Time Dependent Non Adiabatic Markovian Master Equation

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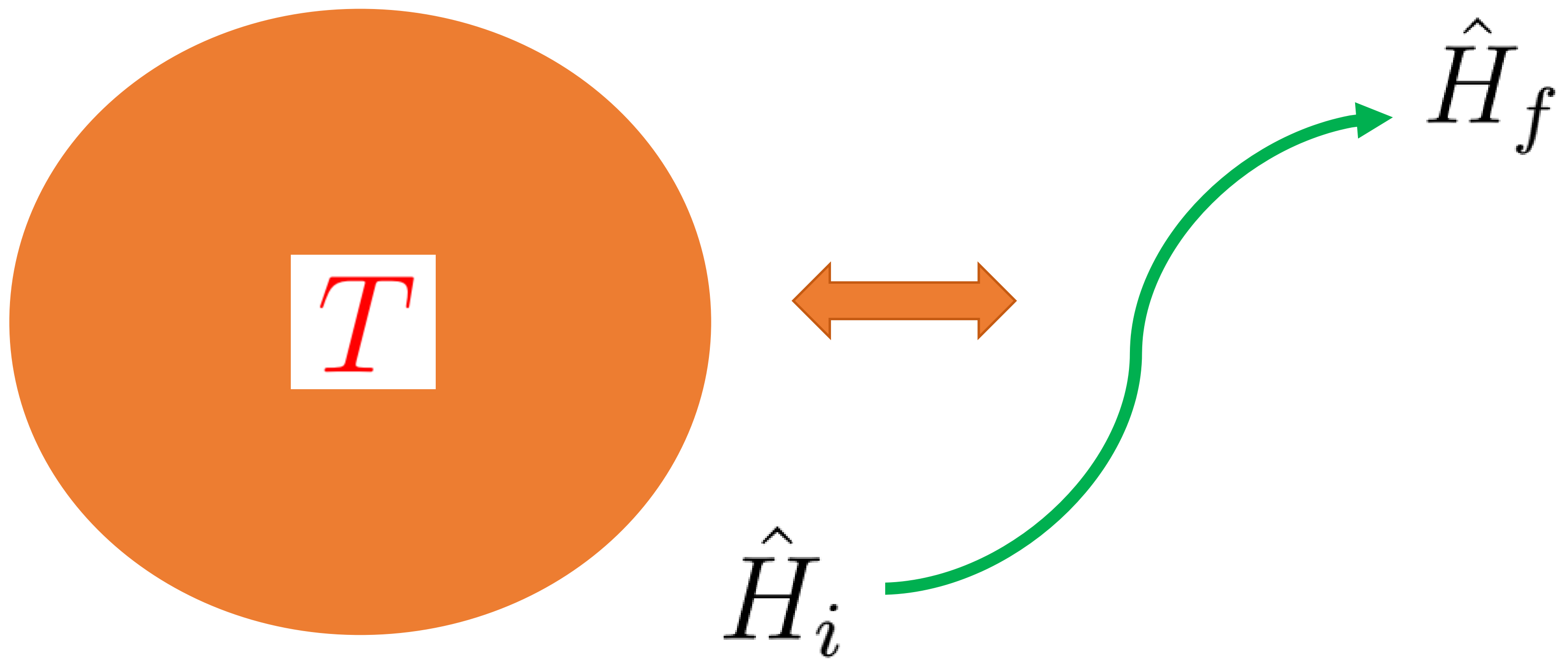
Goal – Non oscillatory time dependent non adiabatic process



Reduced description

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_I$$

Separation of time scales

If the bath timescale is much faster than the system then:

$$\frac{d}{dt}\hat{\rho}_S = \mathcal{L}_S\hat{\rho}_S$$

Where $\mathcal{L}_S$ depends on the bath implicitly.

$$\hbar = 1$$

The theory of open quantum systems

- Complete positive map: for $\hat{\rho}(0) = \hat{\rho}_S \otimes \hat{\rho}_B$

$$\Lambda\hat{\rho} = \sum_j \hat{K}_j^\dagger \hat{\rho} \hat{K}_j$$

Where $\sum_j \hat{K}_j^\dagger \hat{K}_j = \hat{I}$

$$\Lambda_t = e^{\mathcal{L}_S t}$$

The Gorini-Kossakowski-Lindblad-Sudarshan (GKLS) quantum Master equation

$$\frac{d}{dt}\hat{\rho}_S = -i\left[\hat{H}_S, \hat{\rho}_S\right] + \frac{1}{2}\sum_j \left(\left[\hat{V}_j \hat{\rho}_S, \hat{V}_j^\dagger\right] + \left[\hat{V}_j, \hat{\rho}_S \hat{V}_j^\dagger\right]\right) \equiv -i\left[\hat{H}_S, \hat{\rho}_S\right] + \mathcal{L}_S \hat{\rho}_S$$

System and bath are in tensor product form at all times

Lindblad G. *Comm. in Math. Phys.* 1976

Gorini, V., Kossakowski, A., & Sudarshan, E. C. G. (1976).. *Jour. of Math. Phys., 17*(5), 821-825.

Previous derivations

- Davies construction: The weak coupling limit
- Floquet derivation: Periodic Driving
- Quantum Adiabatic Master equation

Davies, E. B. (1974). *Comm. in math. Phys.*, *39*(2).
Alicki, R., Gelbwaser-Klimovsky, D., & Kurizki, G. (2012). *arXiv preprint arXiv:1205.4552*.
Geva, E., Kosloff, R., & Skinner, J. L. (1995). *The Journal of chemical physics*, *102*(21).
Albash, T., Boixo, S., Lidar, D. A., & Zanardi, P. (2012). *New Journal of Physics*, *14*(12).
Cavina, V., Mari, A., & Giovannetti, V. (2017). *PRL*, *119*(5), 050601.

Non Adiabatic Master Equation (NAME)

$$\hat{H}(t) = \hat{H}_s(t) + \hat{H}_B + \hat{H}_I$$

$$\hat{H}_I = \sum_k g_k \hat{A}_k \otimes \hat{B}_k$$

- Following Davies's derivation, the first step is a transformation to the Interaction picture:

$$\tilde{A}_k(t) = \hat{U}_S^\dagger(t,0)\,\hat{A}_k \hat{U}_S(t,0)$$

$$\tilde{B}_k(t) = e^{i\hat{H}_B t}\hat{B}_k e^{-i\hat{H}_B t}$$

Where the system evolution operator is given by,

$$i\frac{\partial \hat{U}_S(t)}{\partial t} = \hat{H}_S(t)\hat{U}_S(t) \;\;, \;\; \hat{U}_S(0) = I$$

$$\hbar = 1$$

Non Adiabatic Master Equation (NAME)

- Second order perturbation theory leads to the Markovian quantum Master equation

$$\frac{d}{dt}\tilde{\rho}_S(t) = \int_0^\infty ds\, \mathrm{tr}_B\left[\hat{H}_I(t), \left[\hat{H}_I(t-s), \tilde{\rho}_S(t)\otimes\hat{\rho}_B\right]\right]$$

$$\frac{d}{dt}\hat{\rho}_S(t) = -i\left[\hat{H}_S(t) + \hat{H}_{LS}(t), \hat{\rho}_S\right]$$
$$+\sum_{k,j}\left(\xi_j^k(t)\right)^2 g_k^2 \gamma\left(\alpha_j^k(t)\right)\left(\hat{F}_j(t)\,\hat{\rho}_S\hat{F}_j^\dagger(t) - \frac{1}{2}\{\hat{F}_j^\dagger(t)\,\hat{F}_j(t), \hat{\rho}_S\}\right)$$

$\hat{H}_{LS}(t)$ is the Lamb shift Hamiltonian given by: $\hat{H}_{LS}(t) = \sum_{k,j} S_{kk}\left(\alpha_j^k(t)\right)\hat{F}_j^\dagger(t)\,\hat{F}_j(t)$

Separation of time scales between the system and the bath

Regime of interest

Four typical time scales:

- $\tau_S = \left(\frac{1}{\omega_i(t)}\right)$ - Typical time scale of the system
- $\tau_B \sim \frac{1}{\Delta\nu}$ - Bath correlations decay time scale
- $\tau_R \propto (g^2)^{-1}$ - Relaxation time scale
- $\tau_d = \min_{j,t}|\theta_j'(t)|^{-1}$ - Driving time scale

$\tau_B \ll \tau_S$ $\quad$ $\tau_B \ll \tau_R$ $\quad$ $\tau_B \ll \tau_d$

The jump operators

Consider the Lie Algebra $$\left[\hat{A}_i, \hat{A}_j\right] = \sum_k C_{ij}^k \hat{A}_k$$

If the Hamiltonian is: $$\hat{H}_S = \sum_j h\left(t\right) \hat{A}_j$$

Then the propagator has the form $$\mathcal{U}\left(t\right) = \Pi_j e^{\alpha_j(t)\left[\hat{A}_j, \cdot\right]}$$

- Heisenberg equations of motion for the algebra are closed.

The eigenoperators of are: $$\mathcal{U}\left(t\right) \hat{F}_m = \hat{F}_m e^{i\lambda_m \theta(t)}$$

If $$\hat{H}_I = \sum_n g_n \hat{A}_n \otimes \hat{B}_n$$ then we can expand in $\{\hat{F}_m\}$

$$\hat{H}_I = \sum_{m,n} g_n \xi_m^n\left(0\right) \hat{F}_m \otimes \hat{B}_n \Longrightarrow \hat{F}_m$$ become the jump operators

Non Adiabatic Master Equation (NAME)

- Inserting $\hat{H}_I$ into the Markovian Master equation $\tilde{A}_k(t) = \sum_j \xi_j^k(t)\, e^{i\theta_j(t)} \hat{F}_j$

$$\frac{d}{dt}\tilde{\rho}_S(t) = \sum_{k,k'j,j'} \int_0^\infty ds\, \xi_j^k(t)\xi_{j'}^{k'}(t-s)\left(\hat{F}_{j'}\tilde{\rho}_S\hat{F}_j + \{\hat{F}_j\hat{F}_{j'},\tilde{\rho}_S\}\right)\times$$

$$e^{i\theta_{j'}(t)}e^{i\theta_j(t-s)}g_{k'}g_k \mathrm{tr}_B\{\tilde{B}_{k'}(t-s)\,\tilde{B}_k(t)\,\hat{\rho}_B\} + \mathrm{h.c}$$

- If $\tau_B \ll \tau_d$, when $s \sim \tau_B$ → $\xi_j^k(t-s) \approx \xi_j^k(t)$

- Expanding $\theta_j(t-s)$ around $s = t$,

$$\alpha_j \equiv -\frac{d}{dt}\theta_j(t-s)\,|_{s=0}$$

$$\theta_j(t-s) \approx \theta_j(t) - \frac{d}{dt}\theta_j(t)\, s$$

- Secular approx., neglecting terms where $\theta_j(t) \neq -\theta_{j'}(t)$

The NAME in the Heisenberg form

In the Heisenberg picture, the reduced dynamics are of the form,

$$\frac{d}{dt}\hat{O} = V^{\dagger}(t,0)\left\{\mathcal{L}^{\dagger}(t)\,\hat{O}\right\}$$

For such a case the adjoint propagator is given by,

$$V^{\dagger}(t,t_0) = \mathcal{T}_{\rightarrow}\exp\left(\int_{t_0}^{t} ds\,\mathcal{L}^{\dagger}(s)\right)$$

Where $\mathcal{T}_{\rightarrow}$ is the anti-chronological time ordering operator.

$V^{\dagger}(t,t_0)$ satisfies the differential equation

$$\frac{\partial}{\partial t}V^{\dagger}(t,t_0) = V^{\dagger}(t,t_0)\,\mathcal{L}^{\dagger}(t)$$

Breuer, H. P., & Petruccione, F. (2002). *The theory of open quantum systems*. (pg. 124-125)

The NAME for the Harmonic oscillator

$$\hat{H}_S = \frac{\hat{P}^2}{2m} + \frac{1}{2} m\omega^2(t)\,\hat{Q}^2$$

Constant non-adiabatic parameter,

$$\mu = \frac{\dot{\omega}}{\omega^2}$$

This determines the driving protocol

$$\omega(t) = \frac{\omega(0)}{1 - \mu\omega(0)\,t}$$

$$\hat{H}_I = g\hat{Q} \otimes \sum_k p_k = ig \sum_k \sqrt{\frac{m\omega_k}{2}}\hat{Q} \otimes \left(\hat{b}_k^\dagger - \hat{b}_k\right)$$

Alhassid, Y., & Levine, R. D. (1978). *Phys. Rev. A*, *18*(1), 89.

Jaynes, E. T. (1957). *Physical review*, *106*(4), 620.

Operators for a Gaussian state

It is convenient to analyze the problem in terms of operators

- Hamiltonian $$\hat{H}_S = \frac{\hat{P}^2}{2m} + \frac{1}{2} m \omega^2 (t) \hat{Q}^2$$
- Lagrangian $$\hat{L} = \frac{\hat{P}^2}{2m} - \frac{1}{2} m \omega^2 (t) \hat{Q}^2$$
- Position and momentum correlation $$\hat{C} = \frac{\omega (t)}{2} \left(\hat{P}\hat{Q} + \hat{Q}\hat{P} \right)$$

The coherence can be identified as, $$Coh \equiv \omega^{-1} \sqrt{\langle \hat{L} \rangle^2 + \langle \hat{C} \rangle^2}$$

Kosloff, R., & Rezek, Y. (2017 *Entropy*, *19*(4), 136.

Solution for the propagator

For $\mu = const$ can be solved in terms of $\{\hat{H}_S, \hat{L}, \hat{C}, \hat{I}\}^T$

$$\mathcal{U}(t,0) = \frac{\omega(t)}{\omega(0)} \frac{1}{\kappa^2} \begin{bmatrix} 4-\mu^2 c & -\mu\kappa s & -2\mu(c-1) & 0 \\ -\mu\kappa s & \kappa^2 c & -2\kappa s & 0 \\ 2\mu(c-1) & 2\kappa s & 4c-\mu^2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

where $s = sin(\kappa\theta(t))$ and $c = cos(\kappa\theta(t))$

$$\kappa = \sqrt{4-\mu^2} \qquad \theta(t) = -\frac{1}{\mu}\log\left(\frac{\omega(t)}{\omega(0)}\right)$$

Kosloff, R., & Rezek, Y. (2017 *Entropy*, *19*(4), 136.

NAME for an Harmonic oscillator

$$\frac{d}{dt}\hat{\rho}_S(t) = -i\left[\hat{H}_S(t) + \hat{H}_{LS}(t), \hat{\rho}_S\right] + |\xi(t)|^2 \gamma(\alpha(t)) \times \left[\left(\hat{F}_+(t)\hat{\rho}_S\hat{F}_-(t) - \frac{1}{2}\{\hat{F}_-(t)\hat{F}_+(t), \hat{\rho}_S\}\right) + e^{-\alpha(t)/k_BT}\left(\hat{F}_-(t)\hat{\rho}_S\hat{F}_+(t) - \frac{1}{2}\{\hat{F}_+(t)\hat{F}_-(t), \hat{\rho}_S\}\right)\right]$$

Where $\hat{F}_+(t) = A\hat{Q}(t) + B\hat{P}(t) = \left(\hat{F}_-(t)\right)^\dagger$ and $A = \frac{1}{2}\left(i\frac{\mu}{\kappa} + 1\right)$ $B = i\frac{1}{m\omega_0\kappa}$

$$\gamma(\alpha(t)) = \pi m J(\alpha(t))(N(\alpha(t)) + 1) \qquad \alpha(t) = \frac{\kappa}{2}\omega(t)$$

$\kappa = \sqrt{4 - \mu^2} \leq 2$ The relaxation rate is slowed down

Comparing the non adiabatic rate to the adiabatic rate

Non adiabatic relaxation rate:

$$\gamma_{N.A}\left(\frac{\kappa}{2}\omega\left(t\right)\right)=\pi mJ\left(\frac{\kappa}{2}\omega\left(t\right)\right)\left(N\left(\frac{\kappa}{2}\omega\left(t\right)\right)+1\right)$$

Adiabatic relaxation rate:

$$\gamma_{adi}\left(\omega\left(t\right)\right)=\pi mJ\left(\omega\left(t\right)\right)\left(N\left(\omega\left(t\right)\right)+1\right)$$

In the low temperature regime and when $J\propto\omega^3$,

$$\gamma_{N.A}\approx\frac{\kappa^3}{8}\gamma_{adi} \qquad \kappa=\sqrt{4-\mu^2}\leq 2$$

Solving the NAME of an HO

Transforming variables in the interaction picture: $\left[\tilde{b}, \tilde{b}^\dagger\right] = 1$

$$\frac{d}{dt}\hat{\rho}_S(t) = k_\downarrow(t)\left(\tilde{b}\tilde{\rho}_S\tilde{b}^\dagger - \frac{1}{2}\{\tilde{b}^\dagger\tilde{b}, \tilde{\rho}_S\}\right) + k_\uparrow(t)\left(\tilde{b}^\dagger\tilde{\rho}_S\tilde{b} - \frac{1}{2}\{\tilde{b}\tilde{b}^\dagger, \tilde{\rho}_S\}\right)$$

Guessing a solution in the form of Generalized Canonical form

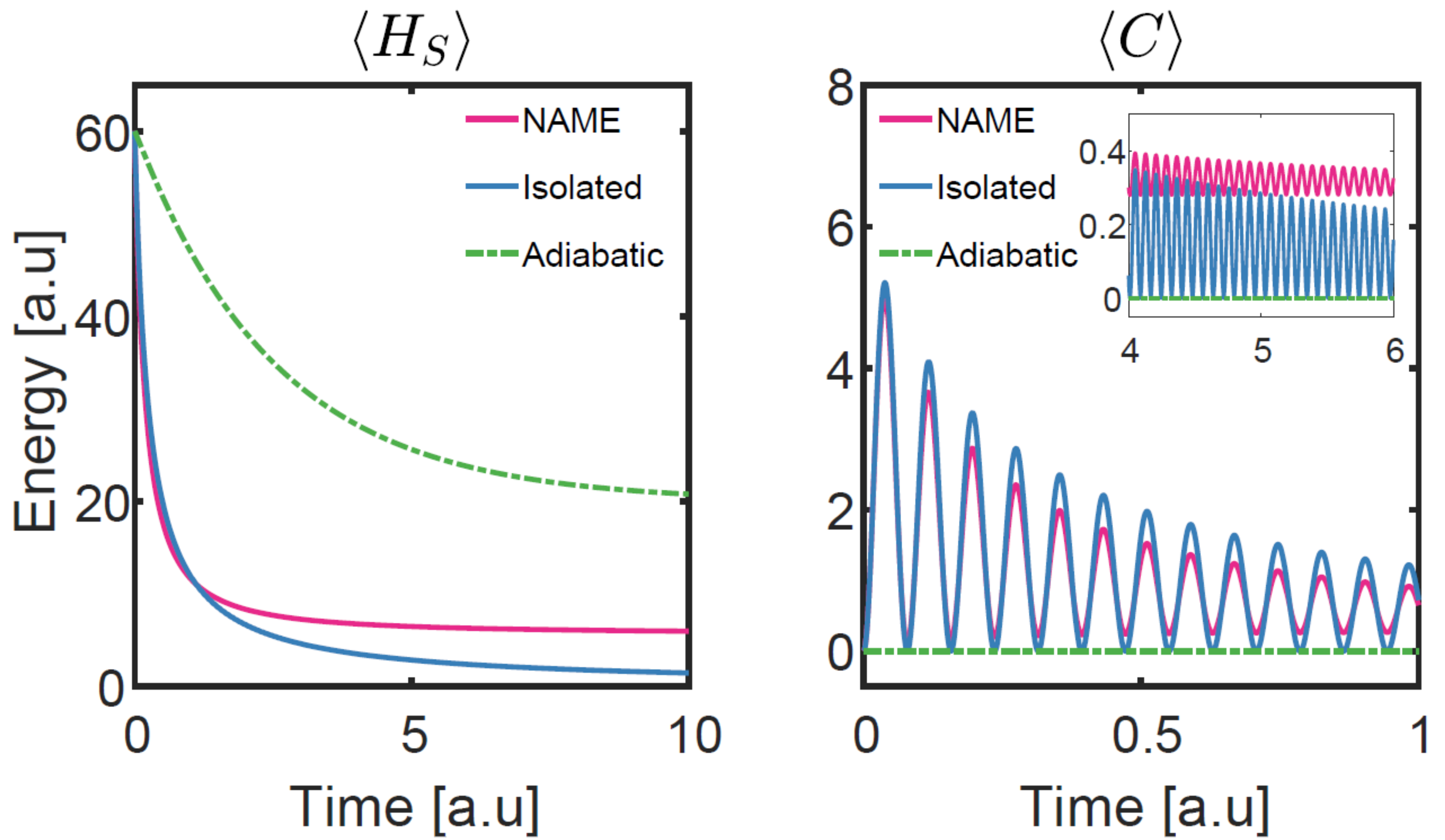
$$\tilde{\rho}_S(t) = (Z(t))^{-1} e^{\gamma(t)\tilde{b}^2} e^{\beta(t)\tilde{b}^\dagger\tilde{b}} e^{\gamma^*(t)\left(\tilde{b}^\dagger\right)^2}$$

$$\dot{\beta} = k_\downarrow\left(e^\beta - 1\right) + k_\uparrow\left(e^{-\beta} - 1 + 4e^\beta|\gamma|^2\right)$$

$$\dot{\gamma} = (k_\downarrow + k_\uparrow)\gamma - 2k_\uparrow\gamma e^{-\beta}$$

Andersen, H. C., Oppenheim, I., Shuler, K. E., & Weiss, G. H. (1964). *Jour. of Math. Phys.*, *5*(4), 522-536.

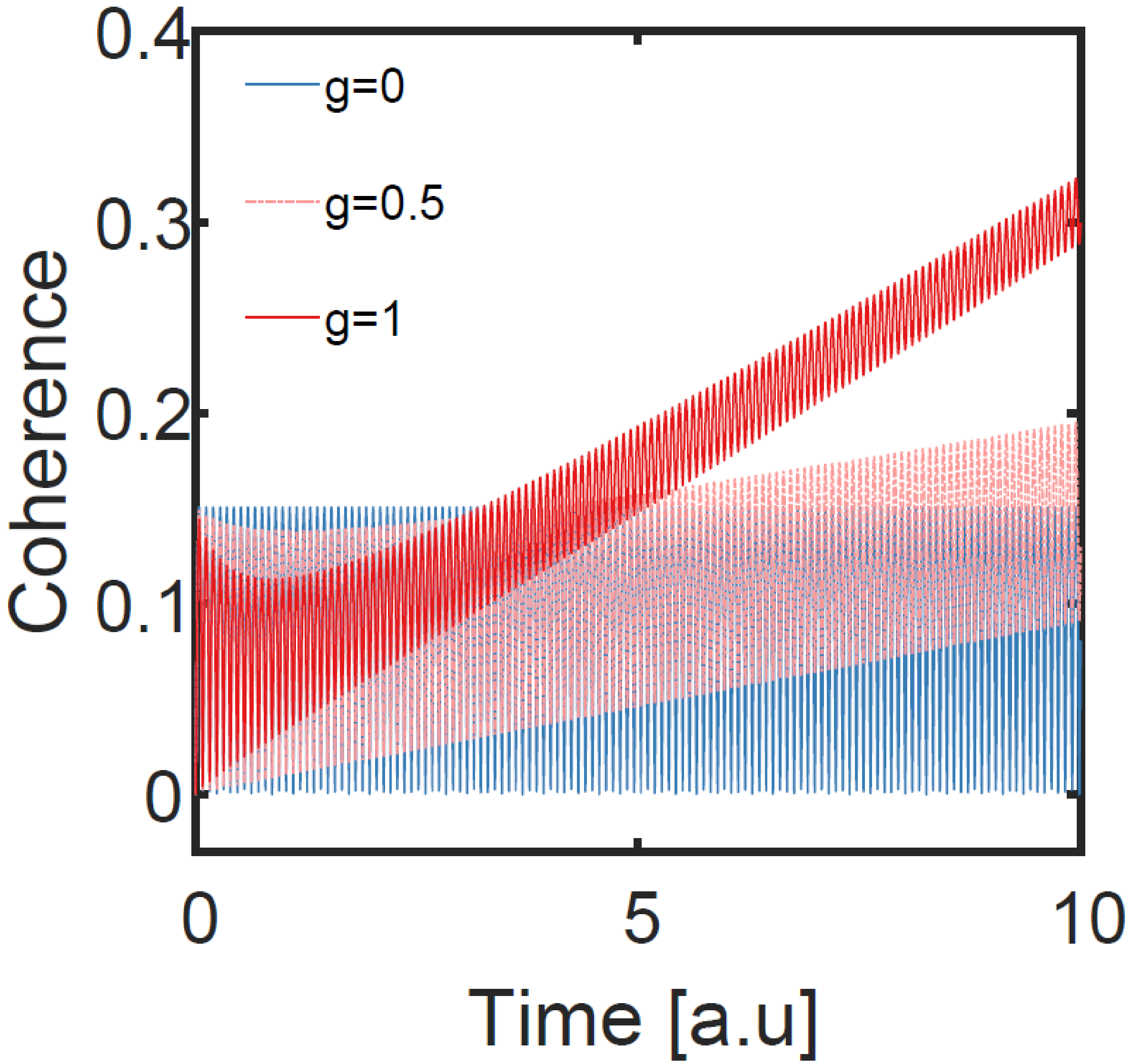
Solution of the NAME for HO



$$\omega(t) = \frac{\omega(0)}{1 - \mu\omega(0)}$$

$$\mu < 0$$

Solution of the NAME for HO



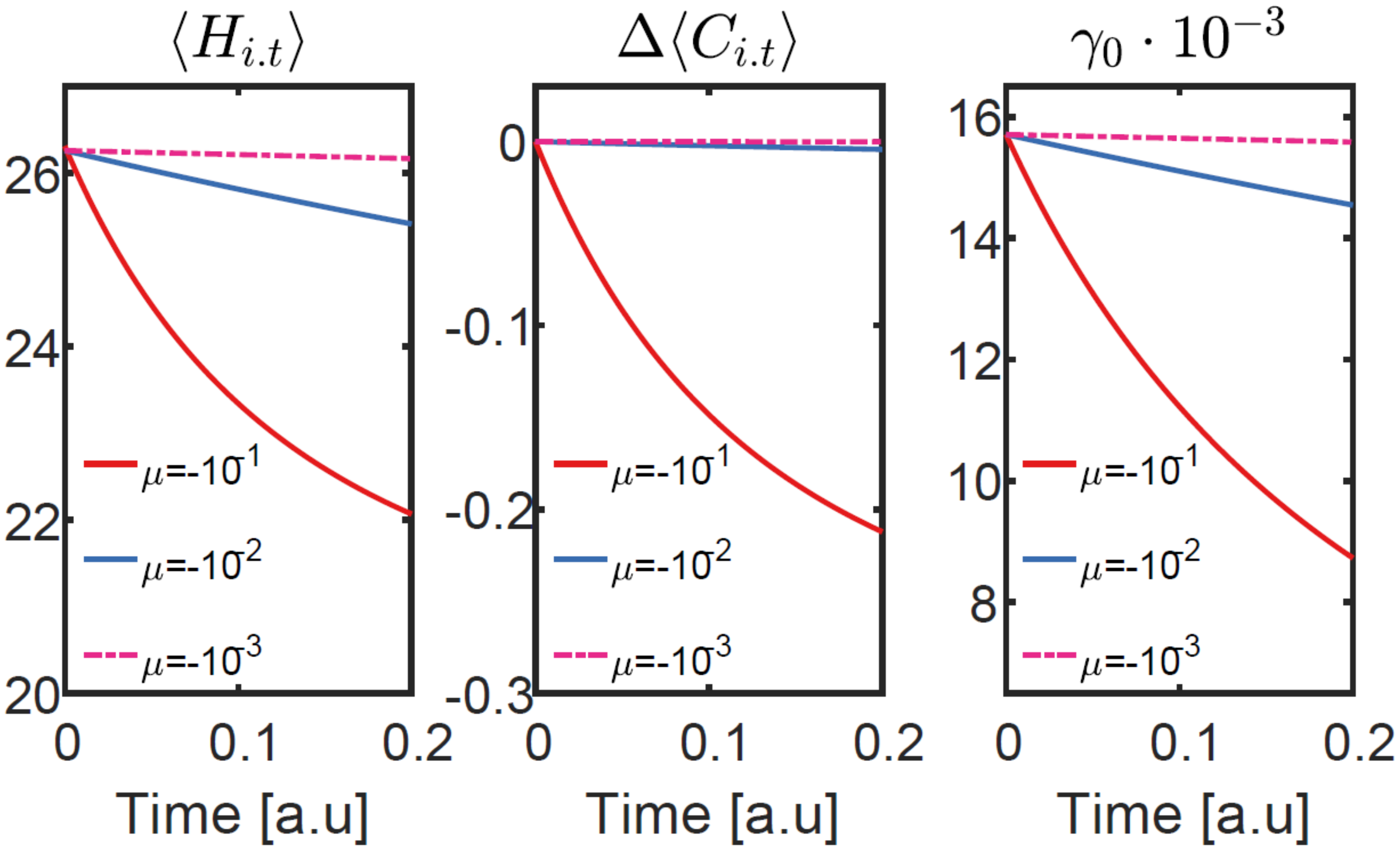
$$Coh \equiv \omega^{-1}\sqrt{\langle\hat{L}\rangle^2 + \langle\hat{C}\rangle^2}$$

Coherence generated by the bath.

Solution of the NAME for HO

Instantaneous Attractor

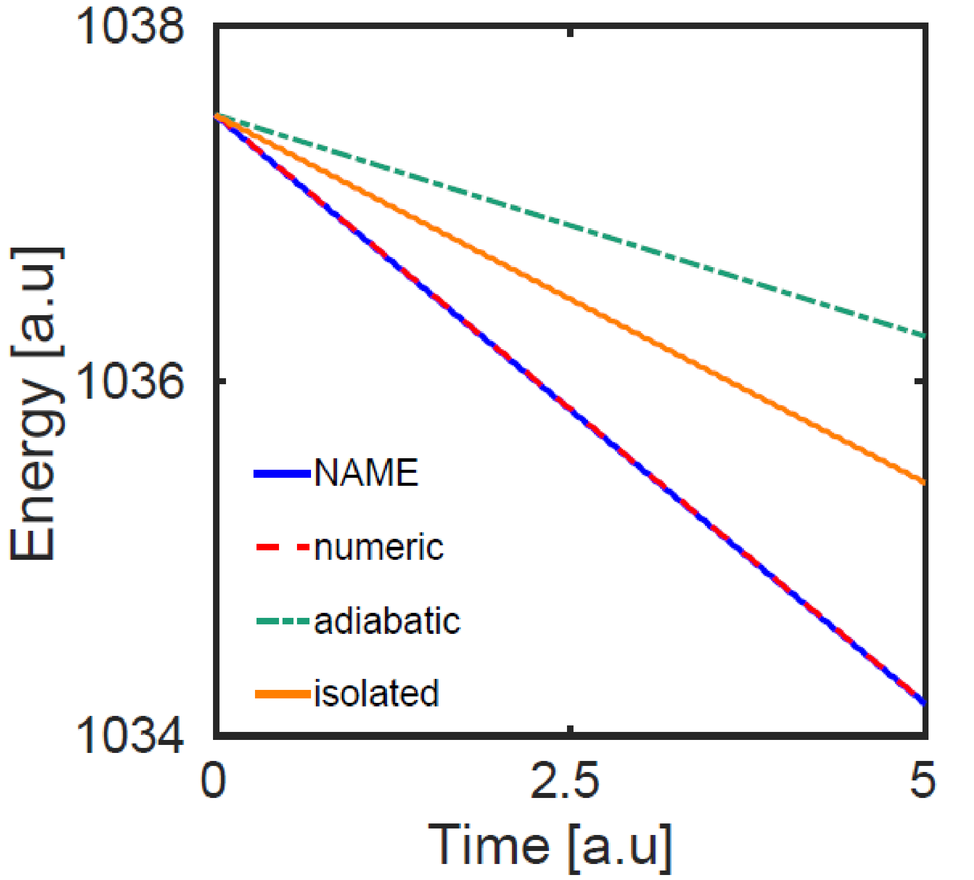
$$\frac{d}{dt} \to 0$$



$$\omega(t) < \omega(0)$$

Solution of the NAME for HO

Comparison to numerical simulation



Comparison to the adiabatic Master equation

- Both equation have a GKLS form, guaranteeing a CPTP map.

- Doppler like shift in the frequency:

$$\alpha\left(t\right)=\frac{\kappa}{2}\omega\left(t\right) \qquad \kappa=\sqrt{4-\mu^{2}}\leq 2$$

Slowing down the relaxation rate and modifying the instantaneous target state.

- The unitary and dissipative terms don’t commute, (resulting from the TD jump operators), mixing energy and coherence.

- Time dependent instantaneous attractor

Carnot cycle for a two-level-system

$$\hat{H}_S(t) = \omega(t)\,\hat{S}_z + \varepsilon \hat{S}_x$$

$$\eta \rightarrow \eta_c$$