624 WE-Heraeus-Seminar “Simulating Quantum Processes and Devices”

Stochastic Description of Quantum Brownian Dynamics

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Outline

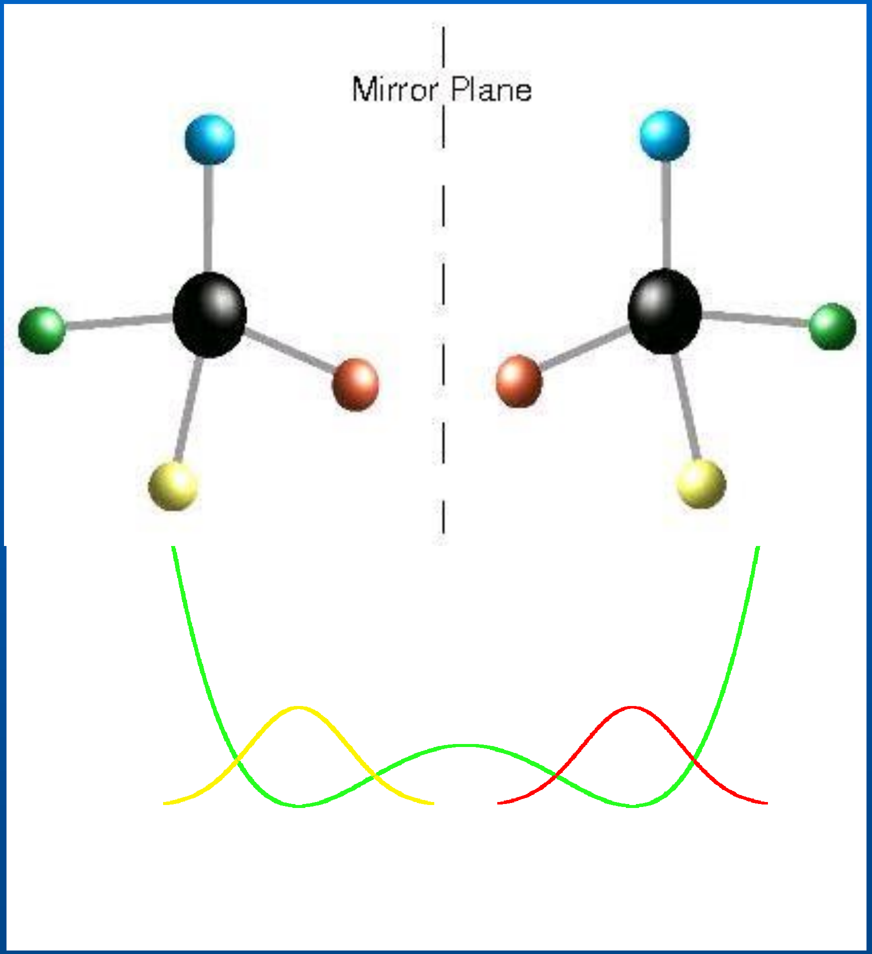
- Motivations
- Stochastic Formulation of Quantum Brownian Motion
- Numerical and Analytical Results
- Functional Integral Equation
- Summary

Solving Multidimensional Quantum Dynamics: Difficulties

- **Schroedinger Eq.** $$i\hbar\partial\left|\Psi(t)\right\rangle/\partial t = H\left|\Psi(t)\right\rangle$$
- **Wave Function** $$\left|\Psi(t)\right\rangle = e^{-iHt/\hbar}\left|\Psi(0)\right\rangle$$
  Memory bottleneck
- **Path Integral** $$\left|\Psi(t)\right\rangle = \int d\mathbf{X}' e^{-iHt/\hbar}\left|\mathbf{X}'\right\rangle\left\langle\mathbf{X}'\middle|\Psi(0)\right\rangle$$
  Sign problem

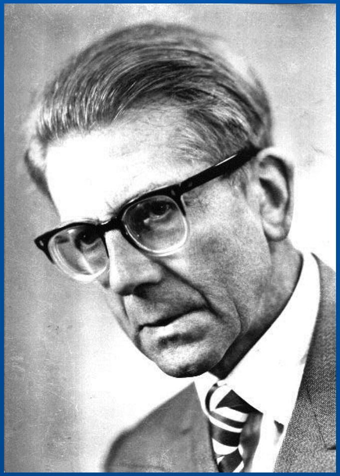
Curse of Dimensionality

Molecular Chirality: Why is it a problem?

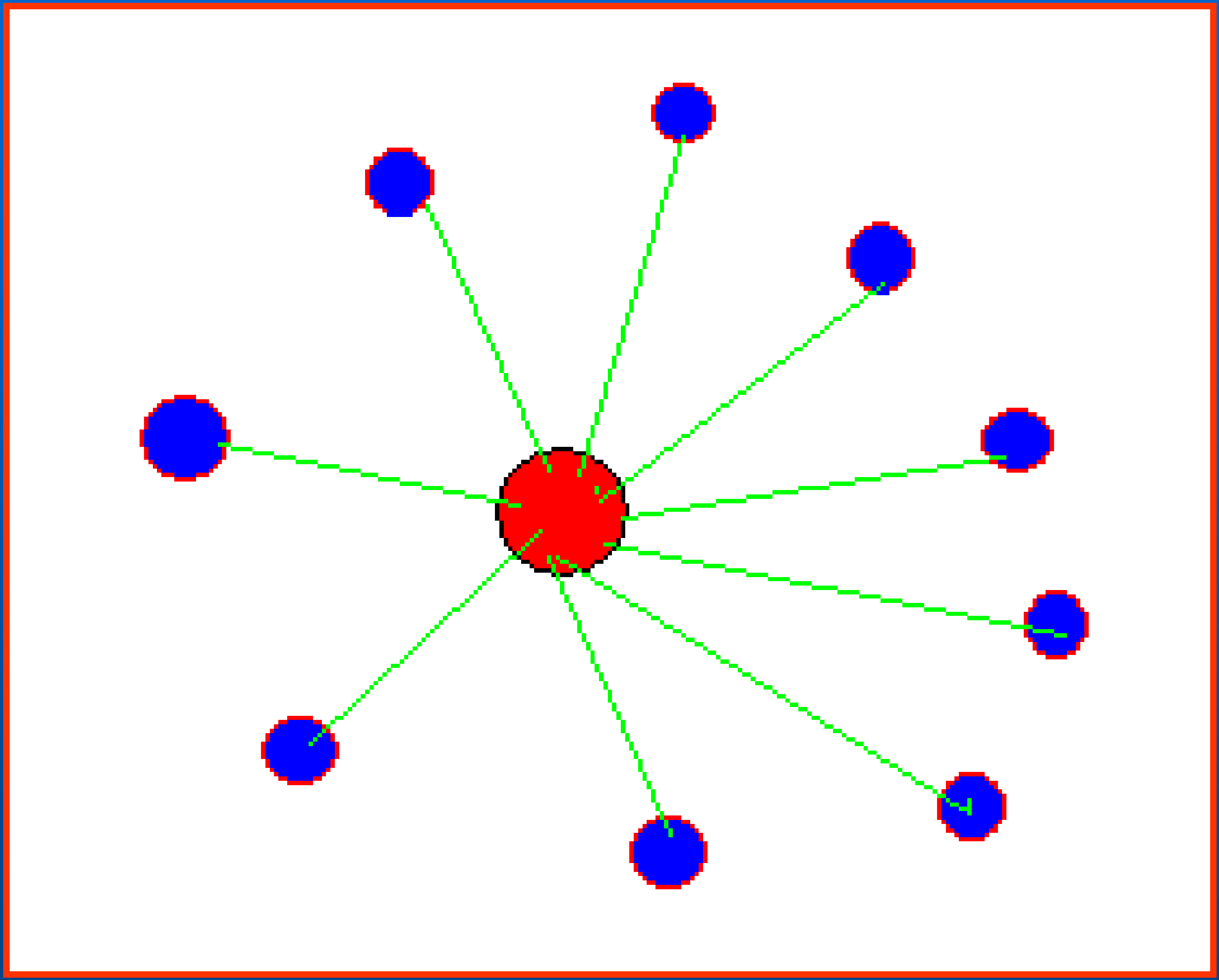


$$P_L = \frac{1}{2} + \frac{1}{2}\cos\left(\frac{2\Delta_0 t}{\hbar}\right)$$

Why are the chiral configurations stable?



Hund



Microscopic Description

- **Hamiltonian** $H = H_s + H_b + H_{\text{int}} = H_s + H_b + f(\hat{s})g(\hat{b})$
- **Liouville Equation** $i\hbar \frac{\partial \rho}{\partial t} = [H, \rho]$
- **Initial Condition** $\rho(0) = \rho_s(0)\rho_b(0)$
- **Decoupling: Put stochastic fields such that**

$$\rho(t) = M_{s.f.}\{\rho_s(t)\rho_b(t)\}$$

Heuristic Way to Decoupling

JS, *JCP* 120, 5053 (2004); Castin, Dalibard, Chomaz

- **Propagator of Whole System**

$$U(t)=e^{-i\left[H_s+H_b+f(\hat{s})g(\hat{b})\right]t/\hbar}=\prod_{j=1}^{N}U(\Delta t),\ \ \Delta t=t/N$$

$$U(\Delta t)=e^{-iH_s\Delta t/\hbar}e^{-iH_b\Delta t/\hbar}e^{-if(\hat{s})g(\hat{b})\Delta t/\hbar}+o(\Delta t^2)$$

$$e^{-if(\hat{s})g(\hat{b})\Delta t/\hbar}\overset{?}{=}\hat{F}(\hat{s},\Delta t)\hat{G}(\hat{b},\Delta t)$$

- **Hubbard-Stratonovich Transformation**

$$e^{\hat{o}^2}=\int_{-\infty}^{\infty}d\mu e^{-\mu^2/2\pm\sqrt{2}\mu\hat{o}}/\sqrt{2\pi}=M\left\{e^{\pm\sqrt{2}\mu\hat{o}}\right\}$$

$$-if(\hat{s})g(\hat{b})\Delta t/\hbar=\left\{\left[-if(\hat{s})+g(\hat{b})\right]^2-\left[-if(\hat{s})-g(\hat{b})\right]^2\right\}\left(\sqrt{\Delta t/\hbar}/2\right)^2$$

Decoupled Propagator

$$U(t) = M\left\{U_s\left[\mu_1(t), \mu_2(t)\right]U_b\left[\mu_1(t), \mu_2(t)\right]\right\}$$

Gaussian Fields

- Statistical Properties for $dB_j = \mu_j(t)dt$

$$M\left\{dB_j(t)\right\} = 0$$

$$M\left\{dB_j(t)dB_k(t')\right\} = \delta_{jk}dt$$

- Separated Hamiltonians

$$\tilde{H}_s(t) = H_s + \sqrt{\hbar/2}\left[\mu_1(t) + i\mu_2(t)\right] f(\hat{s})$$

$$\tilde{H}_b(t) = H_b + \sqrt{\hbar/2}\left[\mu_2(t) + i\mu_1(t)\right] g(\hat{b})$$

Ito Calculus Helps

JS, *CP* 322, 187 (2006); 370, 29 (2010); Li,JS&Wang, *PRE* 84, 051112 (2011)

- **EOM for System**

$$i\hbar d\rho_s = [H_s, \rho_s]dt + \frac{\sqrt{\hbar}}{2}[f(\hat{s}), \rho_s]dW_1 + i\frac{\sqrt{\hbar}}{2}\{f(\hat{s}), \rho_s\}dW_2^*$$

- **EOM for Bath**

$$i\hbar d\rho_b = [H_b, \rho_b]dt + \frac{\sqrt{\hbar}}{2}\left[g(\hat{b}), \rho_b\right]dW_2 + i\frac{\sqrt{\hbar}}{2}\left\{g(\hat{b}), \rho_s\right\}dW_1^*$$

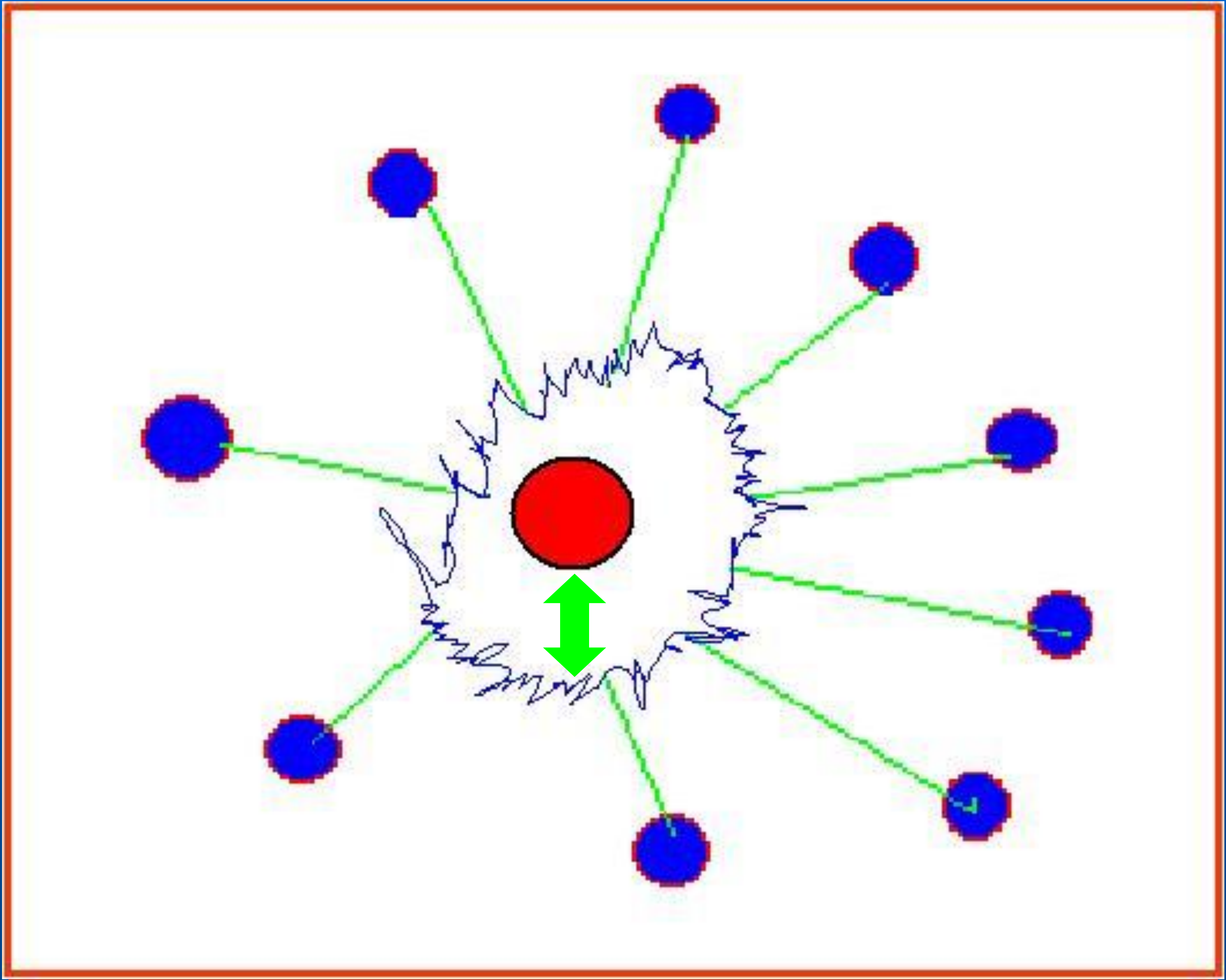
- **Complex Wiener Processes**

$$W_1(t) = \int_0^t dt'[\mu_1(t') + i\mu_4(t')],\ W_2(t) = \int_0^t dt'[\mu_2(t') + i\mu_3(t')]$$

One Can Prove

$$i\hbar dM\left\{\rho_s(t)\rho_b(t)\right\} = \left[H_s + H_b + f(\hat{s})g(\hat{b}), M\left\{\rho_s(t)\rho_b(t)\right\}\right]dt$$

$$M\left\{\rho_s(t)\rho_b(t)\right\} = \rho(t)$$



EOM

- **Initial Condition** $\rho(0)=\rho_s(0)\rho_b(0)$
- **Decoupled Equations of Motion**

$$\rho(t)=U(t)\rho(0)U^{\dagger}(t)\equiv M\{\rho_s(t)\rho_b(t)\},\ \text{where}$$

$$\begin{cases} i\hbar d\rho_s=[H_s,\rho_s]dt+\sqrt{\hbar/2}\left[f(\hat{s})\rho_s dz_1-\rho_s f(\hat{s})dz_2^*\right] \\ i\hbar d\rho_b=[H_b,\rho_b]dt+\sqrt{\hbar/2}i\left[g(\hat{b})\rho_b dz_1^*+\rho_b g(\hat{b})dz_2\right] \end{cases}$$

$$(z_1=B_1+iB_2,\ z_2=B_3+iB_4)$$

which, by a simple change of variables can be recast as what we obtained by virtue of Ito calculus

Reduced Density Matrix

- **Reduced Density Matrix (RDM)**

$$\tilde{\rho}_s(t) \equiv \mathrm{Tr}_b \rho(t) = \mathrm{Tr}_b M\left\{\rho_s(t)\rho_b(t)\right\}$$
$$= M\left\{\rho_s(t)\mathrm{Tr}_b \rho_b(t)\right\}$$

- **Trace of Density Matrix for Bath: Influence on System**

$$\mathrm{Tr}_b \rho_b(t) = \exp\left\{\frac{1}{\sqrt{\hbar}}\int_0^t dt' \bar{g}(t')\left[\mu_1(t') - i\mu_4(t')\right]\right\}$$
$$\bar{g}(t) = \mathrm{Tr}_b\left\{g(\hat{b})\rho_b(t)\right\} / \mathrm{Tr}_b\left\{\rho_b(t)\right\}$$

Girsanov Transformation

- **RDM**

$$\tilde{\rho}_s(t) = M\left\{\rho_s(t)\boxed{\mathrm{Tr}_b\,\rho_b(t)}\right\}$$

- **Change of Variables**

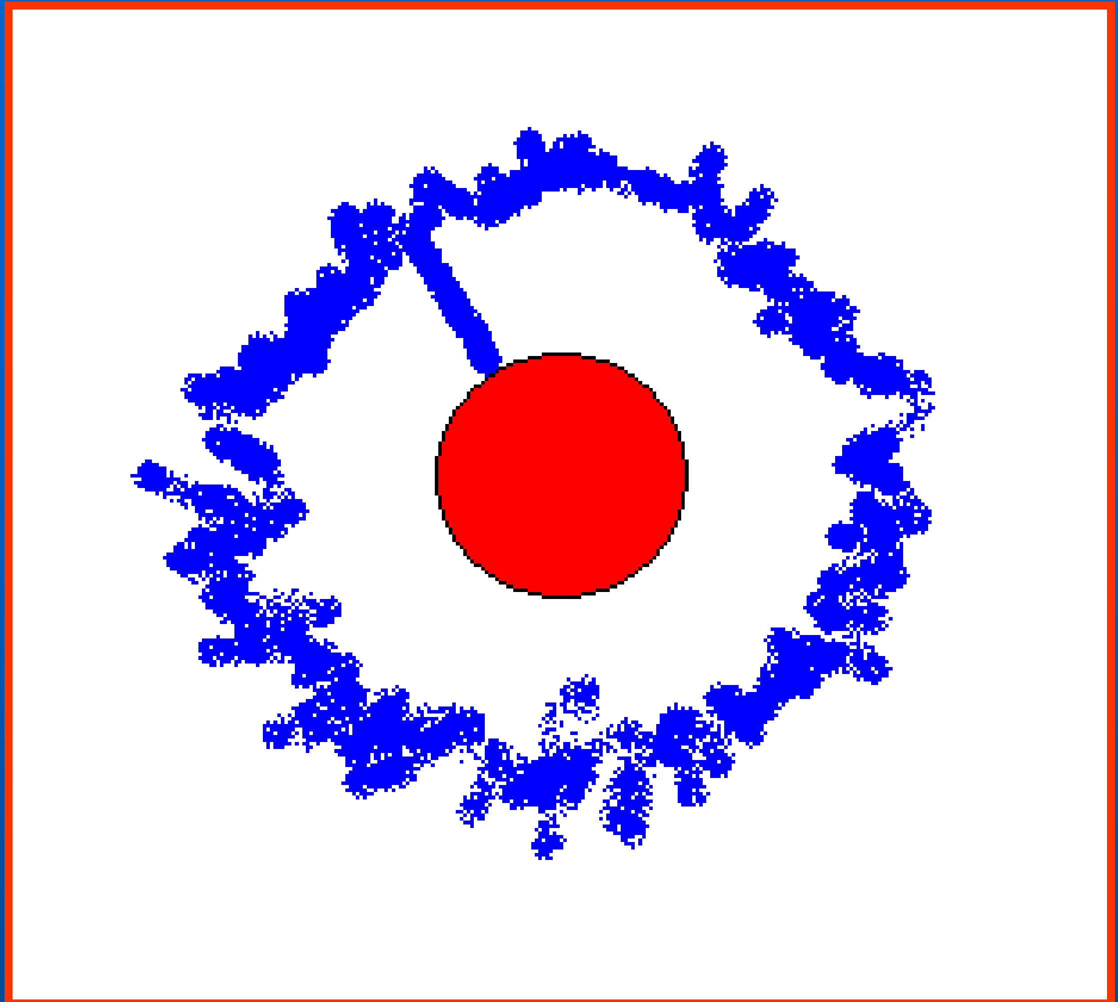
$$\mu_1 \to \mu_1 + 1/\sqrt{\hbar}\int_0^t dt'\bar{g}(t'),\quad \mu_4 \to \mu_4 - i/\sqrt{\hbar}\int_0^t dt'\bar{g}(t')$$

$$\bar{g}(t) = \mathrm{Tr}_b\left\{g(\hat{b})\rho_b(t)\right\}/\mathrm{Tr}_b\left\{\rho_b(t)\right\}$$

- **EOM**

$$i\hbar d\rho_s = \left[H_s + \bar{g}(t) f(\hat{s}), \rho_s\right]dt + \sqrt{\hbar}/2\left\{\left[f(\hat{s}), \rho_s\right]dW_1 + i\left\{f(\hat{s}), \rho_s\right\}dW_2^*\right\}$$

$$\tilde{\rho}_s(t) = M\left\{\rho_s(t)\right\}$$



1. Calculating the bath-induced field

$$i\hbar d\rho_s = \left[H_s + \bar{q}(t) f(\hat{s}), \rho_s\right] dt - \sqrt{\hbar/2}\left\{\left[f(\hat{s}), \rho_s\right] dW_1 + i\left\{f(\hat{s}), \rho_s\right\} dW_2^*\right\}$$

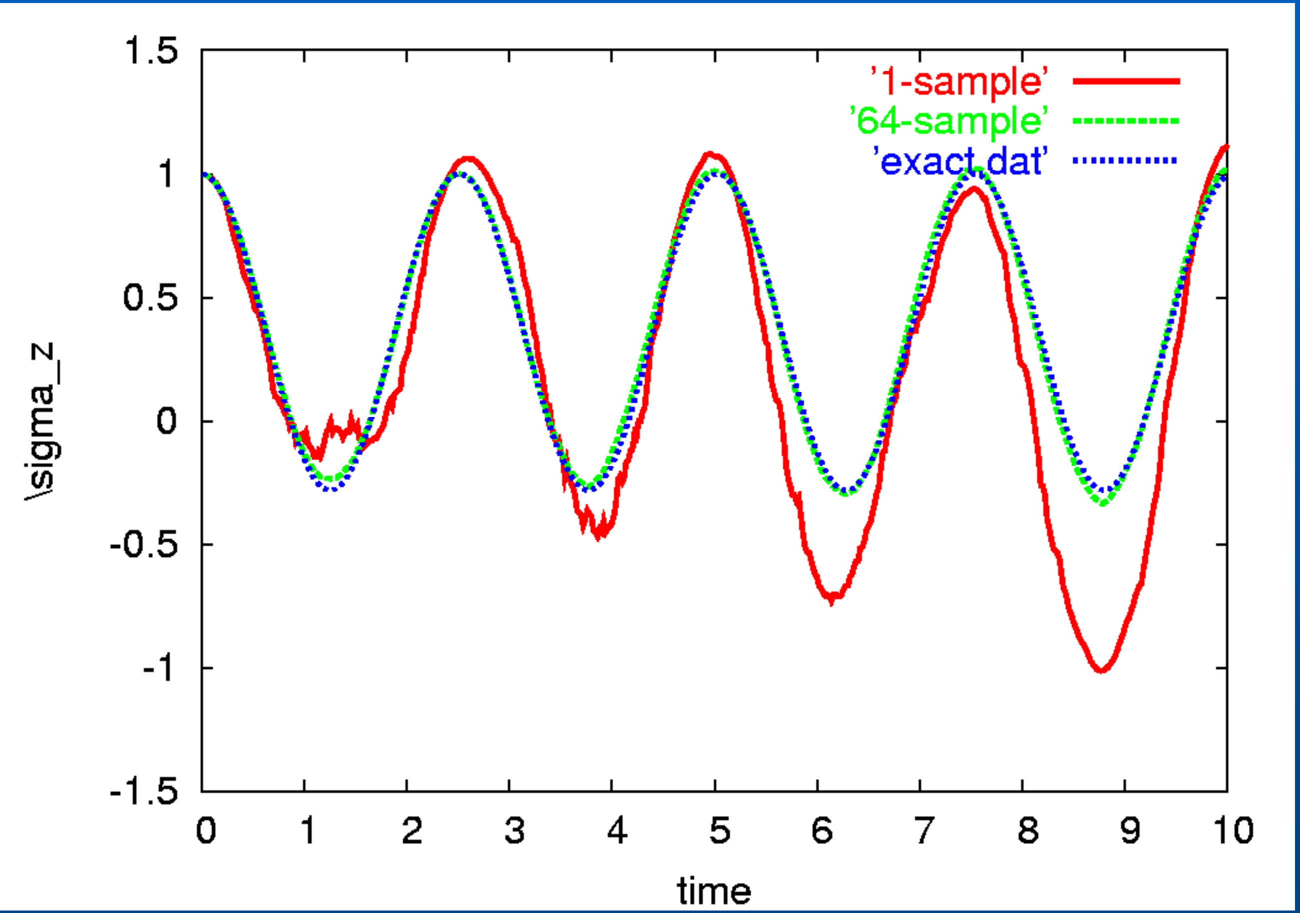
2. Solving the SDE and doing stochastic average

$$\tilde{\rho}_s(t) = M\left\{\rho_s(t)\right\}$$

Toy Model

$$H = \sigma_x + 0.15\sigma_z g \quad \left(H_b = 0,\ f(\hat{s}) = 0.15\sigma_z,\ g(\hat{b}) = 5 \right)$$

$$i\hbar d\rho_s = [\sigma_x + 0.75\sigma_z, \rho_s]dt + 0.075\left\{[\sigma_z, \rho_s]dW_1 + i\{\sigma_z, \rho_s\}dW_2^*\right\}$$



Spontaneous Decay of Two-State Atoms

- **Hamiltonian**

$$H_s = \frac{\omega_0}{2}\sigma_z, \; H_b = \sum_k \omega_k b_k^\dagger b_k,$$

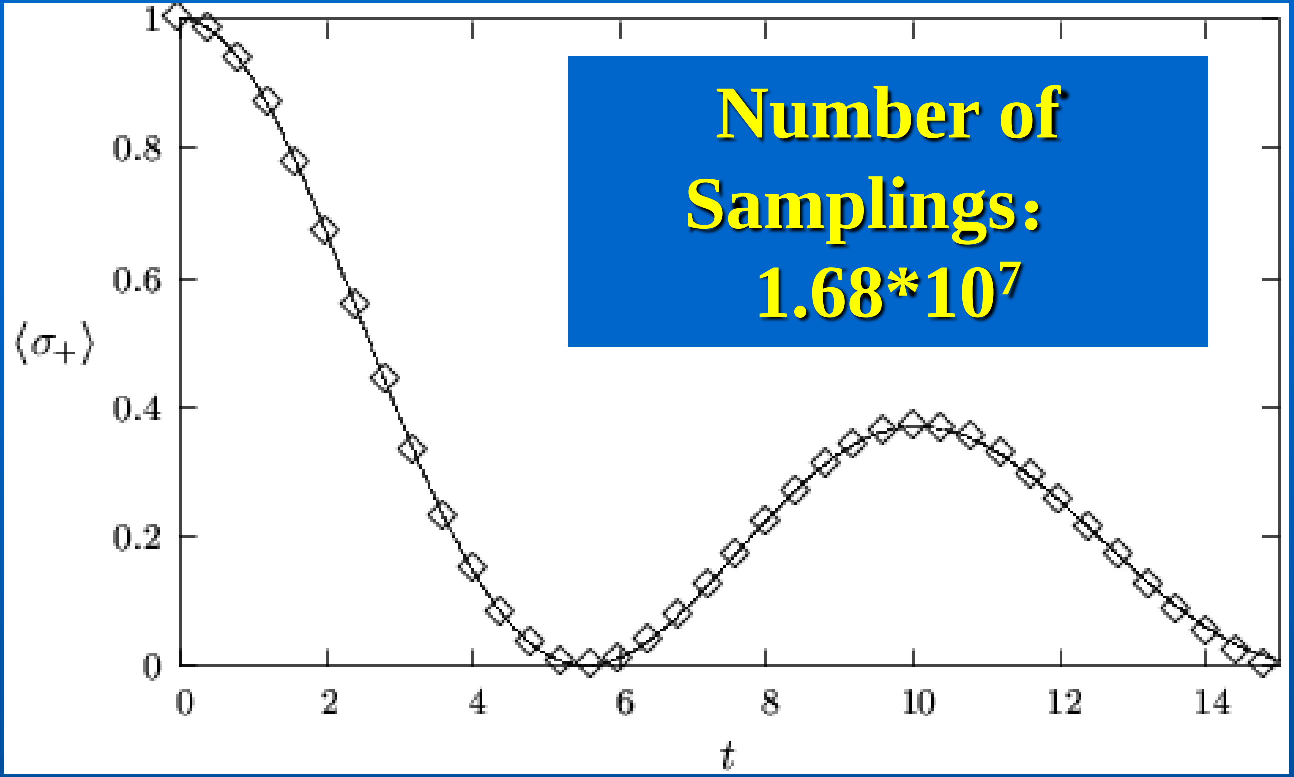
$$H_{sb} = \sigma^- \hat{g}_1 + \sigma^+ \hat{g}_2 \equiv \sigma^- \otimes \sum_k c_k b_k^\dagger + \sigma^+ \otimes \sum_k c_k^* b_k$$

- **Bath-Induced Field**

$$\bar{g}_1(t) = \int_0^t dt' \alpha(t-t')\left[-i\mu_{12}(t') + \mu_{22}(t') + i\mu_{32}(t') - \mu_{42}(t')\right],$$

$$\bar{g}_2(t) = \int_0^t dt' \alpha^*(t-t')\left[i\mu_{11}(t') + \mu_{21}(t') + i\mu_{31}(t') + \mu_{41}(t')\right]$$

$$\alpha(t) = i/\left(2\sqrt{\hbar}\right)\sum_k \left|c_k\right|^2 e^{i\omega_k t}$$



$$\alpha(t) = \alpha_R(t) = \frac{\gamma}{2} e^{-\gamma|t|} \quad (\gamma = 0.1)$$

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Chemical Physics Letters 395 (2004) 216–221

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Hierarchical approach based on stochastic decoupling to dissipative systems

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Abstract

Based on the novel stochastic methodology for describing quantum dynamics of dissipative systems [J. Shao, J. Chem. Phys. 120 (2004) 5053], a hierarchical approach is suggested and applied to the spin–boson model with Debye spectral density function. The algorithm to implement this deterministic technique is expounded and the numerical results for the spin–boson system are explained.

Working Formula

$$i\hbar d\rho_s = \left[H_s + \bar{g}(t) f(\hat{s}), \rho_s\right] dt + \sqrt{\hbar/2}\left\{\left[f(\hat{s}), \rho_s\right] dW_1 + i\left\{f(\hat{s}), \rho_s\right\} dW_2^*\right\}$$

$$\tilde{\rho}_s(t) = M\left\{\rho_s(t)\right\}$$

Hierarchy Approach

Yan, Yang, Liu, & JS, *CPL* 395, 216 (2004), Cao, Tanimura, Yan; Shapiro-Loginov

- **Memory Kernel** $\alpha(t)=\alpha_R(t)=\kappa e^{-\gamma t}$
- **Auxiliary Quantities (due to correlation)**

$$\rho_{s,m}(t)=\bar{g}^m(t)\rho_s(t),\quad \tilde{\rho}_{s,m}(t)=M\{\rho_{s,m}(t)\}$$

- **EOM**

$$i\hbar d\tilde{\rho}_{s,m}(t)/dt=[H_s,\tilde{\rho}_{s,m}(t)]+[f(\hat{s}),\tilde{\rho}_{s,m+1}(t)] +n\hbar\kappa[f(\hat{s}),\tilde{\rho}_{s,m-1}(t)]-in\hbar\gamma\tilde{\rho}_{s,m}(t)$$

- **Truncation** $\tilde{\rho}_{s,m}(t)=0\ (m\geq N_{\min})$

$$\alpha(t) = \kappa e^{-(\gamma_R + i\gamma_I)t}$$

Bath-Induced Field

$$\bar{g}(t) = \bar{g}_1(t) + \bar{g}_2(t)$$

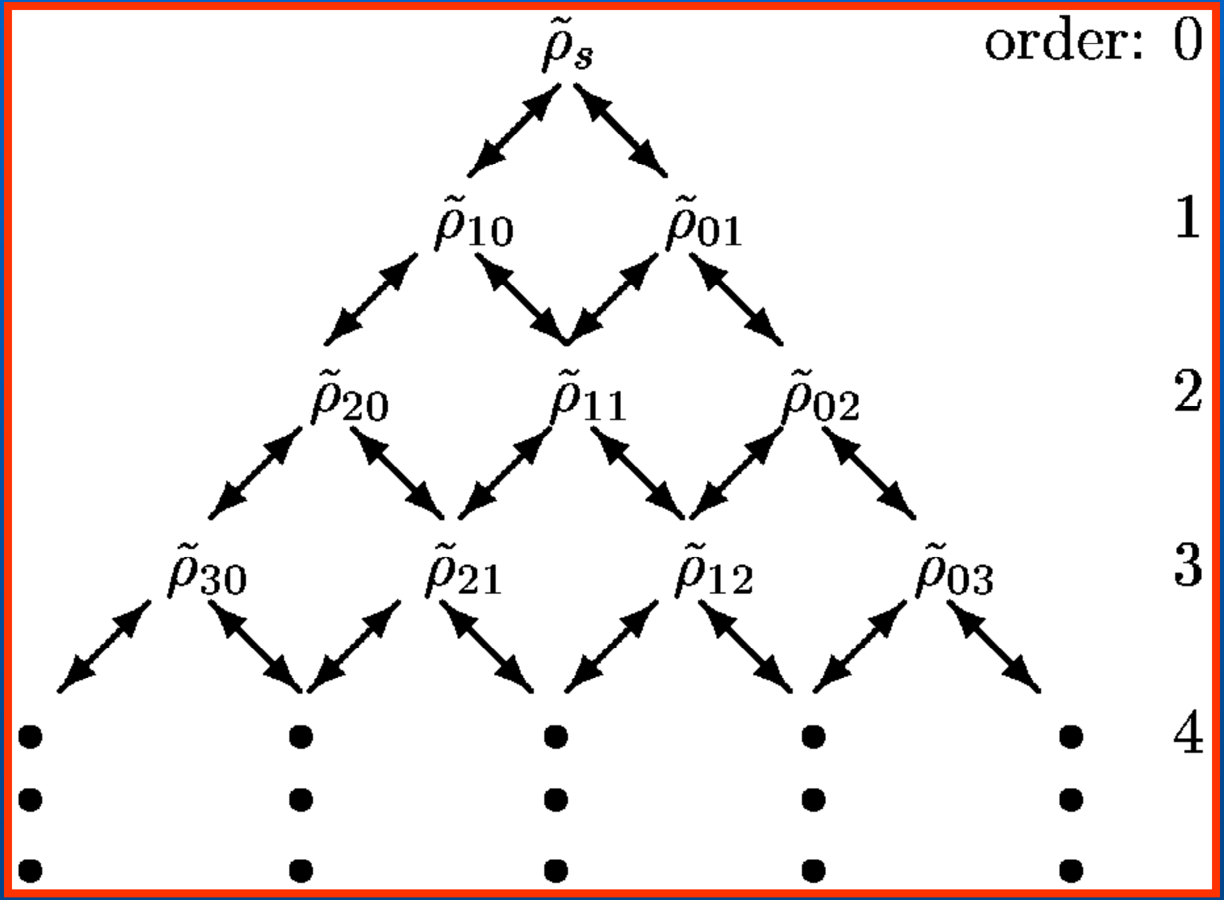
$$\bar{g}_1(t) = \int_0^t dt' \alpha(t-t') \left[\mu_1(t') - i\mu_4(t') - i\mu_2(t') + \mu_3(t') \right],$$

$$\bar{g}_2(t) = \int_0^t dt' \alpha^*(t-t') \left[\mu_1(t') - i\mu_4(t') + i\mu_2(t') - \mu_3(t') \right]$$

Auxiliary Quantities

$$\tilde{\rho}_{mn}(t) = M\{\bar{g}_1^m(t) \bar{g}_2^n(t) \rho_s(t)\}$$

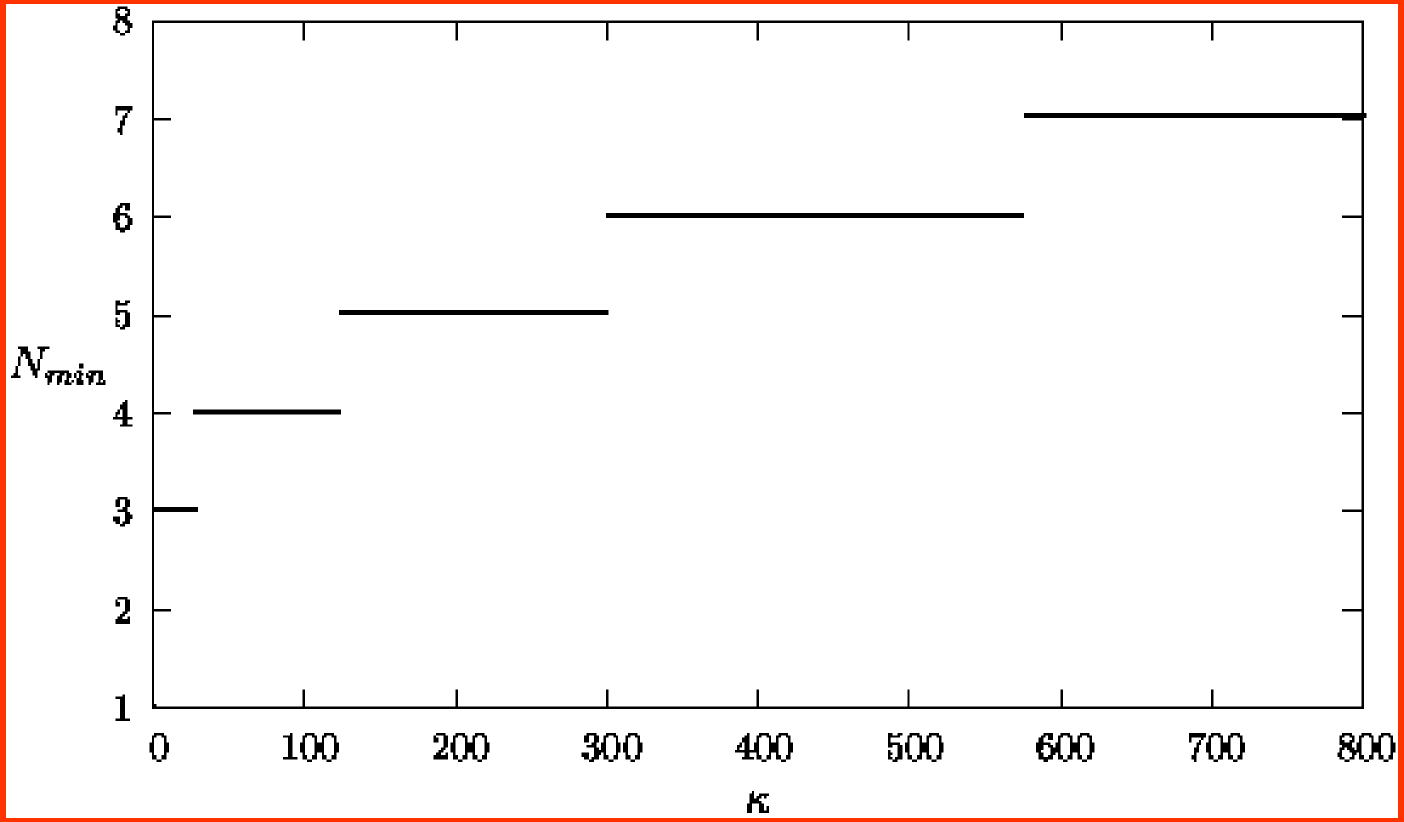
Hierarchical Structure



Truncation vs Dissipation Strength

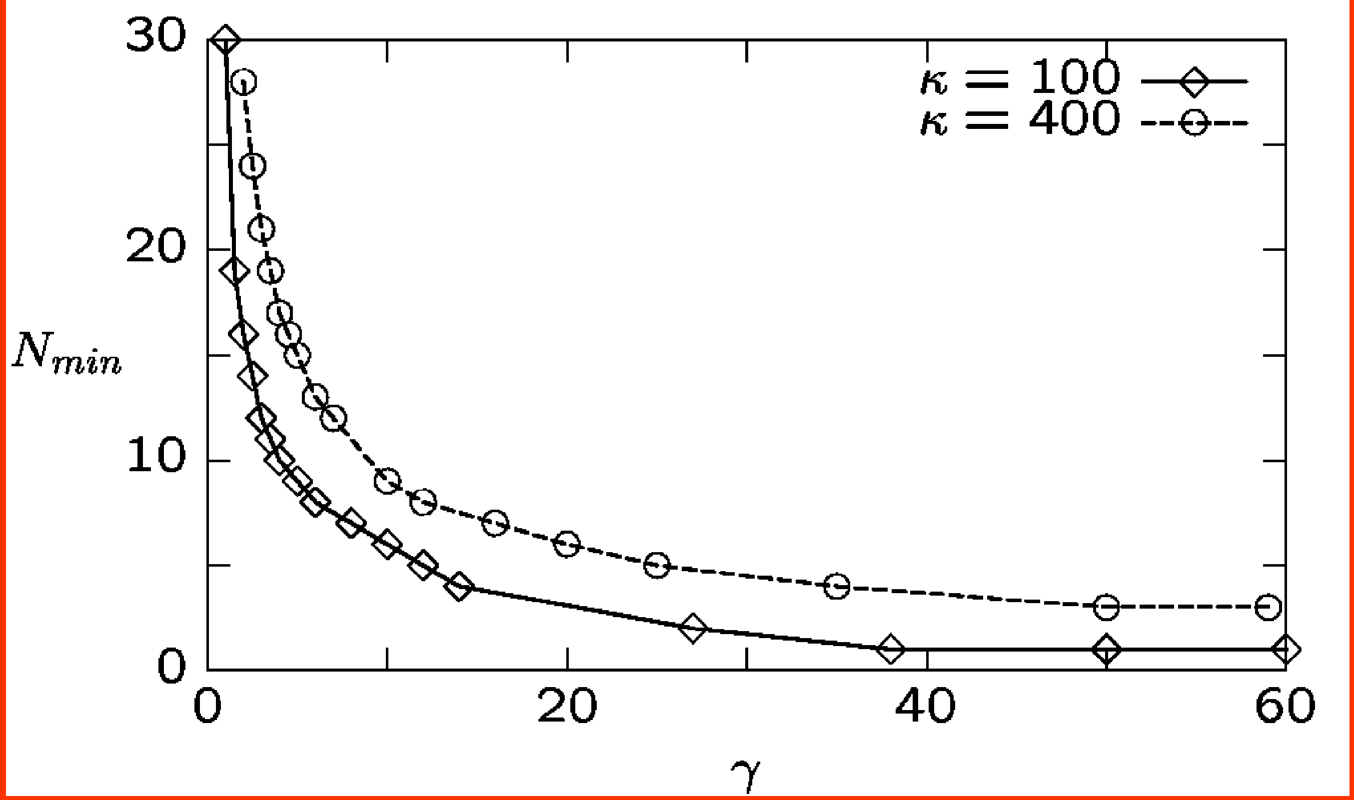
Zhou, Yan & JS, *EPL 72*, 305 (2005), YiJing Yan

$$\alpha(t) = \alpha_R(t) = \kappa e^{-\gamma t} \quad (\gamma = 20)$$



Truncation vs Memory Length

$$\alpha(t) = \alpha_R(t) = \kappa e^{-\gamma t} (\kappa = 100, 400)$$



Electron Transfer

Yan, Yang, Liu, & JS, *CPL* 395, 216 (2004)

Model: $H_s = \Omega\sigma_x + \varepsilon\sigma_z,\ f(\hat{s}) = \sigma_z$

Spectral Density Function

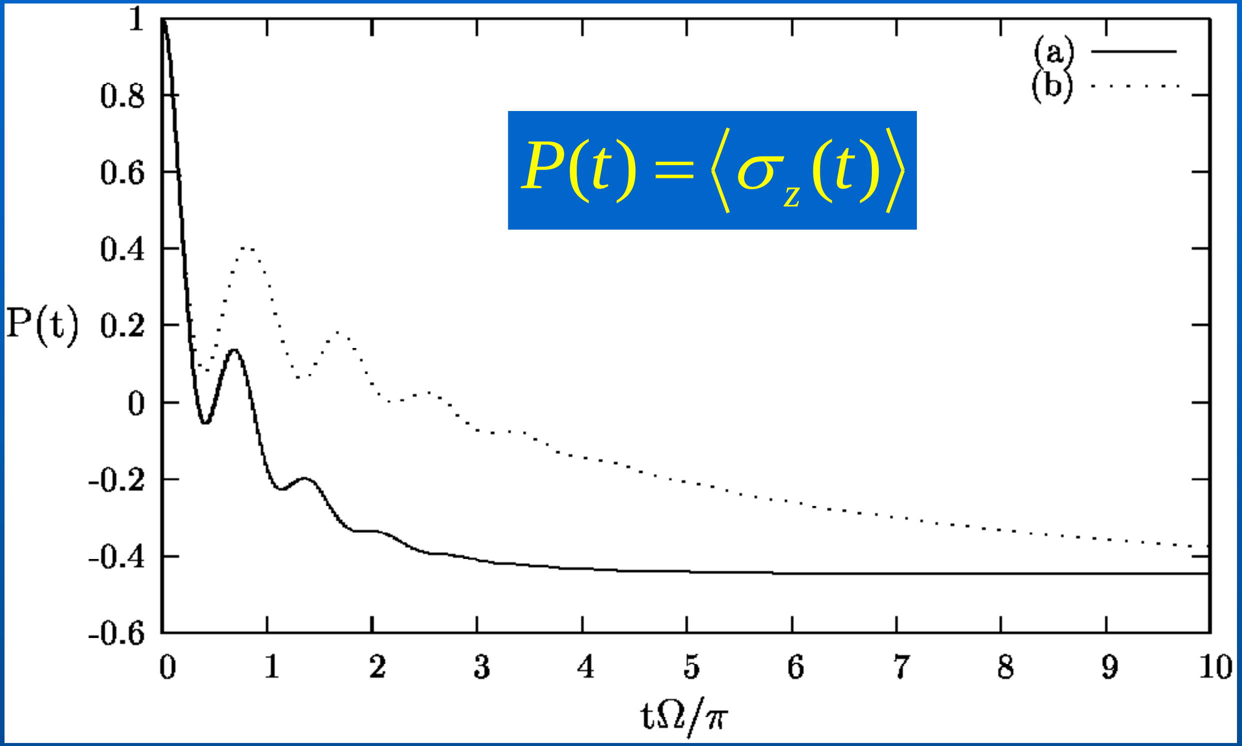
$$J(\omega) = \frac{\pi}{2}\sum \frac{c_j^2}{m_j\omega_j}\delta(\omega-\omega_j) = \eta\omega\frac{\omega_c^2}{\omega_c^2+\omega^2}$$

$$\alpha(t) = \frac{\eta\omega_c^2}{2}\cot\left(\frac{\beta\omega_c}{2}\right)e^{-\omega_c t} + \frac{2\eta\omega_c^2}{\beta}\sum_{n=1}^{\infty}\frac{\nu_n e^{-\nu_n t}}{\nu_n^2-\omega_c^2} - i\frac{\eta\omega_c^2}{2}e^{-\omega_c t}$$

$$\nu_n = \frac{2\pi n}{\hbar\beta}$$

A finite number N_e of exponentials will be used in numerical calculations.

Transient Dynamics

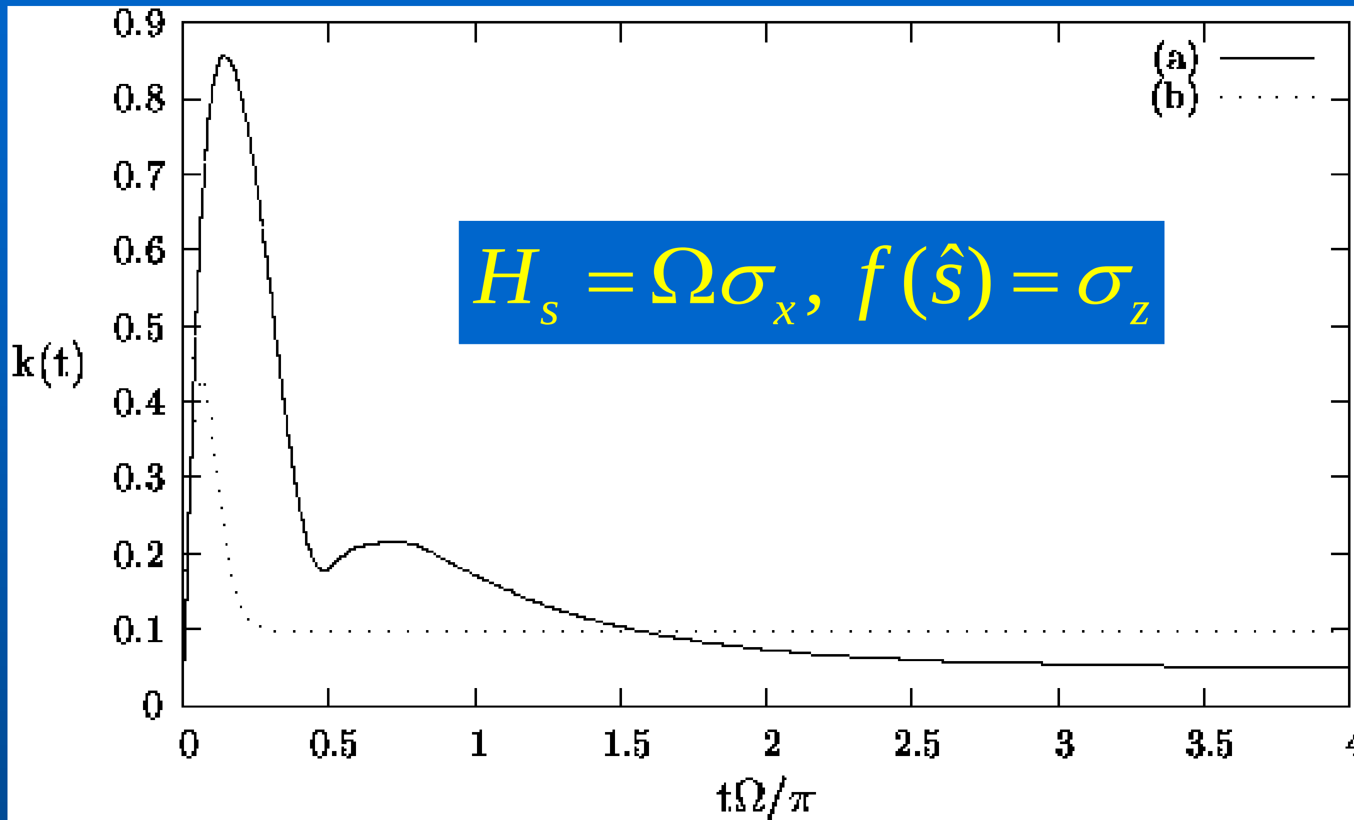


$\varepsilon/\Omega = 1,\ \beta\Omega = 0.5$

$(a)\ \Omega/\omega_c = 4,\ \eta/\Omega = 4,\ N_e = 4,\ N_{\min} = 7$

$(b)\ \Omega/\omega_c = 0.2,\ \eta/\Omega = 0.2,\ N_e = 5,\ N_{\min} = 7$

Rate Constants



$\beta\Omega = 0.5$

$(a)\ \omega_c/\Omega = 5,\ \eta/\Omega = 2;\ (b)\ \omega_c/\Omega = 0.25,\ \eta/\Omega = 40$

Bath-induced Random Field

- Caldeira-Leggett Model

$$H_b + H_{\text{int}} = \sum_j \left\{ \frac{\hat{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left[\hat{x}_j - \frac{c_j f(\hat{s})}{m_j \omega_j^2} \right]^2 \right\}$$

$$\bar{g}(t) = \sqrt{\hbar} \int_0^t dt' \left\{ \alpha_R(t-t') \left[\mu_1(t') - i\mu_4(t') \right] + \alpha_I(t-t') \left[\mu_2(t') + i\mu_3(t') \right] \right\}$$

- Response and Spectral Density Functions

$$\alpha(t) = \sum_j \frac{c_j^2}{2m_j \omega_j} \left[\coth(\hbar\beta\omega_j/2) \cos(\omega_j t) - i \sin(\omega_j t) \right]$$

$$J(\omega) = \frac{\pi}{2} \sum_j \frac{c_j^2}{2m_j \omega_j} \delta(\omega - \omega_j)$$

A Way to Master Equation

- **Furutsu-Novikov Theorem**

$$M\left\{\mu(t')F[\mu]\right\} = M\left\{\delta F[\mu]/\delta\mu(t')\right\}$$

- **Exact "Master Equation"**

$$i\hbar d\rho_s = \left[H_s + \bar{g}(t) f(\hat{s}), \rho_s\right]dt + \sqrt{\hbar}/2\left\{\left[f(\hat{s}), \rho_s\right]dz_1 + i\left\{f(\hat{s}), \rho_s\right\}dz_2^*\right\}$$

$$i\hbar d\tilde{\rho}_s(t)/dt = \left[H_s, \tilde{\rho}_s(t)\right] + \left[f(\hat{s}), \boxed{O(t)}\right], \quad \tilde{O}_{s,R(I)}(t,t') : \text{Disspation Operators}$$

$$O(t) = \sqrt{\hbar}\int_0^t dt'\left[\alpha_R(t-t')\boxed{\tilde{O}_{s,R}(t,t')} + \alpha_I(t-t')\boxed{\tilde{O}_{s,I}(t,t')}\right]$$

$$\boxed{O_{s,R}(t,t')} = \frac{\delta\rho_s(t)}{\delta\mu_1(t')} - i\frac{\delta\rho_s(t)}{\delta\mu_4(t')}, \quad \boxed{O_{s,I}(t,t')} = \frac{\delta\rho_s(t)}{\delta\mu_2(t')} + i\frac{\delta\rho_s(t)}{\delta\mu_3(t')}$$

$$\tilde{O}_{s,R(I)}(t,t') = M\left\{O_{s,R(I)}(t,t')\right\}$$

Formal Solution and Unravelling

JS, *Chem. Phys.* 322, 187 (2006), 370, 29 (2010)

$$\rho_s(t) = U_1(t,0)\rho_s(0)U_2(0,t)$$

$U_{1,2}(t,0)$ **correspond to**

$$H_{1,2}(t) = H_s + \left\{ \bar{g}(t) + \sqrt{\hbar}\left[\mu_1(t) \pm i\mu_2(t) \pm \mu_3(t) + i\mu_4(t)\right]/2 \right\} f(\hat{s})$$
$$\equiv H_s + W_{f,b}(t) f(\hat{s})$$

Natural unravelling for $\rho_s(0) = |\psi\rangle\langle\psi|$

$$\tilde{\rho}_s(t) = M\left\{U_1(t,0)|\psi\rangle\langle\psi|U_2(0,t)\right\} \equiv M\left\{|\psi_1(t)\rangle\langle\psi_2(t)|\right\}$$

Dissipative Operators

- Time-Local Form

$$O_{s,R}(t,t') = -\frac{i}{\sqrt{\hbar}}\left[\hat{f}_1(t,t')\rho_s(t) - \rho_s(t)\hat{f}_2(t,t')\right]$$

$$O_{s,I}(t,t') = \frac{1}{\sqrt{\hbar}}\left[\hat{f}_1(t,t')\rho_s(t) + \rho_s(t)\hat{f}_2(t,t')\right]$$

$$\hat{f}_{1,2}(t,t') = U_{1,2}(t,t') f(\hat{s}) U_{1,2}(t',t)$$

- Time-Nonlocal Form

$$O_{s,R}(t,t') = -\frac{i}{\sqrt{\hbar}}\left[U_1(t,t') f(\hat{s})\rho_s(t')U_2(t',t) - U_1(t,t')\rho_s(t') f(\hat{s})U_2(t',t)\right]$$

$$O_{s,I}(t,t') = \frac{1}{\sqrt{\hbar}}\left[U_1(t,t') f(\hat{s})\rho_s(t')U_2(t',t) + U_1(t,t')\rho_s(t') f(\hat{s})U_2(t',t)\right]$$

Markovian Limit

- **Exact Relation**

$$\begin{cases} \delta\rho_s(t)/\delta\mu_1(t) = -i\left[f(\hat{s}), \rho_s(t)\right] / \left(2\sqrt{\hbar}\right) \\ \delta\rho_s(t)/\delta\mu_2(t) = \left\{ f(\hat{s}), \rho_s(t)\right\} / \left(2\sqrt{\hbar}\right) \end{cases}$$

- **Approximation**

$$\delta\rho_s(t)/\delta\mu_j(t') = \delta\rho_s(t)/\delta\mu_j(t)$$

- **Master Equation**

$$i\hbar d\tilde{\rho}_s = \left[H_s + A_I(t) f^2(\hat{s}), \tilde{\rho}_s \right] dt - iA_R(t)\left[f(\hat{s}), \left[f(\hat{s}), \tilde{\rho}_s \right]\right] dt$$

$$A_{R,I}(t) = \int_0^t dt' \alpha_{R,I}(t')$$

Harmonic Oscillator $f(\hat{s}) = \hat{x}$

H. Li, JS, & S. Wang, *Phys. Rev.* E <u>84</u>, 051112 (2011)

- **Hamiltonian**

$$H_s = \frac{1}{2M}\hat{p}^2 + \frac{1}{2}M\omega_0^2\hat{x}^2,\ H_{s,\mathrm{eff}} = \frac{1}{2M}\hat{p}^2 + \frac{1}{2}M\tilde{\omega}^2\hat{x}^2$$

$$\tilde{\omega}^2 = \omega_0^2 + \frac{1}{M}\frac{2}{\pi}\int_0^\infty d\omega \frac{J(\omega)}{\omega}$$

- **Heisenberg Operators**

$$\hat{f}_{1,2}(t,t') = \cos\tilde{\omega}(t-t')\hat{x} - \frac{\sin\tilde{\omega}(t-t')}{M\tilde{\omega}}\hat{p} - \frac{1}{M\tilde{\omega}}\int_{t'}^{t} dt_1 \sin\tilde{\omega}(t_1-t')W_{1,2}(t_1)$$

- **Dissipation Operators**

$$\tilde{O}_{s,R}(t,t') = -i\cos\tilde{\omega}(t-t')\left[\hat{x},\tilde{\rho}_s(t)\right] + \frac{i}{M\omega}\sin\tilde{\omega}(t-t')\left[\hat{p},\tilde{\rho}_s(t)\right]$$

$$+\frac{2}{M\tilde{\omega}}\int_{t'}^{t} dt_1 \int_{t_1}^{t} dt_2 \sin\tilde{\omega}(t_1-t')\alpha_I(t_1-t_2)\tilde{O}_{s,R}(t,t_2)$$

$$-\frac{2}{M\tilde{\omega}}\int_{t'} dt_1 \int_0 dt_2 \sin\tilde{\omega}(t_1-t')\alpha_I(t_1-t_2)\tilde{O}_{s,I}(t,t_2)$$

Determining Dissipation Operators

Li, JS, & Wang, *PRE* 84, 051112 (2011)

- **Operator Forms**

$$\tilde{O}_{s,R}(t,t') = c_{11}(t,t')\left[\hat{x},\tilde{\rho}_s(t)\right] + c_{12}(t,t')\left[\hat{p},\tilde{\rho}_s(t)\right]$$

$$\tilde{O}_{s,I}(t,t') = c_{21}(t,t')\left\{\hat{x},\tilde{\rho}_s(t)\right\} + c_{22}(t,t')\left\{\hat{p},\tilde{\rho}_s(t)\right\} + c_{23}(t,t')\left[\hat{x},\tilde{\rho}_s(t)\right] + c_{24}(t,t')\left[\hat{p},\tilde{\rho}_s(t)\right]$$

- **Equations of Coefficients**

$$i\hbar d\tilde{\rho}_s(t)/dt = \left[H_s,\tilde{\rho}_s(t)\right] + \left[f(\hat{s}), O(t)\right], \quad \tilde{O}_{s,R(I)}(t,t') : \text{Disspation Operators}$$

$$O(t) = \sqrt{\hbar}\int_0^t dt'\left[\alpha_R(t-t')\tilde{O}_{s,R}(t,t') + \alpha_I(t-t')\tilde{O}_{s,I}(t,t')\right]$$

$$O_{s,R}(t,t') = \frac{\delta\rho_s(t)}{\delta\mu_1(t')} - i\frac{\delta\rho_s(t)}{\delta\mu_4(t')}, \quad O_{s,I}(t,t') = \frac{\delta\rho_s(t)}{\delta\mu_2(t')} + i\frac{\delta\rho_s(t)}{\delta\mu_3(t')}$$

$$\tilde{O}_{s,R(I)}(t,t') = M\left\{O_{s,R(I)}(t,t')\right\}$$

Master Equation of Harmonic Oscillator

Hu, Paz, & Zhang, *PRD* 45, 2843 (1992), Halliwell & Yu

- **Operator Form**

$$i\hbar \frac{\partial \tilde{\rho}_s(t)}{\partial t} = \left[H_{s,\mathrm{eff}}, \tilde{\rho}_s(t) \right] + A_1(t)\left[\hat{x}, \{ \hat{x}, \tilde{\rho}_s(t) \} \right] + A_2(t)\left[\hat{x}, \{ \hat{p}, \tilde{\rho}_s(t) \} \right] + A_3(t)\left[\hat{x}, [\hat{x}, \tilde{\rho}_s(t)] \right] + A_4(t)\left[\hat{x}, [\hat{p}, \tilde{\rho}_s(t)] \right]$$

- **Equations of Coefficients**

$$A_1(t) = \int_0^t dt' \alpha_I(t-t') c_{21}(t,t')$$

$$A_2(t) = \int_0^t dt' \alpha_I(t-t') c_{22}(t,t')$$

$$A_3(t) = \int_0^t dt' \left[\alpha_R(t-t') c_{11}(t,t') + \alpha_I(t-t') c_{23}(t,t') \right]$$

$$A_4(t) = \int_0^t dt' \left[\alpha_R(t-t') c_{12}(t,t') + \alpha_I(t-t') c_{24}(t,t') \right]$$

Deriving Master Equation

JS, *JCP* 120, 5053 (2004), Garraway, Breuer, Petruccione

Exact Equation of Motion

$$\rho_s(t) = U_1(t,0)\rho_s(t)U_2(0,t), H_j(t) = H_s + W_{1j}(t)\sigma^- + W_{2j}(t)\sigma^+ \; (j=1,2)$$

$$i\frac{\partial\tilde{\rho}_s}{\partial t} = \left[H_s, \tilde{\rho}_s(t)\right] + \left[\sigma^-, \int_0^t dt'\alpha(t-t')O_1(t,t')\right] + \left[\sigma^+, \int_0^t dt'\alpha^*(t-t')O_2(t,t')\right]$$

$$O_1(t,t') = M\left\{-i\frac{\delta\rho_s}{\delta\mu_{12}(t')} + \frac{\delta\rho_s}{\delta\mu_{22}(t')} + i\frac{\delta\rho_s}{\delta\mu_{32}(t')} - \frac{\delta\rho_s}{\delta\mu_{42}(t')}\right\} = 2M\left\{\rho_s(t)U_2(t,t')\sigma^+U_2(t',t)\right\}$$

$$O_2(t,t') = M\left\{i\frac{\delta\rho_s}{\delta\mu_{11}(t')} + \frac{\delta\rho_s}{\delta\mu_{21}(t')} + i\frac{\delta\rho_s}{\delta\mu_{31}(t')} + \frac{\delta\rho_s}{\delta\mu_{41}(t')}\right\} = 2M\left\{U_1(t,t')\sigma^-U_1(t',t)\rho_s(t)\right\}$$

Dissipation Operators

$$U_2(t,t')\sigma^+U_2(t',t) = \sigma^+ + i\int_{t'}^t dt_1\left[W_{12}(t_1)U_2(t,t_1)\sigma_z U_2(t_1,t) - \omega_0 U_2(t,t_1)\sigma^+U_2(t_1,t)\right]$$

$$\rho_s(t) = U_1(t,0)\rho_s(t)U_2(0,t), H_j(t) = H_s + W_{1j}(t)\sigma^- + W_{2j}(t)\sigma^+ \; (j=1,2)$$

$$i\frac{\partial\tilde{\rho}_s}{\partial t} = \left[H_s, \tilde{\rho}_s(t)\right] + \left[\sigma^-, \int_0^t dt'\alpha(t-t')O_1(t,t')\right] + \left[\sigma^+, \int_0^t dt'\alpha^*(t-t')O_2(t,t')\right]$$

$$O_1(t,t') = M\left\{-i\frac{\delta\rho_s}{\delta\mu_{12}(t')} + \frac{\delta\rho_s}{\delta\mu_{22}(t')} + i\frac{\delta\rho_s}{\delta\mu_{32}(t')} - \frac{\delta\rho_s}{\delta\mu_{42}(t')}\right\} = 2M\left\{\rho_s(t)U_2(t,t')\sigma^+U_2(t',t)\right\}$$

$$O_2(t,t') = M\left\{i\frac{\delta\rho_s}{\delta\mu_{11}(t')} + \frac{\delta\rho_s}{\delta\mu_{21}(t')} + i\frac{\delta\rho_s}{\delta\mu_{31}(t')} + \frac{\delta\rho_s}{\delta\mu_{41}(t')}\right\} = 2M\left\{U_1(t,t')\sigma^-U_1(t',t)\rho_s(t)\right\}$$

Implementation of Stochastic Processes

Stockburger, JS

- **Total stochastic fields**

$$W_{f,b}(t) = \bar{g}(t) + \frac{\sqrt{\hbar}}{2}\left[\mu_1(t) \pm i\mu_2(t) \pm \mu_3(t) + i\mu_4(t)\right]$$

$$\bar{g}(t) = \sqrt{\hbar}\int_0^t dt' \left\{\alpha_R(t-t')\left[\mu_1(t') - i\mu_4(t')\right] + \alpha_I(t-t')\left[\mu_2(t') + i\mu_3(t')\right]\right\}$$

- **Regrouping**

$$W_{f,b}(t) = \xi(t) + \nu_{1,2}(t)$$

$$\xi(t) = \sqrt{\hbar}\int_0^t dt'\alpha_R(t-t')\left[\mu_1(t') - i\mu_4(t')\right] + \sqrt{\hbar}\left[\mu_1(t) + i\mu_4(t)\right]/2$$

$$\nu_{1,2}(t) = \sqrt{\hbar}\int_0^t dt'\alpha_I(t-t')\left[\mu_2(t') + i\mu_3(t')\right] + \sqrt{\hbar}\left[\pm i\mu_2(t) \pm \mu_3(t)\right]/2$$

$\xi(t)$ is independent of $\nu_{1,2}(t)$, and $\nu_{1,2}(t)$ are dependent on each other.

TABLE I. Summary of results for $P(t) \equiv \langle \sigma_z(t) \rangle$ for bias $\varepsilon = 0$.

$$H = -\tfrac{1}{2}\hbar\Delta\sigma_x + \tfrac{1}{2}q_0\sigma_z \sum_\alpha C_\alpha x_\alpha + H_b(\{m_\alpha\},\{\omega_\alpha\}),$$

$\alpha = \frac{1}{2}$, all T	Exponential decay with a rate $\pi\Delta^2/2\omega_c$ (Toulouse limit) (Sec. V.B)

relevant time scale. In view of these difficulties we must regard the true behavior of $P(t)$ in the regime $T = 0$, $\frac{1}{2} < \alpha \le 1$ as a currently unresolved problem.

$s > 2$	Weakly damped oscillations (Sec. VI.B)

For results for $\varepsilon \neq 0$, see Sec. VII.

Rev. Mod. Phys. 59, 1 (1987)

already in Section 3.2. The relevant Hamiltonian is given in Eq. (3.75) or Eq. (3.76).

Despite its apparent simplicity, the spin-boson model cannot be solved exactly by any known method (apart from some limited regimes of the parameter space). Not only is the spin-boson model nontrivial mathematically, it is also nontrivial physically.

The environment acts on the TSS by a fluctuating force $\xi(t) = \sum_\alpha c_\alpha x_\alpha(t)$. For a bath with linear response, the modes $x_\alpha(t)$ obey Gaussian statistics. Therefore the dynamics of the bath is fully characterized by the force autocorrelation function in thermal equilibrium $\langle \xi(t)\xi(0)\rangle_\beta$, which is simply a superposition of harmonic oscillator correlation functions [cf. Eq. (5.33)]. In the formal path integral expression for the reduced density matrix, the environment reveals itself through an influence functional $\mathcal{F}$. In Chapters 4 and 5 we have given several useful forms for $\mathcal{F}$ applicable to thermodynamics and dynamics, respectively.

Statistics of New Gaussian Processes

- **The Real**

$$M\left\{\xi(t)\right\}=0,\ \ M\left\{\xi(t)\xi(t')\right\}=\hbar\alpha_R(t-t')$$

- **The "Imaginary"**

$$M\left\{\nu_{1,2}(t)\right\}=0,\ \ M\left\{\nu_1(t)\nu_2(t')\right\}=i\hbar\alpha_I(t-t')$$

$$M\left\{\nu_1(t)\nu_1(t')\right\}=-M\left\{\nu_2(t)\nu_2(t')\right\}=i\hbar\left[\theta(t-t')-\theta(t'-t)\right]\alpha_I(t-t')$$

- **Example: Spin-Boson (Ohmic case at zero temperature)**

$$J(\omega)=2\pi\alpha\omega\left[1+\left(\omega/\omega_c\right)^2\right]^{-2},\ \ \alpha(t)=\pi^{-1}\int_0^\infty d\omega J(\omega)e^{-i\omega t}$$

$$\alpha_I(t)=-\frac{1}{2}\pi\alpha\omega_c^3 t e^{-\omega_c t}$$

Problem and Solution

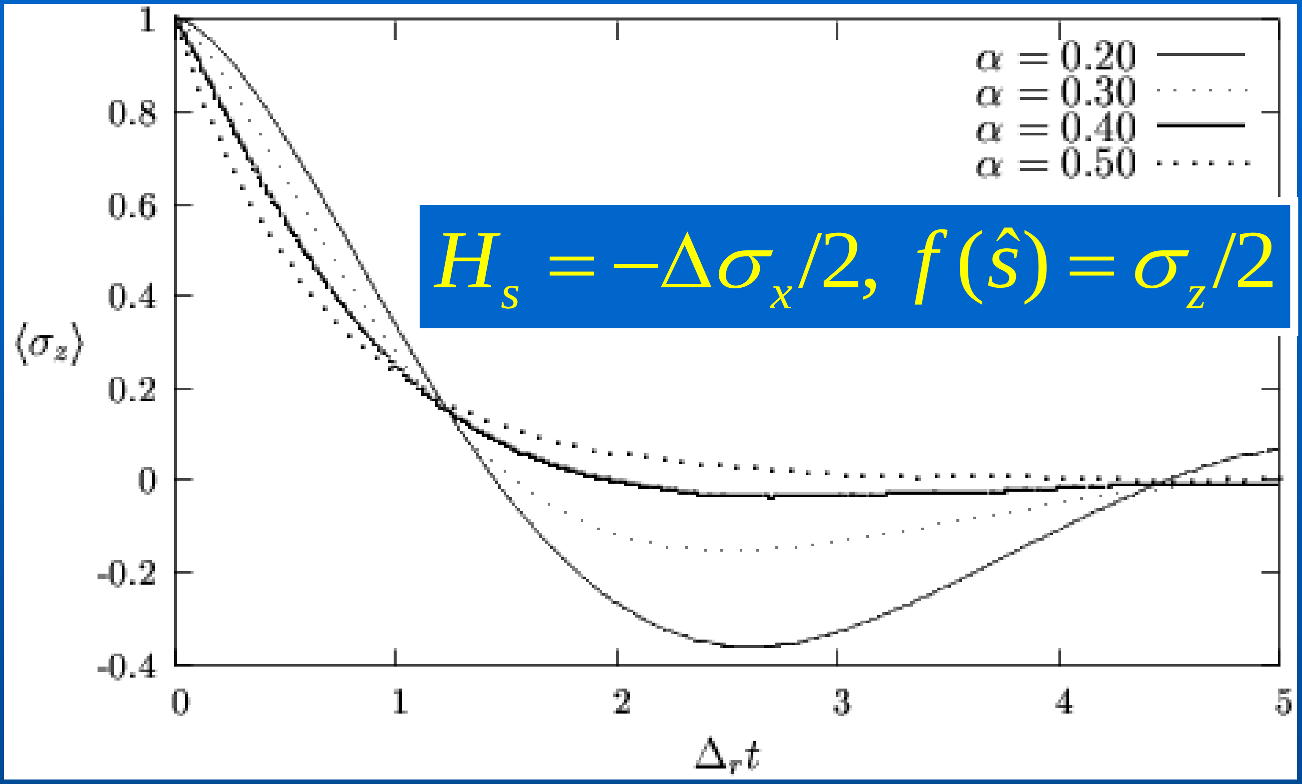
P: The real stochastic field is long-ranged in time and numerical convergence of averaging is very slow.

S: Combining the hierarchical equations of motion method and stochastic simulation is very useful.

Other better solutions?

Mixed Random-Hierarchy Approach

Zhou, Yan & JS, *EPL* 72, 334 (2005)

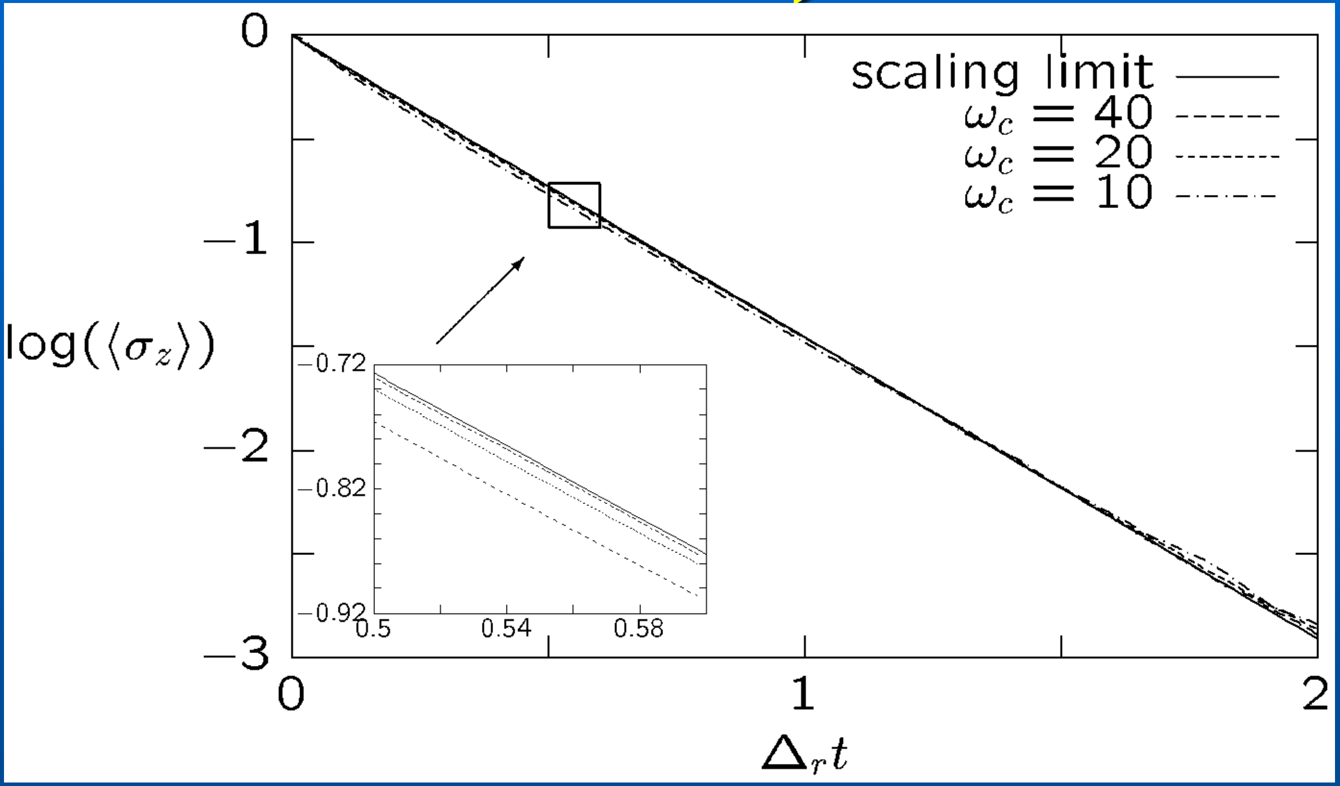


$$H_s = -\Delta\sigma_x/2,\ f(\hat{s}) = \sigma_z/2$$

$$J(\omega) = 2\pi\alpha\omega\frac{\omega_c^4}{(\omega_c^2+\omega^2)^2};\ \Delta_r = \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}, \omega_c = 20\Delta$$

$$\alpha(t) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)e^{-i\omega t}, \alpha_I(t) = -\frac{1}{2}\alpha\pi t\omega_c^3 e^{-\omega_c t}$$

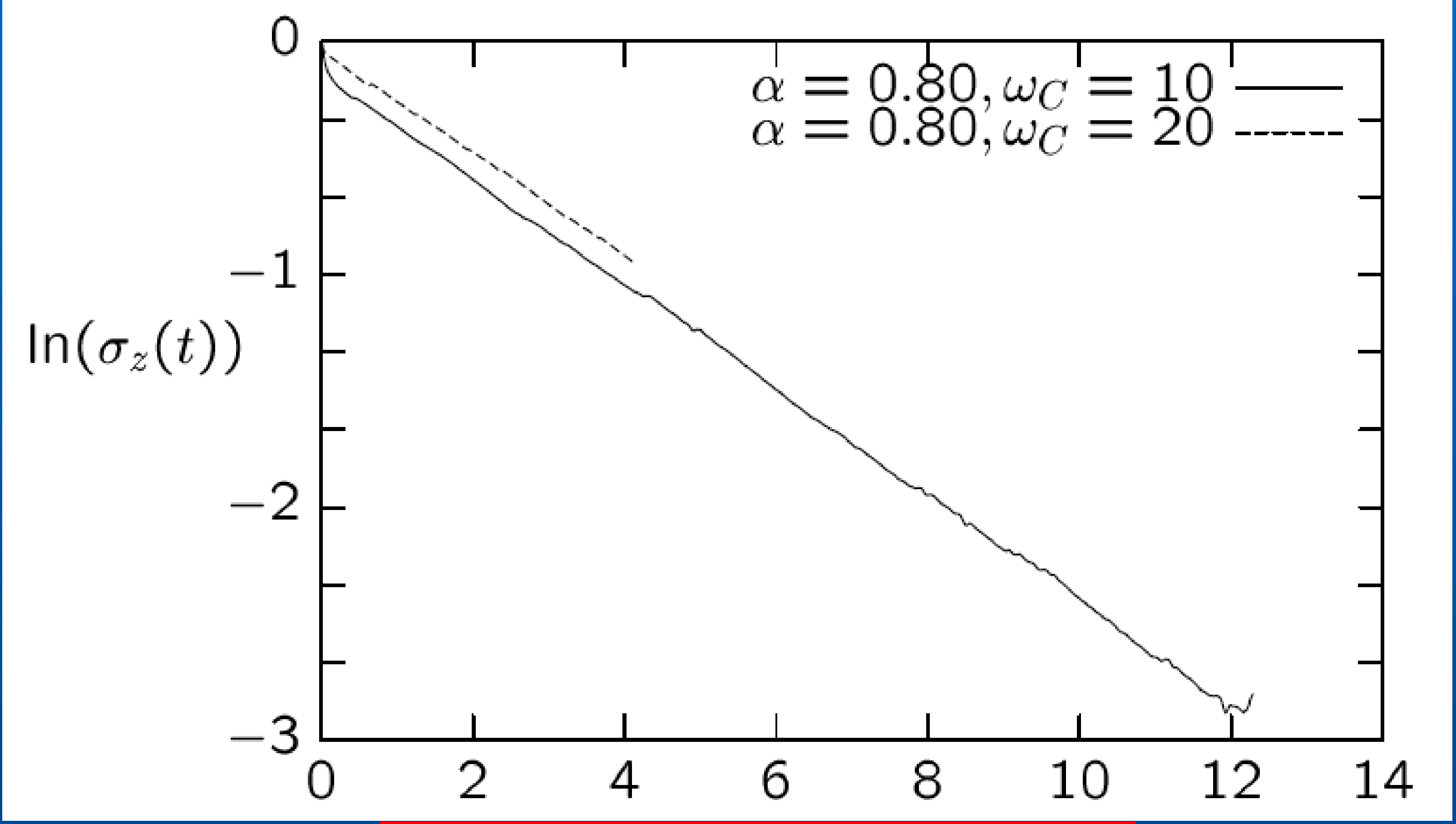
Special Case (α= 0.5, Toulouse Limit)



$$\Delta_r = \Delta(\Delta / \omega_c)$$

Decay Dynamics (α> 0.5)

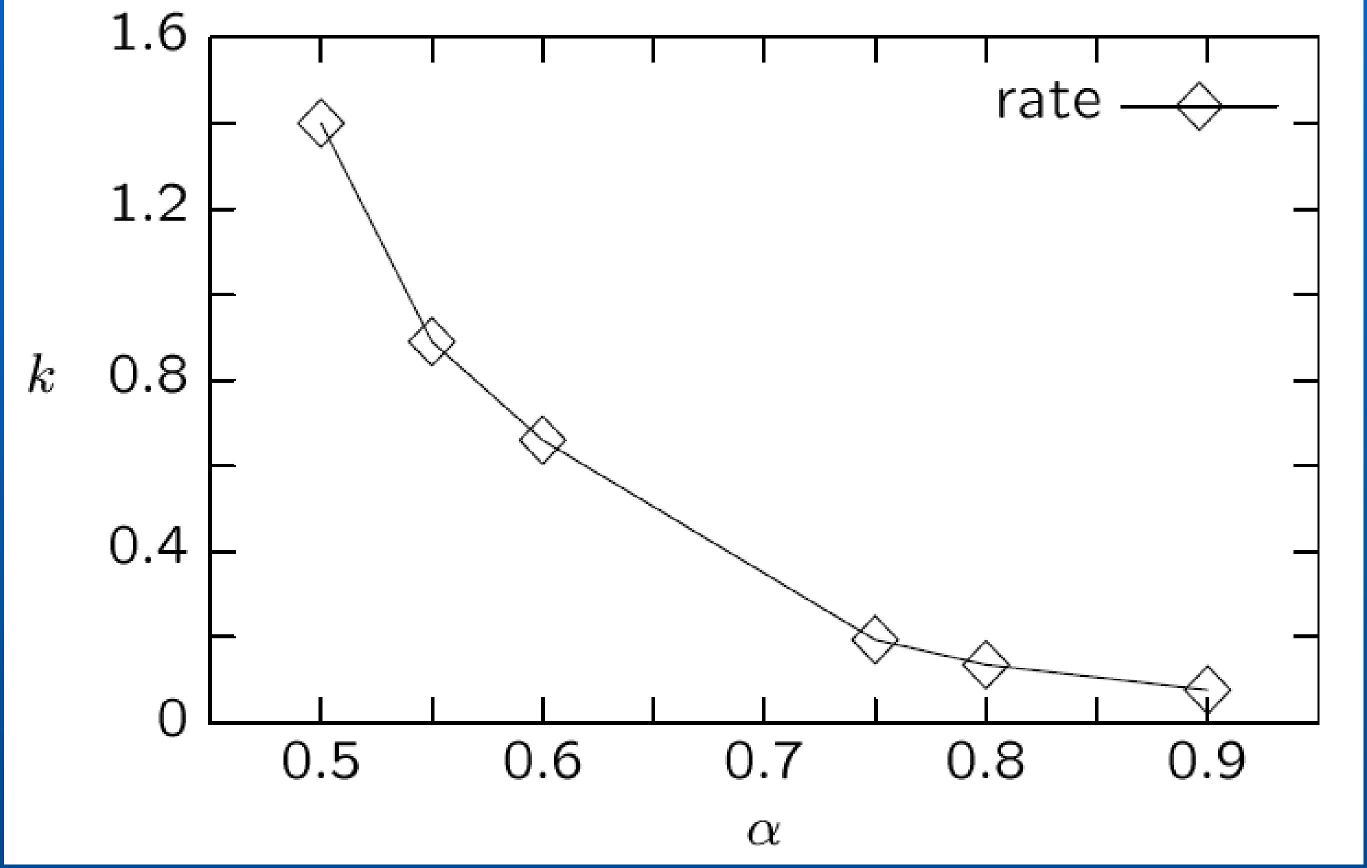
Zhou & JS, *JCP* 128, 034106 (2008)



time scale: $\Delta(\Delta/\omega_c)t \neq \Delta_r t$

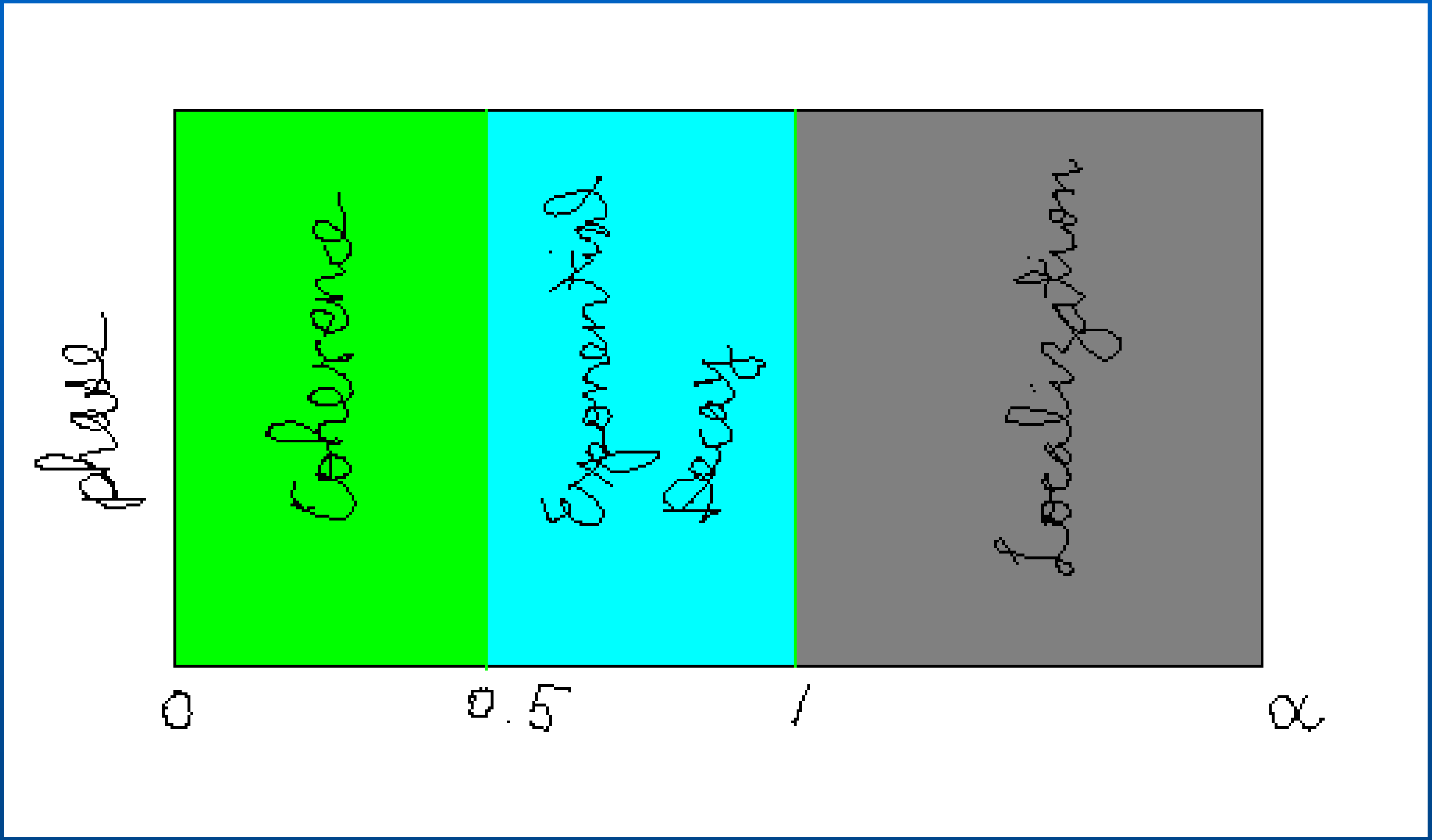
$$\Delta_r = \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}$$

Decay Rate



$$\sigma_z(t) = \exp(-kt/\omega_c)$$

Phase Diagram



SBM: From Operator Eq to Scalar One

Define: $I(t) = \mathrm{Tr}\{\rho_s(t)\}$, $x(t) = \mathrm{Tr}\{\rho_s(t)\sigma_x\}$,
$y(t) = \mathrm{Tr}\{\rho_s(t)\sigma_y\}$, $z(t) = \mathrm{Tr}\{\rho_s(t)\sigma_z\}$

$$\frac{dI}{dt} = -\frac{i}{\hbar}\Gamma_2(t)z(t)$$
$$\frac{dx}{dt} = -\frac{1}{\hbar}\Gamma_2(t)y(t)$$
$$\frac{dy}{dt} = \Delta z(t) + \frac{1}{\hbar}\Gamma_1(t)x(t)$$
$$\frac{dz}{dt} = -\Delta y(t) - \frac{i}{\hbar}\Gamma_2(t)I(t)$$

$$\Gamma_1(t) = 2\bar{g}(t) + \sqrt{\hbar}\left[\mu_1(t) + i\mu_2(t)\right],\ \Gamma_2(t) = \sqrt{\hbar}\left[\mu_4(t) + i\mu_3(t)\right]$$
$$\left\langle \Gamma_1(t)\Gamma_1(t')\right\rangle = 4\hbar\alpha_R\left(|t-t'|\right),\ \left\langle \Gamma_2(t)\Gamma_2(t')\right\rangle = 0,$$
$$\left\langle \Gamma_1(t)\Gamma_2(t')\right\rangle = \theta(t-t')\alpha_I\left(t-t'\right).$$

Integral Equation for *z*(*t*)

$$z(t) = e^{-\frac{i}{\hbar}\int_0^t ds\Gamma_2(s)} - \Delta^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \cos\left[\frac{1}{\hbar}\int_{t_1}^t ds\Gamma_2(s)\right]\cos\left[\frac{1}{\hbar}\int_{t_2}^{t_1} ds\Gamma_1(s)\right] z(t_2)$$

$$z(t) = e^{-\frac{i}{\hbar}\int_0^t ds\Gamma_2(s)} z_1(t)$$

$$= e^{\frac{1}{\sqrt{\hbar}}\int_0^t ds[\mu_3(s) - i\mu_4(s)]} z_1(t)$$

$$z_1(t) = 1 - \Delta^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \cos\left[\frac{1}{\hbar}\int_{t_1}^t ds\Gamma_2(s)\right]\cos\left[\frac{1}{\hbar}\int_{t_2}^{t_1} ds\Gamma_1(s)\right] e^{\frac{i}{\hbar}\int_{t_2}^t ds\Gamma_2(s)} z_1(t_2)$$

Girsanov Transformation

$$\mu_3(t) \to \mu_3(t) + 1/\sqrt{\hbar},\ \mu_4(t) \to \mu_4(t) - i/\sqrt{\hbar}$$

Stochastic average of *z*(*t*) is equal to that of the transformed *z₁*(*t*), $\tilde{z}(t)$

$$\tilde{z}(t) = 1 - \Delta^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \cos\left[\frac{1}{\hbar}\int_{t_1}^{t} ds\Gamma_2(s)\right] \cos\left[\frac{1}{\hbar}\int_{t_2}^{t_1} ds\tilde{\Gamma}_1(s)\right] e^{\frac{i}{\hbar}\int_{t_2}^{t} ds\Gamma_2(s)} \tilde{z}(t_2)$$

$$\tilde{\Gamma}_1(s) = \Gamma_1(s) + 4\int_{-\infty}^{s} ds'\alpha_I(s-s') \equiv \Gamma_1(s) + A(s)$$

As $\langle \tilde{z}(t) \rangle = \langle z(t) \rangle$, no confusion will arise if $\tilde{z}(t)$ is simply denoted as $z(t)$.

Introduce two deterministic functions A_1 and A_2 and define

$\Theta_1 = \tilde{\Gamma}_1(t) + A_1$ and $\Theta_2 = \Gamma_2(t) + A_2$.

From IE to Functional Equation

JS, Klyatskin

$$\left\langle z\left(\left[\Theta_1,\Theta_2\right],t\right)\right\rangle = 1-\frac{\Delta^2}{2}\int_0^t dt_1\int_0^{t_1} dt_2 \left\langle \cos\left[\frac{1}{\hbar}\int_{t_1}^{t} ds\Theta_2(s)\right] e^{\frac{i}{\hbar}\int_{t_1}^{t} ds\Theta_2(s)} \right\rangle$$

$$\left[F_1(t_1,t_2)Z_1(t_1,t_2)+F_2(t_1,t_2)Z_2(t_1,t_2)\right]$$

$$F_{1,2}(t_1,t_2) = \left\langle e^{\pm\frac{i}{\hbar}\int_{t_2}^{t_1} ds\left\{2\int_{t_2}^{s} ds_1 Y(s,s_1)+\sqrt{\hbar}\left[\mu_1(s)+i\mu_2(s)\right]+A(s)+A_1(s)\right\}} e^{\frac{i}{\hbar}\int_{t_2}^{t_1} ds\Theta_2(s)} \right\rangle$$

$$Y(t,t') = \sqrt{\hbar}\left\{\alpha_R(t-t')\left[\mu_1(t')-i\mu_2(t')\right]+\alpha_I(t-t')\left[\mu_3(t')+i\mu_4(t')\right]\right\}$$

$$F_{1,2}(t_1,t_2) = e^{-\frac{4}{\hbar}\int_{t_2}^{t_1} ds\int_{t_2}^{s} ds'\left[\alpha_R(s-s')\pm i\alpha_I(s-s')\right]} e^{\frac{i}{\hbar}\int_{t_2}^{t_1} ds\left[\pm A(s)\pm A_1(s)+A_2(s)\right]}$$

$$\equiv C_{\pm}(t_1,t_2)e^{\frac{i}{\hbar}\int_{t_2}^{t_1} ds\left[\pm A_1(s)+A_2(s)\right]}$$

Girsanov Transformation Again

$$Z_{1,2}(t_1,t_2) = \left\langle e^{\pm 2\frac{i}{\sqrt{\hbar}}\int_{-\infty}^{t_2} ds \int_{t_2}^{s} ds_1 Y(s,s_1)} z\left(\left[\Theta_1,\Theta_2\right],t_2\right)\right\rangle$$

$$= \left\langle z\left(\left[\Theta_1 \pm 4iA_{R,t_1,t_2},\Theta_2 \pm 4A_{I,t_1,t_2}\right],t_2\right)\right\rangle$$

The self-induced field during the evolution:

$$A_{t_1,t_2}(t) = \int_{t_2}^{t_1} dt'\alpha(t'-t)$$

$$Z\left(\left[A_1,A_2\right],t\right) \equiv \left\langle z\left(\left[\Theta_1,\Theta_2\right],t\right)\right\rangle$$

Functional Integral Equation

$$Z_{1,2}(t_1,t_2) = \left\langle e^{\pm 2\frac{i}{\sqrt{\hbar}}\int_{-\infty}^{t_2} ds \int_{t_2}^{s} ds_1 Y(s,s_1)} z\left(\left[\Theta_1,\Theta_2\right],t_2\right)\right\rangle$$

$$= \left\langle z\left(\left[\Theta_1 \pm 4iA_{R,t_1,t_2},\Theta_2 \pm 4A_{I,t_1,t_2}\right],t_2\right)\right\rangle$$

$$Z\left(\left[A_1,A_2\right],t\right) = 1 - \frac{\Delta^2}{4}\int_0^t dt_1 \int_0^{t_1} dt_1 \left[1 + e^{2\frac{i}{\hbar}\int_{t_1}^{t} ds A_2(s)}\right]\left\{C_+(t_1,t_2) e^{\frac{i}{\hbar}\int_{t_2}^{t_1} ds\left[A_1(s)+A_2(s)\right]}\right.$$

$$Z\left(\left[A_1 + 4iA_{R,t_1,t_2},A_2 + 4A_{I,t_1,t_2}\right],t_2\right)$$

$$\left. + C_+(t_1,t_2) e^{-\frac{i}{\hbar}\int_{t_2}^{t_1} ds\left[A_1(s)-A_2(s)\right]} Z\left(\left[A_1 - 4iA_{R,t_1,t_2},A_2 - 4A_{I,t_1,t_2}\right],t_2\right)\right\}$$

Formal Equation of Motion

$$\langle z(t)\rangle = Z\left(\left[0,0\right],t\right)$$

$$= 1 - \frac{\Delta^2}{4}\int_0^t dt_1 \int_0^{t_1} dt_1 \left\{ C_+(t_1,t_2)\, Z\left(\left[4iA_{R,t_1,t_2}, 4A_{I,t_1,t_2}\right], t_2\right)\right.$$

$$\left. + C_+(t_1,t_2) Z\left(\left[-4iA_{R,t_1,t_2}, -4A_{I,t_1,t_2}\right], t_2\right)\right\}$$

Non-interacting Blip Approximation

Neglecting the self-induced field:

$$\langle z(t)\rangle = 1 - \frac{\Delta^2}{4}\int_0^t dt_1 \int_0^{t_1} dt_1 \left[C_+(t_1,t_2) + C_+(t_1,t_2)\right]\langle z(t_2)\rangle$$

Stochastic Formulation

- Alleviating or transforming the curse of dimensionality
- Designing numerical techniques
- Studying spin-boson model
- Obtaining the functional integral equation for the spin-boson model

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