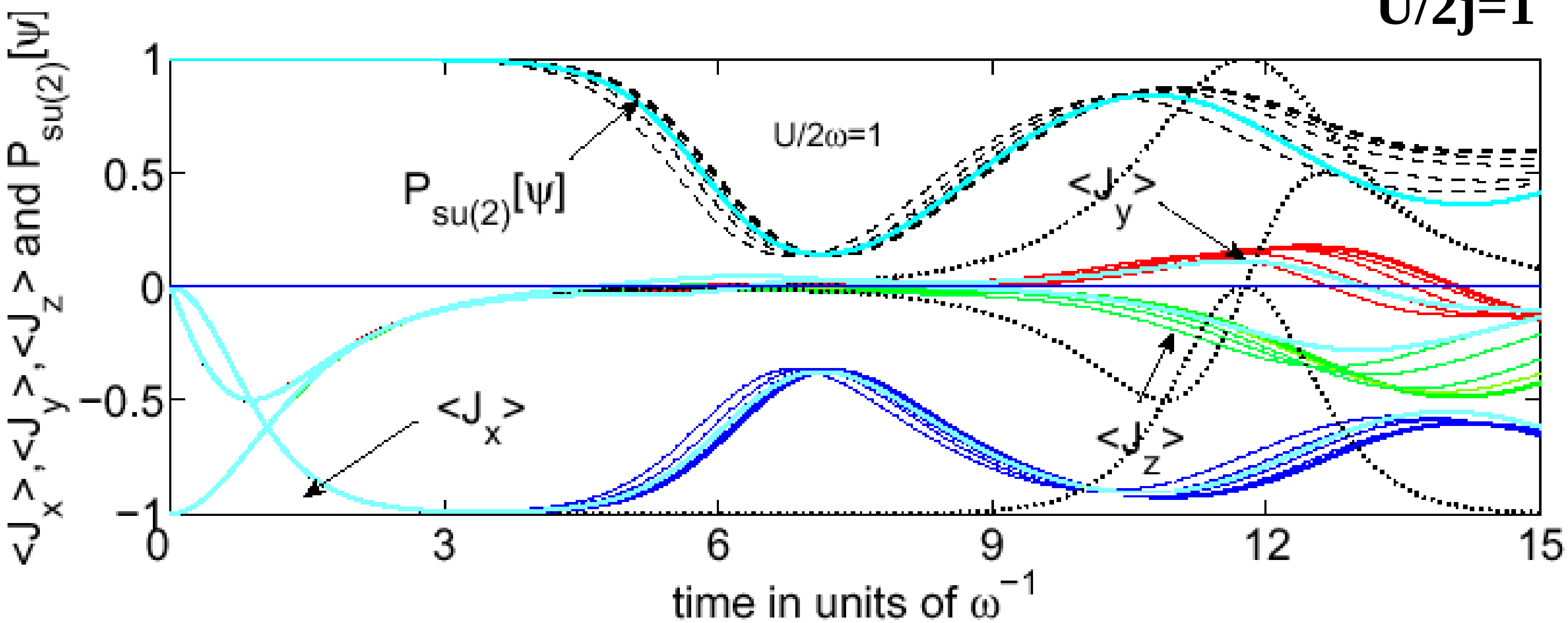
Then: $\frac{U}{2\omega} = \frac{2j}{2j-1} = 1 + \frac{1}{2j} + O(j^{-2}),$ **~1**

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



Surrogate Dynamics

Flowchart

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 ψ_k

Averaging

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

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

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!

Controllability of quantum systems

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \sum_i u_i(t)\hat{\mathrm{X}}_i \qquad \left[\mathfrak{g}, \hat{\mathrm{H}}_0\right] = \mathfrak{su}(N)$$

Noise on the controls

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \sum_i \left[u_i(t) + \xi_i(t)\right]\hat{\mathrm{X}}_i$$

$$\langle \xi_i(t) \rangle = 0 \qquad \langle \xi_i(t)\xi_j(t') \rangle = \gamma_i \delta_{ij} \delta(t - t').$$

$$\dot{\hat{\rho}} = -i\left[\hat{\mathrm{H}}_0 + \sum_i u_i(t)\hat{\mathrm{X}}_i, \hat{\rho}\right] - \frac{1}{2}\sum_i \gamma_i \left[\hat{\mathrm{X}}_i, \left[\hat{\mathrm{X}}_i, \hat{\rho}\right]\right].$$

Total uncertainty $\Delta[\psi] \equiv \sum_i \left\langle \left(\hat{X}_i - \langle \hat{X}_i \rangle \right)^2 \right\rangle$

$$\Delta_{min} \leq \Delta[\psi] \leq \Delta[\psi]_{max} = C_{\mathcal{H}},$$

$$\Gamma_{dec} = \gamma \Delta[\psi].$$

$$u_i \gg \gamma \Delta[\psi]_{max},$$

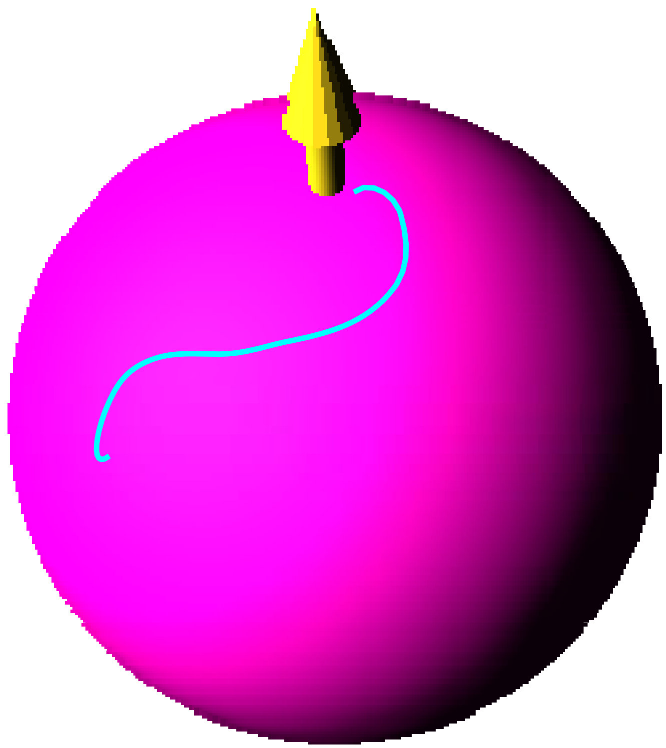
This leads to the conditions on the controls

$$\frac{\gamma}{u_i} \ll \Delta[\psi]^{-1}_{max} = C^{-1}_{\mathcal{H}}.$$

$C_{\mathcal{H}}$ = j(j+1) for SU(2)

The errors have to decrease with the size of the representation

Thank you



For $\mathfrak{g} = \oplus_{i=1}^{n} \mathfrak{su}(2)$ $C_{\mathcal{H}} = 3n/4.$

$$\frac{\gamma}{u_i} \ll \frac{4}{3n}.$$

For Bose-Hubbard model for the n-modes BEC

M bosons in optical lattice is $\mathfrak{su}(n)$ subulgebra of the single particles observables

$$c_{\mathcal{H}} = \frac{n-1}{2n} M(M+n).$$

$$\frac{\gamma}{u_i} \ll \Delta[\psi]_{max}^{-1} = \frac{2n}{(n-1)(M+n)M} = O\left(M^{-2}\right)$$