Open Quantum Systems

Noise, dissipation, memory

$$\rho_n = T_1\,\rho_{n-1} + T_2\,\rho_{n-2} + T_3\,\rho_{n-3} + \cdots$$

Quantum Thermodynamics for Young Scientists

Bad Honnef, February 3, 2020

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Universidad Politécnica de Cartagena

Massachusetts Institute of Technology

Technische Universität Berlin

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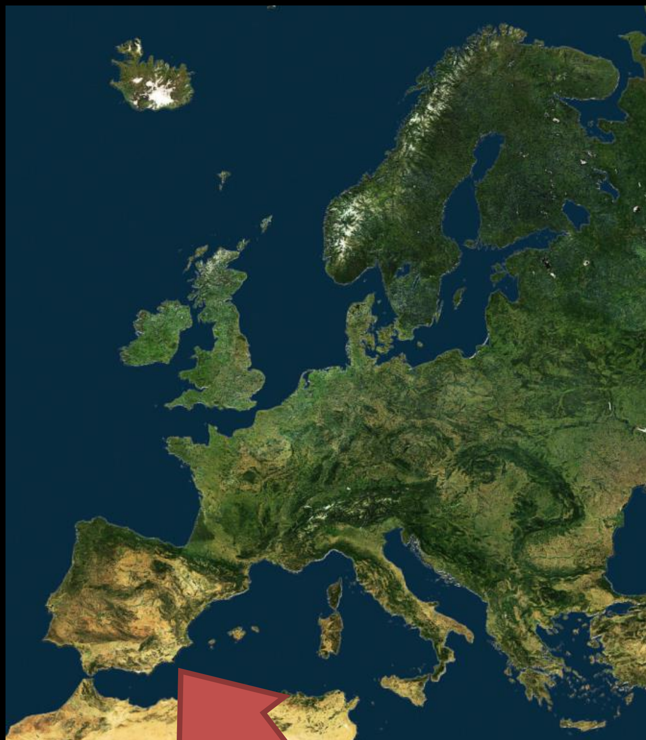
Cartagena?




Universidad


GALLAECIA
TARRACONENSIS
CARTHAGINENSIS
LUSITANIA
BALEARICA
BAETICA

Open Quantum Systems

Noise, dissipation, memory

- Approaches to Complex Open Quantum Systems
- Reaction Coordinate and Thermal Function
- Hierarchy of Equations of Motion and Full Counting Statistics
- Memory and the Transfer Tensor Method
- Chain Mapping
- Initial System-Bath Correlations and Temperature Measurements

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Simulation of complex open quantum systems

Non-Markovian, strong-coupling, time-dependence, initial system-bath correlations…

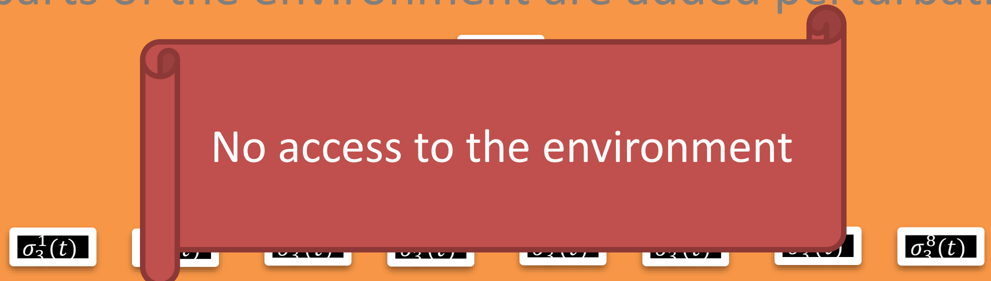
Markovian-embedding techniques

Enlarging the System to include environmental degrees of freedom

Reaction-coordinate, chain-mapping techniques, matrix-product states, MCTDH…

Integrability-embedding techniques

Integrable parts of the environment are added perturbatively to the system



Feynman-Vernon Influence Functional, Hierarchy of equation of motion, Quasi adiabatic path integral (QUAPI), stochastics methods..

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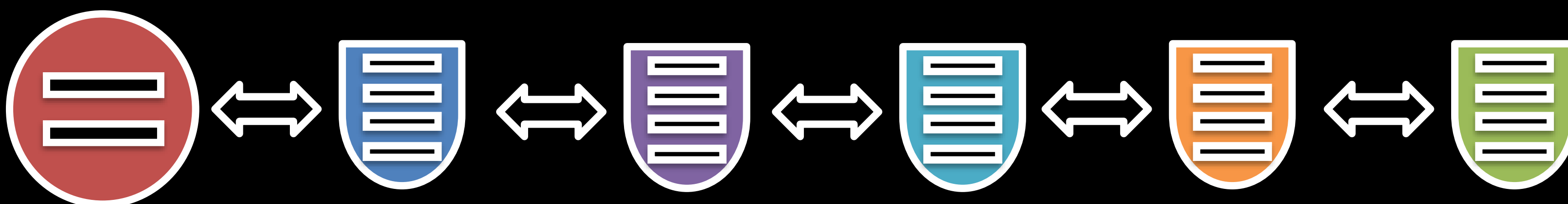
Chain mapping and orthogonal polynomials

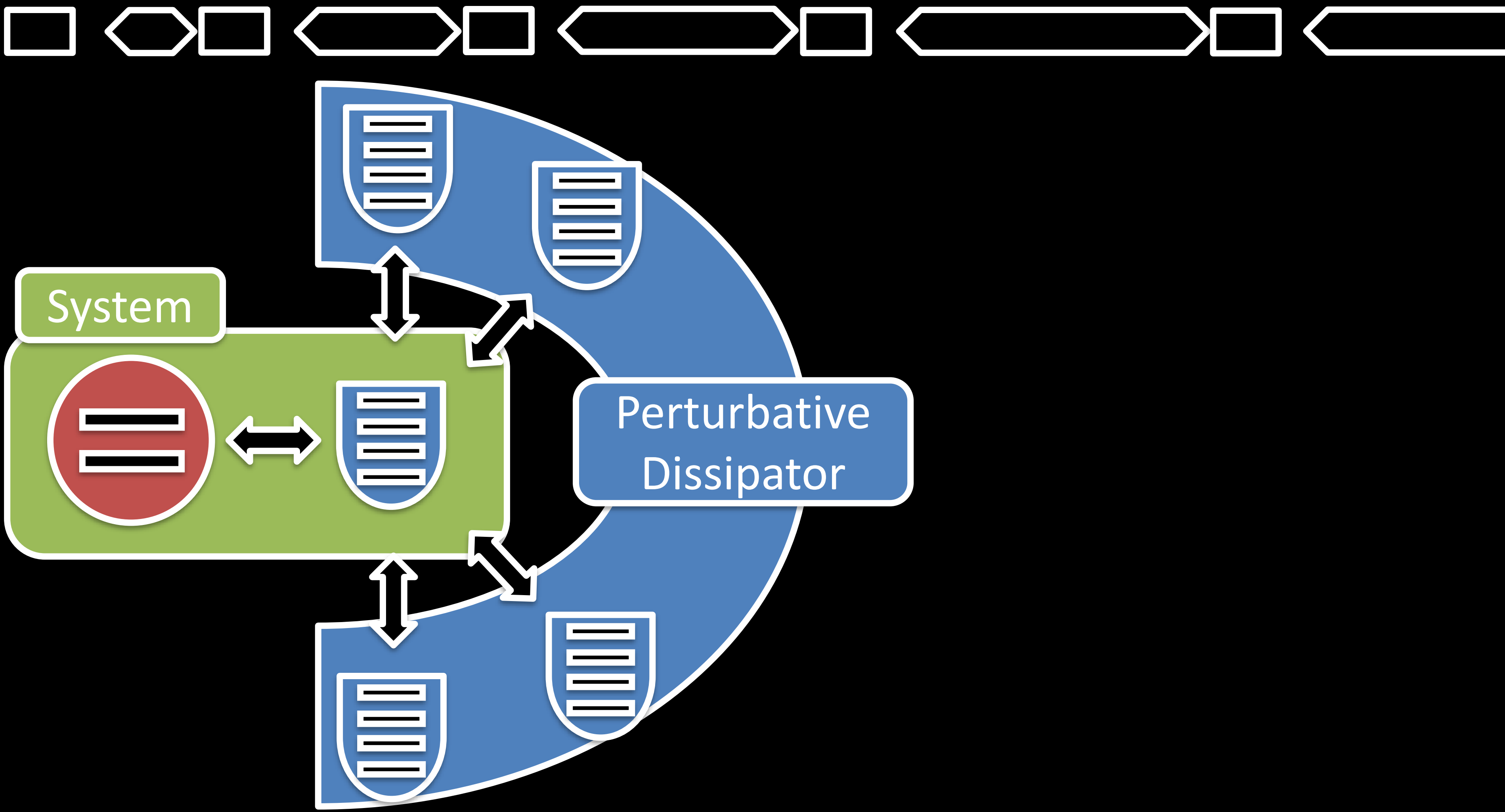
A Chin, A Rivas, S Huelga, M Plenio, *J. Math. Phys.* **51**, (2010).



+ Simulation with Matrix Product States/DMRG

Time Evolving Density matrix using Orthogonal Polynomial Algorithm
TEDOPA

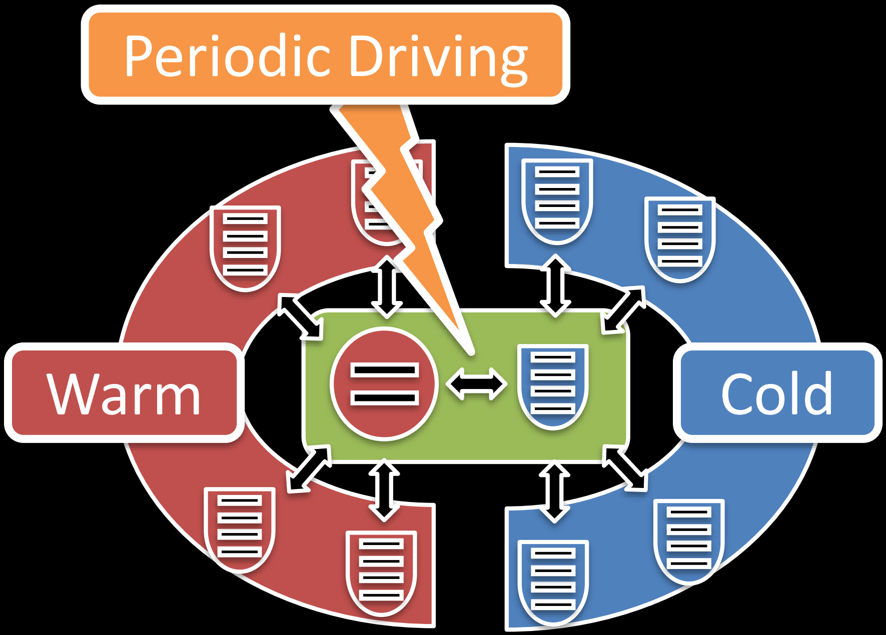
Reaction Coordinate



R. Martinazzo, B. Vacchini, K. H. Hughes, and I. Burghardt, *J. Chem. Phys.* **134**, 011101 (2011).
J. Iles-smith, N. Lambert, and A. Nazir, *Phys. Rev. A* **90**, 032114 (2014).

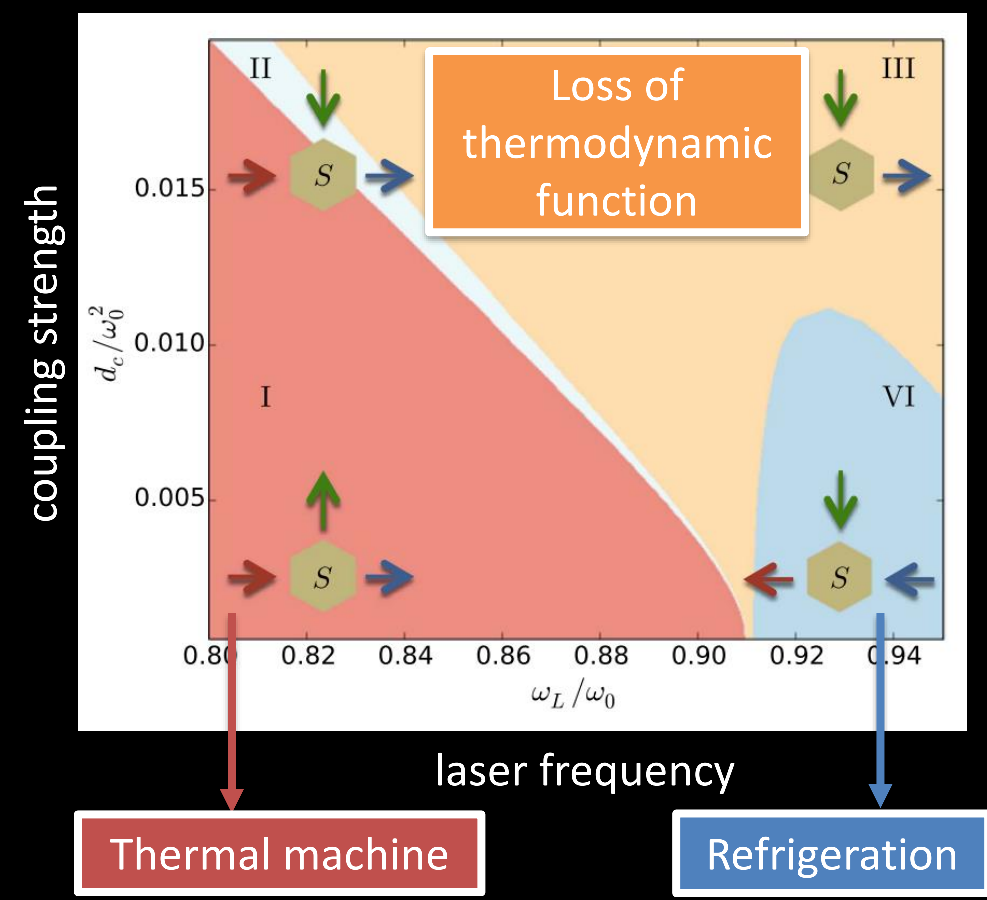
Reaction Coordinate – Strong coupling thermodynamics

S. Restrepo, J. Cerrillo, P. Strasberg, and G. Schaller, *New J. Phys.* **20**, 053063 (2018).



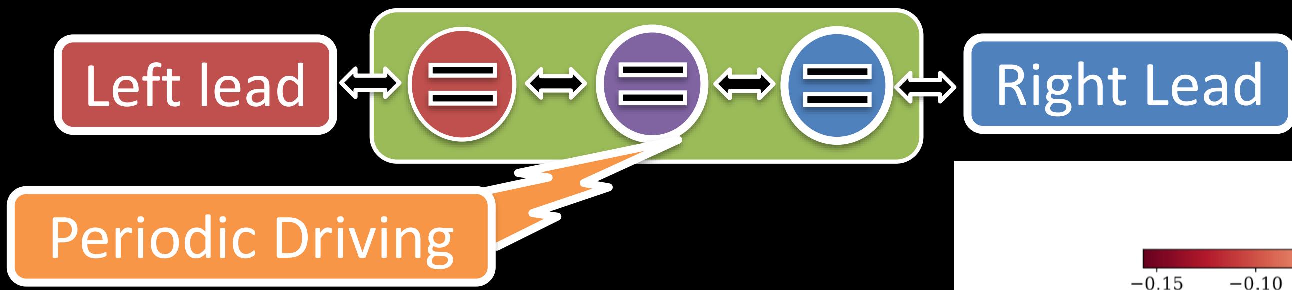
+ Floquet-Markov
+ Full counting statistics

Thermodynamics of laser cooling in strong-coupling regime



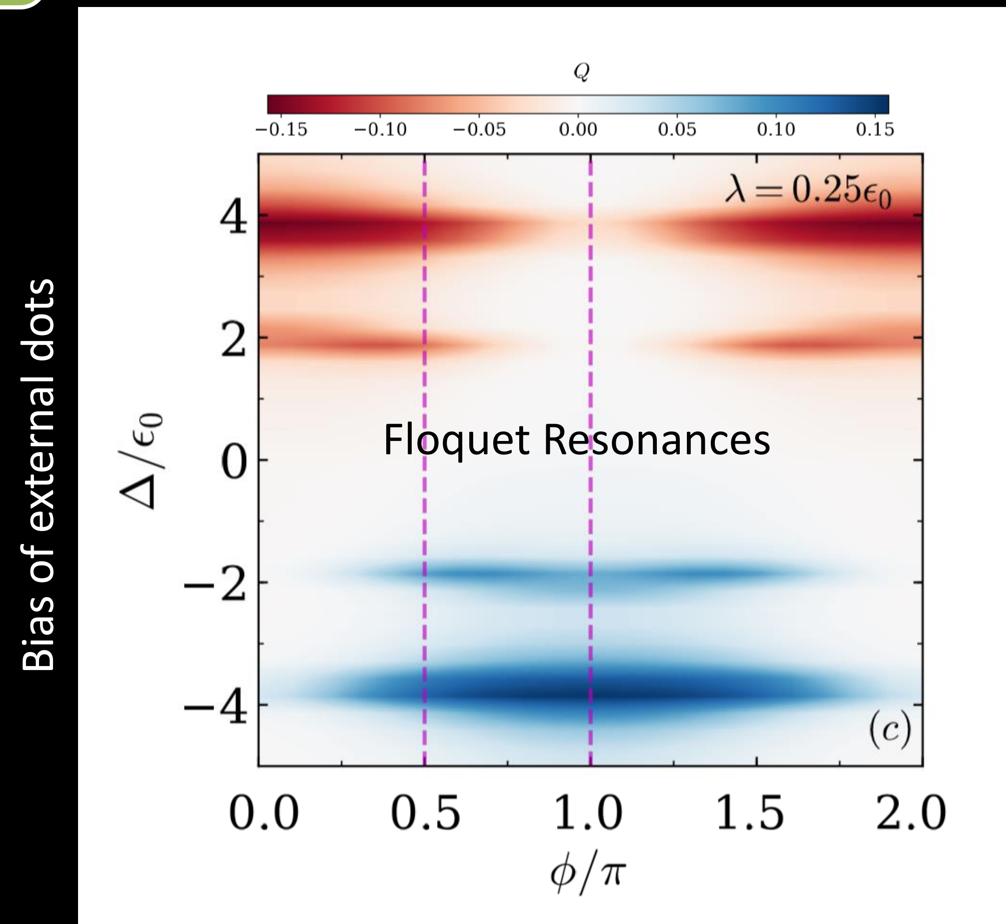
Reaction Coordinate – Electron pumping

S. Restrepo, S. Boehling, J. Cerrillo and G. Schaller, *Phys. Rev. B* **100**, 035109 (2019).



+ Floquet-Markov
+ Full counting statistics

Goal:
pump electrons from one lead to the other without potential bias, by the effect of driving alone.



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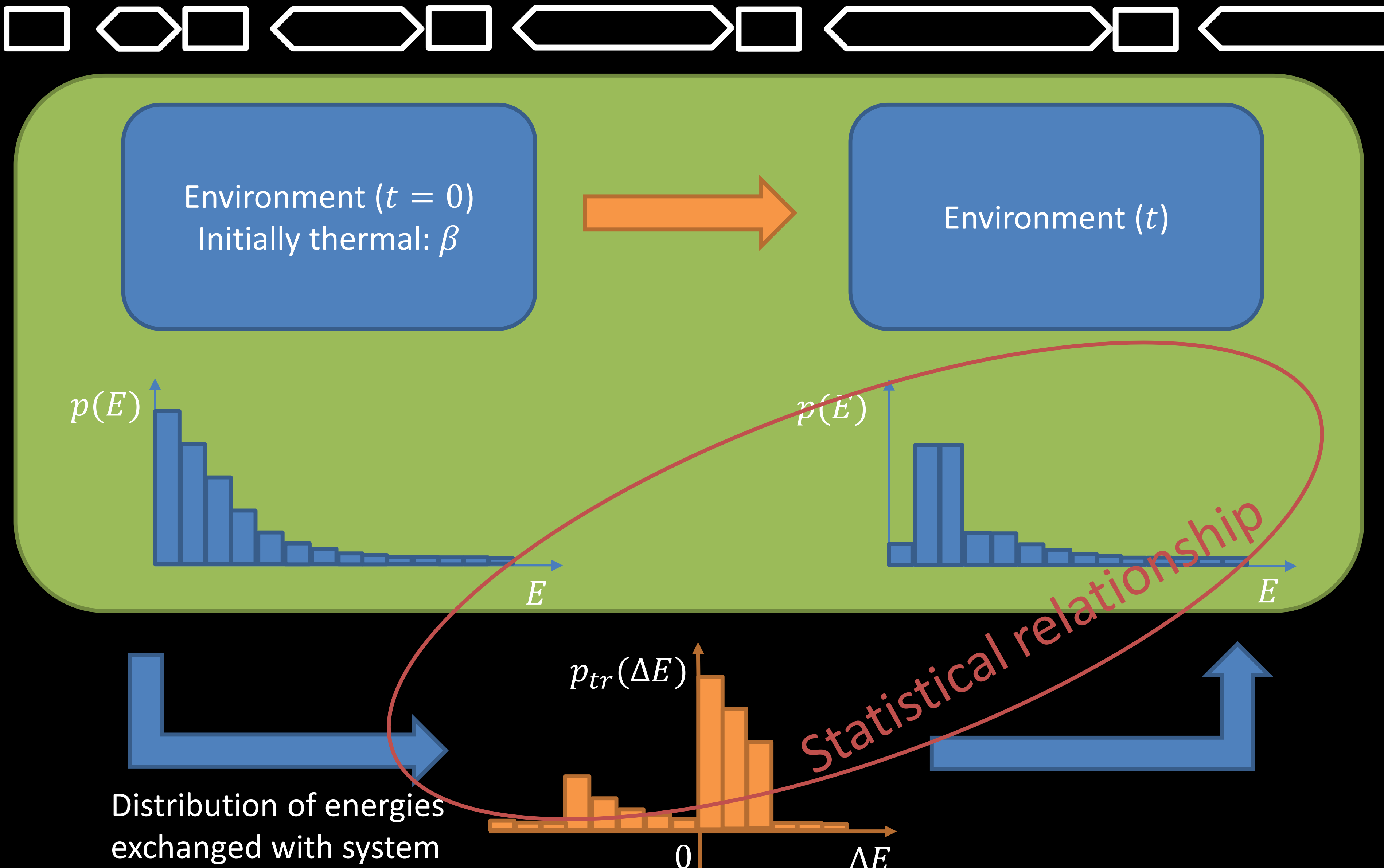
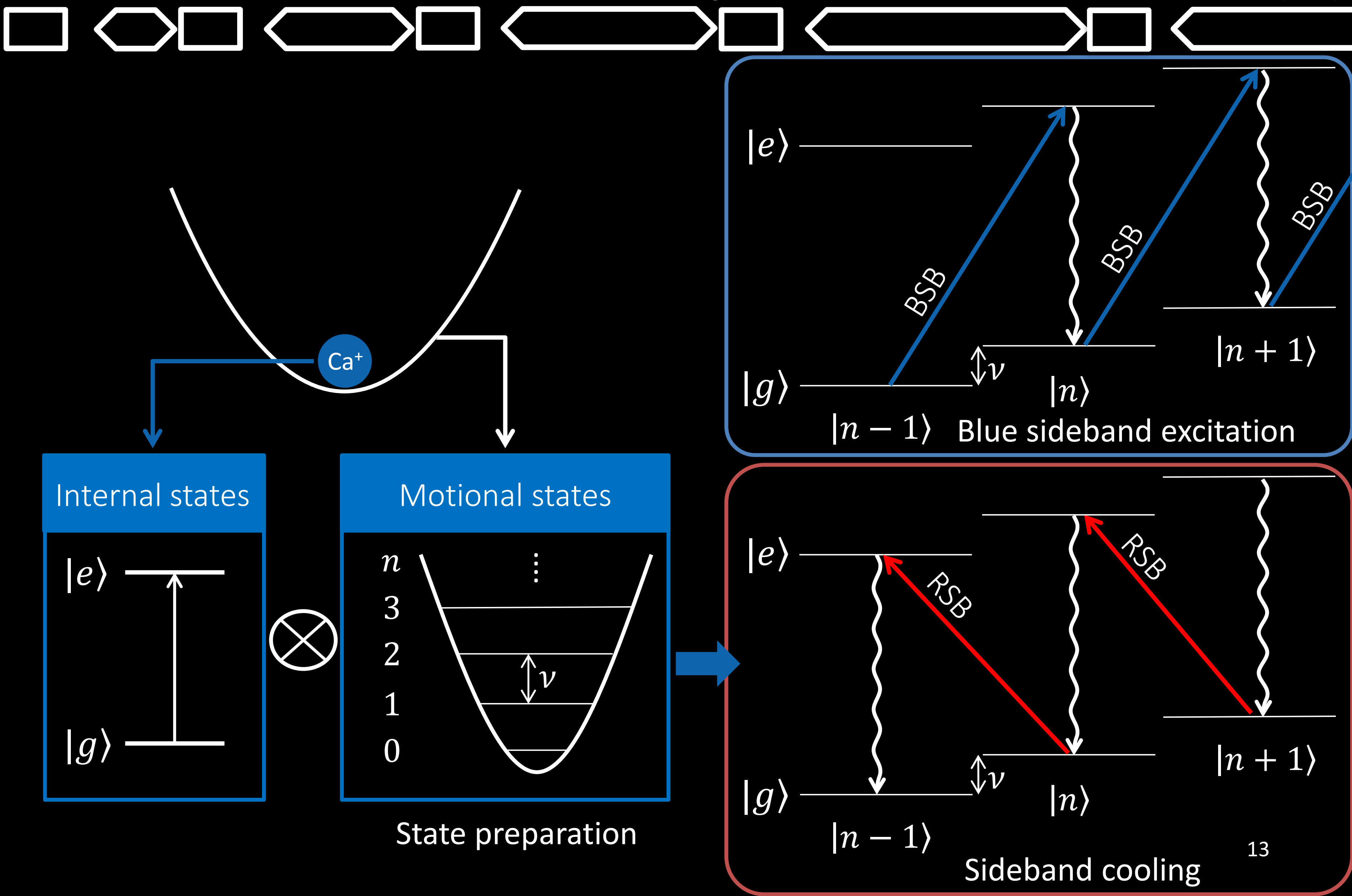
Full Counting Statistics

J. Cerrillo, M. Buser and T. Brandes, *Phys. Rev. B* **94**, 214308 (2016).



Atomic clock preparation

C. Monroe, D. M. Meekhof, B. E. King, S. R. Jefferts, W. M. Itano, and D. J. Wineland, PRL **75**, 4011 (1995).



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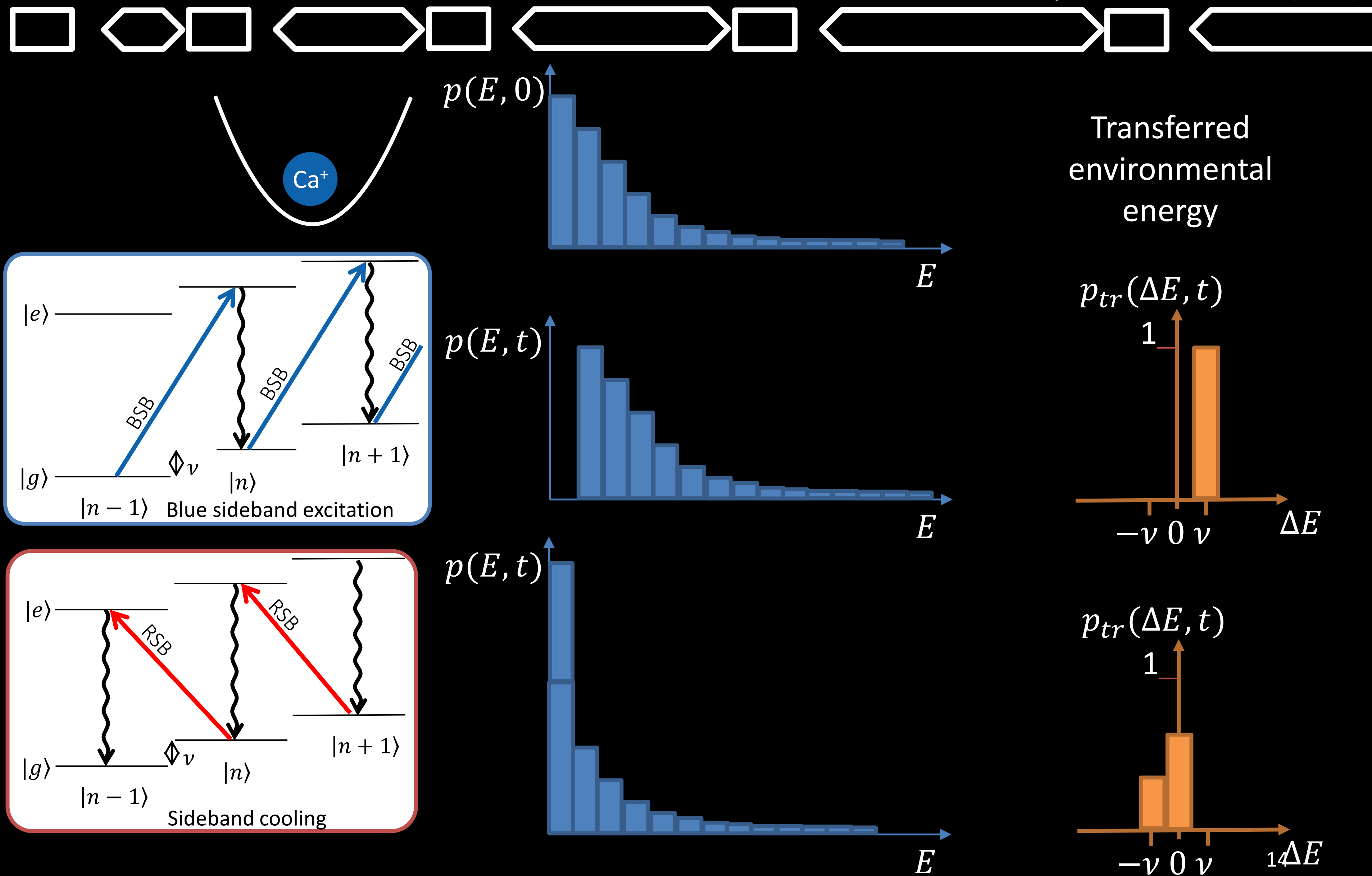
J. Cerrillo, M. Buser and T. Brandes, *Phys. Rev. B* **94**, 214308 (2016).



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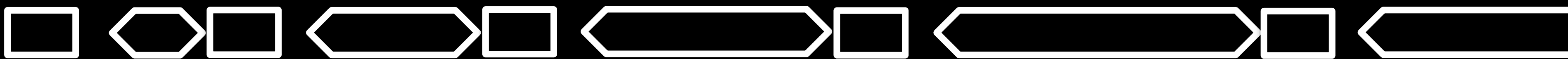
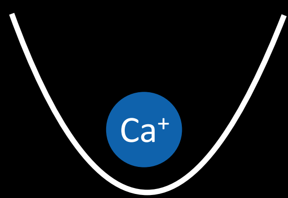
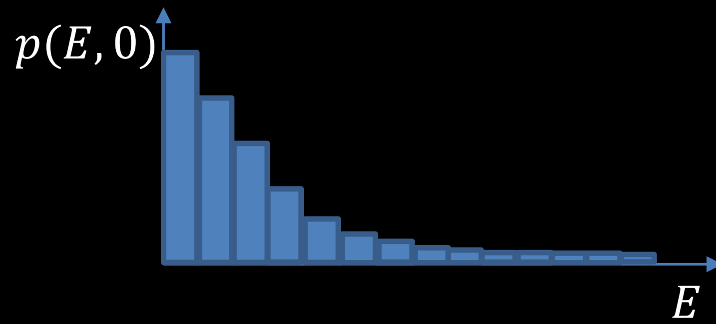
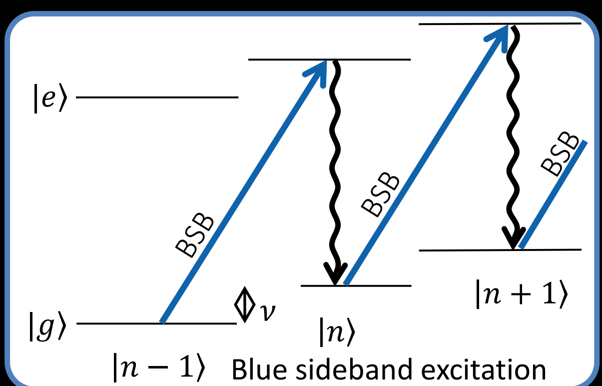
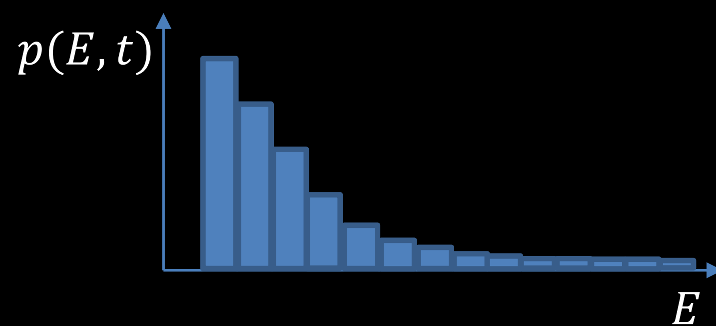


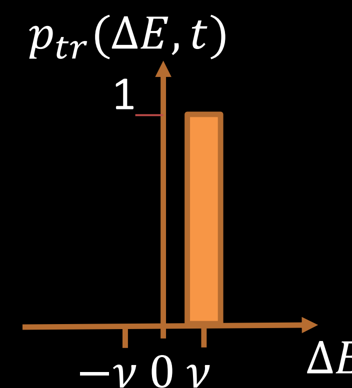




Transferred environmental energy







$$\frac{\int e^{i\chi E} p(E,t)dE}{\int e^{i\chi E} p(E,0)dE} = \int e^{i\chi \Delta E}\, p_{tr}(\Delta E,t)dE\Big|_{\beta=\beta-i\chi}$$

In terms of cumulant generating functions $\lambda(\chi,t,\beta)$:

$$\lambda_{tr}(\chi,t,\beta-i\chi) - \lambda(\chi,t,\beta) = F(\beta-i\chi) - F(\beta)$$

Properties

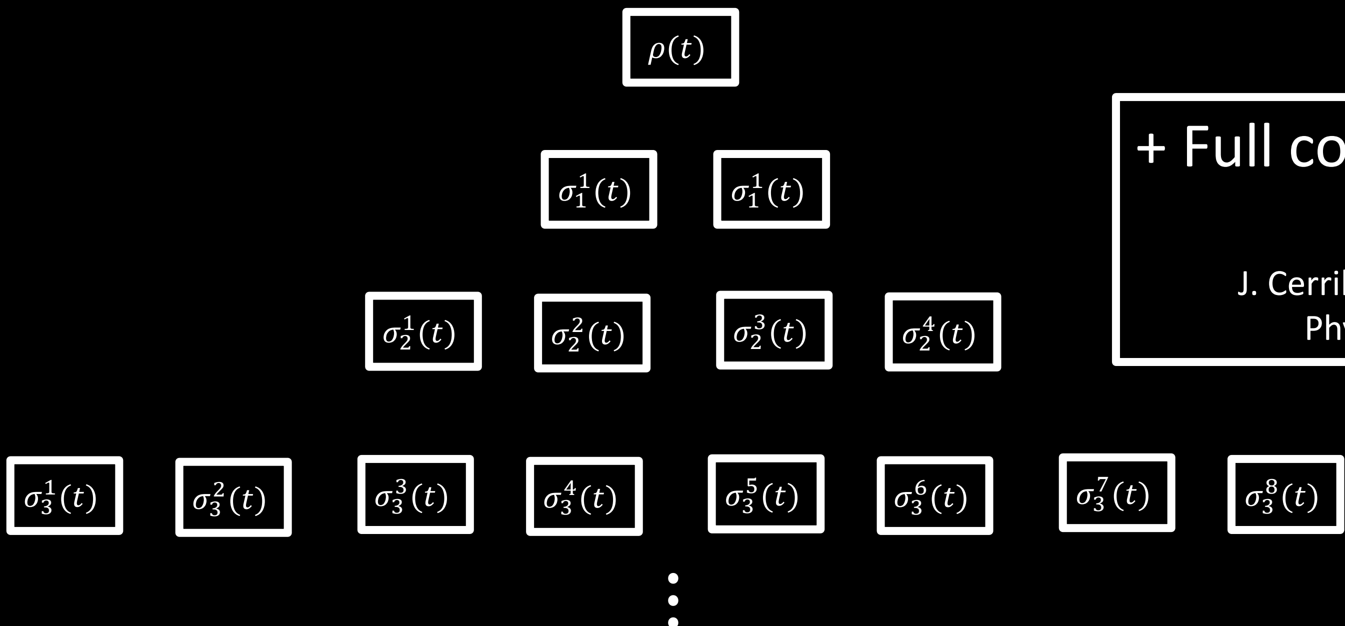
J. Cerrillo, M. Buser and T. Brandes, *Phys. Rev. B* **94**, 214308 (2016).

$$\lambda_{tr}(\chi, t, \beta - i\chi) - \lambda(\chi, t, \beta) = F(\beta - i\chi) - F(\beta)$$

- Relates two non-equilibrium distributions
  - statistics of energy transfer $\lambda_{tr}(\chi, t, \beta)$ to
  - final energy distribution $\lambda(\chi, t, \beta)$.
- Relation holds for
  - **strong coupling** to **non-Markovian** environments
  - **non-thermal** states in the environment ρ_{Env}

Hierarchy of equations of motion

Y. Tanimura and R. Kubo, *J. Phys. Soc. Japan* **58**, 101 (1989).



+ Full counting statistics

J. Cerrillo, M. Buser, and T. Brandes, Phys. Rev. B **94**, 214308 (2016).

$$G_{\Delta E}(\chi, \beta - i\chi, t) = \frac{G_E(\chi, \beta, t)}{G_E(\chi, \beta, 0)}$$

The time propagator of the bath energy pdf $p(E, \beta, t)$ is the analytic continuation of the fluctuation MGF $G_{\Delta E}(\chi, \beta, t)$.

Valid for any coupling strength, degree of non-Markovianity, environmental state…

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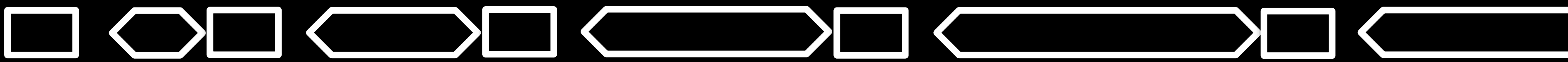
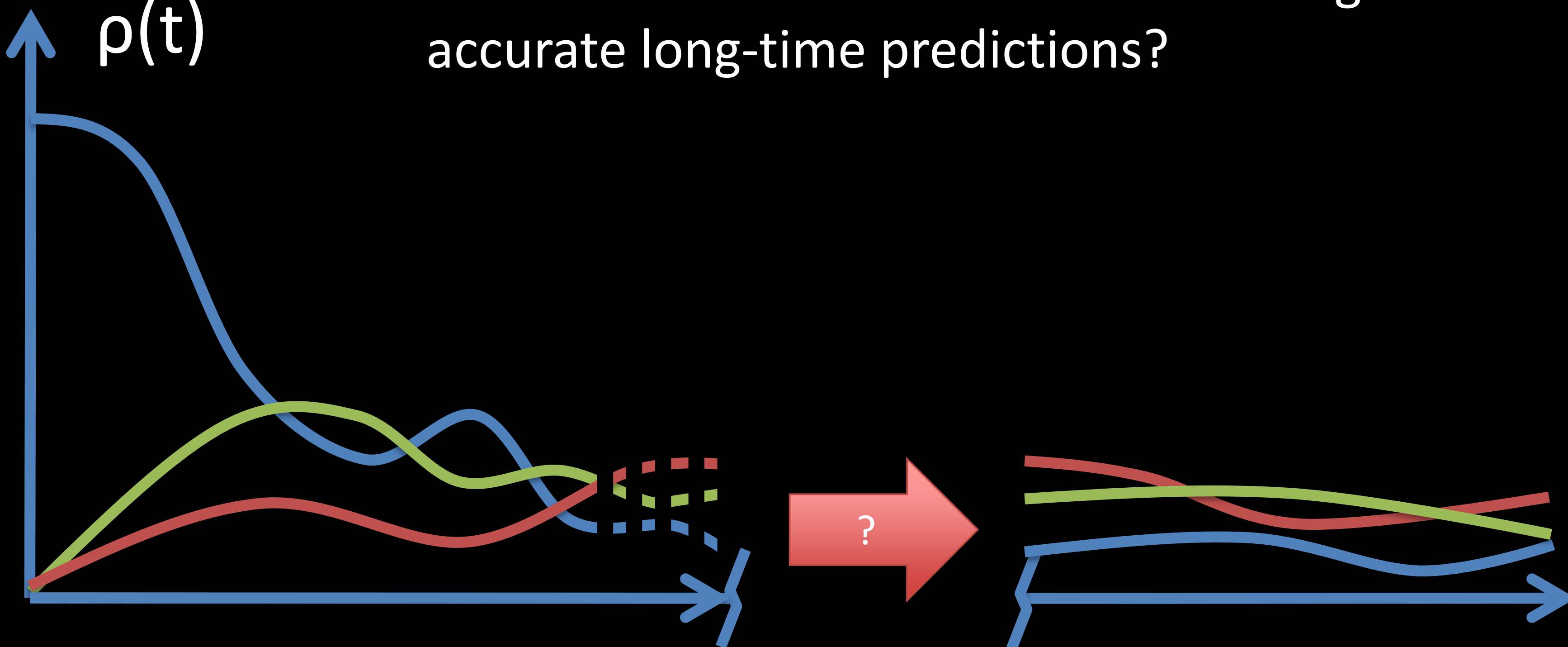
Simulation of general open quantum systems

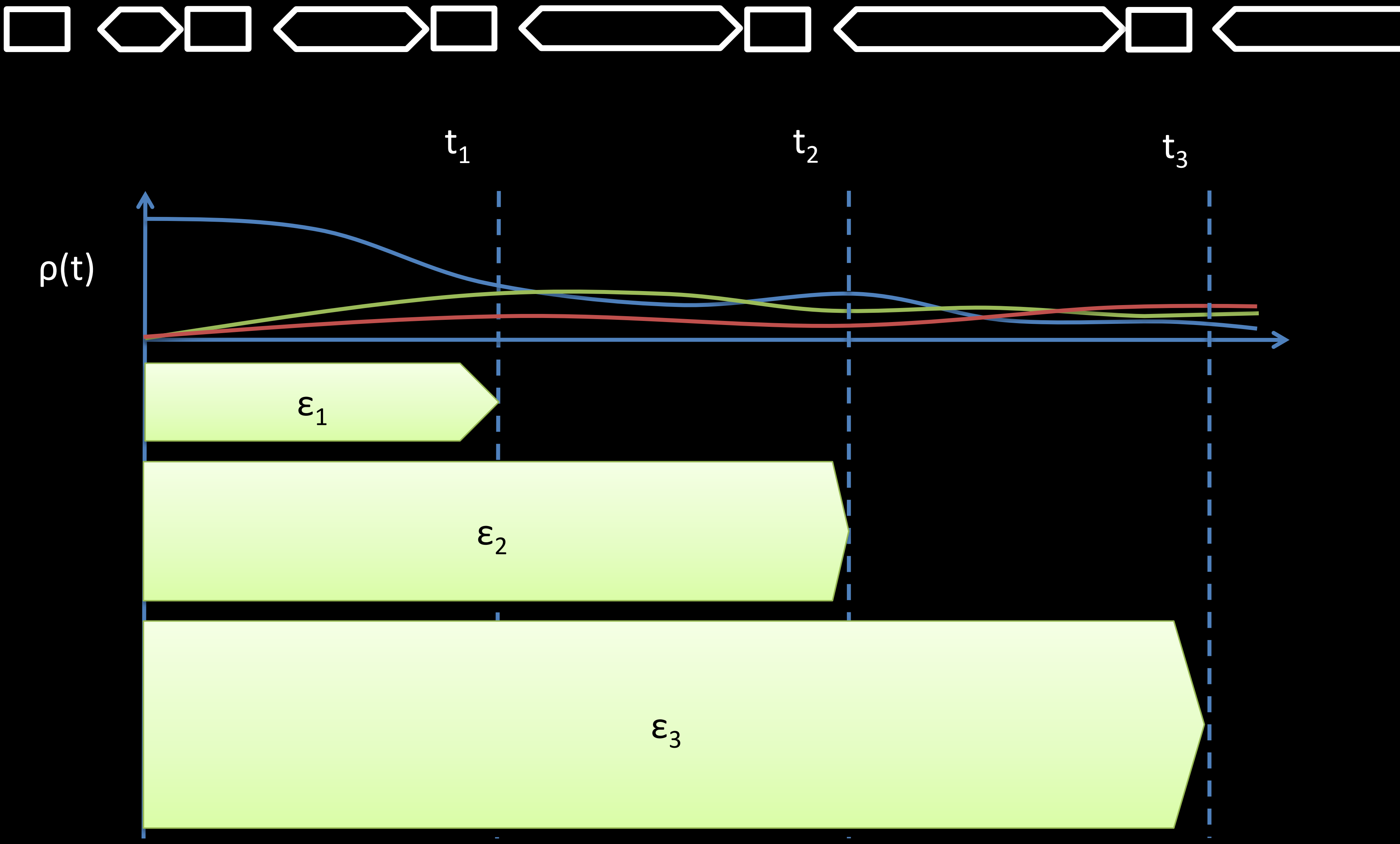


- Easy and accurate for short times
- Demanding and uncertain for long times
- Can one use information short time to generate accurate long-time predictions?



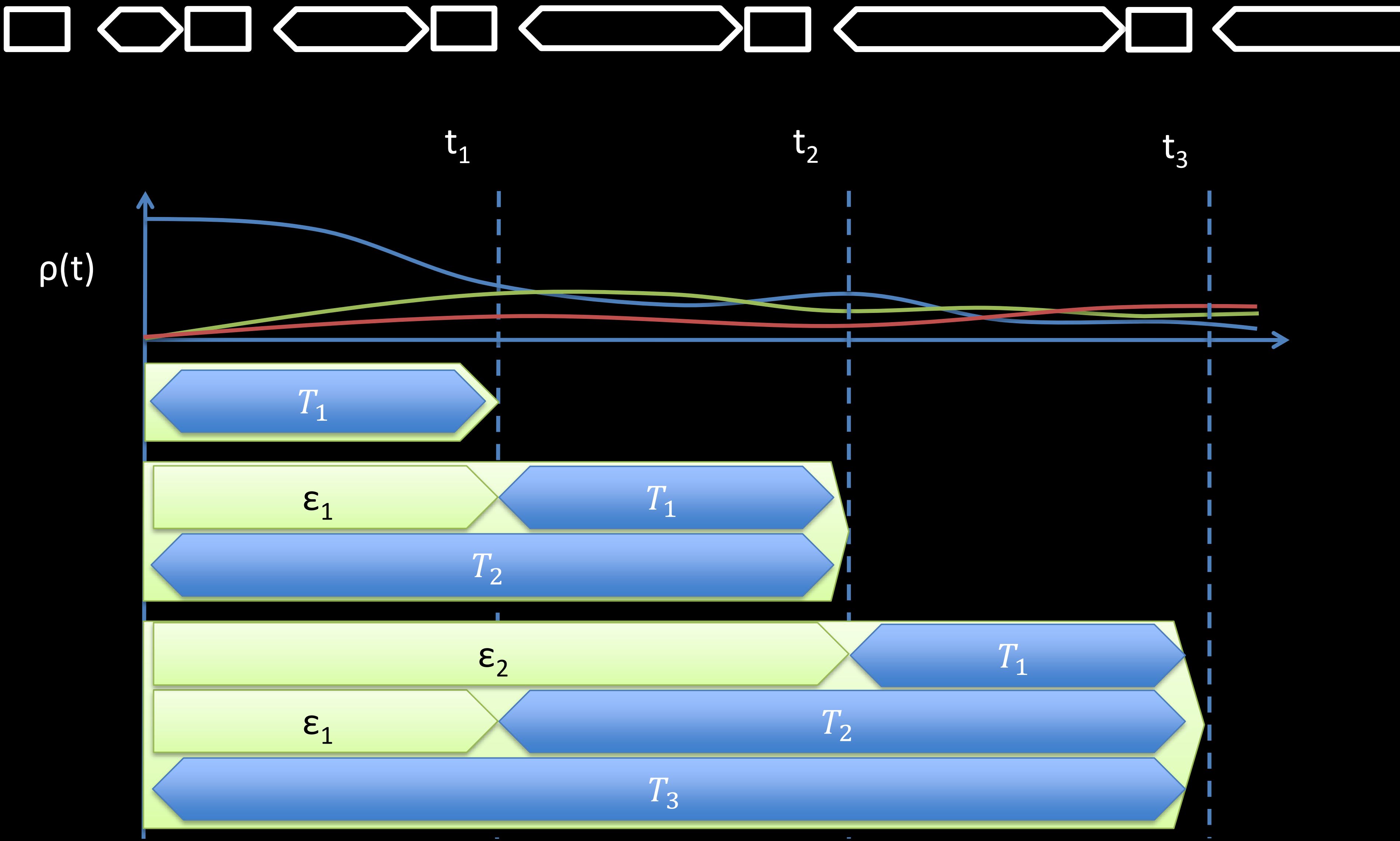
Transfer-Tensor Method

J. Cerrillo, J. Cao, *Phys. Rev. Lett.* **112**, 110401 (2014).



Transfer-Tensor Method

J. Cerrillo, J. Cao, *Phys. Rev. Lett.* **112**, 110401 (2014).



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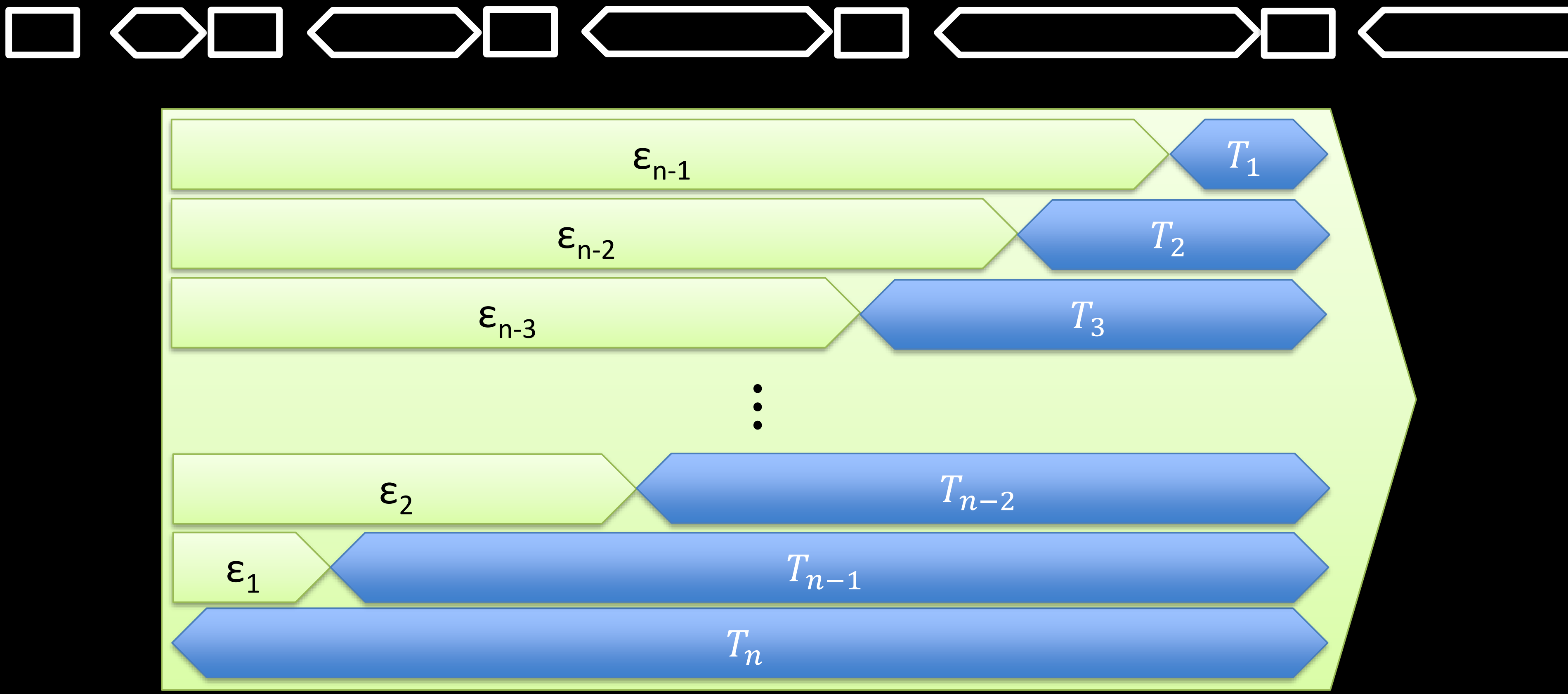
J. Cerrillo, J. Cao, *Phys. Rev. Lett.* **112**, 110401 (2014).

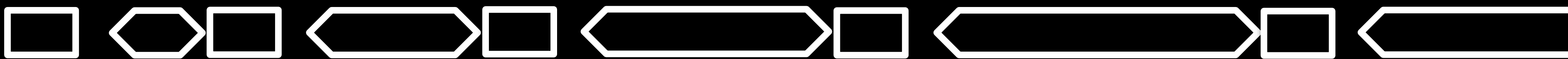


Convolution:

$$\mathcal{E}_n = \sum_{k=1}^{n} T_n \mathcal{E}_{n-k} \quad \Longrightarrow \quad \boxed{\rho(t_n) = \sum_{k=1}^{n} T_n \rho(t_{n-k})}$$

Transfer-Tensor Method

J. Cerrillo, J. Cao, *Phys. Rev. Lett.* **112**, 110401 (2014).



$$\rho(t_n) = \sum_{k=1}^{n} T_n \rho(t_{n-k})$$

Can be understood as a discretization of the

Nakajima-Zwanzig Equation

$$\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t) + \int_0^t \mathcal{K}(t-s)\rho(s)ds$$

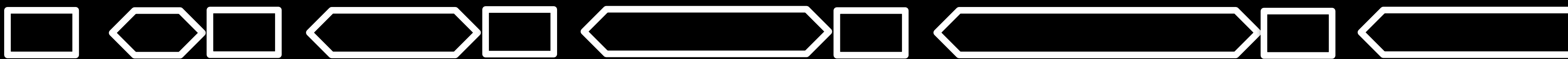
⇕

Memory Kernel

- Transfer Tensors provide the <u>memory effects</u> induced by interaction with the environment.
- For memory effects of finite range one can <u>define a cutoff</u> K above which $T_{k>K} = 0$.
- A <u>multiplicative propagator</u> allows us to efficiently reach long-time simulations.

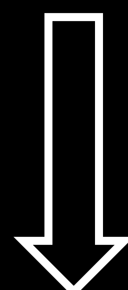
Transfer-Tensor Method

J. Cerrillo, J. Cao, *Phys. Rev. Lett.* **112**, 110401 (2014).



$$\rho(t_n) = \sum_{k=1}^{n} T_n \rho(t_{n-k})$$

$$\rho_n = T_1 \, \rho_{n-1} + T_2 \, \rho_{n-2} + T_3 \, \rho_{n-3} + \cdots$$

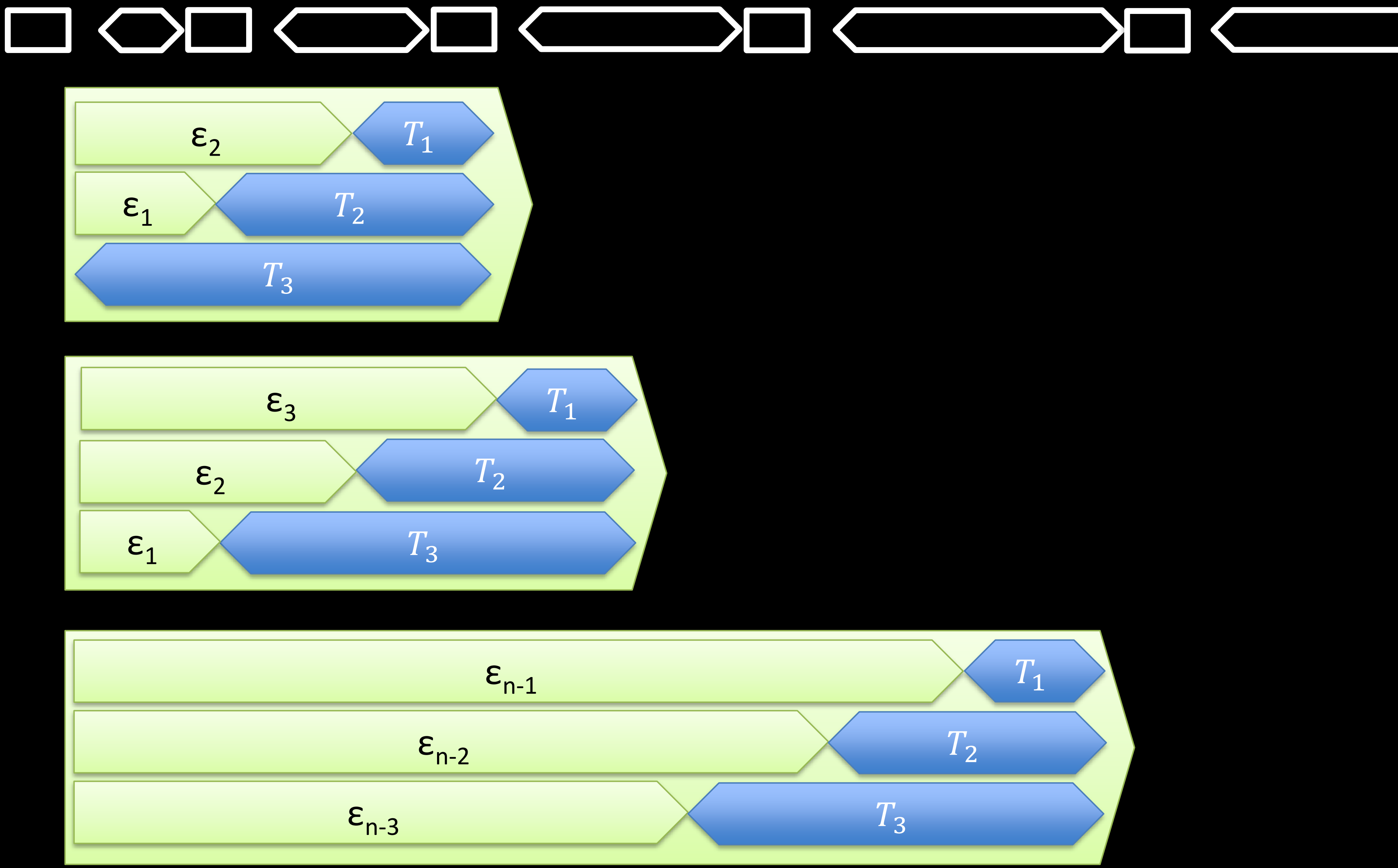


Cutoff K

$$\rho(t_n) = \begin{pmatrix} T_1 & T_2 & T_3 & \cdots & T_K \end{pmatrix} \begin{pmatrix} \rho(t_{n-1}) \\ \rho(t_{n-2}) \\ \rho(t_{n-3}) \\ \vdots \\ \rho(t_{n-K}) \end{pmatrix}$$

Transfer-Tensor Method

J. Cerrillo, J. Cao, *Phys. Rev. Lett.* **112**, 110401 (2014).



QUasi Adiabatic Path Integration (QUAPI)

N. Makri and D. E. Makarov, *J. Chem. Phys.* **102**, 4600 (1995).

QUAPI is a…

- discretization of the path integral of an open quantum system coupled to a

Propagator size for a D dimensional open quantum system and K memory steps

QUAPI	D^{4K}
Transfer Tensors	$D^4 \times K$

TTM is exponentially smaller

- Gaussian environment (Feynman-Vernon Influence Functional).

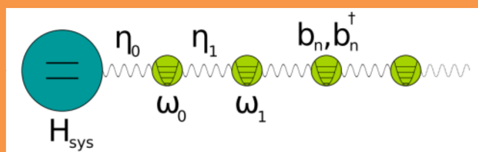
TTM applies to all sorts of environments

- Transfer tensors can be used to compress QUAPI propagator.

Applications

J. Cerrillo, J. Cao, *Phys. Rev. Lett.* **112**, 110401 (2014).

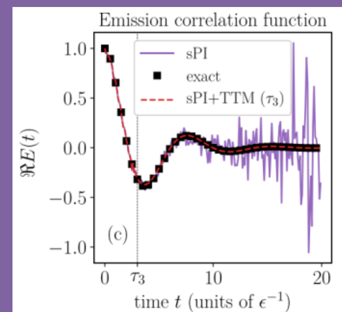
TEDOPA



Chain mapping and DMRG

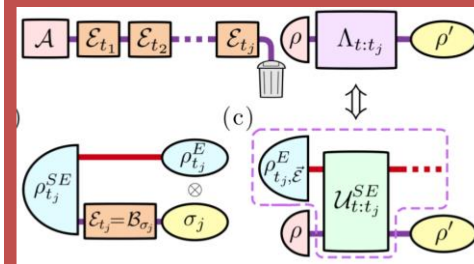
R. Rosenbach, J. Cerrillo, S. F. Huelga, J. Cao, and M. B. Plenio, *New J. Phys.* **18**, 23035 (2016).

Stochastic Methods



M. Buser, J. Cerrillo, G. Schaller, and J. Cao, *Phys. Rev. A* **96**, 062122 (2017).

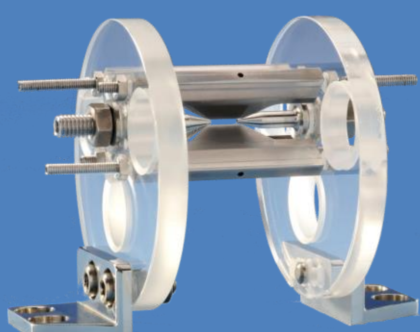
Process tensor



Generalizations of dynamical maps

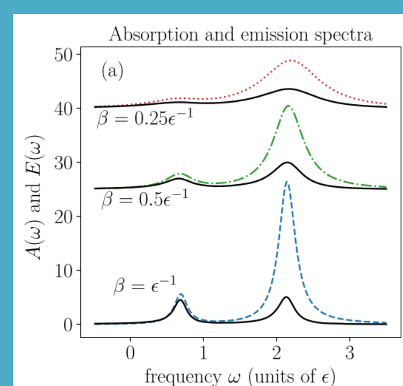
F. A. Pollock, K. Modi, *Quantum* **2**, 76 (2018).

Anharmonic Environments

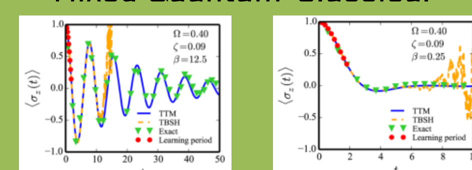


N. Scharnhorst, J. Cerrillo, J. Kramer, I. Leroux, J. Wübbena, A. Retzker, P. O. Schmidt, *PRA* **98**, 023424 (2018).

System-Bath Correlations



Mixed Quantum-Classical



A. A. Kananenka, C.-Y. Hsieh, J. Cao, and E. Geva, *J. Phys. Chem. Lett.* **7**, 4809 (2016).

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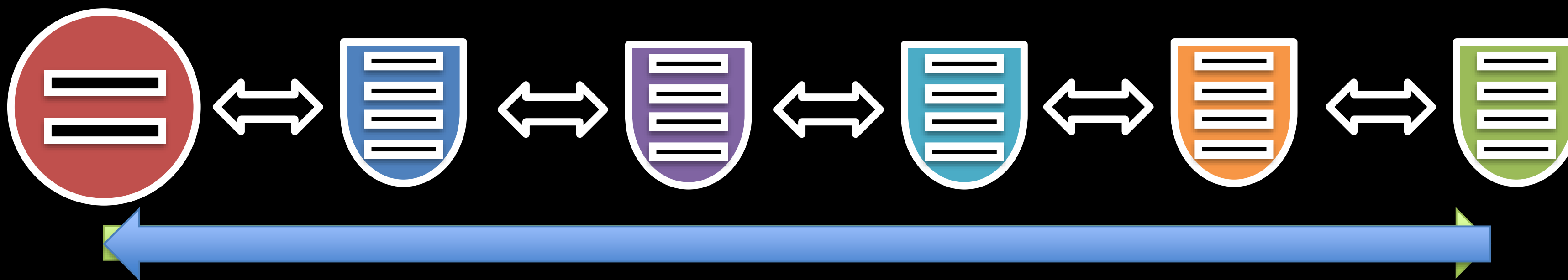
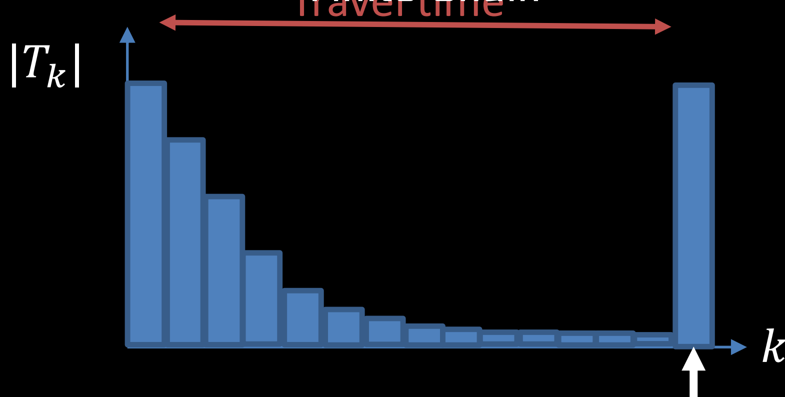
TEDOPA + Transfer Tensors

R. Rosenbach, J. Cerrillo, S. F. Huelga, J. Cao, and M. B. Plenio, *New J. Phys.* **18**, 23035 (2016).

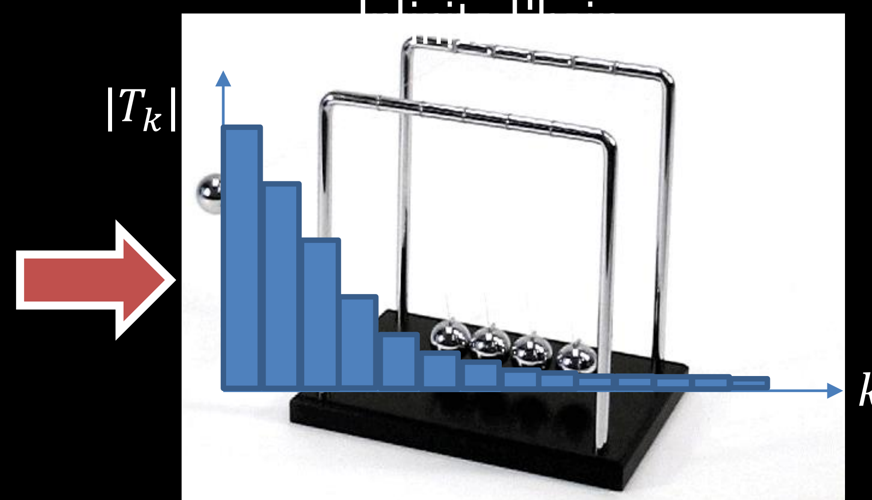
TEDOPA facilitates the study of general spectral densities



Finite Chain



Newton´s cradle effect



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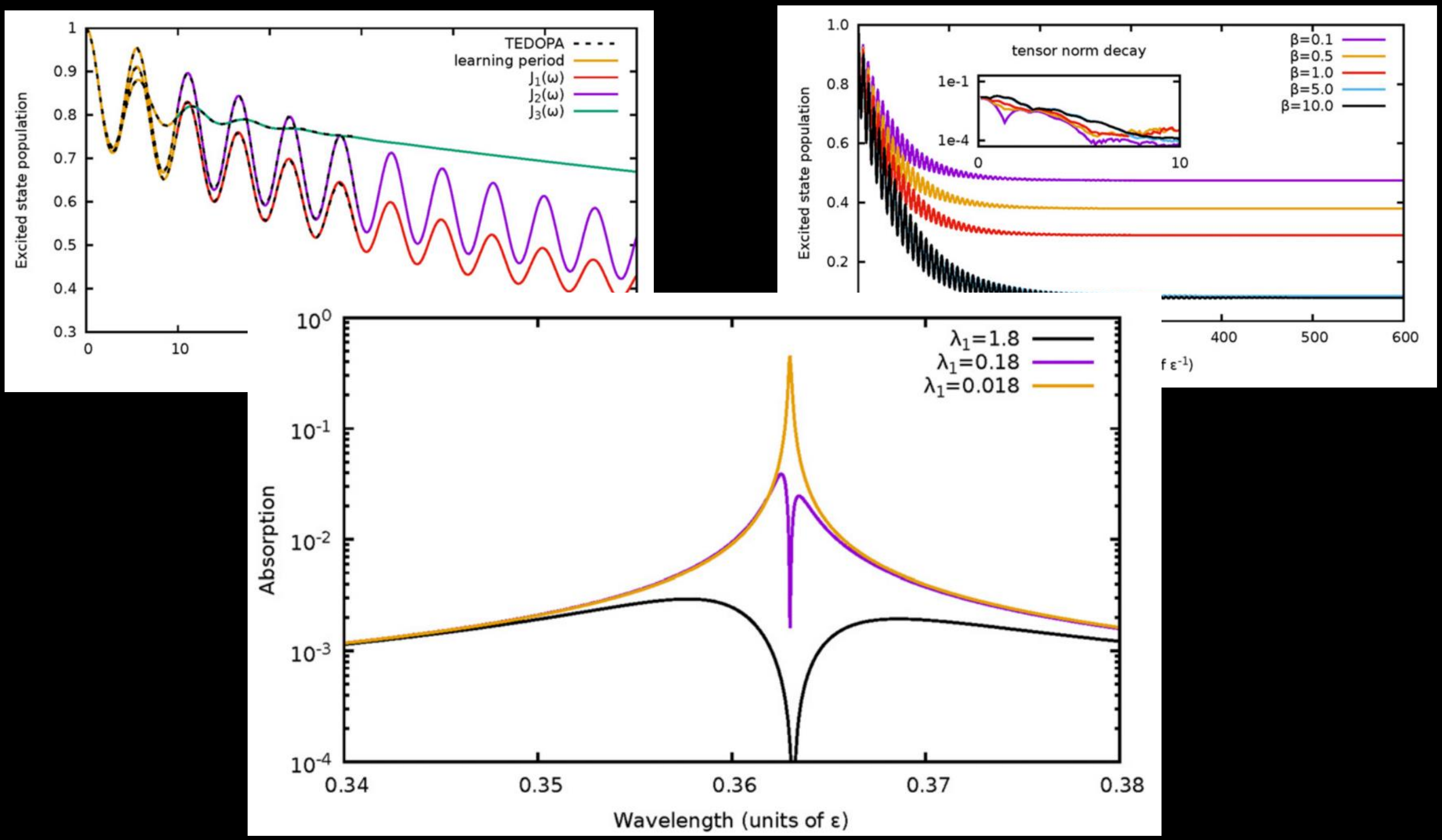

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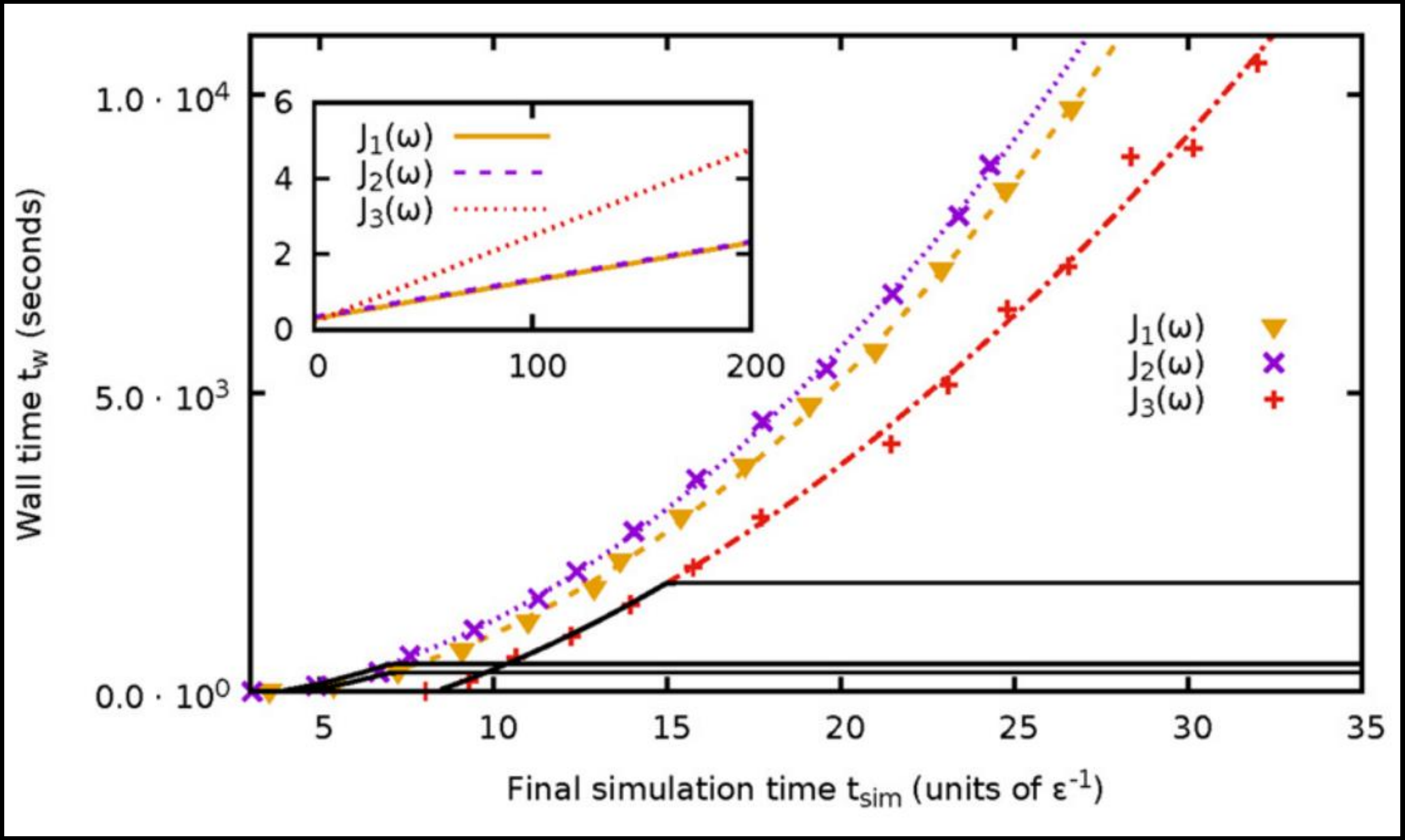

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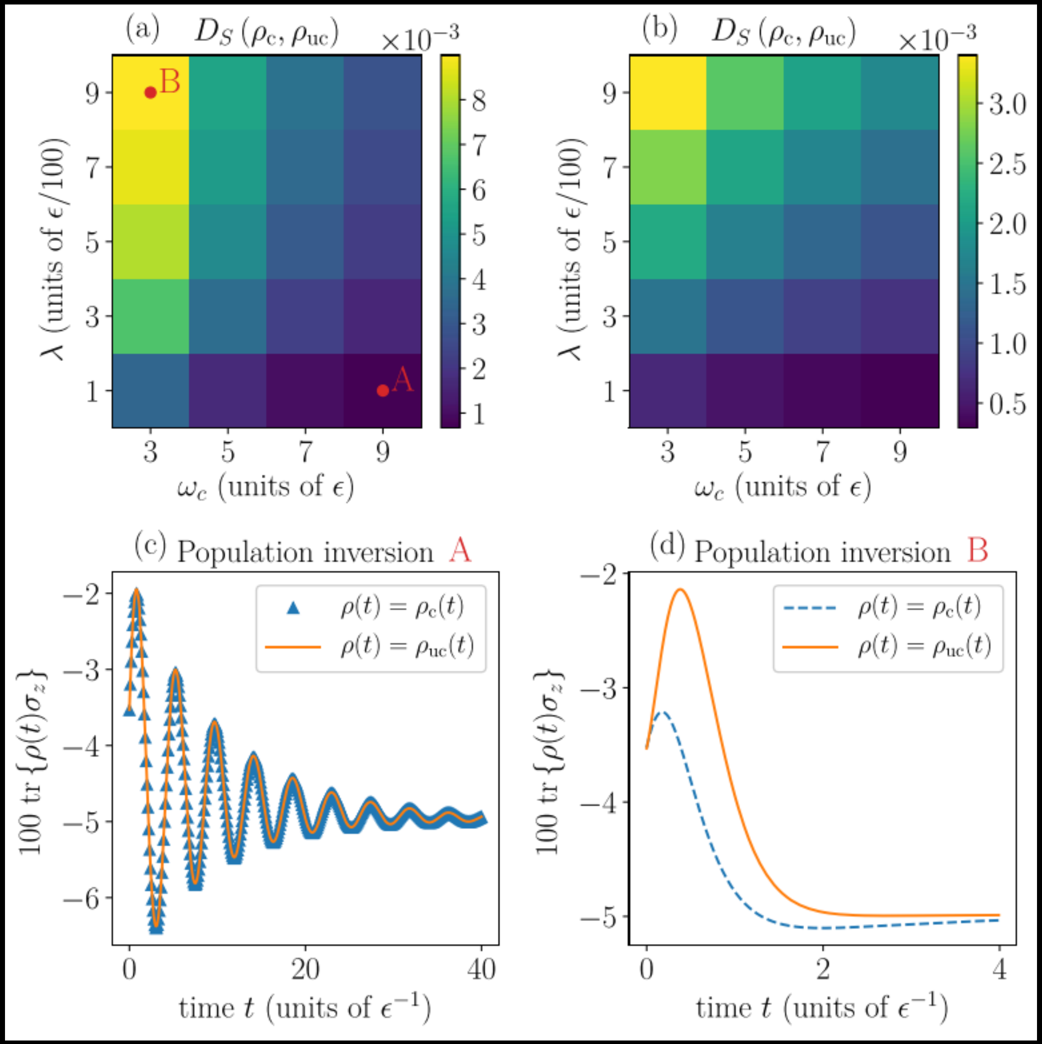
Initial Correlations

M. Buser, J. Cerrillo, G. Schaller, and J. Cao, *Phys. Rev. A* **96**, 062122 (2017).



Effect of dropping initial correlations for:

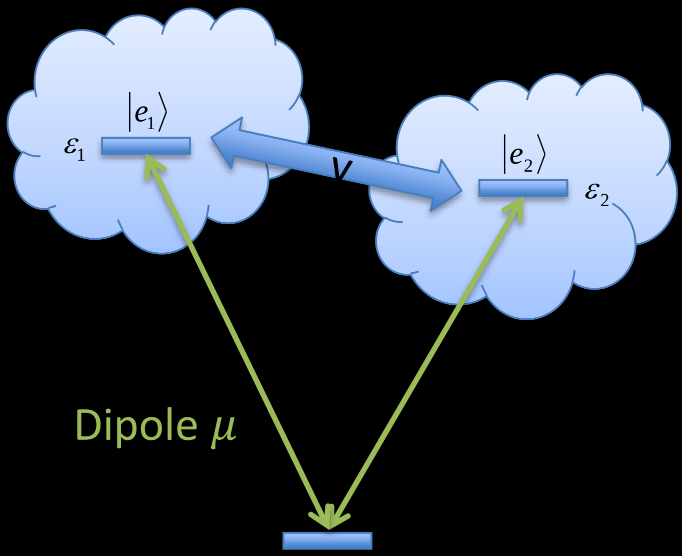
- Global Gibbs state involving system and environment with
  a) unitary in the system
  b) measurement in the system

- Deviations for strong coupling and small bath cutoff frequency, since initial state becomes less separable.

Emission spectra

M. Buser, J. Cerrillo, G. Schaller, and J. Cao, *Phys. Rev. A* **96**, 062122 (2017).

Excitonic dimer with independent baths



Absorption

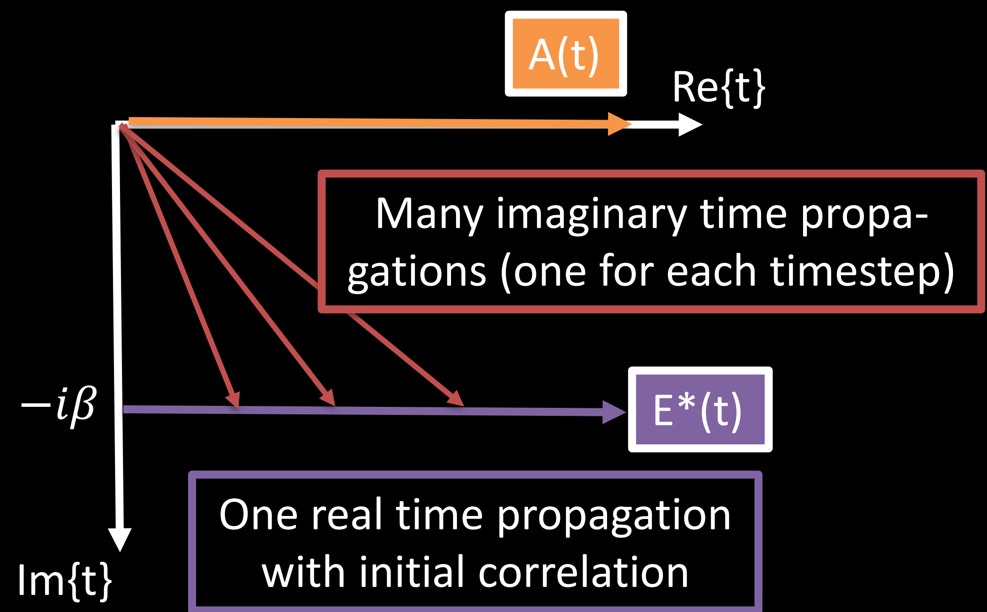
$$A(t) = Tr\{\mu(t)\mu P_g \rho_{ss}\}$$

Emission

$$E(t) = Tr\{\mu(t)\mu P_e \rho_{ss}\}$$

Detailed balance

$$E^*(t) = A(t - i\beta)$$

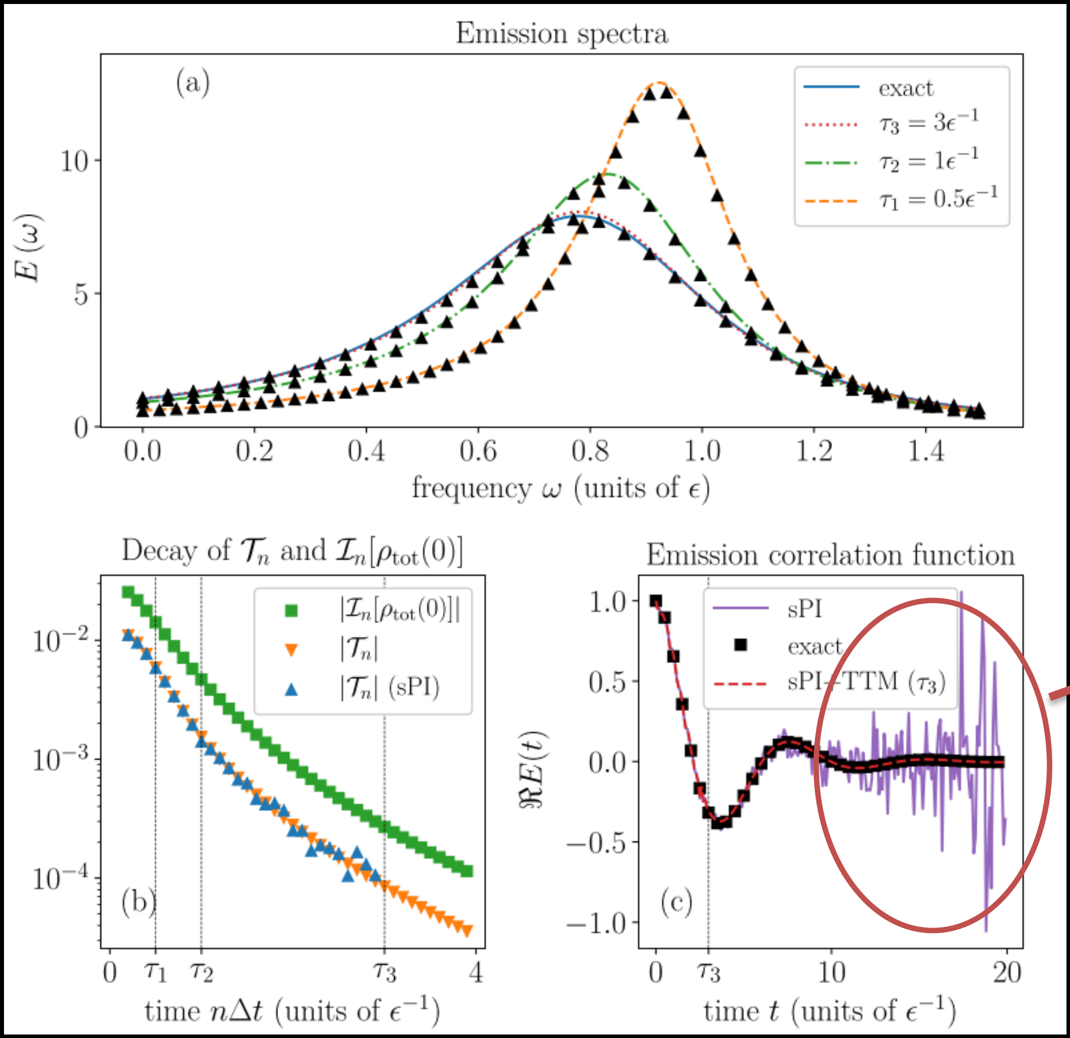


Solution:

Use absorption transfer tensors for emission

Emission spectra

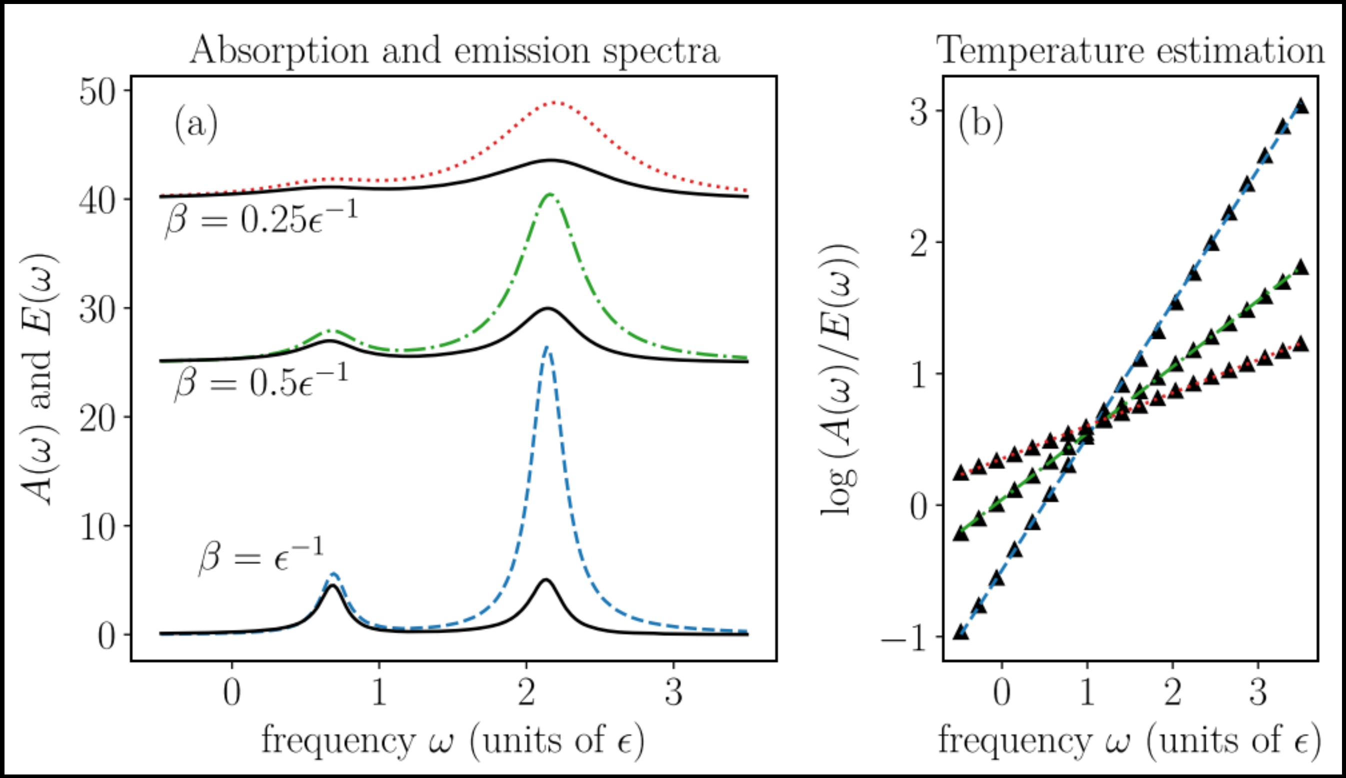
M. Buser, J. Cerrillo, G. Schaller, and J. Cao, *Phys. Rev. A* **96**, 062122 (2017).



Beat stochastic noise

Thermometry

M. Buser, J. Cerrillo, G. Schaller, and J. Cao, *Phys. Rev. A* **96**, 062122 (2017).



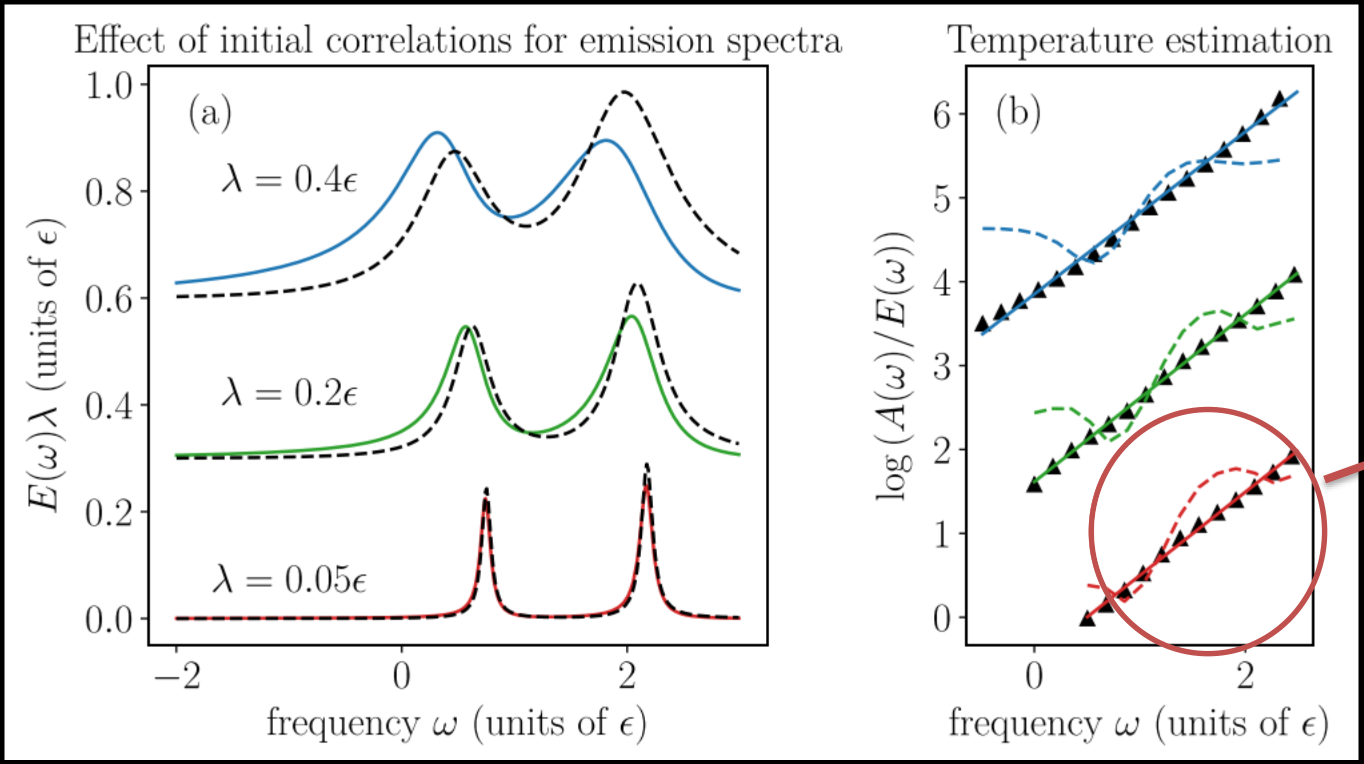
Detailed balance

$$E(-\omega) = e^{-\beta\omega} A(\omega)$$

Thermometry

M. Buser, J. Cerrillo, G. Schaller, and J. Cao, *Phys. Rev. A* **96**, 062122 (2017).

Neglecting initial correlations

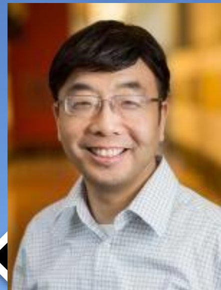


Failure even for weak coupling, where initial correlations are almost negligible

Detailed balance

$$E(-\omega) = e^{-\beta\omega} A(\omega)$$

Summary

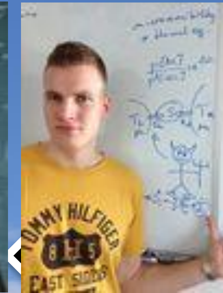

Jianshu Cao


Martin B. Plenio

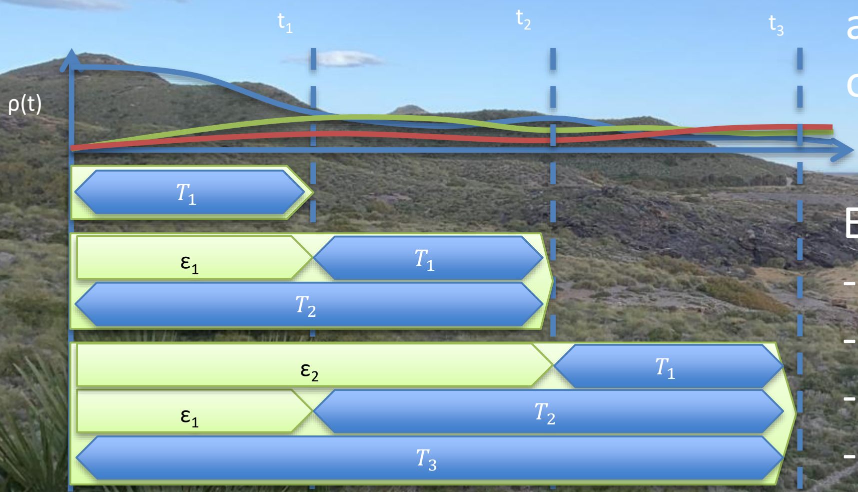

Tobias Brandes


Susana Huelga


Gernot Schaller


Philipp Strasberg

Transfer-Tensor Method



General purpose analysis and propagation tool for open quantum systems.

Especially useful for:
- -Non-Markovian systems
- -Strong-coupling
- -Initial system-bath corr.
- -Long time simulations


Robert Rosenbach


Max Buser


Sebastián Restrepo


Sina Böhling

Thank you for your attention

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