Memory Effects in Micro and Nanoscale Systems

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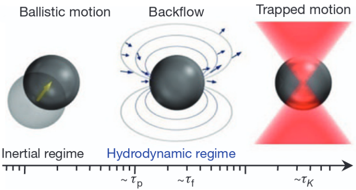
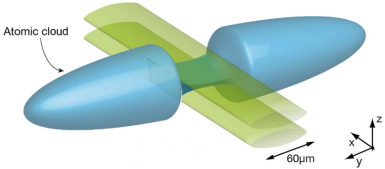
Brownian motion

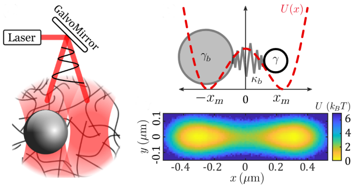


➸ T. Franosch et al., Nature **478** 85 (2011).

Finite-size reservoirs

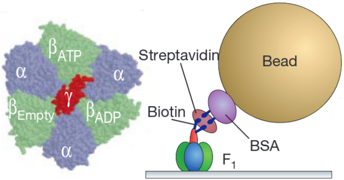


➸ S. Krinner et al., J. Phys. Condens. Matter **29** 343003 (2017).



➸ F. Ginot et al., PRL **128** 028001 (2022).

Hidden degrees of freedom



➸ R. Yasuda et al., Nature **410** 898 (2001).

Basic Approach

Step 1: Microscopic model

$\dot{X}_t = \mathsf{W} X_t$

X_t . . . state vector

W . . . microscopic generator

- local in time

Step 2: Coarse graining

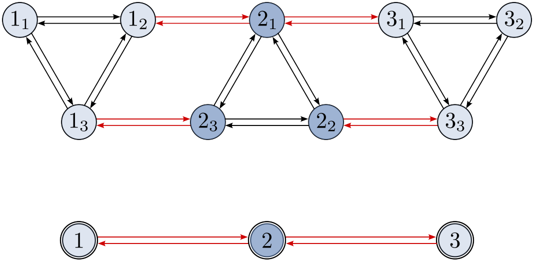
$$\dot{x}_t = \mathsf{V} x_t + \int_0^t dt' \; \mathsf{K}_{t'} x_{t-t'}$$

x_t . . . reduced state vector

V . . . adiabatic generator

K_t . . . memory kernel

- non-local in time
- fully systematic



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- non-local in time
- fully systematic

Step 3: Short memory approximation

$\dot{x}_t \simeq L x_t$

L . . . effective generator

Adiabatic approximation

$L^0 = V$

Markov approximation

$$L^1 = V + \int_0^\infty dt \; K_t e^{-Vt}$$

➸ M. Esposito, PRE **85** 041125 (2012).

➸ G. Hummer, A. Szabo, J. Phys. Chem. B **119** 9029 (2015).

- local in time
- generally non-systematic
- requires sharp separation of time scales

Basic Approach

Step 1: Microscopic model

$\dot{X}_t = \mathrm{W} X_t$

X_t . . . state vector

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- local in time

Step 2: Coarse graining

$\dot{x}_t = \mathrm{V} x_t + \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'}$

x_t . . . reduced state vector

V . . . adiabatic generator

K_t . . . memory kernel

- non-local in time
- fully systematic

Step 3: Short memory approximation

$\dot{x}_t \simeq \mathrm{L} x_t$

L . . . effective local generator

- local in time
- generally non-systematic
- requires sharp separation of time scales

Questions

1. When and in what sense does a local approximation exist?
2. Can its error be bounded?
3. How to construct it systematically?
4. Is it unique?

Formalization

Starting point

$$\dot{x}_t = \mathrm{V} x_t + \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'}$$

$x_t \in \mathbb{C}^N$

$\mathrm{V}, \mathrm{K}_t \in \mathbb{C}^{N \times N}$

Initial condition

$x_{t=0} = x_0$

Weak memory condition

$\|\mathrm{K}_t\| \leq M e^{-kt} \quad \text{for} \quad t \geq 0$

Aim

$\mathrm{L} \in \mathbb{C}^{N \times N}$ and $y_0 \in \mathbb{C}^N$ so that

$\dot{y}_t = \mathrm{L} y_t \quad \text{and} \quad x_t \simeq y_t$

Short time expansion

$$x_t = x_0 + \mathrm{V} x_0 \cdot t + \frac{\mathrm{V}^2 + \mathrm{K}_0}{2} x_0 \cdot t^2 + \mathcal{O}(t^3)$$

$$y_t = y_0 + \mathrm{L} y_0 \cdot t + \frac{\mathrm{L}^2}{2} y_0 \cdot t^2 + \mathcal{O}(t^3)$$

- $x_t \neq y_t$ for short times in general

Formalization

Starting point

$$\dot{x}_t = Vx_t + \int_0^t dt' \; K_{t'} x_{t-t'}$$

$$x_t \in \mathbb{C}^N$$

$$V, K_t \in \mathbb{C}^{N\times N}$$

Initial condition

$$x_{t=0} = x_0$$

Weak memory condition

$$\|K_t\| \le Me^{-kt} \quad \text{for} \quad t \ge 0$$

Aim

$L \in \mathbb{C}^{N\times N}$ and $y_0 \in \mathbb{C}^N$ so that

$$\dot{y}_t = Ly_t \quad \text{and} \quad x_t \simeq y_t$$

Ansatz

$$x_t = e^{Lt} A_t x_0, \quad \lim_{t\to\infty} A_t = D, \quad \det[D] \neq 0$$

$$y_t = e^{Lt} y_0, \quad y_0 = Dx_0, \quad \lim_{t\to\infty} |x_t - y_t| = 0$$

A_t . . . reduced propagator

D . . . slippage matrix

y_t . . . long time approximation

Questions

1. When does such a generator L exist?
2. Can $|x_t - y_t|$ be bounded?

First Approach

Scalar Model

$$\dot{x}_t = V x_t + \int_0^t dt' \; K_{t'} x_{t-t'}$$

$$V = -v \qquad \leq 0$$

$$K_t = -M e^{-kt} \leq 0$$

$$x_0 = 1$$

Solution

$$x_t = \frac{k-\rho}{\eta-\rho} e^{-\rho t} - \frac{k-\eta}{\eta-\rho} e^{-\eta t}$$

$$\rho = \frac{k+v-\sqrt{(k-v)^2-4M}}{2}$$

$$\eta = \frac{k+v+\sqrt{(k-v)^2-4M}}{2}$$

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Observation

If $4M < (k-v)^2$:

$$L = -\rho, \qquad A_t = e^{-Lt} x_t \to \frac{k-\rho}{\eta-\rho} = D \neq 0$$

$$y_t = e^{Lt} D, \qquad |x_t - y_t| = \frac{k-\eta}{\eta-\rho} e^{-\eta t} \to 0$$

If $4M = (k-v)^2$:

$$x_t = \big(1 + (k-\rho)t\big) e^{-\rho t}$$

If $4M > (k-v)^2$:

$$x_t = \left(\cos[\omega t] + \frac{k-v}{2\omega} \sin[\omega t]\right) e^{-\delta t}$$

$$\omega = \frac{|\eta-\rho|}{2}, \qquad \delta = \frac{|\eta+\rho|}{2}$$

- The condition $4M < (k-v)^2$ is necessary for the existence of an effective generator.

Theorem

Setting

$$\dot{x}_t = \mathsf{V}x_t + \int_0^t dt' \ \mathsf{K}_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$x_t \in \mathbb{C}^N, \quad \mathsf{V}, \mathsf{K}_t \in \mathbb{C}^{N \times N}, \quad x_{t=0} = x_0$$

Weak memory conditions

$$\|\mathsf{K}_t\| \leq Me^{-kt}, \quad \|V\| = v < k, \quad \frac{4M}{(k-v)^2} \leq 1$$

$$M, k > 0, \qquad v \geq 0$$

Theorem

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Existence of effective generators

There exists a unique pair of generators $\mathrm{L}, \mathrm{R} \in \mathbb{C}^{N\times N}$ so that

$$x_t = e^{\mathrm{L}t}\mathrm{A}_t x_0 = \mathrm{B}_t e^{\mathrm{R}t} x_0,$$

$$\lim_{t\to\infty} \mathrm{A}_t = \lim_{t\to\infty} \mathrm{B}_t = \mathrm{D}, \quad \det[\mathrm{D}] \neq 0.$$

The slippage matrix D satisfies LD $=$ DR and

$$\mathrm{D} = \left[1 + \int_0^\infty dt \int_0^\infty dt' \; e^{-\mathrm{R}t}\mathrm{K}_{t+t'}e^{-\mathrm{L}t'}\right]^{-1}.$$

Theorem

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Fixed point equations

L and R are unique attractive solutions of

$$L = V + \int_0^\infty dt \; K_t e^{-Lt},$$

$$R = V + \int_0^\infty dt \; e^{-Rt} K_t,$$

$$\|L\|, \|R\| \leq \rho = \frac{k + v - \sqrt{(k-v)^2 - 4M}}{2}.$$

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$$D = \left[1 + \int_0^\infty dt \int_0^\infty dt' \; e^{-Rt} K_{t+t'} e^{-Lt'}\right]^{-1}.$$

Long time approximation

For any vector norm $|\cdot|$ consistent with the matrix norm $\|\cdot\|$ we have

$$y_t = e^{Lt} D = De^{Rt}, \quad |x_t - y_t| \leq \frac{k-\eta}{\eta-\rho} e^{-\eta t} \quad ,$$

$$\eta = \frac{k + v + \sqrt{(k-v)^2 - 4M}}{2}.$$

Fixed point equations

L and R are unique attractive solutions of

$$L = V + \int_0^\infty dt \; K_t e^{-Lt},$$

$$R = V + \int_0^\infty dt \; e^{-Rt} K_t,$$

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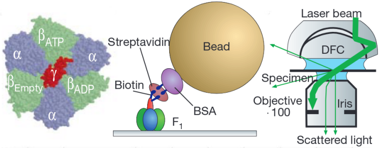
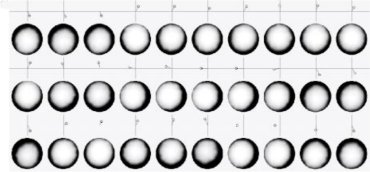
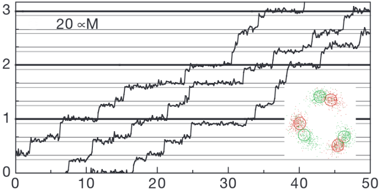
F_1-ATPase

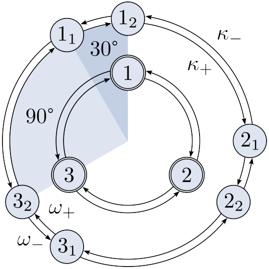






➼ R. Yasuda et al., Nature **410** 898 (2001).

Model



$$x_t = [p_t^1, p_t^2, p_t^3]^T, \qquad \dot{x}_t = Vx_t + \int_0^t dt' \; K_{t'} x_{t-t'}$$

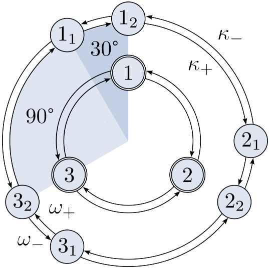
$$V = \sigma_+(S-1) + \sigma_-(S^T - 1)$$

$$K_t = (\zeta_+(S-1) + \zeta_-(S^T - 1))\, e^{-(V+\nu)t}$$

$$S = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \qquad S^T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

Example 1 : Molecular Motor

Model



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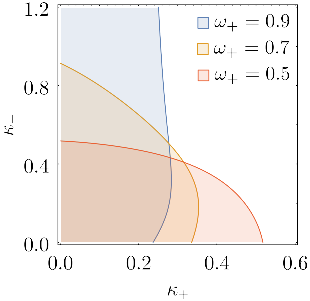
Weak memory conditions



$$\|K_t\|_2 \leq M e^{-kt},$$

$$\|V\|_2 = v < k, \qquad \frac{4M}{(k-v)^2} \leq 1$$

➤ No sharp separation of time scales required.

$[\omega_+ + \omega_- = 1]$

Example 1 : Molecular Motor

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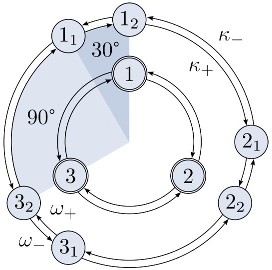

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$$V = \sigma_+(S - 1) + \sigma_-(S^T - 1)$$

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Effective generators

Fixed point equations

$$L = V + \int_0^\infty dt \; K_t e^{-Lt}$$

$$R = V + \int_0^\infty dt \; e^{-Rt} K_t$$

Solution

$$L = R = \lambda_+(S - 1) + \lambda_-(S^T - 1)$$

Slippage matrix

$$D = \left[1 + \int_0^\infty dt \int_0^\infty dt' e^{-Rt} K_{t+t'} e^{-Lt}\right]^{-1}$$

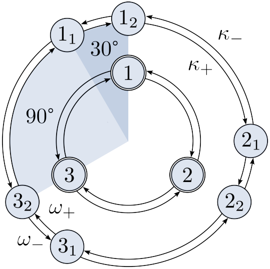
$$= \left[1 + K_0 [L + V + \kappa]^{-2}\right]^{-1}$$

Long time approximation

$$y_t = e^{Lt} D x_0$$

Example 1 : Molecular Motor

Model



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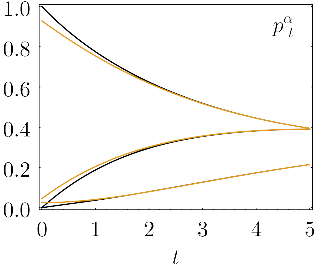
Long time approximation



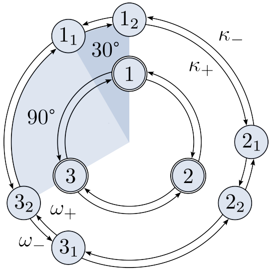
$$y_t = e^{Lt} D x_0$$

$[\omega_+ = 0.8, \ \omega_- = 0.2, \ \kappa_+ = 0.3, \ \kappa_- = 0.2]$

$[v/k \simeq 0.42, \ 4M/(k - v)^2 \simeq 0.89]$

Example 1 : Molecular Motor

Model



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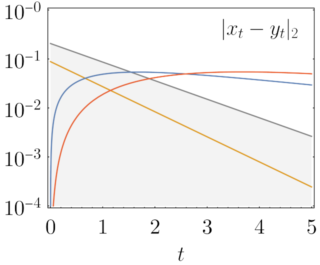

$$|x_t - y_t|_2 \le \frac{k-\eta}{\eta-\rho} e^{-\eta t}$$

$$|x_t - y_t^M|_2, \quad y_t^M = e^{L^1 t} x_0$$

$$L^1 = V + \int_0^\infty dt \; K_t e^{-Vt}$$

$$|x_t - y_t^0|_2, \quad y_t^0 = e^{Vt} x_0$$

Questions

1. When and in what sense does a local approximation exist?
2. Can its error be bounded?
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4. Is it unique?

Perturbation Theory

Setting

$$\dot{x}_t = V x_t + \int_0^t dt' \; K_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|K_t\| \leq M e^{-kt}, \qquad \|V\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = e^{Lt} A_t x_0$$

Memory function

$$\dot{x}_t = L x_t + E_t x_0 , \qquad E_t = e^{Lt} \dot{A}_t$$

$$\dot{E}_t = K_t + E_t V + \int_0^t dt' \; E_{t'} K_{t-t'} , \qquad E_0 = V - L$$

Rescaling

$$s = kt, \quad \bar{E}_s = E_{s/k}/k, \quad \bar{V} = V/k, \quad \bar{K}_s = K_{s/k}/M$$

$$\|\bar{K}_s\| \leq e^{-s}$$

$$\frac{d}{ds} \bar{E}_s = \varphi \bar{K}_s + \bar{E}_s \bar{V} + \varphi \int_0^s ds' \; \bar{E}_{s'} \bar{K}_{s-s'} , \qquad \varphi = \frac{M}{k^2}$$

Perturbation Theory

Setting

$$\dot{x}_t = Vx_t + \int_0^t dt' \; K_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|K_t\| \leq Me^{-kt}, \qquad \|V\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = e^{Lt} A_t x_0$$

Memory function

$$\dot{x}_t = Lx_t + E_t x_0, \qquad E_t = e^{Lt}\dot{A}_t$$

$$\dot{E}_t = K_t + E_t V + \int_0^t dt' \; E_{t'} K_{t-t'}, \qquad E_0 = V - L$$

Rescaling

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$$\|\bar{K}_s\| \leq e^{-s}$$

$$\frac{d}{ds}\bar{E}_s = \varphi \bar{K}_s + \bar{E}_s \bar{V} + \varphi \int_0^s ds' \; \bar{E}_{s'} \bar{K}_{s-s'}, \qquad \varphi = \frac{M}{k^2}$$

Perturbation theory

Ansatz

$$\bar{E}_s = \sum_{n=1}^{\infty} \varphi^n \bar{E}_s^{(n)}, \qquad \lim_{s\to\infty} \bar{E}_s^{(n)} e^{-\bar{V}s} = 0$$

Recursion relations

$$E_t^{(n)} = -\int_t^{\infty} dt' \int_0^{t'} dt'' \; E_{t''}^{(n-1)} K_{t'-t''} e^{V(t-t')}$$

$$E_t^{(1)} = -\int_t^{\infty} dt' \; K_{t'} e^{V(t-t')}$$

Approximations

$$E_t^n = \sum_{m=1}^{n} E_t^{(m)}, \qquad L^n = V - \sum_{m=1}^{n} E_0^{(m)}$$

$$A_t^n = 1 + \int_0^t dt' \; e^{-L^n t'} E_{t'}^n$$

$$x_t^n = e^{L^n t} A_t^n x_0$$

Perturbation Theory

Setting

$$\dot{x}_t = \mathrm{V}x_t + \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|\mathrm{K}_t\| \leq Me^{-kt}, \qquad \|V\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = e^{\mathrm{L}t}\mathrm{A}_t x_0$$

$$\dot{x}_t = \mathrm{L}x_t + \mathrm{E}_t x_0, \qquad \mathrm{E}_t = e^{\mathrm{L}t}\dot{\mathrm{A}}_t$$

Perturbation theory

$$\mathrm{E}_t^n = \sum_{m=1}^n \mathrm{E}_t^{(m)}, \qquad \mathrm{L}^n = \mathrm{V} - \sum_{m=1}^n \mathrm{E}_0^{(m)}$$

$$\mathrm{E}_t^{(n)} = -\int_t^\infty dt' \int_0^{t'} dt'' \; \mathrm{E}_{t''}^{(n-1)} \mathrm{K}_{t'-t''} e^{\mathrm{V}(t-t')}$$

$$\mathrm{E}_t^{(1)} = -\int_t^\infty dt' \; \mathrm{K}_{t'} e^{\mathrm{V}(t-t')}$$

$$\mathrm{A}_t^n = 1 + \int_0^t dt' \; e^{-\mathrm{L}^n t'} \mathrm{E}_{t'}^n$$

$$x_t^n = e^{\mathrm{L}^n t}\mathrm{A}_t^n x_0 \qquad \varphi = \frac{M}{k^2}$$

Convergence

$$\|\mathrm{E}_t - \mathrm{E}_t^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\frac{M}{k-v}e^{-\mu t}$$

$$\|\mathrm{L} - \mathrm{L}^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\frac{M}{k-v}$$

$$\|\mathrm{A}_t - \mathrm{A}_t^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\alpha$$

$$|x_t - x_t^n| \leq \frac{\varepsilon^n}{1-\varepsilon}(\alpha + \beta t)|x_0|e^{\rho t}$$

$$\varepsilon = \frac{4M}{(k-v)^2} < 1 \qquad \mu = \frac{k+v}{2}$$

$$\alpha = \frac{(1+3\sqrt{1-\varepsilon})\varepsilon}{8(1-\varepsilon)}$$

$$\beta = \frac{(1+\sqrt{1-\varepsilon})\varepsilon}{8\sqrt{1-\varepsilon}}(k-v)$$

$$\rho = \frac{k+v-\sqrt{(k-v)^2-4M}}{2}$$

Perturbation Theory

Setting

$$\dot{x}_t = \mathrm{V}x_t + \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|\mathrm{K}_t\| \leq Me^{-kt}, \qquad \|V\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = e^{\mathrm{L}t}\mathrm{A}_t x_0$$

$$\dot{x}_t = \mathrm{L}x_t + \mathrm{E}_t x_0, \qquad \mathrm{E}_t = e^{\mathrm{L}t}\dot{\mathrm{A}}_t$$

Perturbation theory

$$\mathrm{E}_t^n = \sum_{m=1}^n \mathrm{E}_t^{(m)}, \qquad \mathrm{L}^n = \mathrm{V} - \sum_{m=1}^n \mathrm{E}_0^{(m)}$$

$$\mathrm{E}_t^{(n)} = -\int_t^\infty dt' \int_0^{t'} dt'' \; \mathrm{E}_{t''}^{(n-1)} \mathrm{K}_{t'-t''} e^{\mathrm{V}(t-t')}$$

$$\mathrm{E}_t^{(1)} = -\int_t^\infty dt' \; \mathrm{K}_{t'} e^{\mathrm{V}(t-t')}$$

$$\mathrm{A}_t^n = 1 + \int_0^t dt' \; e^{-\mathrm{L}^n t'} \mathrm{E}_{t'}^n$$

$$x_t^n = e^{\mathrm{L}^n t}\mathrm{A}_t^n x_0 \qquad \varphi = \frac{M}{k^2}$$

Convergence

$$\|\mathrm{E}_t - \mathrm{E}_t^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\frac{M}{k-v}e^{-\mu t}$$

$$\|\mathrm{L} - \mathrm{L}^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\frac{M}{k-v}$$

$$\|\mathrm{A}_t - \mathrm{A}_t^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\alpha$$

$$|x_t - x_t^n| \leq \frac{\varepsilon^n}{1-\varepsilon}(\alpha + \beta t)|x_0|e^{\rho t}$$

$$\mathrm{L}^0 = \mathrm{V}$$

$$\mathrm{L}^1 = \mathrm{V} + \int_0^\infty dt \; \mathrm{K}_t e^{-\mathrm{V}t}$$

- Adiabatic and Markov generators recovered in zeroth and first order.

Perturbation Theory

Setting

$$\dot{x}_t = \mathrm{V}x_t + \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|\mathrm{K}_t\| \leq Me^{-kt}, \qquad \|V\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = e^{\mathrm{L}t}\mathrm{A}_t x_0$$

$$\dot{x}_t = \mathrm{L}x_t + \mathrm{E}_t x_0, \qquad \mathrm{E}_t = e^{\mathrm{L}t}\dot{\mathrm{A}}_t$$

Perturbation theory

$$\mathrm{E}_t^n = \sum_{m=1}^n \mathrm{E}_t^{(m)}, \qquad \mathrm{L}^n = \mathrm{V} - \sum_{m=1}^n \mathrm{E}_0^{(m)}$$

$$\mathrm{E}_t^{(n)} = -\int_t^\infty dt' \int_0^{t'} dt'' \; \mathrm{E}_{t''}^{(n-1)} \mathrm{K}_{t'-t''} e^{\mathrm{V}(t-t')}$$

$$\mathrm{E}_t^{(1)} = -\int_t^\infty dt' \; \mathrm{K}_{t'} e^{\mathrm{V}(t-t')}$$

$$\mathrm{A}_t^n = 1 + \int_0^t dt' \; e^{-\mathrm{L}^n t'} \mathrm{E}_{t'}^n$$

$$x_t^n = e^{\mathrm{L}^n t}\mathrm{A}_t^n x_0 \qquad \varphi = \frac{M}{k^2}$$

Convergence

$$\|\mathrm{E}_t - \mathrm{E}_t^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\frac{M}{k-v}e^{-\mu t}$$

$$\|\mathrm{L} - \mathrm{L}^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\frac{M}{k-v}$$

$$\|\mathrm{A}_t - \mathrm{A}_t^n\| \leq \frac{\varepsilon^n}{1-\varepsilon}\alpha$$

$$|x_t - x_t^n| \leq \frac{\varepsilon^n}{1-\varepsilon}(\alpha + \beta t)|x_0|e^{\rho t}$$

Further bounds

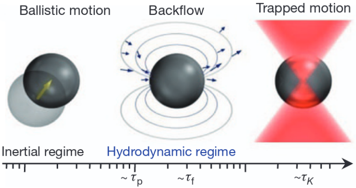
MF: $\|\mathrm{E}_t\|, \|\mathrm{E}_t^n\| \leq (k-\eta)e^{-\eta t}$

LTA: $y_t^n = e^{\mathrm{L}^n t}\mathrm{A}_\infty^n x_0$

$$|x_t^n - y_t^n| \leq \frac{k-\eta}{\eta-\rho}|x_0|e^{-\eta t}$$

Example 2 : Generalized Langevin Equations

Non-Markovian Brownian motion



➻ T. Franosch et al., Nature **478** 85 (2011).

Model

$$\dot{x}_t = V x_t + \int_0^t dt' \; K_{t'} x_{t-t'} + f_t$$

$$x_t = [x_t, v_t]^T, \qquad \langle x_0^2 \rangle_{eq} = \langle v_0^2 \rangle_{eq} = 1$$

$$V = \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix}, \quad K_t = \begin{bmatrix} 0 & 0 \\ 0 & -\Gamma_t \end{bmatrix}, \quad f_t = \begin{bmatrix} 0 \\ \xi_t \end{bmatrix}$$

x_t . . . particle position

v_t . . . particle velocity

ω . . . trap frequency

Γ_t . . . friction kernel

ξ_t . . . stochastic force

$$\Gamma_t = M e^{-kt}, \qquad M > 0, \; k = 1$$

Example 2 : Generalized Langevin Equations

Model

$$\dot{x}_t = \mathsf{V} x_t + \int_0^t dt' \; \mathsf{K}_{t'} x_{t-t'} + f_t$$

$$x_t = [\mathrm{x}_t, \mathrm{v}_t]^{\mathsf{T}}, \qquad \langle \mathrm{x}_0^2 \rangle_{eq} = \langle \mathrm{v}_0^2 \rangle_{eq} = 1$$

$$\mathsf{V} = \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix}, \quad \mathsf{K}_t = \begin{bmatrix} 0 & 0 \\ 0 & -\Gamma_t \end{bmatrix}, \quad f_t = \begin{bmatrix} 0 \\ \xi_t \end{bmatrix}$$

- x_t . . . particle position
- v_t . . . particle velocity
- ω . . . trap frequency
- Γ_t . . . friction kernel
- ξ_t . . . stochastic force

$$\Gamma_t = M e^{-kt}, \qquad M > 0, \; k = 1$$

Weak memory conditions

$$v = \|\mathsf{V}\|_\infty = \omega < 1, \qquad \frac{4M}{(\omega - 1)^2} < 1$$

Equilibrium correlation matrix

$$\mathsf{Z}_t = \langle x_t x_0^{\mathsf{T}} \rangle_{eq} [\langle x_0 x_0^{\mathsf{T}} \rangle_{eq}]^{-1}$$

$$\dot{\mathsf{Z}}_t = \mathsf{V}\mathsf{Z}_t + \int_0^t dt' \; \mathsf{K}_{t'} \mathsf{Z}_{t-t'}, \qquad \mathsf{Z}_0 = 1$$

$$\mathsf{Z}_t = e^{\mathsf{L}t} \mathsf{A}_t = e^{\mathsf{L}t} + \int_0^t dt' \; e^{\mathsf{L}(t-t')} \mathsf{E}_{t'}$$

General solution

$$x_t = \mathsf{Z}_t x_0 + \int_0^t dt' \; \mathsf{Z}_{t'} f_{t-t'}$$

Model

$$\dot{x}_t = \mathrm{V}x_t + \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'} + f_t$$

$$x_t = [\mathrm{x}_t, \mathrm{v}_t]^\mathrm{T}, \qquad \langle \mathrm{x}_0^2 \rangle_{eq} = \langle \mathrm{v}_0^2 \rangle_{eq} = 1$$

$$\mathrm{V} = \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix}, \quad \mathrm{K}_t = \begin{bmatrix} 0 & 0 \\ 0 & -\Gamma_t \end{bmatrix}, \quad f_t = \begin{bmatrix} 0 \\ \xi_t \end{bmatrix}$$

$$\Gamma_t = Me^{-kt}, \qquad M > 0, \; k = 1$$

Weak memory conditions

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Equilibrium correlation matrix

$$\mathrm{Z}_t = \langle x_t x_0^\mathrm{T} \rangle_{eq} [\langle x_0 x_0^\mathrm{T} \rangle_{eq}]^{-1}$$

$$\mathrm{Z}_t = e^{\mathrm{L}t}\mathrm{A}_t = e^{\mathrm{L}t} + \int_0^t dt' \; e^{\mathrm{L}(t-t')}\mathrm{E}_{t'}$$

Perturbation theory

$$\mathrm{E}_t^1 = \mathrm{H}_{11} e^{-t}, \qquad \mathrm{L}^1 = \mathrm{V} - \mathrm{H}_{11}$$

$$\mathrm{E}_t^2 = \left(\mathrm{H}_{21} + \mathrm{H}_{22} t\right) e^{-t}, \qquad \mathrm{L}^2 = \mathrm{V} - \mathrm{H}_{21}$$

$$\mathrm{H}_{11} = \frac{M}{1+\omega^2} \begin{bmatrix} 0 & 0 \\ \omega & 1 \end{bmatrix}$$

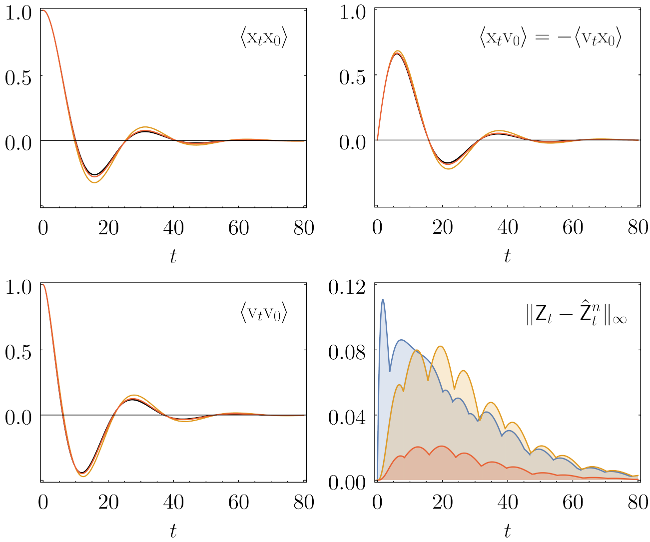
$$\mathrm{H}_{21} = \mathrm{H}_{11} + \frac{M^2}{(1+\omega^2)^3} \begin{bmatrix} 0 & 0 \\ 2\omega & 1-\omega^2 \end{bmatrix}$$

$$\mathrm{H}_{22} = \frac{M}{1+\omega^2} \mathrm{H}_{11}$$

$$\mathrm{Z}_t^M = e^{\mathrm{L}^1 t}$$

$$\mathrm{Z}_t^n = e^{\mathrm{L}^n t}\mathrm{A}_t^n = e^{\mathrm{L}^n t} + \int_0^t dt' \; e^{\mathrm{L}^n (t-t')}\mathrm{E}_{t'}^n$$

Example 2 : Generalized Langevin Equations



$Z_t^M = e^{L^1 t}$

$Z_t^1 = e^{L^1 t} A_t^1$

$Z_t^2 = e^{L^2 t} A_t^2$

[$\omega = 0.2$, $M = 0.15$, $k = 1$, $4M/(1-\omega^2) \simeq 0.94$]

Questions

1. When and in what sense does a local approximation exist?
2. Can its error be bounded?
3. How to construct it systematically?
4. Is it unique?

Uniqueness

Setting

$$\dot{x}_t = Vx_t + \int_0^t dt'\ K_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|K_t\| \leq Me^{-kt}, \qquad \|V\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = Z_t x_0$$

Two-sided factorization

$$\lim_{t\to\infty} e^{-Lt} Z_t = \lim_{t\to\infty} Z_t e^{-Rt} \stackrel{!}{=} D, \qquad \det[D] \stackrel{!}{\neq} 0$$

$\Rightarrow$ L, R uniquely determined.

One-sided factorization

$$\lim_{t\to\infty} e^{-L't} Z_t \stackrel{!}{=} D', \qquad \det[D'] \stackrel{!}{\neq} 0$$

$$\Rightarrow L' = SLS^{-1}, \quad D' = SD$$

$$\lim_{t\to\infty} e^{Lt} S^{-1} e^{-Lt} = 1, \qquad \det[S] \neq 0$$

Uniqueness

Setting

$$\dot{x}_t = \mathsf{V}x_t + \int_0^t dt' \; \mathsf{K}_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|\mathsf{K}_t\| \leq Me^{-kt}, \qquad \|\mathsf{V}\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = \mathsf{Z}_t x_0$$

Two-sided factorization

$$\lim_{t\to\infty} e^{-\mathsf{L}t}\mathsf{Z}_t = \lim_{t\to\infty} \mathsf{Z}_t e^{-\mathsf{R}t} \stackrel{!}{=} \mathsf{D}, \qquad \det[\mathsf{D}] \stackrel{!}{\neq} 0$$

$\Rightarrow$ L, R uniquely determined.

One-sided factorization

$$\lim_{t\to\infty} e^{-\mathsf{L}'t}\mathsf{Z}_t \stackrel{!}{=} \mathsf{D}', \qquad \det[\mathsf{D}'] \stackrel{!}{\neq} 0$$

$$\Rightarrow \mathsf{L}' = \mathsf{SLS}^{-1}, \qquad \mathsf{D}' = \mathsf{SD}$$

$$\lim_{t\to\infty} e^{\mathsf{L}t}\mathsf{S}^{-1}e^{-\mathsf{L}t} = 1, \qquad \det[\mathsf{S}] \neq 0$$

Fixed point equations

$$\mathsf{L} \stackrel{!}{=} \mathsf{V} + \int_0^\infty dt \; \mathsf{K}_t e^{-\mathsf{L}t}, \qquad \|\mathsf{L}\| \stackrel{!}{\leq} \rho$$

$$\mathsf{R} \stackrel{!}{=} \mathsf{V} + \int_0^\infty dt \; e^{-\mathsf{R}t}\mathsf{K}_t, \qquad \|\mathsf{R}\| \stackrel{!}{\leq} \rho$$

$\Rightarrow$ L, R uniquely determined.

Memory functions

$$\dot{\mathsf{Z}}_t = \mathsf{L}\mathsf{Z}_t + \mathsf{E}_t = \mathsf{Z}_t\mathsf{R} + \mathsf{F}_t$$

$$\|\mathsf{E}_t\|, \|\mathsf{F}_t\| \stackrel{!}{\leq} (k-\eta)e^{-\eta t}$$

$\Rightarrow$ L, R uniquely determined.

For any $\mathsf{L}' \neq \mathsf{L}$, $\mathsf{R}' \neq \mathsf{R}$ and $\sigma > \rho$:

$$\dot{\mathsf{Z}}_t = \mathsf{L}'\mathsf{Z}_t + \mathsf{E}'_t = \mathsf{Z}_t\mathsf{R}' + \mathsf{F}'_t$$

$$\lim_{t\to\infty} \|\mathsf{E}'_t\| e^{\sigma t} = \lim_{t\to\infty} \|\mathsf{F}'_t\| e^{\sigma t} = \infty \qquad (\rho < \eta)$$

Uniqueness

Setting

$$\dot{x}_t = \mathsf{V}x_t + \int_0^t dt' \; \mathsf{K}_{t'} x_{t-t'} \qquad (t \geq 0)$$

$$\|\mathsf{K}_t\| \leq Me^{-kt}, \qquad \|\mathsf{V}\| = v < k, \qquad \frac{4M}{(k-v)^2} < 1$$

$$x_t = \mathsf{Z}_t x_0$$

Two-sided factorization

$$\lim_{t\to\infty} e^{-\mathsf{L}t}\mathsf{Z}_t = \lim_{t\to\infty} \mathsf{Z}_t e^{-\mathsf{R}t} \overset{!}{=} \mathsf{D}, \qquad \det[\mathsf{D}] \overset{!}{\neq} 0$$

$\Rightarrow$ L, R uniquely determined.

One-sided factorization

$$\lim_{t\to\infty} e^{-\mathsf{L}'t}\mathsf{Z}_t \overset{!}{=} \mathsf{D}', \qquad \det[\mathsf{D}'] \overset{!}{\neq} 0$$

$$\Rightarrow \mathsf{L}' = \mathsf{S}\mathsf{L}\mathsf{S}^{-1}, \qquad \mathsf{D}' = \mathsf{S}\mathsf{D}$$

$$\lim_{t\to\infty} e^{\mathsf{L}t}\mathsf{S}^{-1}e^{-\mathsf{L}t} = 1, \qquad \det[\mathsf{S}] \neq 0$$

Fixed point equations

$$\mathsf{L} \overset{!}{=} \mathsf{V} + \int_0^\infty dt \; \mathsf{K}_t e^{-\mathsf{L}t}, \qquad \|\mathsf{L}\| \overset{!}{\leq} \rho$$

$$\mathsf{R} \overset{!}{=} \mathsf{V} + \int_0^\infty dt \; e^{-\mathsf{R}t}\mathsf{K}_t, \qquad \|\mathsf{R}\| \overset{!}{\leq} \rho$$

$\Rightarrow$ L, R uniquely determined.

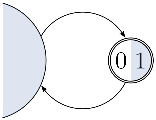
Memory functions

$$\dot{\mathsf{Z}}_t = \mathsf{L}\mathsf{Z}_t + \mathsf{E}_t = \mathsf{Z}_t\mathsf{R} + \mathsf{F}_t$$

$$\|\mathsf{E}_t\|, \|\mathsf{F}_t\| \overset{!}{\leq} (k-\eta)e^{-\eta t}$$

$\Rightarrow$ L, R uniquely determined.

- The proper generators lead to the fastest decaying memory functions.



Waiting time distribution $(\kappa > 4)$

$$\psi_t = \frac{2\gamma\kappa}{\sqrt{\kappa(\kappa-2)}} \sinh\left[\sqrt{\kappa(\kappa-2)}\gamma t\right] e^{-\kappa\gamma t}$$

Master equation

$$\dot{x}_t = \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'}\,, \qquad x_t = [p_t^0, p_t^1]^\mathrm{T}$$

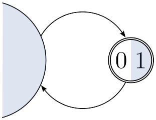
$$\mathrm{K}_t = M e^{-kt}\mathrm{H}_1, \quad M = 4\kappa\gamma^2, \quad k = 2\kappa\gamma$$

$$\mathrm{H}_1 = \frac{1}{2}\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}, \qquad \|\mathrm{H}_1\|_1 = 1$$

$$\rho = \gamma\left(\kappa - \sqrt{\kappa(\kappa-4)}\right)$$

$$\eta = \gamma\left(\kappa + \sqrt{\kappa(\kappa-4)}\right) > \rho$$

Example 3 : Semi-Markov Jump Process



Waiting time distribution $(\kappa > 4)$

$$\psi_t = \frac{2\gamma\kappa}{\sqrt{\kappa(\kappa-2)}} \sinh\left[\sqrt{\kappa(\kappa-2)}\gamma t\right] e^{-\kappa\gamma t}$$

Master equation

$$\dot{x}_t = \int_0^t dt' \; K_{t'} x_{t-t'}, \qquad x_t = [p_t^0, p_t^1]^T$$

$$K_t = M e^{-kt} H_1, \quad M = 4\kappa\gamma^2, \quad k = 2\kappa\gamma$$

$$H_1 = \frac{1}{2}\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}, \qquad \|H_1\|_1 = 1$$

$$\rho = \gamma\left(\kappa - \sqrt{\kappa(\kappa-4)}\right)$$

$$\eta = \gamma\left(\kappa + \sqrt{\kappa(\kappa-4)}\right) > \rho$$

Modified generator

$$L = \rho H_1$$

$$\lim_{t\to\infty} e^{Lt} S^{-1} e^{Lt} = 1 \quad \Rightarrow \quad S = S_\alpha = 1 + \alpha H_2$$

$$H_1 = \frac{1}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}, \qquad \alpha \in \mathbb{C}$$

$$L_\alpha = S_\alpha L S_\alpha^{-1} = \rho H_1 - \alpha\rho H_2$$

Modified memory function

$$E_{\alpha,t} = -\rho e^{-\eta t} H_1 + \frac{\alpha\rho}{\eta-\rho}\left(\eta e^{-\rho t} - \rho e^{-\eta t}\right) H_2$$

For $\alpha = 0$:

$$\|E_t\| = \rho e^{-\eta t} = (k-\eta) e^{-\eta t}$$

For $\alpha \neq 0$:

$$\|E_{\alpha,t}\| = \rho e^{-\eta t} + \frac{\alpha\rho}{\eta-\rho}\left(\eta e^{-\rho t} - \rho e^{-\eta t}\right)$$

Questions

1. When and in what sense does a local approximation exist?
2. Can its error be bounded?
3. How to construct it systematically?
4. Is it unique?

Earlier Results

Time Convolutionless Method

TCL approach

$$\dot{x}_t = \mathrm{V} x_t + \int_0^t dt' \; \mathrm{K}_{t'} x_{t-t'}$$

$$\rightarrow \; \dot{x}_t = \mathrm{L}_t^{TCL} x_t$$

Present approach

$$\rightarrow \; \dot{x}_t = \mathrm{L} + \mathrm{E}_t x_0$$

Under WM conditions:

$$\lim_{t\to\infty} \mathrm{L}_t^{TCL} = \lim_{t\to\infty} \dot{\mathrm{Z}}_t \mathrm{Z}_t^{-1} = \mathrm{L}$$

- M. Tokuyama and H. Mori., Prog. Theor. Phys. **55** 411 (1976).
- F. Shibata and T. Arimitsu, J. Phys. Soc. Jpn. **49** 891 (1980).

Slippage matrix

$$e^{\mathrm{L}^1 t} x_0 \rightarrow e^{\mathrm{L}^1 t} \mathrm{D} x_0$$

- F. Haake and M. Lewenstein, PRA **28** 3606 (1983).
- P. Gaspard and M. Nagaoka, J. Chem. Phys. **111** 5668 (1999).

Fixed point equations

$$\mathrm{L}_t^{TCL} = \mathrm{V}\mathrm{L}_t^{TCL} + \int_0^t dt' \; \mathrm{K}_{t'} \mathcal{T} \exp\left[- \int_0^{t'} dt'' \; \mathrm{L}_{t-t''}^{TCL} \right]$$

If $\mathrm{L}_t^{TCL} \rightarrow \mathrm{L}$ for $t \rightarrow \infty$:

$$\rightarrow \mathrm{L} = \mathrm{V}\mathrm{L} + \int_0^\infty dt \; \mathrm{K}_t e^{-\mathrm{L}t}$$

- K. Nestmann et al., PRX **11** 021041 (2021).
- K. Nestmann, M. R. Wegewijs, PRB **104** 155407 (2021).
- V. Bruch et al., SciPost Phys. **11** 053 (2021).

Memory expansions

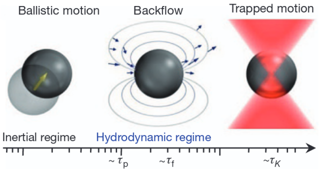
$$\mathrm{L} = \sum_{n=0}^{\infty} \mathrm{L}^{(n)}$$

Assuming convergence:

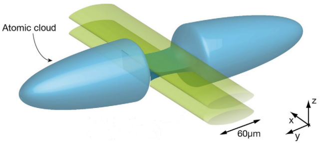
$$\rightarrow \mathrm{L} = \mathrm{V}\mathrm{L} + \int_0^\infty dt \; \mathrm{K}_t e^{-\mathrm{L}t}$$

- L. D. Contreras-Pulido et al., PRB **85** 075301 (2012).
- C. Karlewski and M. Marthaler, PRB **90** 104302 (2014).

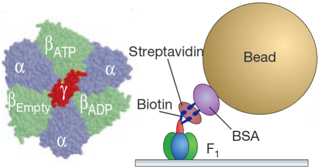
Summary



➸ T. Franosch et al., Nature **478** 85 (2011).



➸ S. Krinner et al., JP CM **29** 343003 (2017).



➸ R. Yasuda et al., Nature **410** 898 (2001).

Key results

$$\dot{x}_t = V x_t + \int_0^t dt' \; K_{t'} x_{t-t'}$$

Weak memory condtions

$$\|K_t\| \leq M e^{-kt}, \quad \|V\| = v < k, \quad \frac{4M}{(k-v)^2} < 1$$

Factorization

$$x_t = e^{Lt} A_t x_0, \quad \lim_{t\to\infty} A_t = D, \quad \det[D] \neq 0$$

Long time approximation

$$y_t = e^{Lt} D x_0, \quad |y_t - x_t| \leq \frac{k-\eta}{\eta-\rho} e^{-\eta t}$$

Quasi local time evolution equation

$$\dot{x}_t = L x_t + E_t x_0, \quad \|E_t\| \leq (k-\eta) e^{-\eta t}$$

Convergent perturabtion scheme

$$\bar{X} = \sum_{n=0}^{\infty} \varphi^n \bar{X}^{(n)}, \quad X = L, E_t \quad \varphi = \frac{M}{k^2} A_t$$