Complete positivity of non-Markovian quantum dynamics

Florian Mintert

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Björn Witt

Łukasz Rudnicki

$$i\frac{\partial|\Psi\rangle}{\partial t} = \mathcal{H}|\Psi\rangle$$

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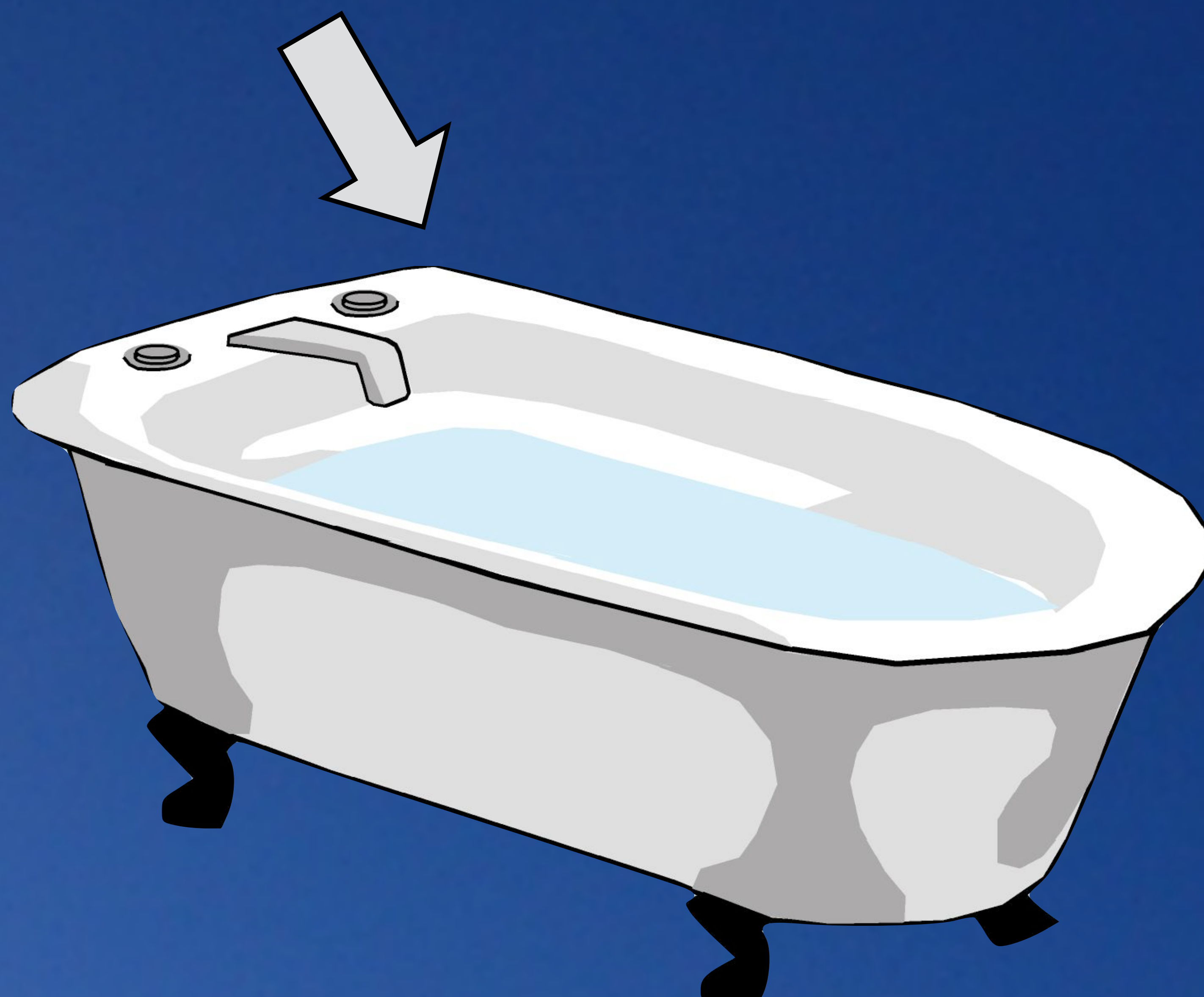
$$|\Psi\rangle$$



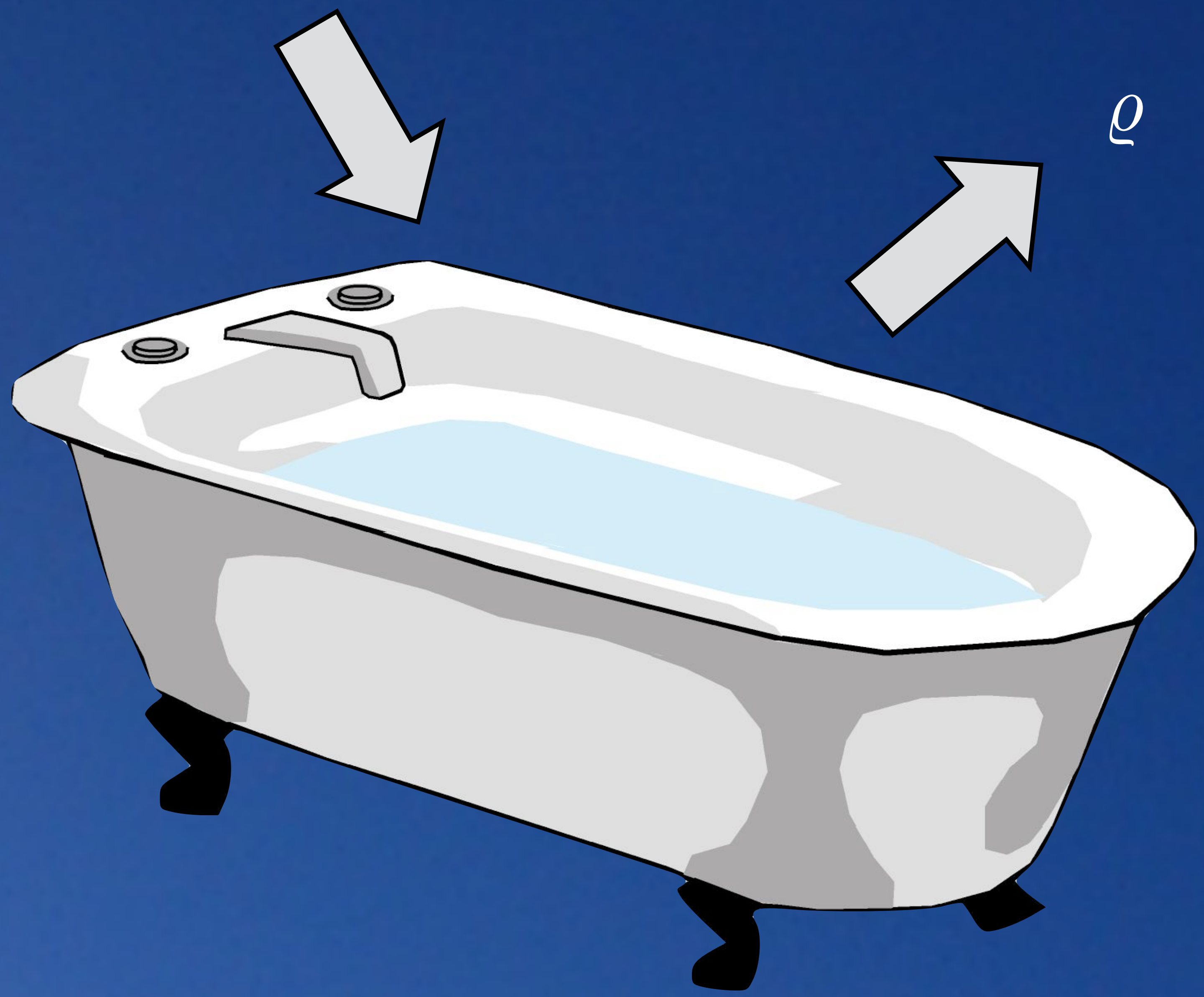
$$i\frac{\partial|\Psi\rangle}{\partial t} = \mathcal{H}|\Psi\rangle$$

$|\Psi\rangle$

ϱ

$\dot{\varrho} = ?$

$\dot{\varrho} = \mathcal{L}\varrho$



Equations of motion

completely positive
if and only if

$$\dot{\varrho} = \mathcal{L}\varrho \quad \Longleftrightarrow \quad \mathcal{L}\varrho = i[\rho, \mathcal{H}] + \sum_{ij} \gamma_{ij} (\sigma_i \varrho \sigma_j^\dagger - \frac{1}{2}\{\varrho, \sigma_j^\dagger \sigma_i\})$$

positive

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positive (γ_{ij})

hierarchical equation of motion (HEOM)

$$\begin{aligned}
\dot{\varrho} &= \mathcal{L}_{00}\varrho + \mathcal{L}_{01}\varrho_1 \\
\dot{\varrho}_1 &= \mathcal{L}_{10}\varrho + \mathcal{L}_{11}\varrho_1 + \mathcal{L}_{12}\varrho_2 \\
\dot{\varrho}_2 &= \mathcal{L}_{20}\varrho + \mathcal{L}_{21}\varrho_2 + \mathcal{L}_{22}\varrho_2 + \mathcal{L}_{23}\varrho_3 \\
&\vdots
\end{aligned}$$

R. Kubo, Adv. Chem. Phys. 15, 101 (1969)

Y. Tanimura, J. Phys. Soc. Jpn. 75, 082001 (2006)

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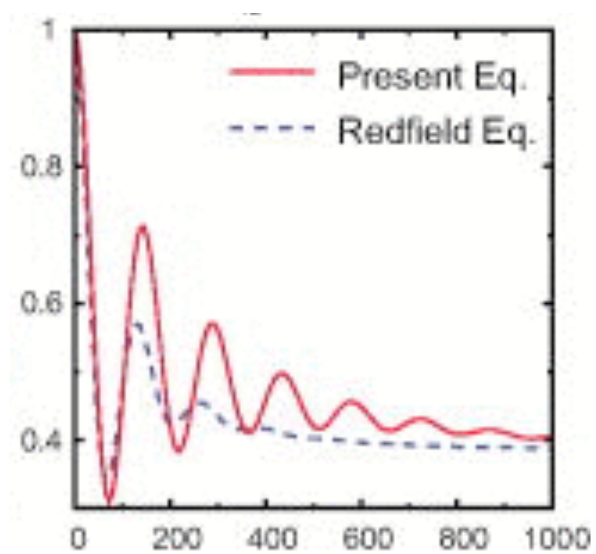
Equations of motion

exciton dynamics



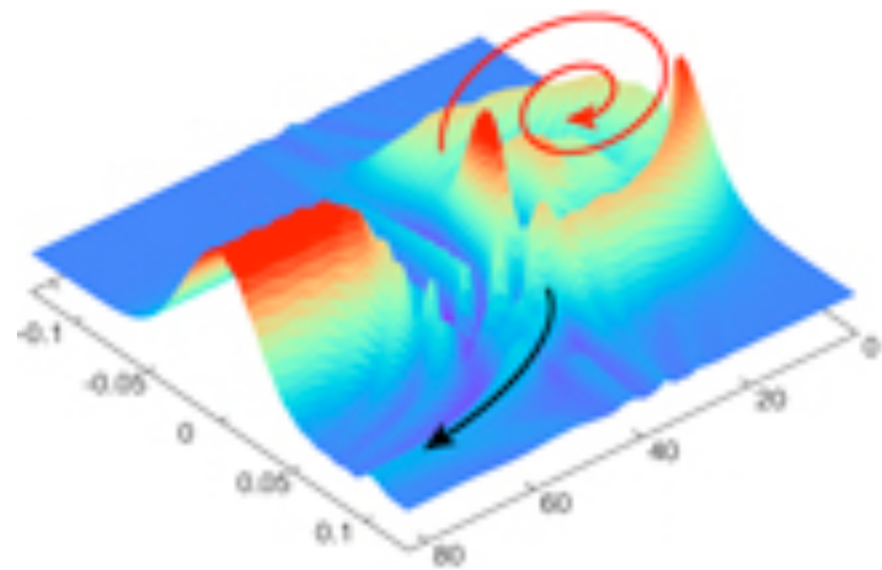
A. Ishizaki & G. Fleming
J. Chem. Phys. 130, 234111 (2009)

itive

f

$$\mathcal{L}\varrho = i[\rho, \mathcal{H}] + \ldots$$

electron currents



A. Sakurai & Y. Tanimura
N.J. Phys. 16, 015002 (2014)

notion (HEOM)

$$+ \quad \mathcal{L}_{01}\varrho_1$$

$$+ \quad \mathcal{L}_{11}\varrho_1 \quad + \quad \mathcal{L}_{12}\varrho_2$$

$$\dot{\varrho}_2 \quad = \quad \mathcal{L}_{20}\varrho \quad + \quad \mathcal{L}_{21}\varrho_2 \quad + \quad \mathcal{L}_{22}\varrho_2 \quad + \quad \mathcal{L}_{23}\varrho_3$$

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Equations of motion

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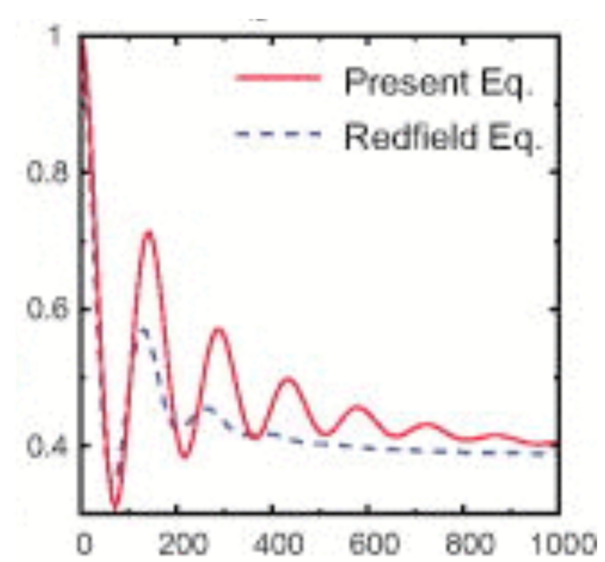

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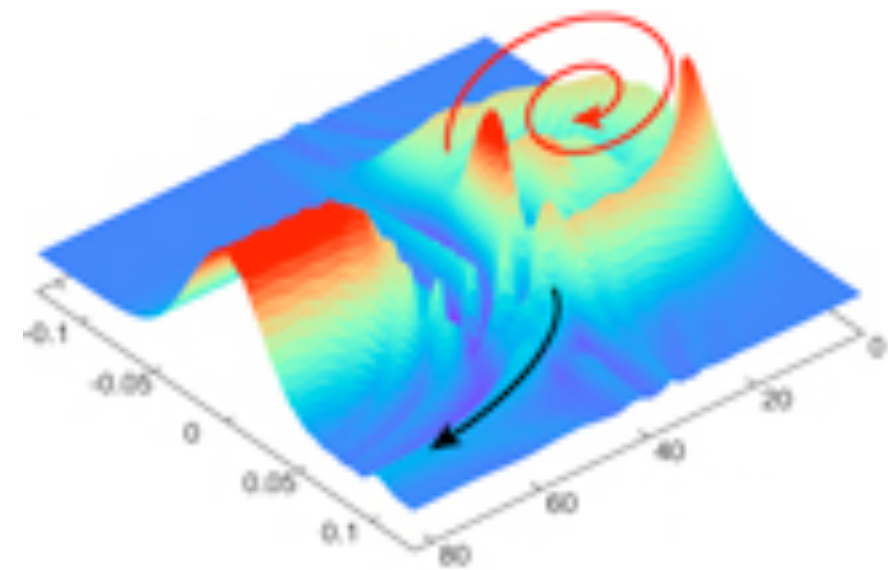
...itive

...f

$$\mathcal{L}\varrho = i[\rho, \mathcal{H}] + \sum ...$$

electron currents



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$$+ \quad \mathcal{L}_{01}\varrho_1$$

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conditions on $\mathcal{L}_{ij}$ for $\Lambda_t(\varrho(0)) = \varrho(t)$ to be CP ?!

Channels instead of states

$$
\begin{aligned}
\varrho(t) &= \Lambda(t)\varrho(0) \\
\varrho_1(t) &= \Lambda_1(t)\varrho(0) \\
\varrho_2(t) &= \Lambda_2(t)\varrho(0) \\
&\vdots
\end{aligned}
$$

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initial conditions $\Lambda(0) = \mathbf{1}$

$$\Lambda_k(0) = \mathbf{0}$$

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dynamical map $\Lambda(t)$

extended dynamical map $\vec{\Lambda} = \begin{bmatrix} \Lambda \\ \vdots \\ \Lambda_k \\ \vdots \end{bmatrix}$

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equation of motion $\dot{\vec{\Lambda}} = L\vec{\Lambda}$

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Does $\Lambda\varrho = \sum_{ij} \eta_{ij}\ \sigma_i \varrho \sigma_j^\dagger$ satisfy $\eta \geq 0$?

Channels instead of states

$$\begin{aligned} \varrho(t) &= \Lambda(t)\varrho(0) \\ \varrho_1(t) &= \Lambda_1(t)\varrho(0) \\ \varrho_2(t) &= \Lambda_2(t)\varrho(0) \\ &\vdots \end{aligned}$$

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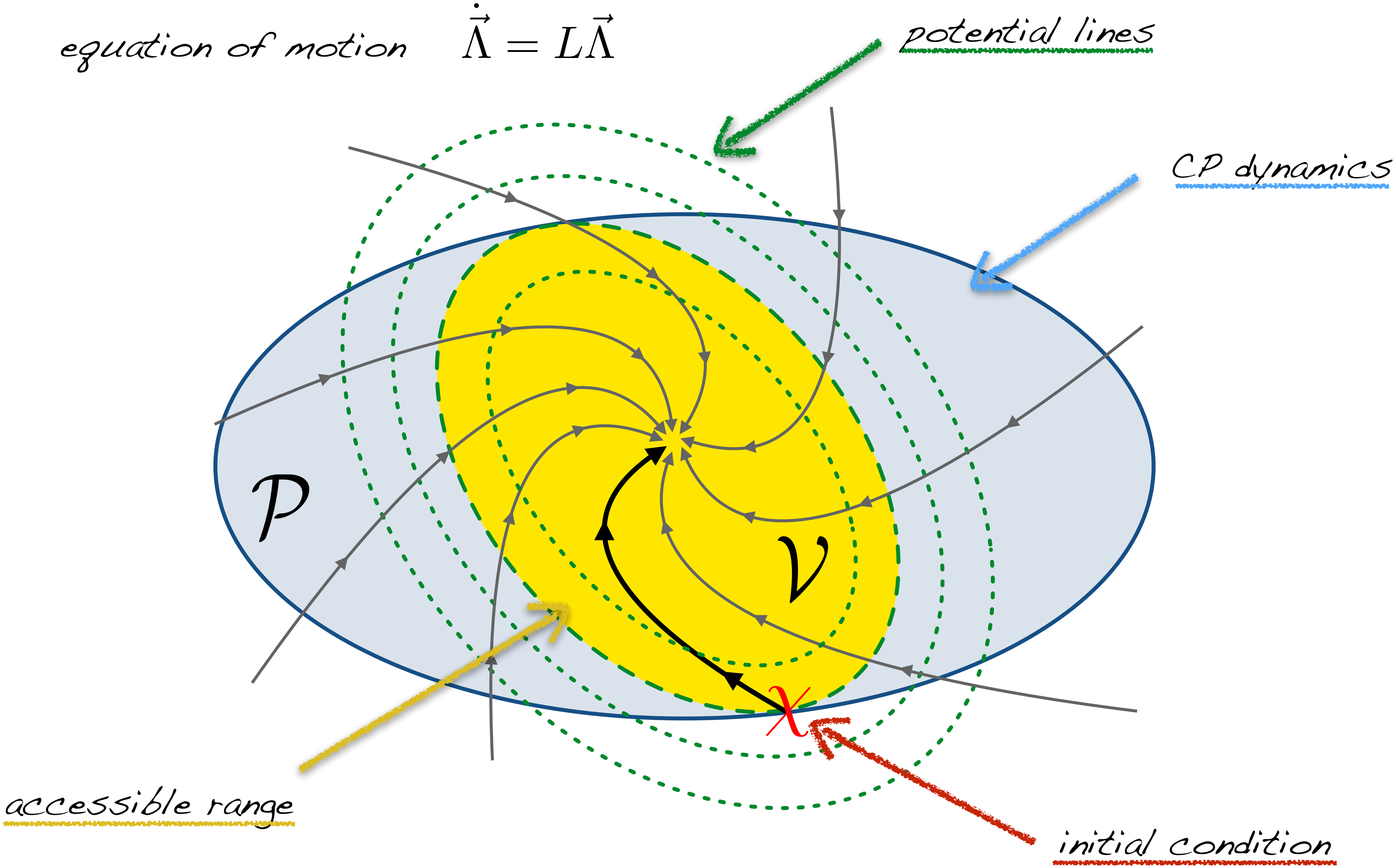
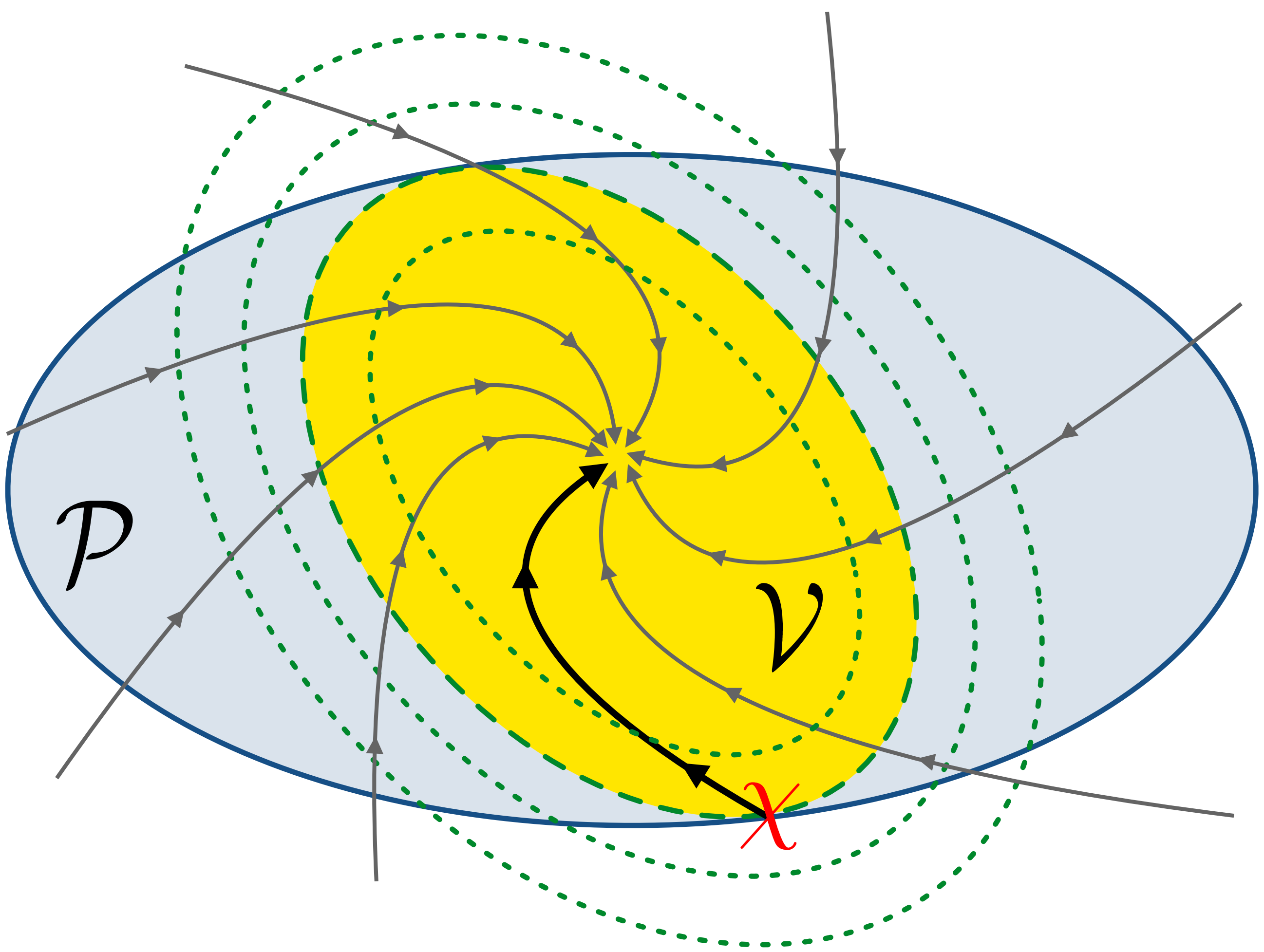
Does $\Lambda\varrho = \sum_{ij} \eta_{ij}\, \sigma_i \varrho \sigma_j^\dagger$ satisfy $\eta \geq 0$?

monitor $\det \eta(t)$!

Underlying geometry



Monotone function



find monotone

$$\vec{\Lambda}(t) R \vec{\Lambda}(t) < \vec{\Lambda}(0) R \vec{\Lambda}(0)$$

monotonic decay

$$\frac{\partial}{\partial t} \vec{\Lambda} R \vec{\Lambda} = \vec{\Lambda}(L^T R + RL) \vec{\Lambda} < 0$$

require that

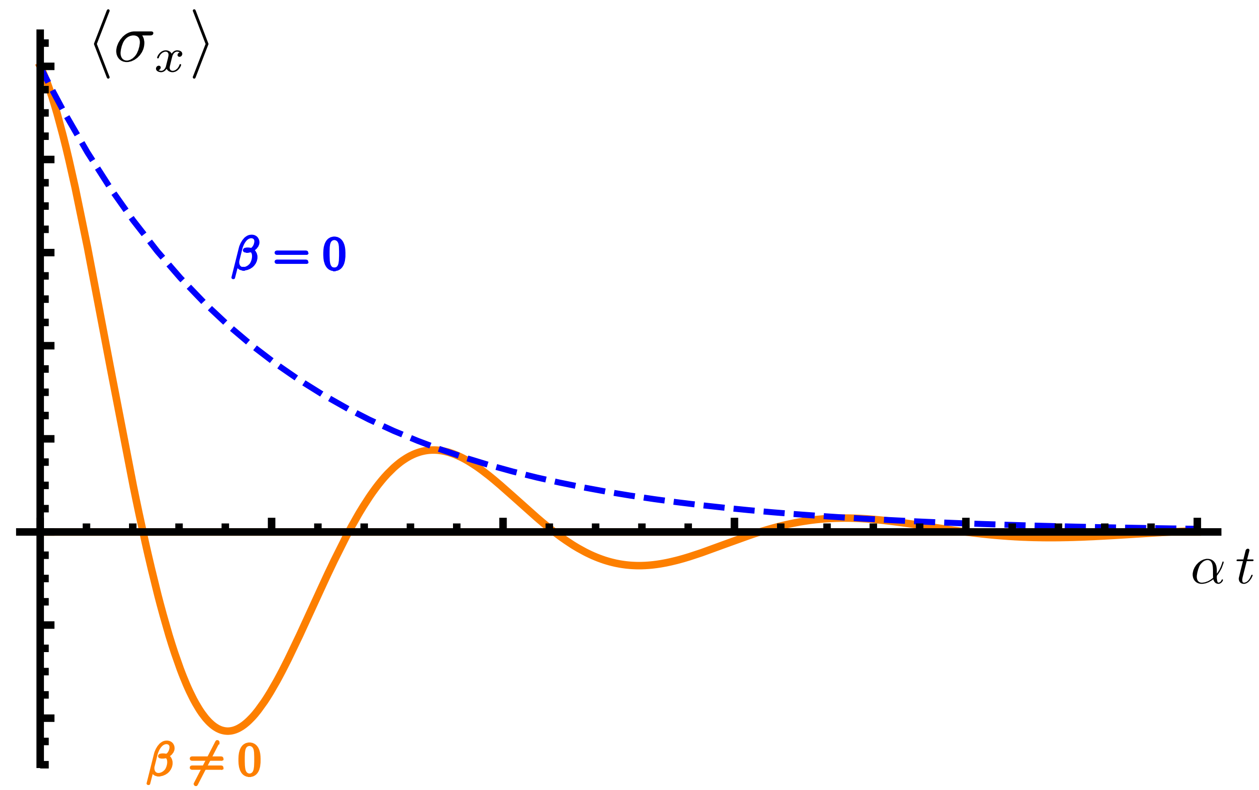
$$Q = L^T R + RL \leq 0$$

A simple example

$$\dot{\varrho} = \frac{\alpha}{2}\mathcal{D}\varrho + \varrho_1$$

$$\dot{\varrho}_1 = \beta\mathcal{D}\varrho + \alpha\sigma_z\varrho_1\sigma_z$$

$$\mathcal{D}\varrho = \sigma_z\varrho\sigma_z - \sigma_z$$



dynamical map

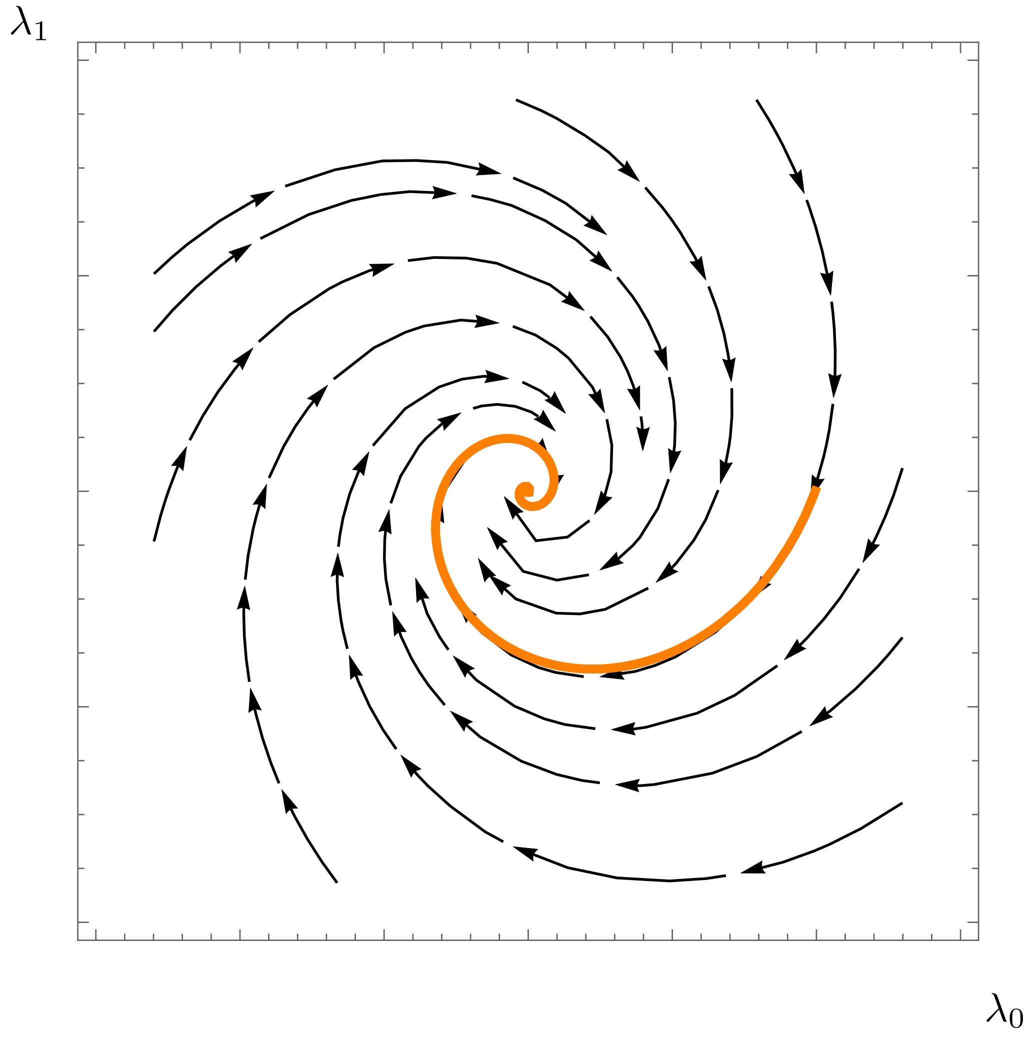
$$\Lambda(\varrho) = (1 - \lambda_0(t))\varrho + (1 + \lambda_0(t))\sigma_z\varrho\sigma_z$$

$$\Lambda_1(\varrho) = (1 - \lambda_1(t))\varrho + (1 + \lambda_1(t))\sigma_z\varrho\sigma_z$$

equation of motion

$$\begin{bmatrix} \dot{\lambda}_0 \\ \dot{\lambda}_1 \end{bmatrix} = \begin{bmatrix} -\alpha & 0 \\ -2\beta & -\alpha \end{bmatrix} \begin{bmatrix} \lambda_0 \\ \lambda_1 \end{bmatrix}$$

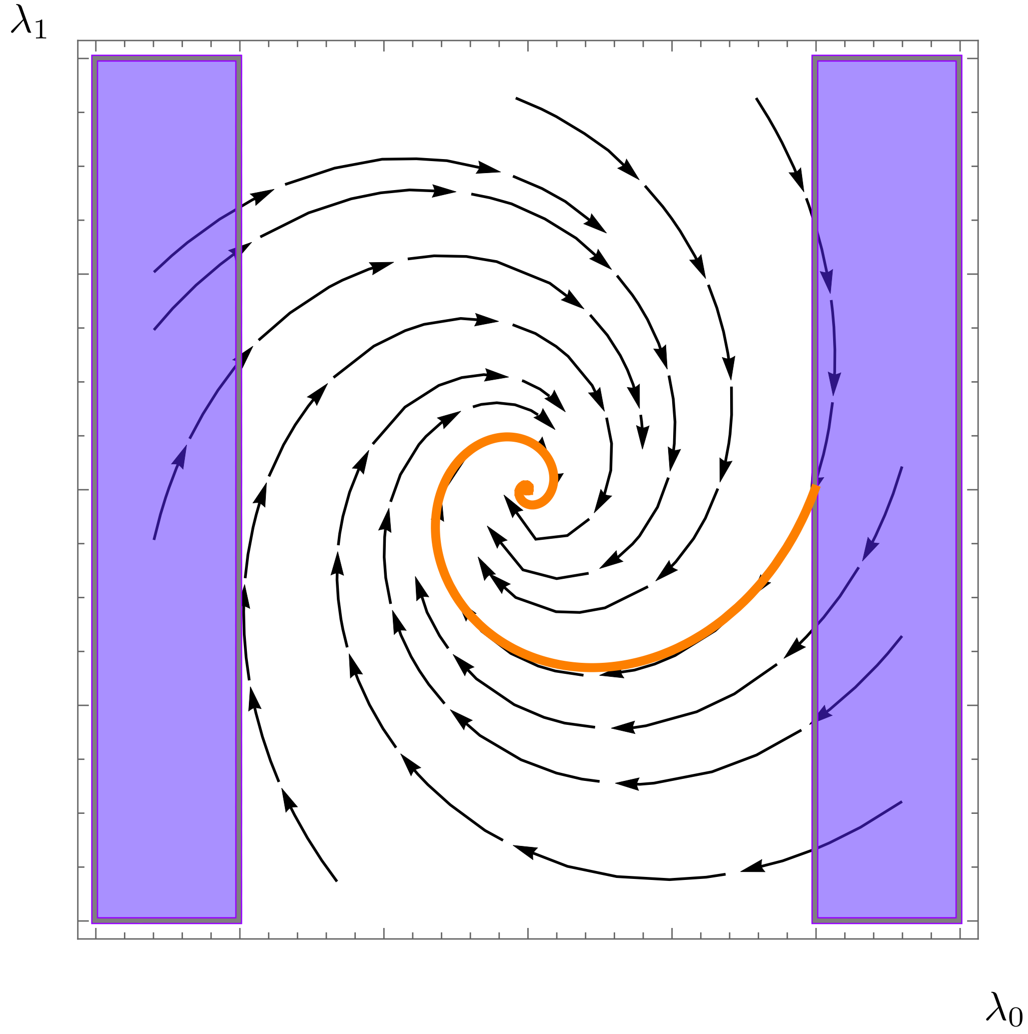
A simple example



A simple example

CP violation

$$P = 1 - \lambda_0^2 \leq 0$$



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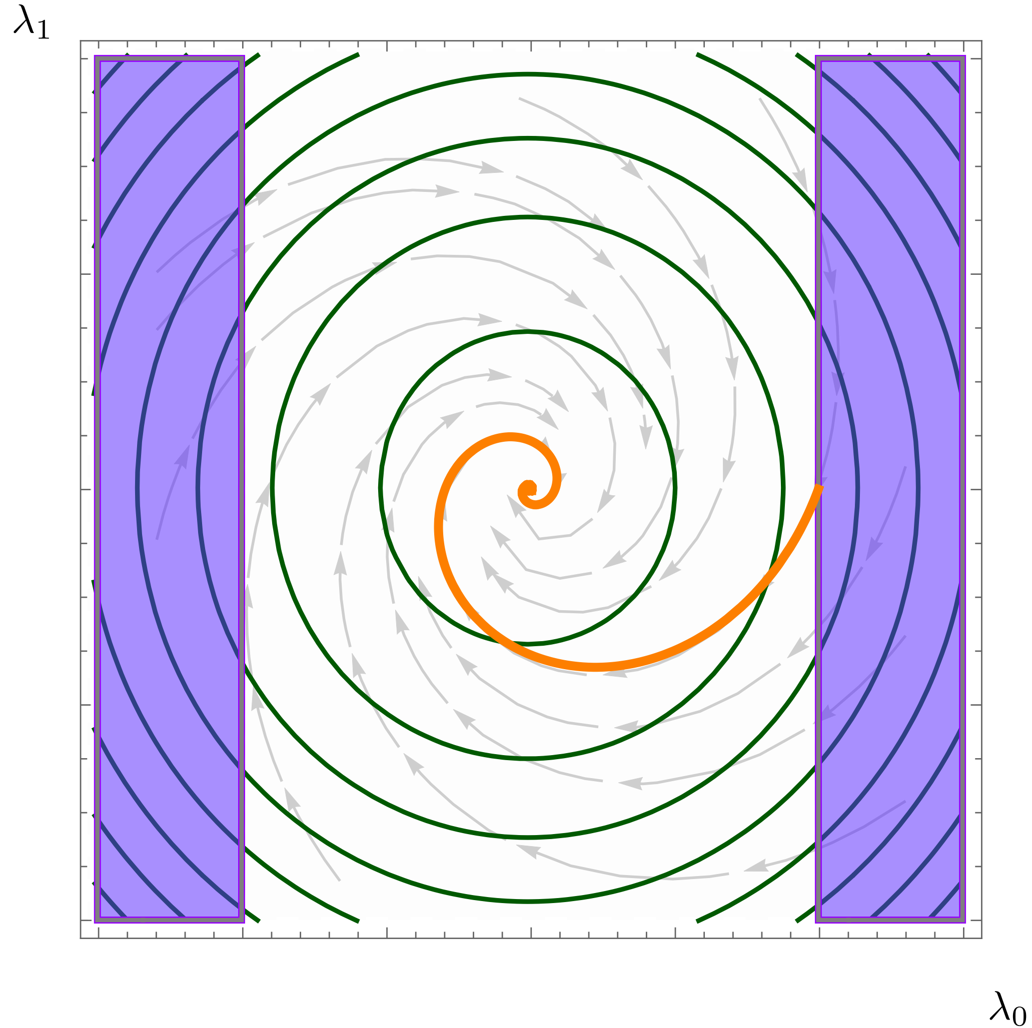

metric

$$R = R^T \geq 0$$

$$Q = L^T R + RL \leq 0$$

$$R = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{\beta} \end{bmatrix}$$

$$Q = -2\alpha R$$

A simple example

CP violation

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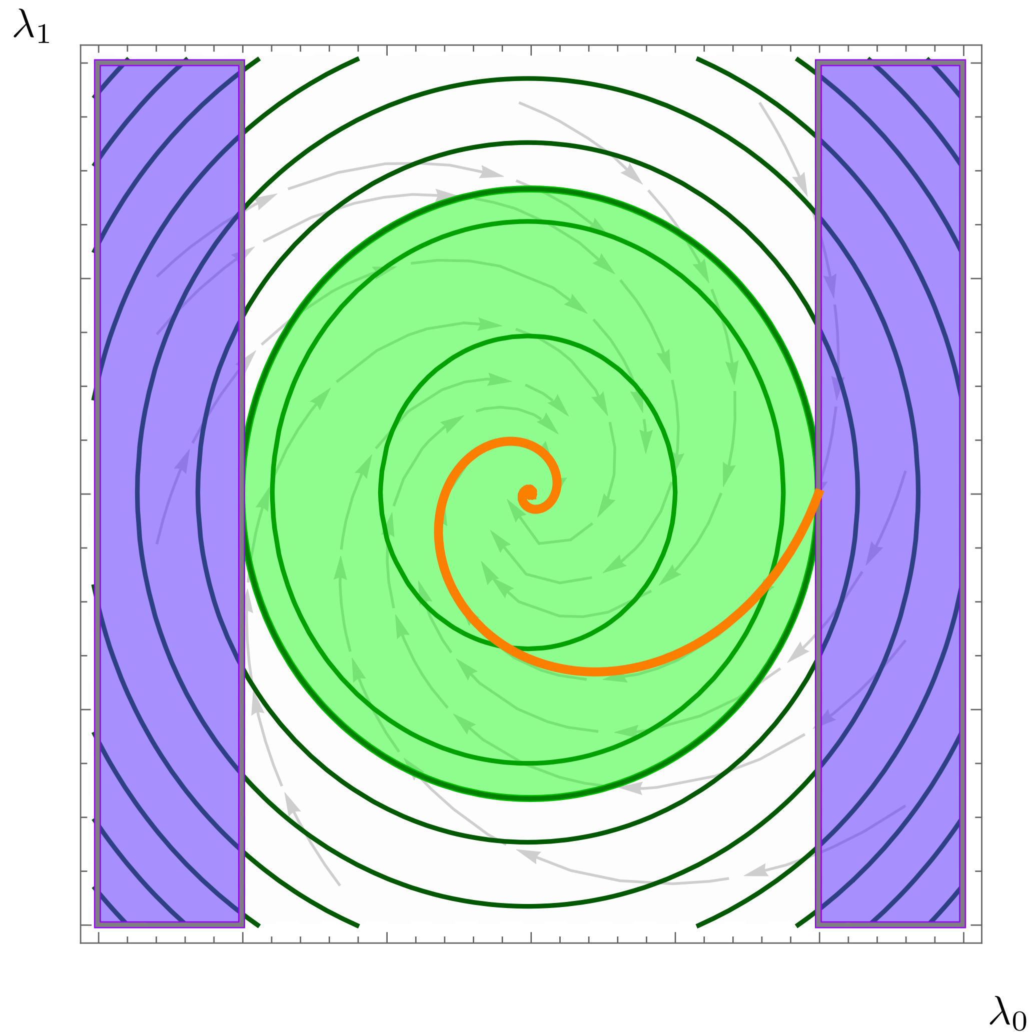

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$$R = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{\beta} \end{bmatrix}$$

$$Q = -2\alpha R$$

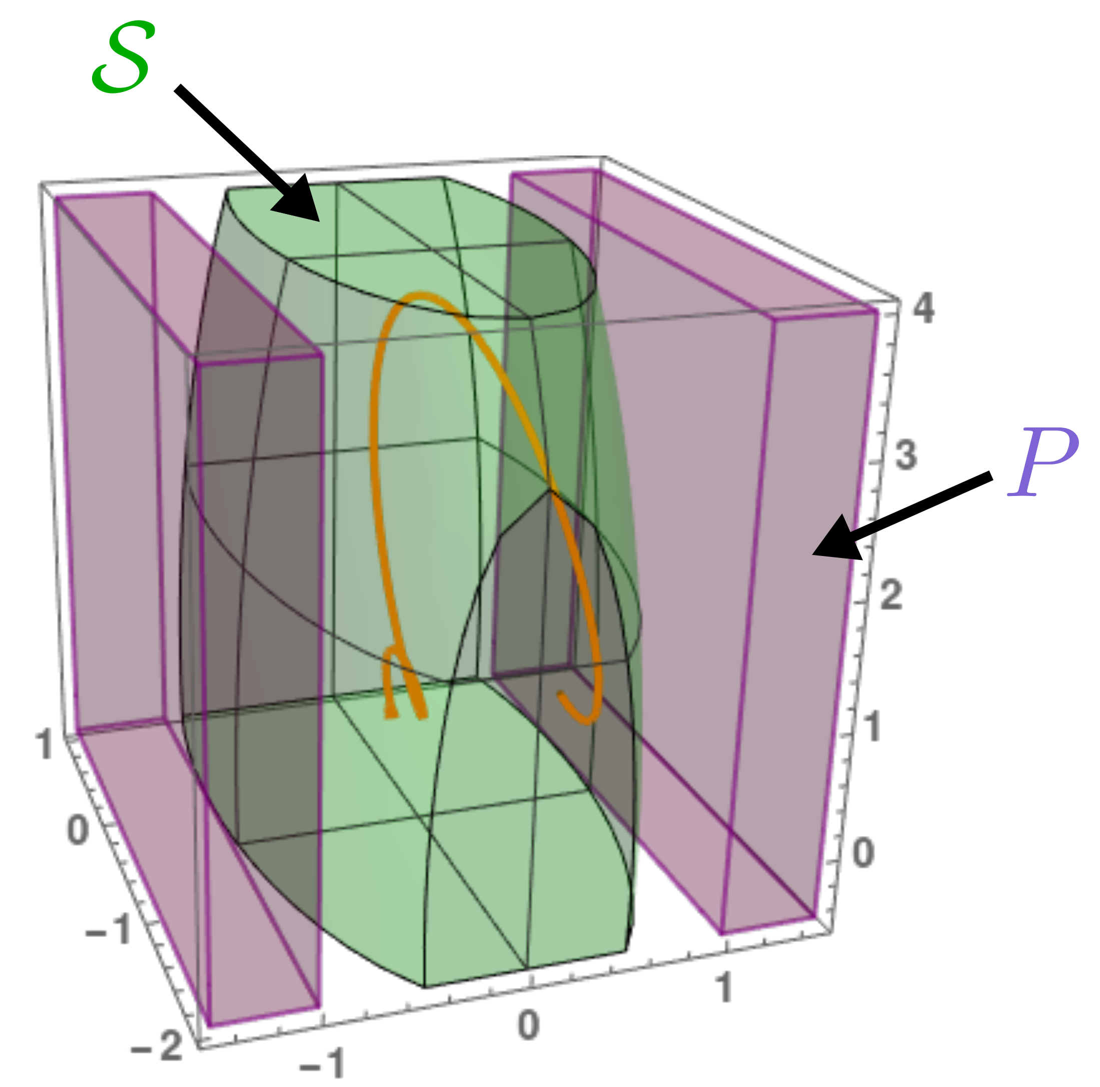
CP for $\alpha, \beta \geq 0$ necessary and sufficient !

A bit more involved

$$\dot{\varrho} = \frac{\alpha}{2}\mathcal{D}\varrho + \varrho_1$$

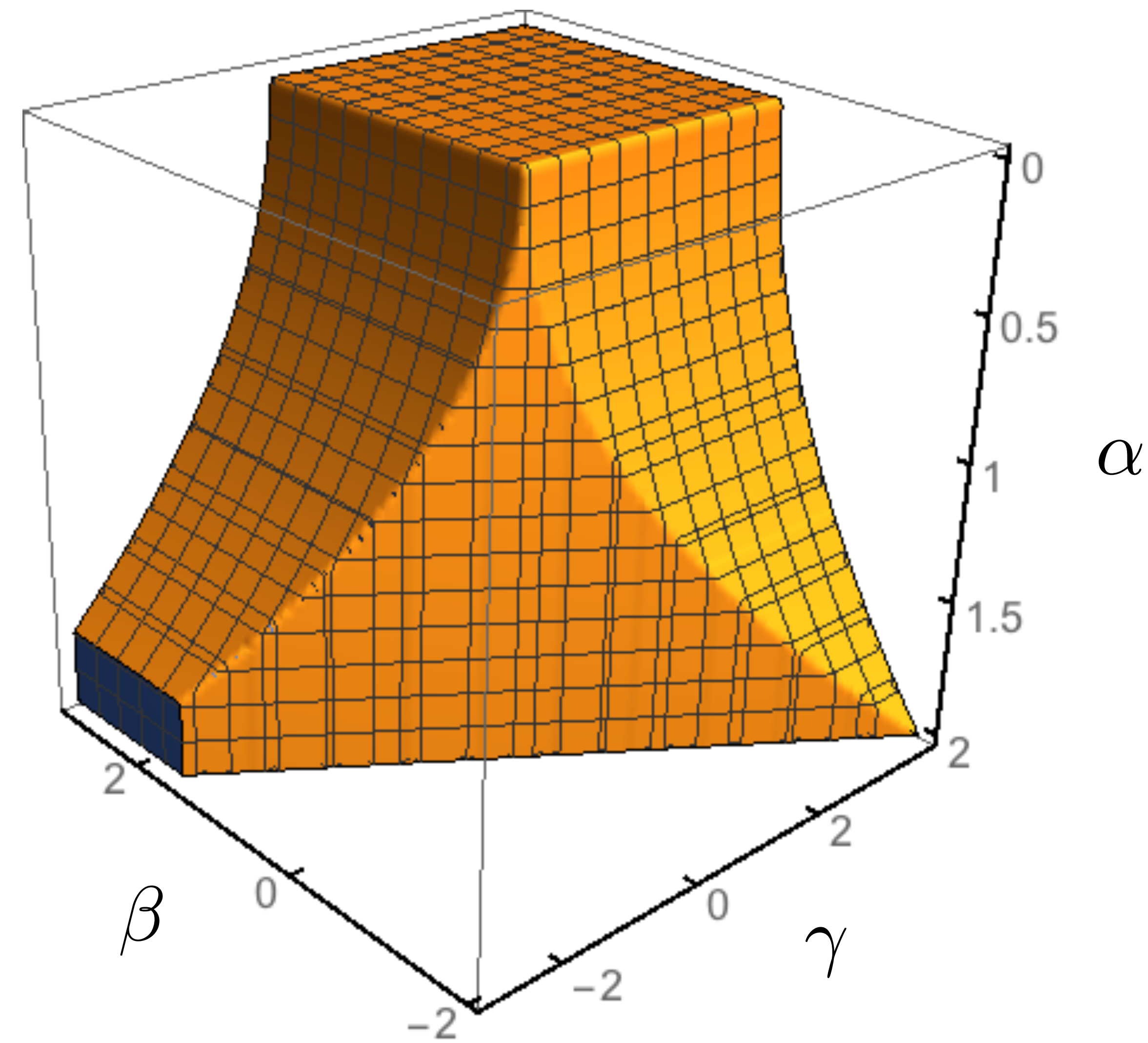
$$\dot{\varrho}_1 = \beta\mathcal{D}\varrho + \alpha\sigma_z\varrho_1\sigma_z + \varrho_2$$

$$\dot{\varrho}_2 = \gamma\sigma_z\varrho_1\varrho_z + \alpha\sigma_z\varrho_2\sigma_z$$

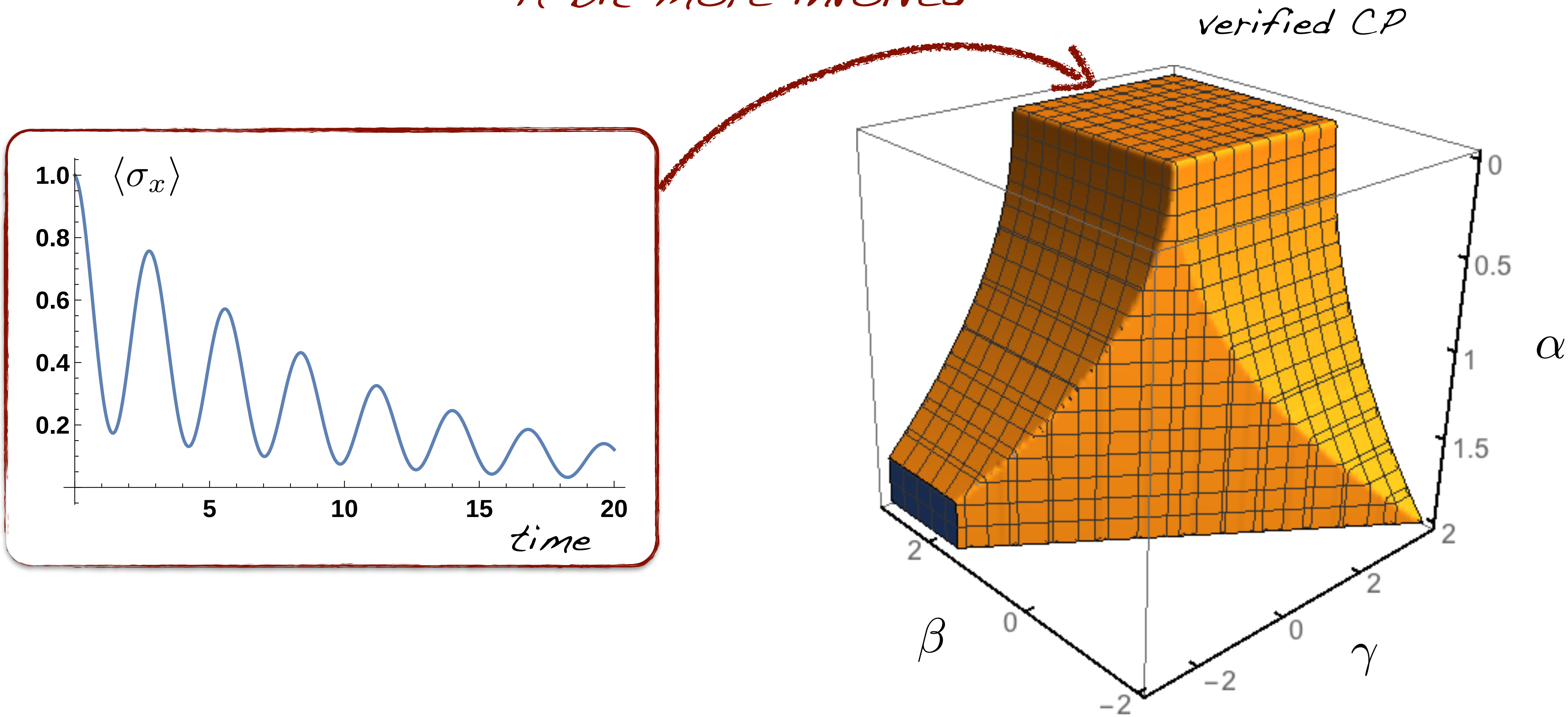


A bit more involved

verified CP



A bit more involved



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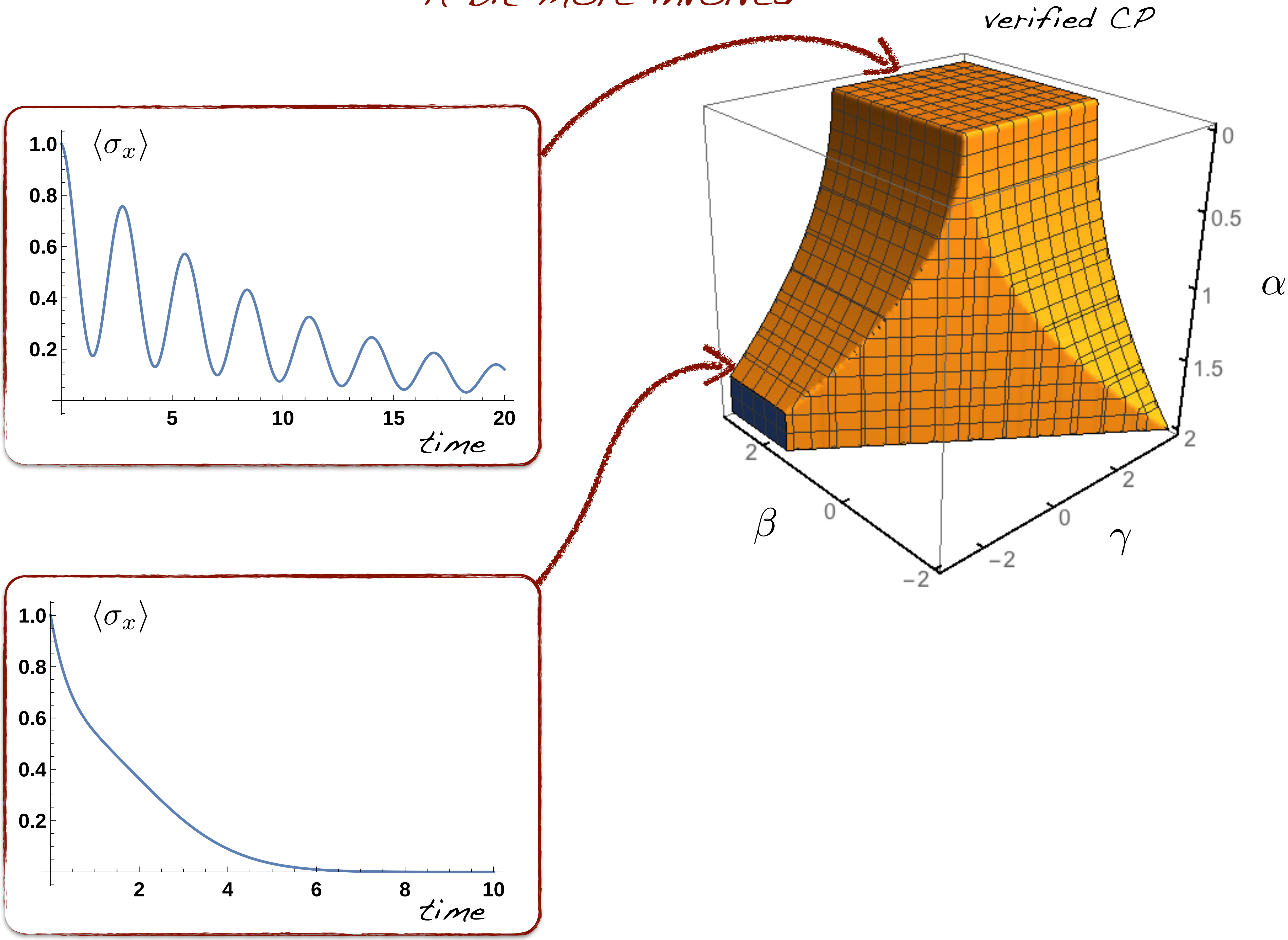
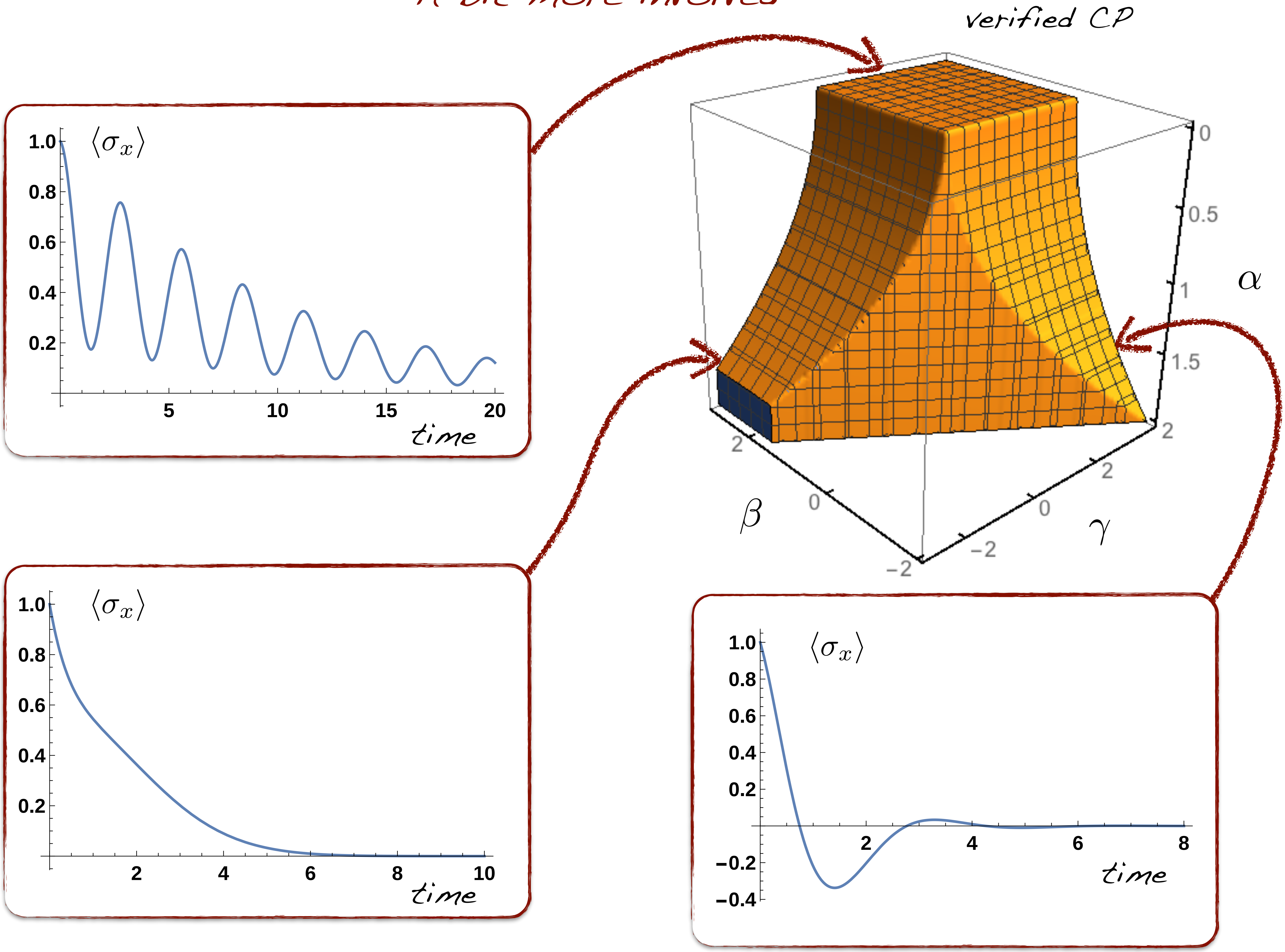
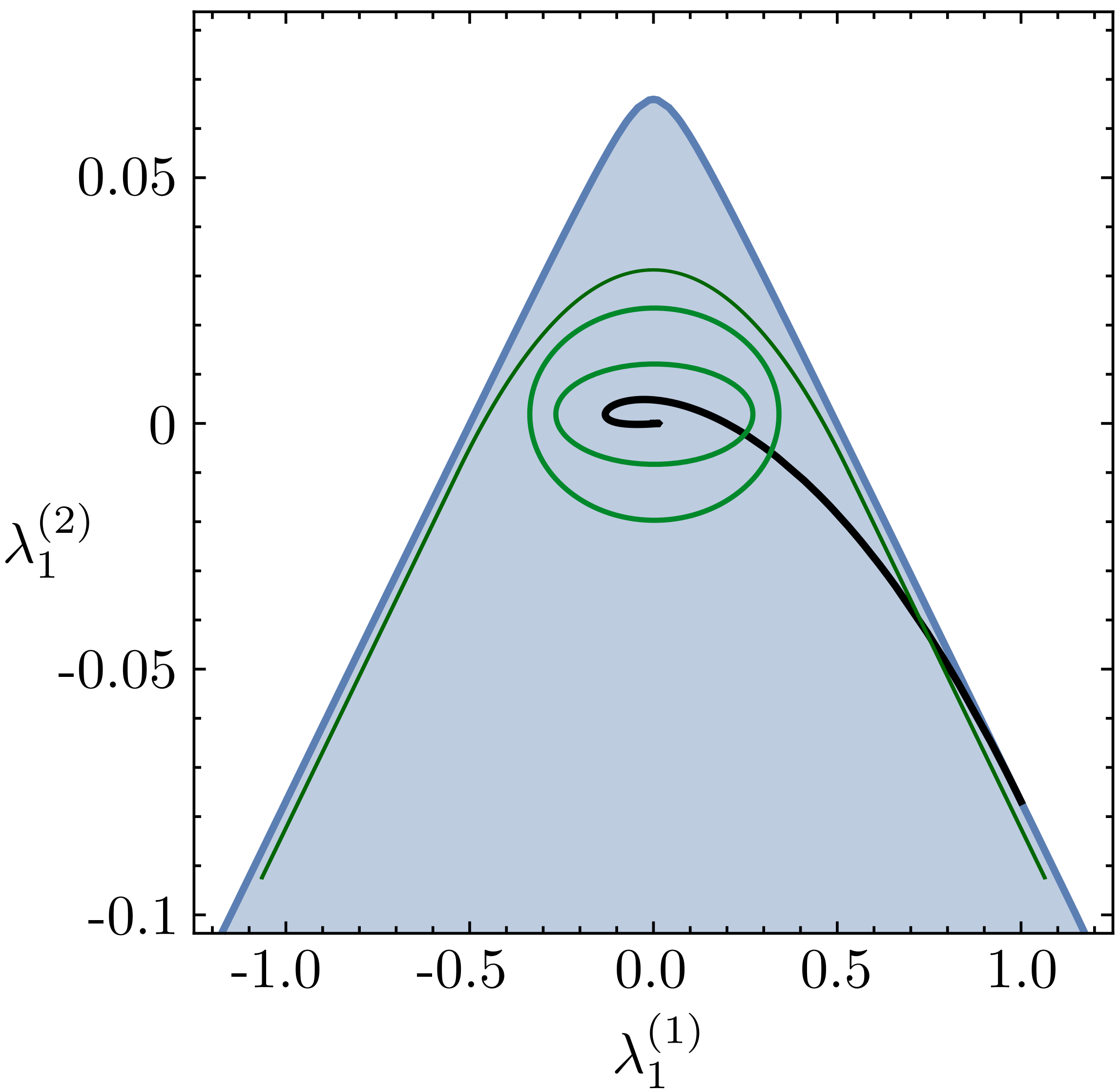


A bit more involved



Finite temperature environment

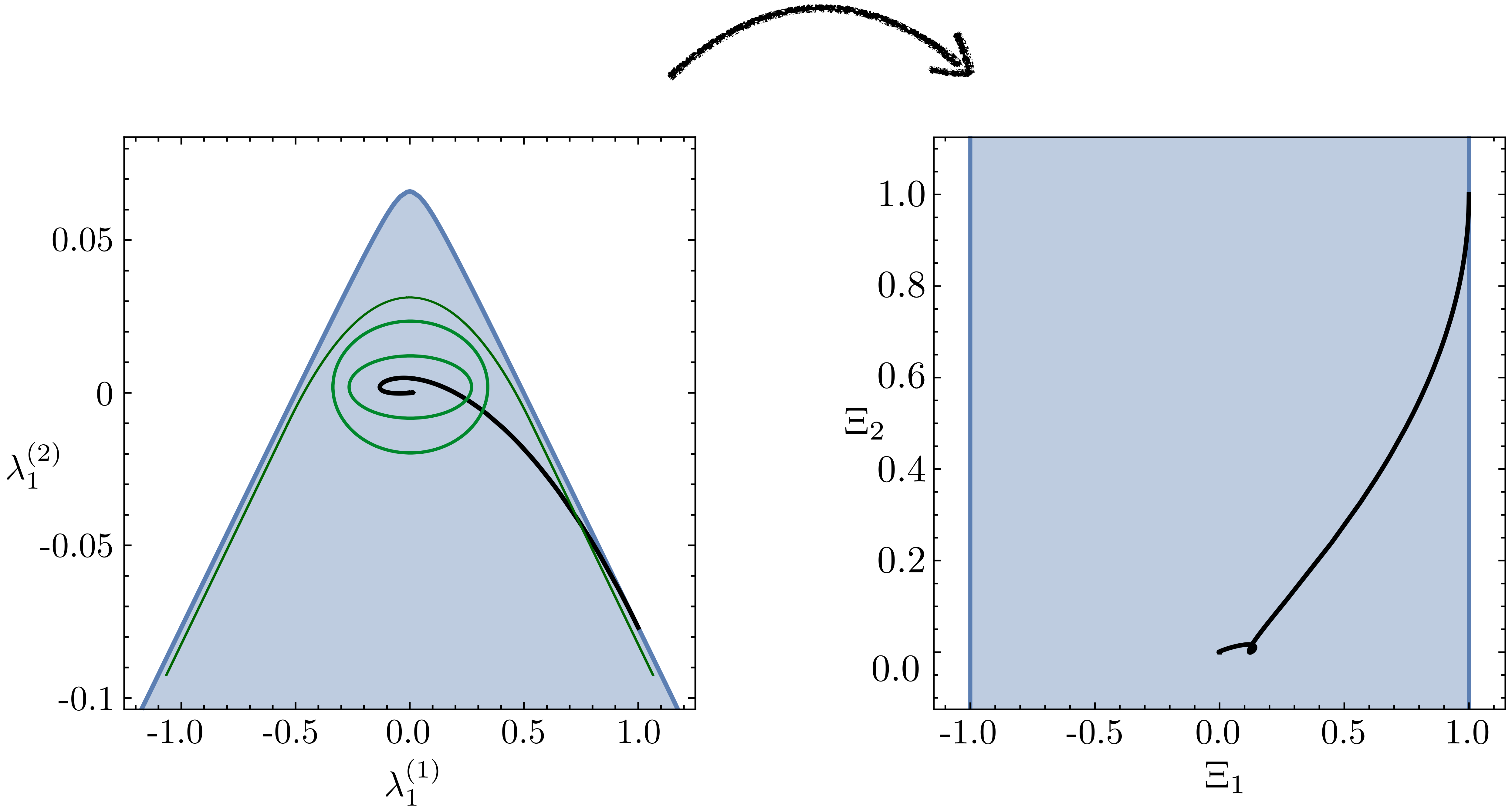
$$\dot{\varrho} = \gamma_+ \left(\sigma_+ \varrho \sigma_- - \frac{1}{2} \{ \sigma_- \sigma_+, \varrho \} \right) + \gamma_- \left(\sigma_- \varrho \sigma_+ - \frac{1}{2} \{ \sigma_+ \sigma_-, \varrho \} \right)$$



... can not find suitable potential

Finite temperature environment

nno-linear coordinate transformation



... can not find suitable potential

Non-linear coordinate transformation

$$\vec{\Lambda} \longrightarrow \vec{\Xi}$$

$$\Xi_1 = \det \chi - c \longrightarrow$$ very simple geometry ...

$$c = \lim_{t \to \infty} \det \chi$$

Non-linear coordinate transformation

$$\vec{\Lambda} \quad \Rightarrow \quad \vec{\Xi}$$

$$\Xi_1 = \det \chi - c$$

$\Longrightarrow$ very simple geometry ...

$$c = \lim_{t \to \infty} \det \chi$$

... but non-linear equation of motion.

$$\dot{\Xi}_1 = \alpha_1 \Xi_1 + \alpha_2 \Xi_2 + \alpha_3 \Xi_2^2 + \ldots$$

Non-linear coordinate transformation

$$\vec{\Lambda} \longrightarrow \vec{\Xi}$$

$$\Xi_1 = \det \chi - c \longrightarrow$$ very simple geometry ...

$$c = \lim_{t \to \infty} \det \chi$$

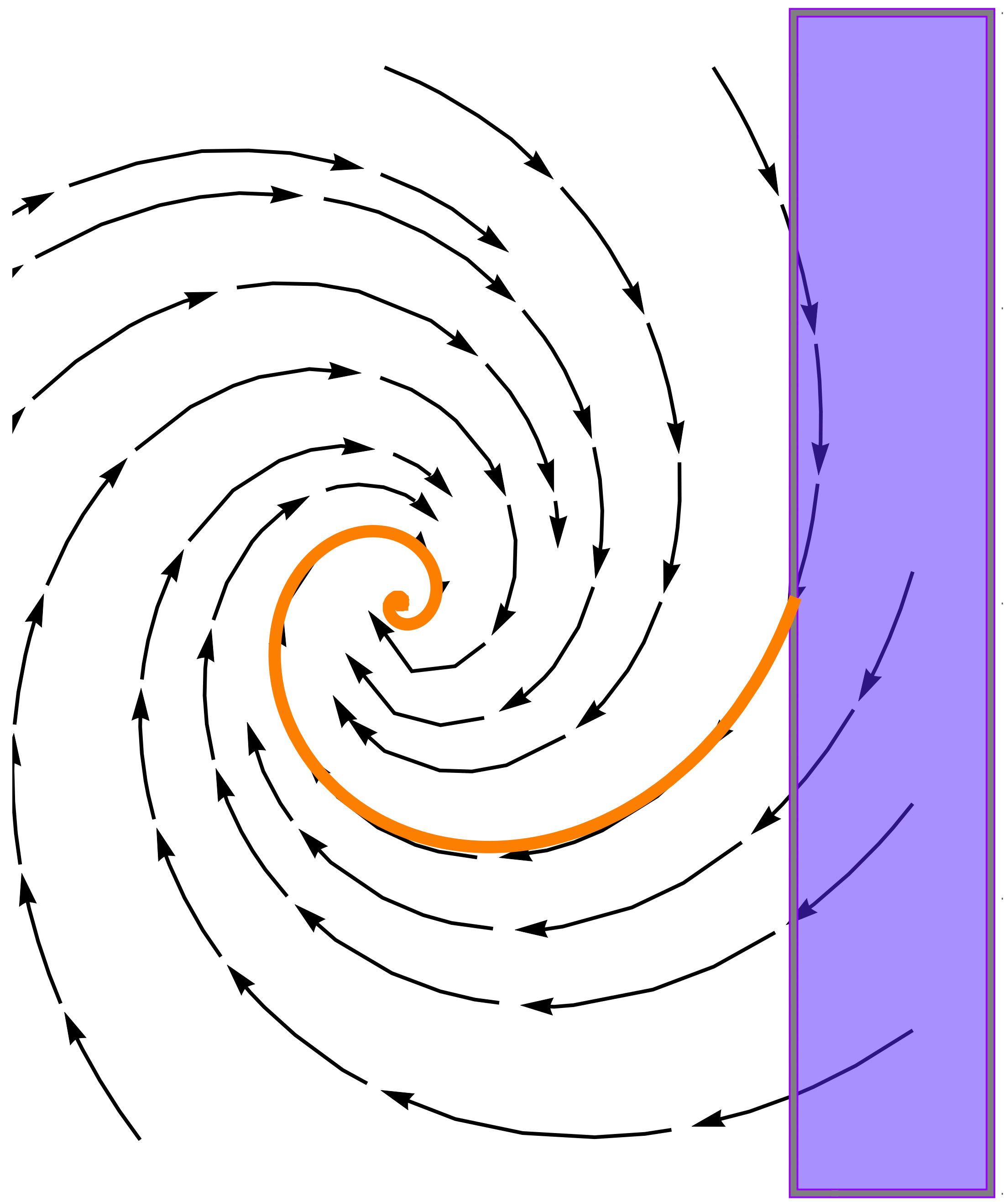
... but non-linear equation of motion.

$$\dot{\Xi}_1 = \alpha_1 \Xi_1 + \alpha_2 \Xi_2 + \alpha_3 \Xi_2^2 + \dots$$

treat as independent variable Ξ_3

Linear equation of motion, but increased dimension!

Standard geometry



...'just' high dimensional!!!

Finding the solution

metric, consistent with CP conditions

$$Q = L^T R + RL \leq 0$$

minimise v such that $$\begin{bmatrix} v\mathbf{1} - Q & 0 \\ 0 & R \end{bmatrix} \geq 0$$

semi-definite program (efficient and reliable)

if $v_{min} < 0$ then $Q \leq 0$ then CP !

Spin-Boson model

$$\dot{\varrho} = -i\frac{\omega}{2}[\sigma_z, \varrho] - i\Delta[\sigma_x, \varrho_1]$$

$$\dot{\varrho}_1 = -i\Delta[\sigma_x, \varrho] - \frac{\Delta\beta\gamma}{2}\{\sigma_x, \varrho\} - i\omega[\sigma_z, \varrho_1] - \gamma\varrho_1$$

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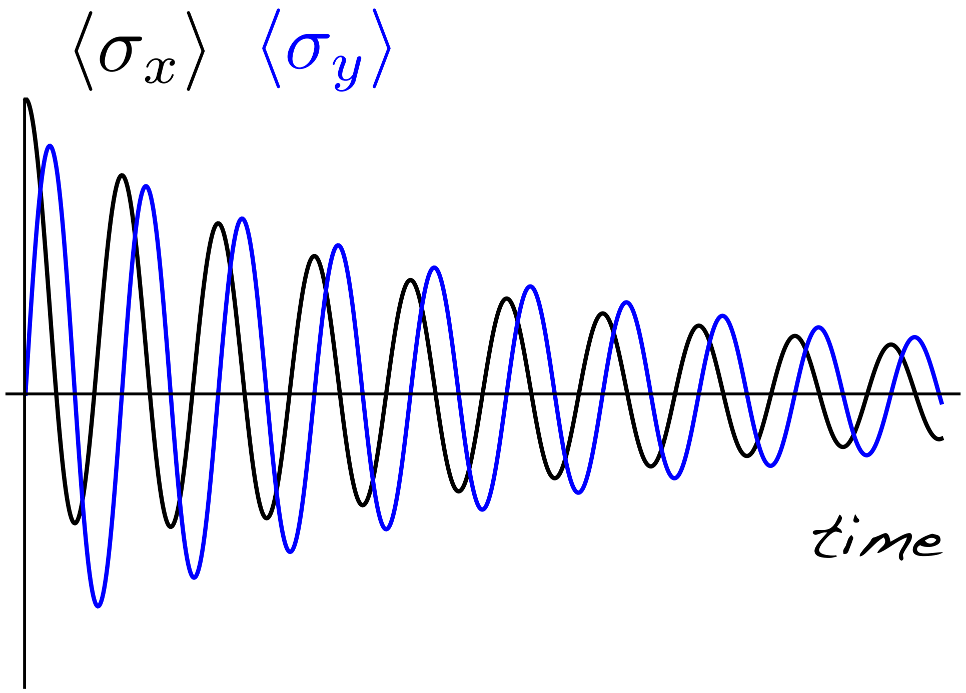
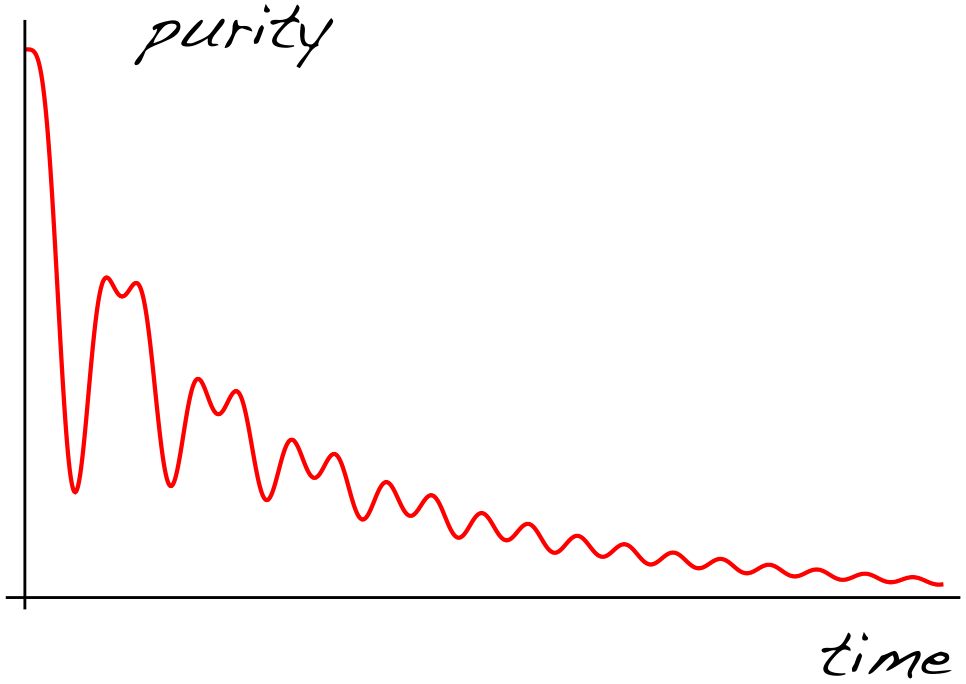




Spin-Boson model

negative eigenvalue $\sim -\beta^2\gamma^2\Delta^2\omega^2 t^4$ nearly never CP

two possible routes :

short time violation CP for $t \geq t_c$

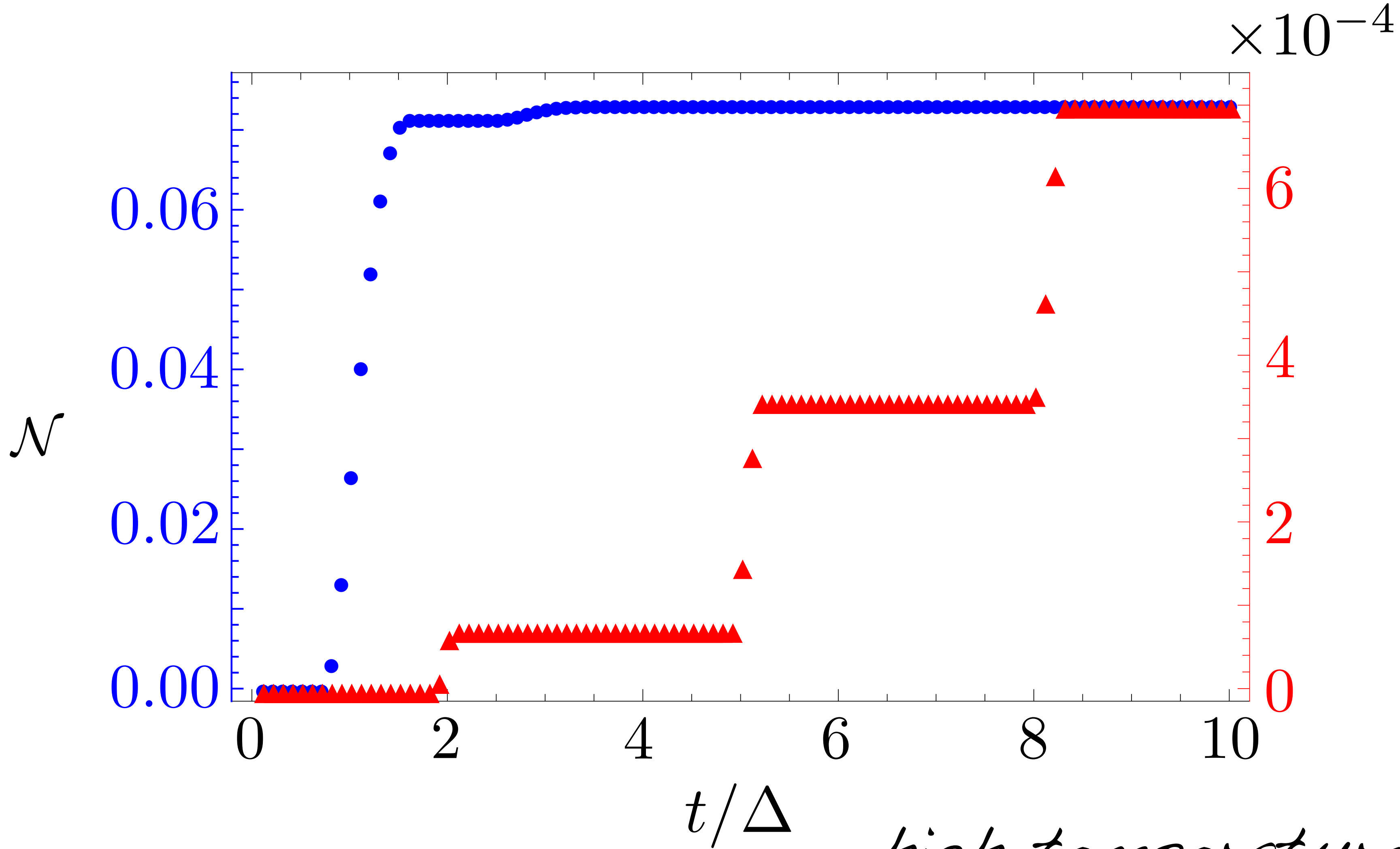
weak violation $\det \chi \geq c$ for $t \geq 0$

non-Markovian Spin-Boson dynamics

low temperature

short time violation

$$\frac{t_c}{\Delta} \simeq 0.6$$



high temperature

weak violation $\det \chi > 10^{-2}$

H.-P. Breuer, E. M. Laine & J. Piilo, PRL 103, 210401 (2009)

Markovianity

$$
\begin{aligned}
\dot{\varrho} &= \mathcal{L}_{00}\varrho + \mathcal{L}_{01}\varrho_1 \\
\dot{\varrho}_1 &= \mathcal{L}_{10}\varrho + \mathcal{L}_{11}\varrho_1 + \mathcal{L}_{12}\varrho_2 \\
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&\vdots
\end{aligned}
$$

Is $\dot{\varrho} = \mathcal{L}(t)\varrho$ satisfied ?

Markovianity

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$$

Is $\dot{\varrho} = \mathcal{L}(t)\varrho$ satisfied ?

linear relation : $\varrho_k(t) = \mathcal{Q}_k(t)\varrho(t)$

Ricatti equation : $\dot{\vec{Q}} = A\vec{Q} + \vec{Q}B + C + \vec{Q}^T D\vec{Q}$

Markovianity

$$\begin{aligned}\dot{\varrho} &= \mathcal{L}_{00}\varrho + \mathcal{L}_{01}\varrho_1 \\ \dot{\varrho}_1 &= \mathcal{L}_{10}\varrho + \mathcal{L}_{11}\varrho_1 + \mathcal{L}_{12}\varrho_2 \\ \dot{\varrho}_2 &= \mathcal{L}_{20}\varrho \\ &\vdots\end{aligned}$$

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$$\mathcal{L}(t)\varrho = (\mathcal{L}_{00} + \mathcal{L}_{01}Q_1)\varrho = i[\rho, \mathcal{H}] + \sum_{ij}\gamma_{ij}(\sigma_i\varrho\sigma_j^\dagger - \frac{1}{2}\{\varrho, \sigma_j^\dagger\sigma_i\})$$

follow positivity

Markovianity

$$\dot{\varrho} = \frac{\alpha}{2}\mathcal{D}\varrho + \varrho_1$$

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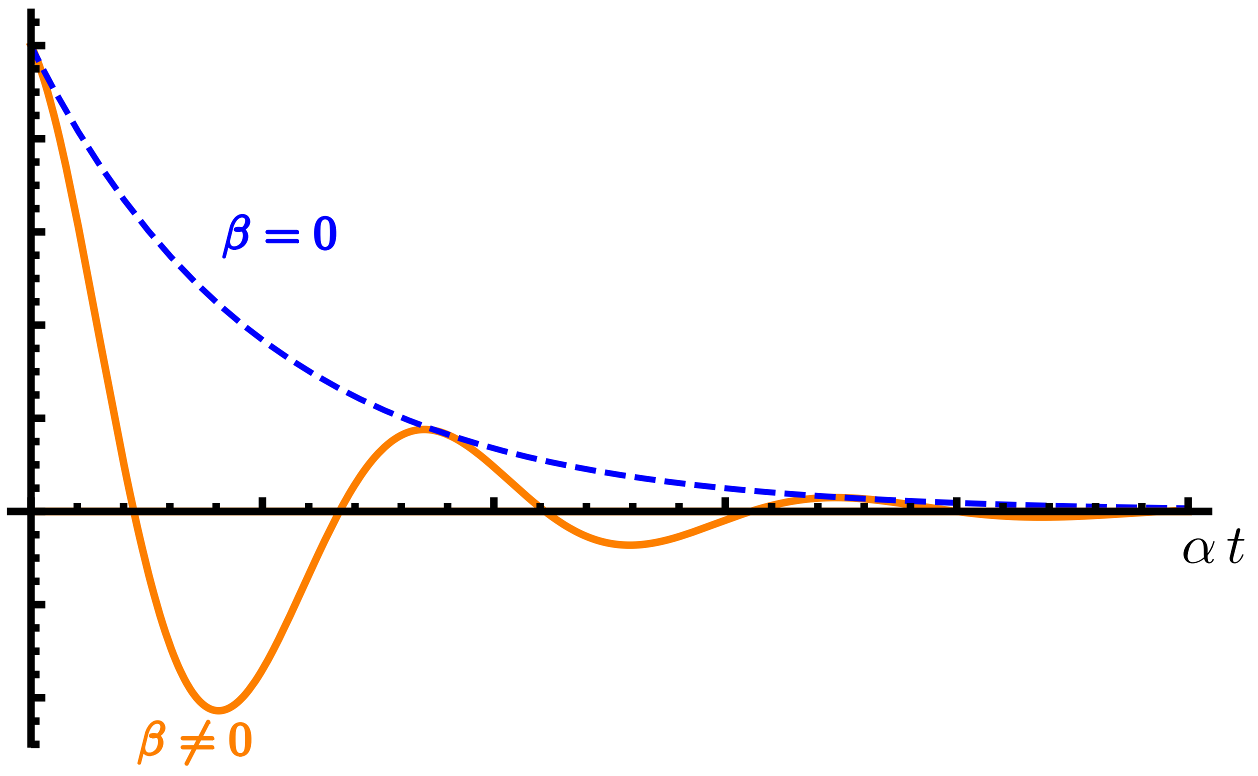
$$\mathcal{D}\varrho = \sigma_z\varrho\sigma_z - \sigma_z$$



Markovian only for $\beta = 0$

Markovianity

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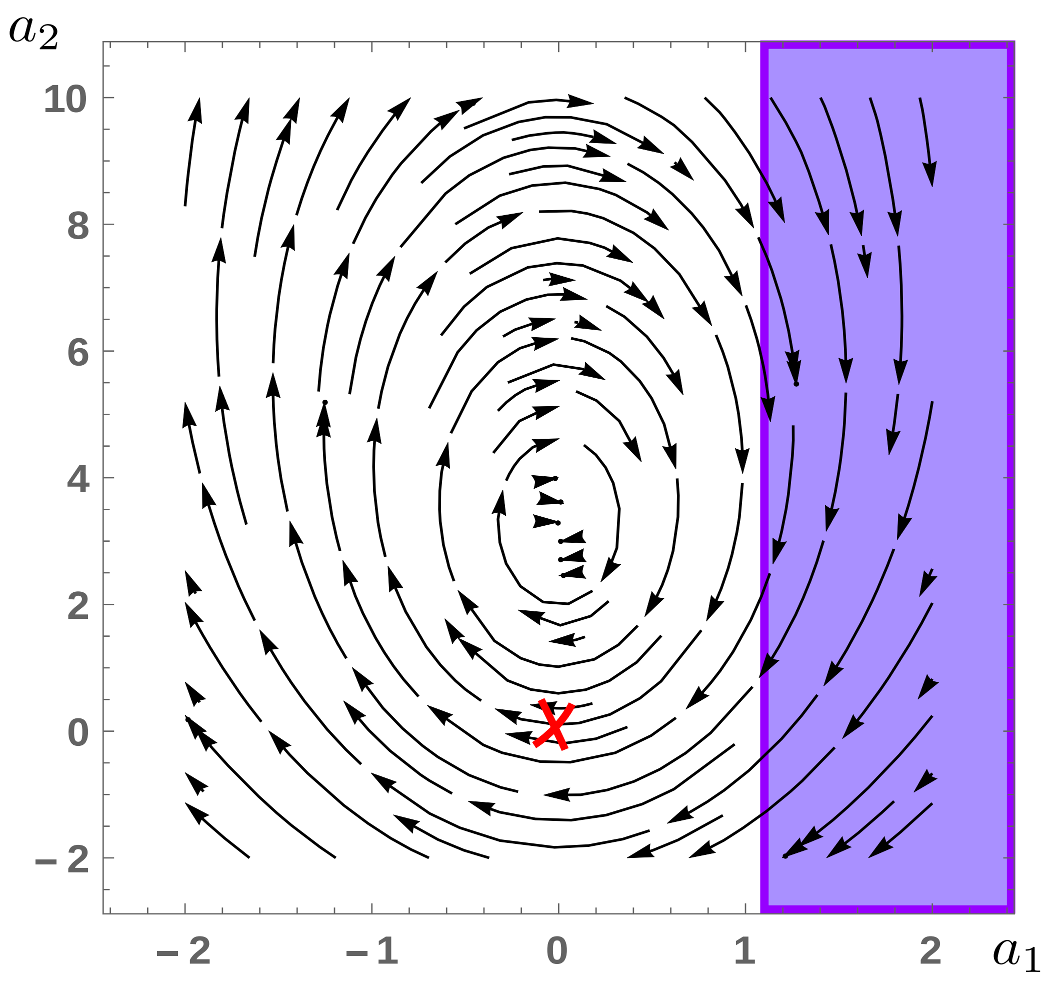

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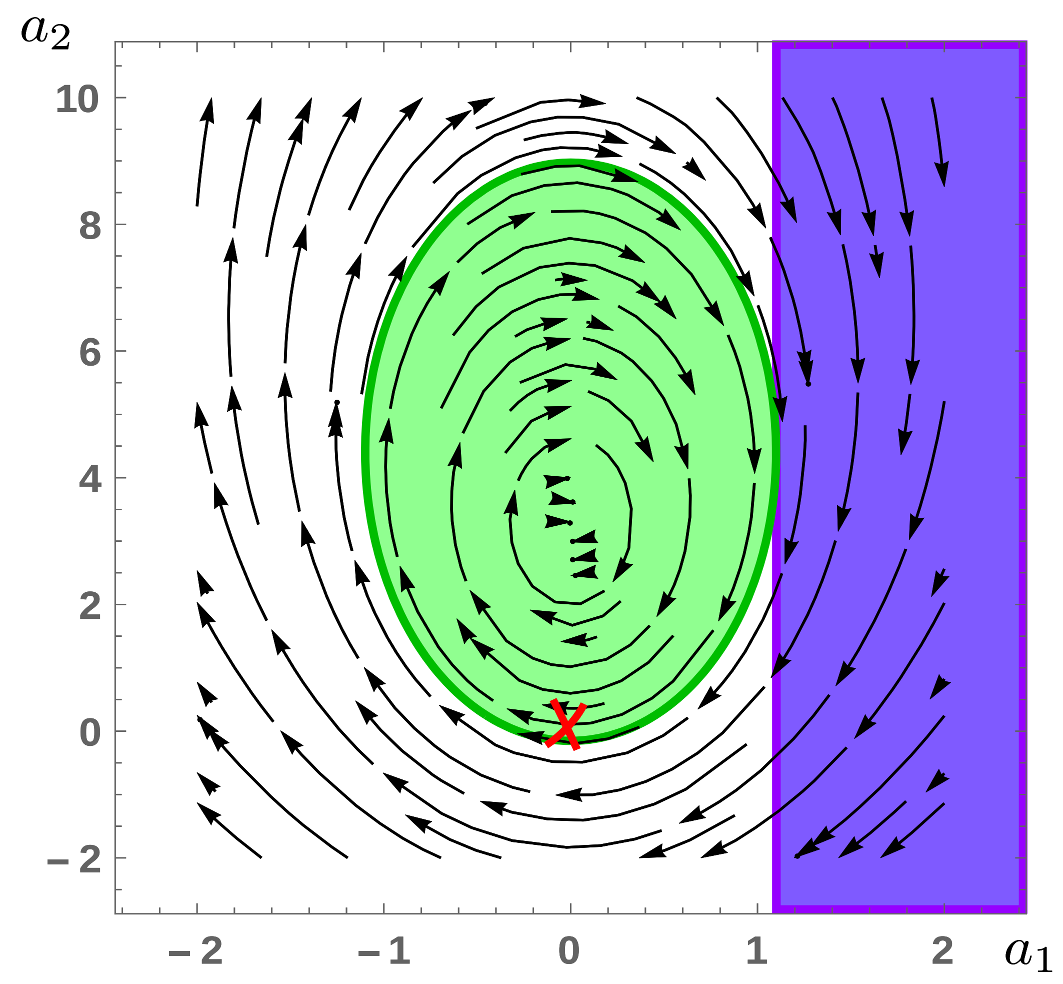

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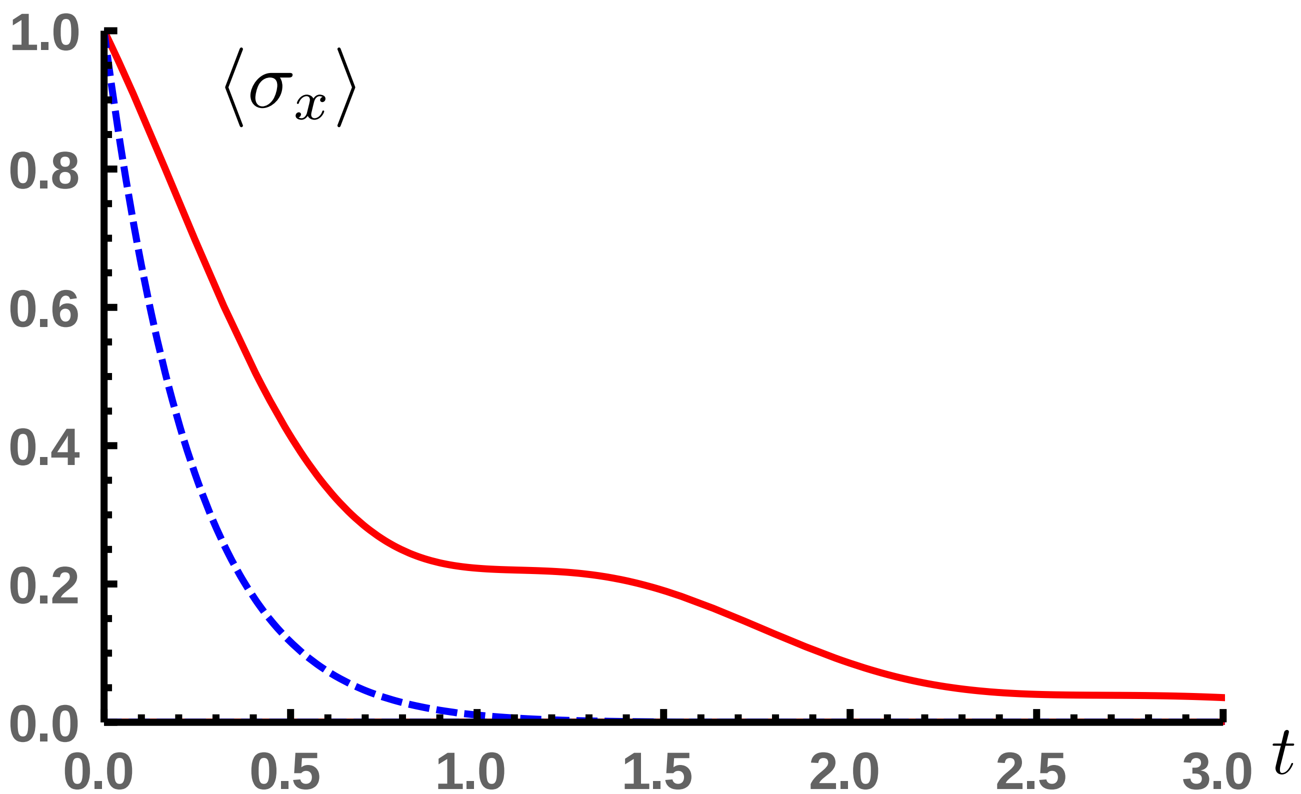
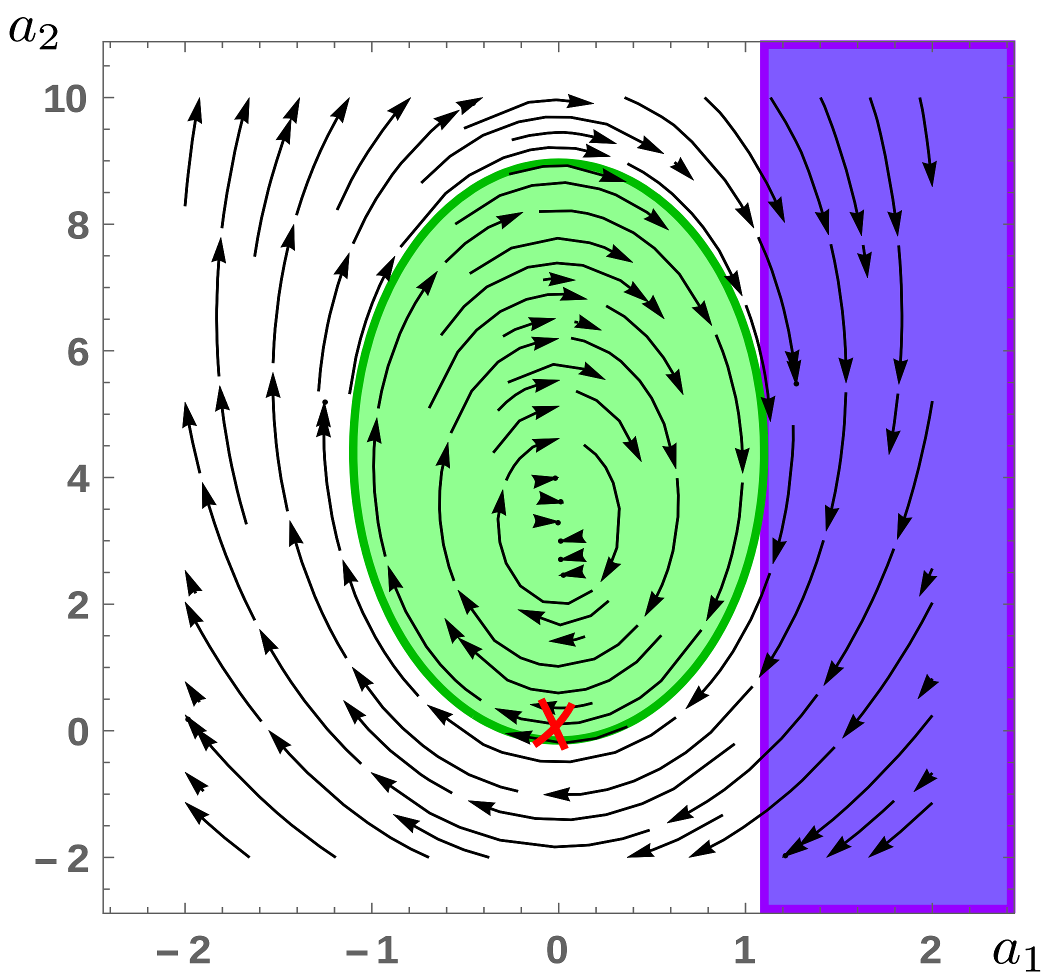
\dot\varrho &= \frac{\alpha}{2}\mathcal{D}\varrho + \varrho_1 \\
\dot\varrho_1 &= \beta\mathcal{D}\varrho + \alpha\sigma_z\varrho_1\sigma_z + \varrho_2 \\
\dot\varrho_2 &= \gamma\sigma_z\varrho_1\varrho_z + \alpha\sigma_z\varrho_2\varrho_z
\end{aligned}$$





$$-\alpha\sqrt{\alpha^2+2\beta+\gamma}+\alpha^2+2\beta\leq 0$$

necessary and sufficient !

Outlook

Initial system bath correlations $\varrho_k(0) \neq 0$

$$\Lambda_k(0) \neq \mathbf{0}$$

Include non-linear transformation in SDP

Model non-Markovian dynamics with valid hom

Find corrections for microscopically derived hom

Björn Witt, Łukasz Rudnicki & FM arXiv:1506.03638