Università degli Studi di Milano, Istituto Nazionale di Fisica Nucleare

CHARACTERIZATION OF HEAT IN NON-MARKOVIAN OPEN QUANTUM SYSTEMS

GIACOMO GUARNIERI

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Contents

- HEAT IN OPEN QUANTUM SYSTEMS
- FULL – COUNTING STATISTICS
- HEAT BACKFLOW: OCCURRENCE AND QUANTIFIER
  - SPIN – BOSON
  - QUANTUM BROWNIAN MOTION
- RELATIONSHIP WITH THE NON-MARKOVIANITY
- CONCLUSIONS

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Heat in open quantum systems

Change in the internal energy $\Delta U(t) = \mathrm{Tr}\left[\mathcal{H}(t)\rho(t)\right] - \mathrm{Tr}\left[\mathcal{H}(0)\rho(0)\right]$

$$\begin{aligned}\Delta U(t) &= \int_0^t d\tau \, \frac{d}{d\tau}\left(\mathrm{Tr}\left[\mathcal{H}(\tau)\rho(\tau)\right]\right) \\ &= \int_0^t d\tau \left(\mathrm{Tr}\left[\frac{d\mathcal{H}(\tau)}{d\tau}\rho(\tau)\right] + \mathrm{Tr}\left[\mathcal{H}(\tau)\frac{d\rho(\tau)}{d\tau}\right]\right) \\ &\equiv \int_0^t d\tau \left[\delta W(\tau) + \delta Q(\tau)\right],\end{aligned}$$

$$W(t) \equiv \int_{t_0}^t d\tau \, \delta W(\tau), \quad Q(t) \equiv \int_{t_0}^t d\tau \, \delta Q(\tau)$$

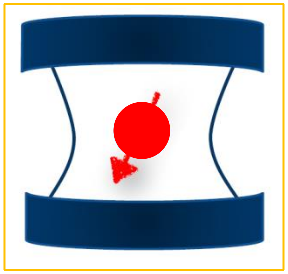
Work
(no change in system's entropy)

Heat
(no change in the Hamiltonian)

$$\Delta U(t) = W(t) + Q(t)$$

First law of thermodynamics

Heat in open quantum systems



Open quantum systems

$$\mathcal{H}(t) = \mathcal{H}_S(t) + \mathcal{H}_E + \mathcal{H}_{SE}(t)$$

Work

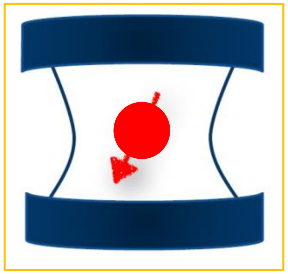
$$W_E(t) = \int_0^t d\tau \, \mathrm{Tr}_E \left[\frac{d\mathcal{H}_E}{dt} \rho_E(t) \right] = 0$$

Heat

$$Q_E(t) \equiv \mathrm{Tr}_E \left[\mathcal{H}_E \left(\rho_E(t) - \rho_E(0) \right) \right] = \int_0^t d\tau \, \mathrm{Tr}_E \left[\mathcal{H}_E \frac{d\rho_E(t)}{dt} \right]$$

Heat in open quantum systems

Open quantum systems



$$\mathcal{H}(t) = \mathcal{H}_S(t) + \mathcal{H}_E + \mathcal{H}_{SE}(t)$$

Work $W_E(t) = \int_0^t d\tau \, \mathrm{Tr}_E \left[\frac{d\mathcal{H}_E}{dt} \rho_E(t) \right] = 0$

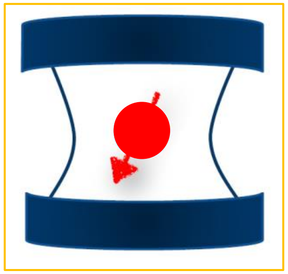
Heat $Q_E(t) \equiv \mathrm{Tr}_E [\mathcal{H}_E \boxed{(\rho_E(t)} -$

$\int^t_0 d\tau \, \mathrm{Tr}_E \left[\mathcal{H}_E \frac{d\rho_E(t)}{dt} \right]$

Heat in open quantum systems

Open quantum systems

$$\mathcal{H}(t) = \mathcal{H}_S(t) + \mathcal{H}_E + \mathcal{H}_{SE}(t)$$



Work

$$W_E(t) = \int_0^t d\tau\, \mathrm{Tr}_E\left[\frac{d\mathcal{H}_E}{dt}\rho_E(t)\right] = 0$$

Heat

$$\boxed{Q_E(t)} \equiv \mathrm{Tr}_E\,[\mathcal{H}_E\,(\boxed{\rho_E(t)} -$$

$$\int_0^t d\tau\, \mathrm{Tr}_E\left[\mathcal{H}_E \frac{d\rho_E(t)}{dt}\right]$$

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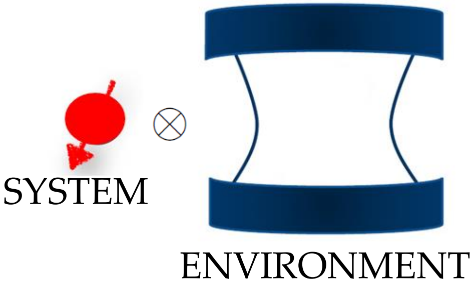
Full – Counting Statistics

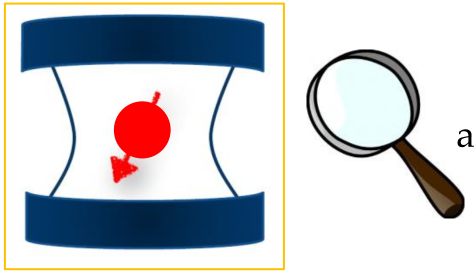
①



Consider a composite system starting in a product state:

$$\rho_{SE}(0) = \rho_S(0) \otimes \rho_E$$

②



Perform a measurement of an environmental observable A at initial time

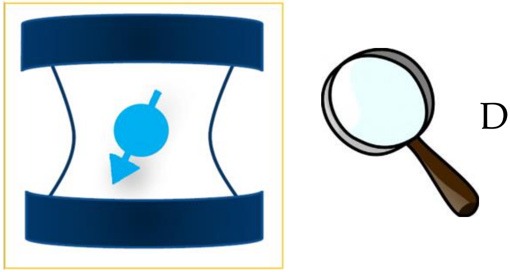
$$\rho'_{SE}(0) = \frac{\Pi_{q_0}\rho_{SE}\Pi_{q_0}}{\mathrm{Tr}_{SE}\left\{\rho_{SE}\Pi_{q_0}\right\}}$$

③

Let the overall system undergo the coupled evolution $U(t,0)$

$$\rho'_{SE}(t) = U(t,0)\rho'_{SE}(0)U^\dagger(t,0)$$

④



Detatch S and E and perform Another measurement of the same observable A at time t

$$\rho''_{SE}(t) = \frac{\Pi_{q_t}\rho'_{SE}(t)\Pi_{q_t}}{\mathrm{Tr}_{SE}\left\{\rho'_{SE}(t)\Pi_{q_t}\right\}}$$

Esposito, Harbola, Mukamel, Rev. Mod. Phys. **81**, 1665 (2009)

Full – Counting Statistics

- The probability distribution $p_t(\Delta a)$ for a change $\Delta a \equiv a_t - a_0$ to occur between time 0 and time t is given by

$$p_t(\Delta a) = \sum_{a_0, a_t} \mathbb{P}_t\left[a_t; a_0\right] \delta(\Delta a - a_t + a_0)$$

where $\mathbb{P}_t\left[a_t; a_0\right] = \mathrm{Tr}\left[\hat{\Pi}_{a_t} \hat{U}(t,0) \hat{\Pi}_{a_0} \rho(0) \hat{\Pi}_{a_0} \hat{U}^{\dagger}(t,0) \hat{\Pi}_{a_t}\right]$

- Upon introducing the cumulant generating function

$$\Theta(\eta, t) \equiv \ln\langle e^{i\eta\Delta a}\rangle_t = \ln \int d(\Delta a)\, p_t(\Delta a) e^{i\eta\Delta a}$$

the cumulants of Δa are obtained by derivation as

$$\langle(\Delta a)^n\rangle_t = (-i)^n \frac{\partial^n}{\partial\eta^n} \Theta(\eta, t)|_{\eta=0}$$

Full – Counting Statistics

- **MAIN POINT:** The cumulant generating can be written as

$$\boxed{\Theta(\eta,t) = \ln \mathrm{Tr}_S\left[\rho_S(\eta,t)\right]}$$

where

System’s operator

$$\rho_S(\eta,t) \equiv \mathrm{Tr}_E\left\{U_{\eta/2}(t,0)\rho_{SE}(0)U^{\dagger}_{-\eta/2}(t,0)\right\}$$

with $$\hat{U}_\eta(t,0) = e^{i\eta\hat{A}(t)}\hat{U}(t,0)e^{-i\eta\hat{A}(0)}$$

Modified evolution operator: usual evolution conditioned on a two-time measurement of the observable A.

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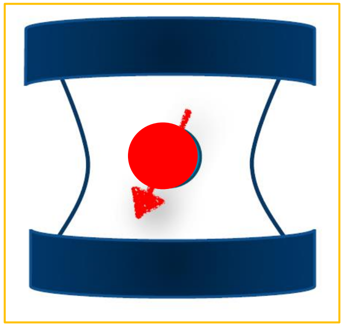
Heat Backflow: occurrence and quantifier



$$\Theta(\eta, t) = \ln \mathrm{Tr}_S \left[\rho_S(\eta, t)\right]$$

- $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E$
- Weak coupling between S and E
- $\frac{d}{dt}\rho_S(\eta, t) = \Xi^{\eta}(t)\rho_S(\eta, t)$

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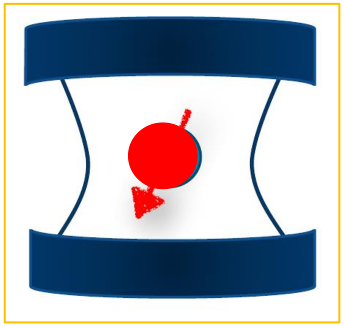
$$\Theta(\eta,t) = \ln \mathrm{Tr}_S\left[\rho_S(\eta,t)\right]$$



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FINITE DIMENSIONAL SYSTEMS

$$\rho_S(\eta,t) = T_+ \exp\left[\int_0^t d\tau \Xi^\eta(\tau)\right]\rho_S(0). \rightarrow |\rho_S(\eta,t)\rangle = T_+ \exp\left[\int_0^t d\tau \mathbf{\Xi}^\eta(\tau)\right]|\rho_S(0)\rangle \equiv \mathbf{\Lambda}^\eta(t,0)\,|\rho_S(0)\rangle$$

$$\rightarrow \quad \langle\Delta q\rangle_t = \int_0^t d\tau\theta(\tau) \qquad \theta(t) \equiv \langle\mathbb{1}|\,\frac{\partial\mathbf{\Xi}^\eta(t)}{\partial(i\eta)}\Big|_{\eta=0}|\rho_S(t)\rangle$$

Heat Backflow: occurrence and quantifier

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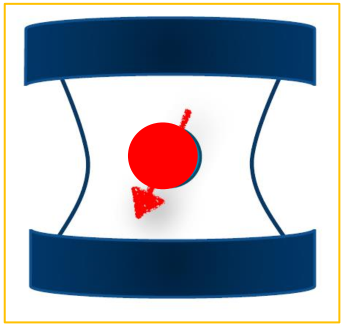

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INFINITE DIMENSIONAL SYSTEMS

$$\chi\left[\rho_S(\eta,t)\right](\lambda,\lambda^*) \equiv \chi^{(\eta)}(\lambda,\lambda^*,t) = \mathrm{Tr}_S\left[\rho_S(\eta,t)e^{\lambda a^\dagger - \lambda^* a}\right]$$

$$\Theta(\eta,t) = \ln \mathrm{Tr}_S\left[\rho_S(\eta,t)\right] = \ln \chi^{(\eta)}(0,0,t)$$

$$\rightarrow \quad \langle \Delta q \rangle_t = \frac{\partial \chi^{(\eta)}(0,0,t)}{\partial(i\eta)}\Big|_{\eta=0} \qquad \theta(t) = \frac{\partial \dot{\chi}^{(\eta)}(0,0,t)}{\partial(i\eta)}\Big|_{\eta=0}$$

Heat Backflow: occurrence and quantifier

Born-Markov and RWA approximations

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}\;\rho(t) = -i[H\,,\rho(t)] + \sum_m \Delta_m\left[C_m\,\rho C_m^\dagger - \frac{1}{2}\left\{C_m^\dagger C_m\,,\rho\right\}\right]$$

Time-independent GKSL master equation

Heat Backflow: occurrence and quantifier

Born-Markov and RWA approximations

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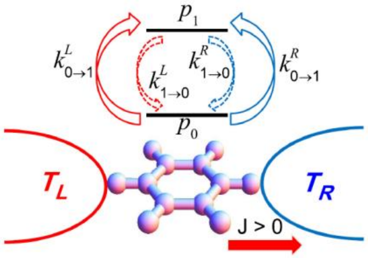

$$\vartheta(\eta) \;=\; lim_{t\to+\infty}\Theta(\eta,t)/t \quad\longrightarrow\quad \langle\Delta q\rangle_t \approx \langle\Delta q\rangle t$$

Temperature-induced **steady** heat flow from hot to cold subsystem

Esposito *et al.*, RMP **81**, 1665 (2009); Ren *et al.*, PRL **104**, 170601 (2010); C. Uchiyama PRE **89**, 052108 (2014)

Heat Backflow: occurrence and quantifier

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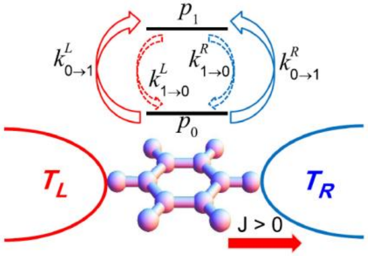

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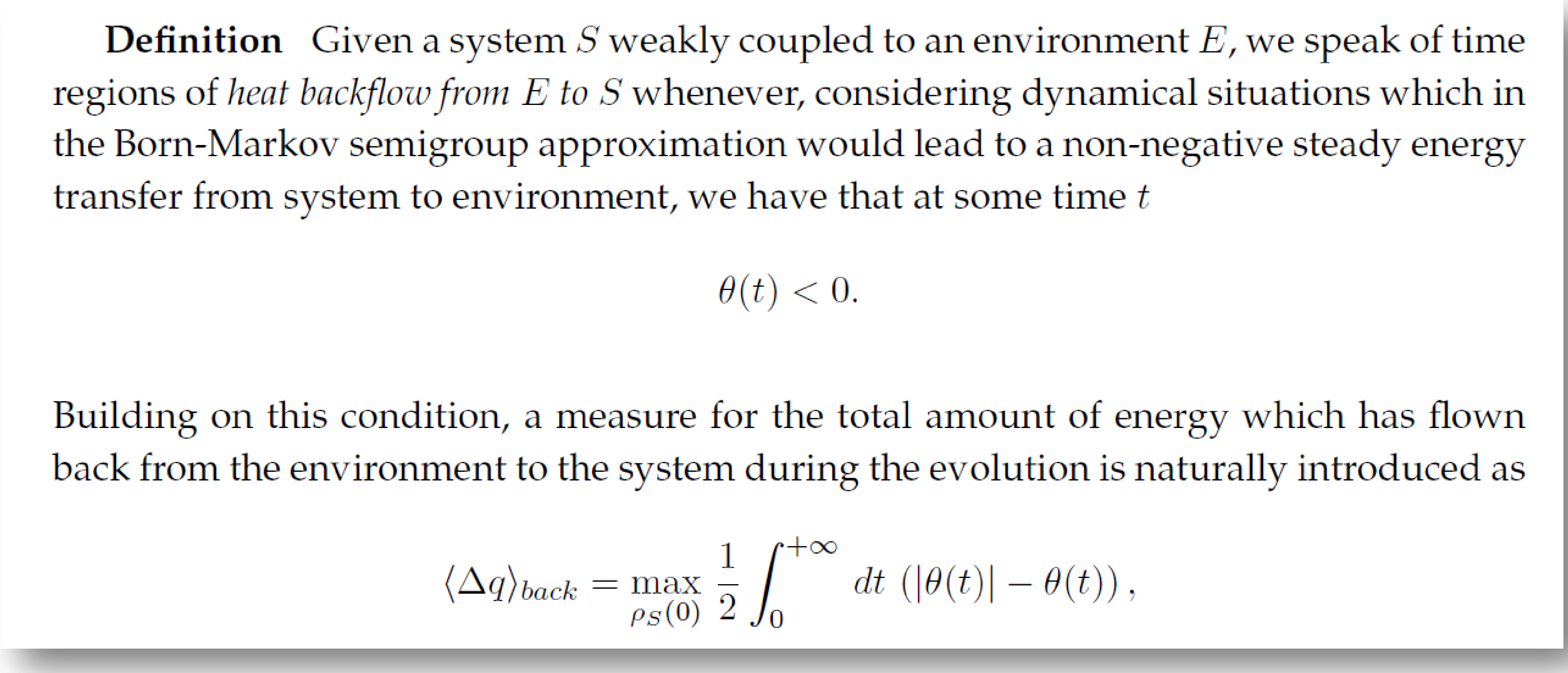
Beyond GKSL

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}_t\rho(t) = -i[H(t), \rho(t)] + \sum_m \Delta_m(t) \left[C_m(t)\rho C_m^\dagger(t) - \frac{1}{2}\left\{C_m^\dagger(t) C_m(t), \rho\right\}\right]$$

$$\Theta(\eta,t) = \ln \mathrm{Tr}_S\left[\rho_S(\eta,t)\right]$$

$$\langle\Delta q\rangle_t = \int_0^t d\tau\theta(\tau)$$

Heat Backflow: occurrence and quantifier



Definition Given a system S weakly coupled to an environment E, we speak of time regions of *heat backflow from E to S* whenever, considering dynamical situations which in the Born-Markov semigroup approximation would lead to a non-negative steady energy transfer from system to environment, we have that at some time t

$$\theta(t) < 0.$$

Building on this condition, a measure for the total amount of energy which has flown back from the environment to the system during the evolution is naturally introduced as

$$\langle \Delta q \rangle_{back} = \max_{\rho_S(0)} \frac{1}{2} \int_0^{+\infty} dt \, \left(|\theta(t)| - \theta(t) \right),$$

G. Guarnieri, C. Uchiyama, B. Vacchini, PRA **93**, 012118 (2016)

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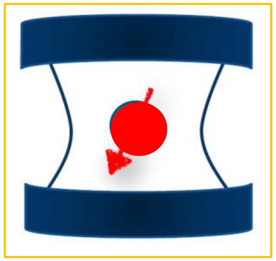
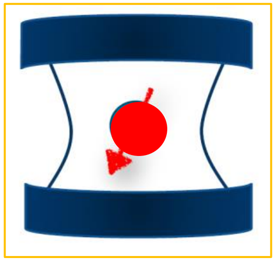
Application to the Spin – boson model



- The two – level system is coupled to an environment consisting of an infinite number of bosonic modes.
- The Hamiltonian is $\mathcal{H} = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sigma_x \otimes B_E$

$$B_E \equiv \sum_k \left(g_k b_k^\dagger + g_k^* b_k \right)$$

Application to the Spin – boson model



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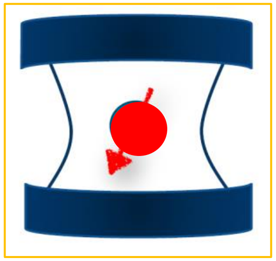
$$B_E \equiv \sum_k \left(g_k b_k^\dagger + g_k^* b_k \right)$$

- The ME obtained through second – order TCL expansion of the generator has the form $\frac{d}{dt}\rho^\eta(t) = \Xi^{(\eta)}(t)\rho^\eta(t)$
- The energy flow per unit of time has the form $\theta(t) \equiv \langle 1|\frac{\partial \boldsymbol{\Xi}^{(\eta)}(t)}{\partial(i\eta)}|\rho_S(t)\rangle_{|\eta=0}$

Application to the Spin – boson model



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$$\Xi^\eta(t) = -\int_0^t d\tau \begin{pmatrix} V_+(\tau) & 0 & 0 & W_+^\eta(\tau) \\ 0 & Y_+(\tau) & Z_+^\eta(\tau) & 0 \\ 0 & Z_-^\eta(\tau) & Y_-(\tau) & 0 \\ W_-^\eta(\tau) & 0 & 0 & V_-(\tau) \end{pmatrix}$$

$$V_\pm(\tau) = \Phi(\tau)e^{\mp i\omega_0\tau} + \Phi(-\tau)e^{\pm i\omega_0\tau},$$

$$W_\pm^\chi(\tau) = -\left[\Phi(\tau-\chi)e^{\pm i\omega_0\tau} + \Phi(-\tau-\chi)e^{\mp i\omega_0\tau}\right],$$

$$Y_\pm(\tau) = 2Re\left[\Phi(\tau)\right]e^{\mp i\omega_0\tau},$$

$$Z_\pm^\chi(\tau) = -\left[\Phi(\tau-\chi) + \Phi(-\tau-\chi)\right]e^{\pm i\omega_0\tau}.$$

Environmental correlation function

$$\Phi(\tau) = \int_0^{+\infty} d\omega\, J(\omega) \left[\coth\left(\frac{\omega}{2T_E}\right)\cos(\omega\tau) - i\sin(\omega\tau)\right]$$

Application to the Spin – boson model

- Assuming the spetral density to be of the form $J(\omega) = \lambda \omega e^{-\frac{\omega}{\Omega}}$
- $\rho_S(0) = Z^{-1}\left(|0\rangle\langle 0| + e^{-\omega_0/T_S}|1\rangle\langle 1|\right) , \quad Z = 1+e^{-\omega_0/T_S}$
- $T_S \geq T_E$

Application to the Spin – boson model

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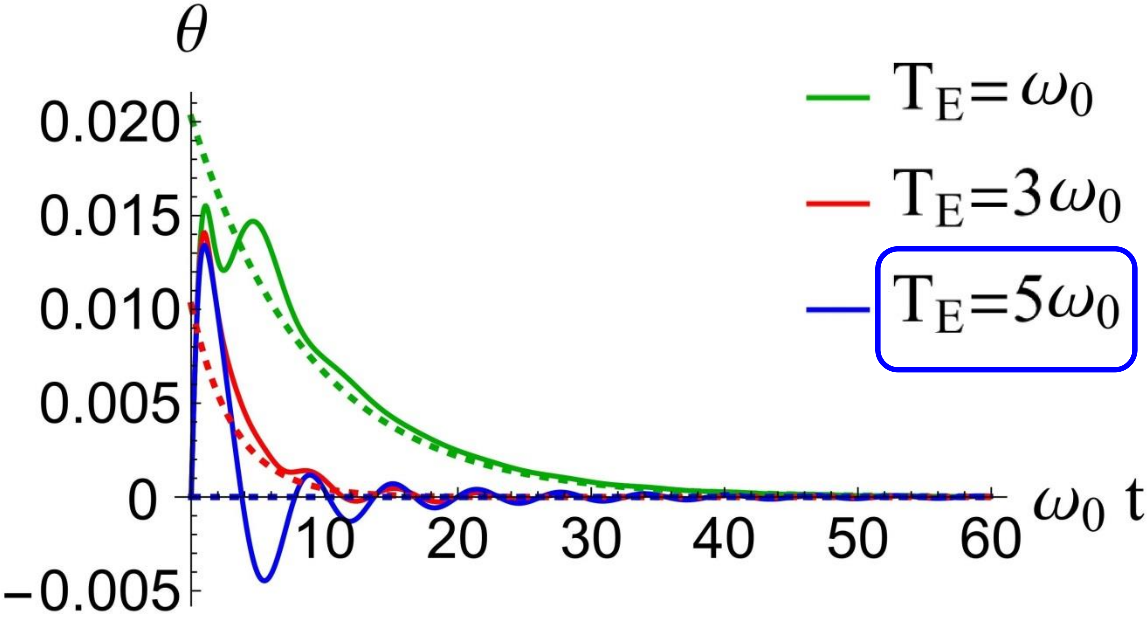


$\Omega = 0.4\,\omega_0$

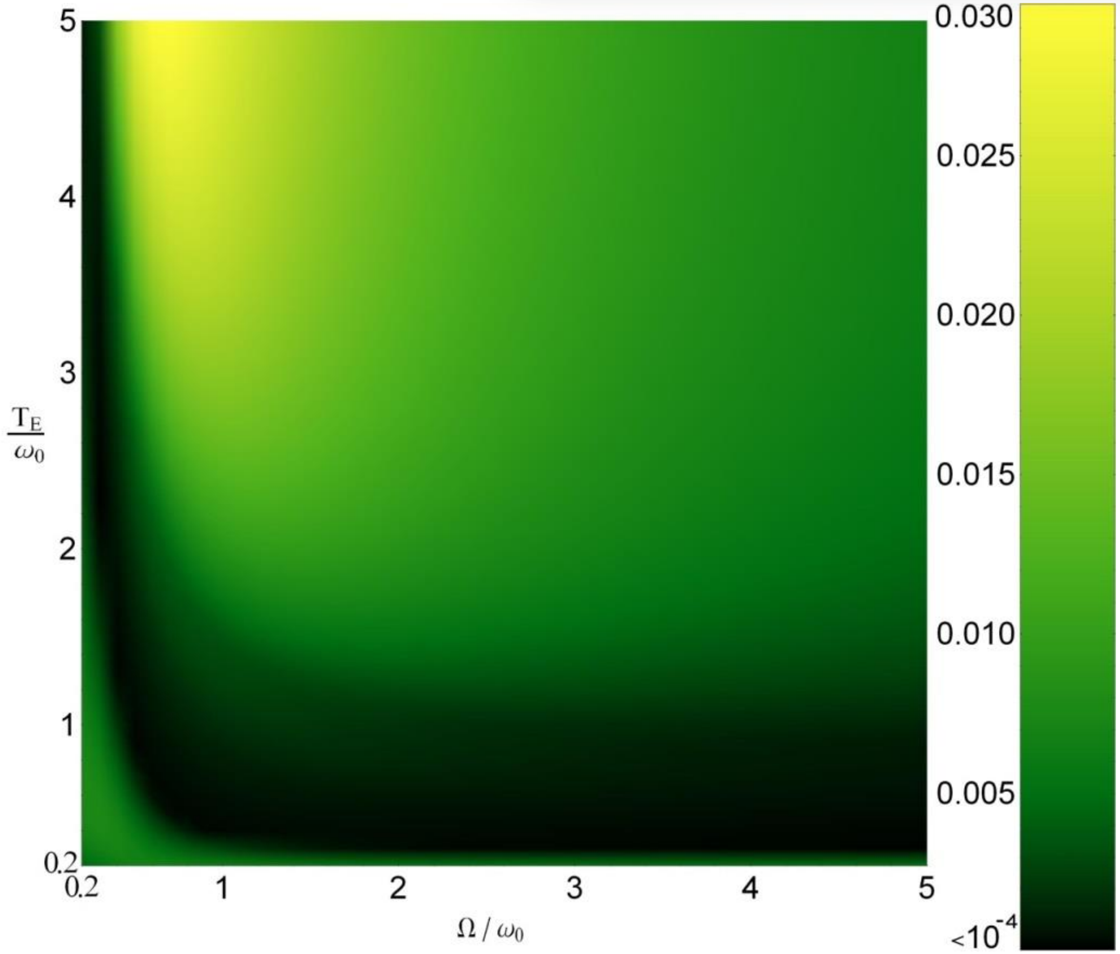
$\lambda = 0.1$

$\boxed{T_S = 5\omega_0}$

For every value of λ, Ω and T_E the heat backflow is maximized by the choice $T_S = T_E$

Application to the Spin – boson model

$$\langle \Delta q \rangle_{back} = \max_{\rho_S(0)} \frac{1}{2} \int_0^{+\infty} dt \, \left(|\theta(t)| - \theta(t) \right)$$



- $\lambda = 0.1$
- $T_S = T_E$
- Region of max heat backflow
- Region of absent heat backflow

G. Guarnieri, C. Uchiyama, B. Vacchini, PRA **93**, 012118 (2016)

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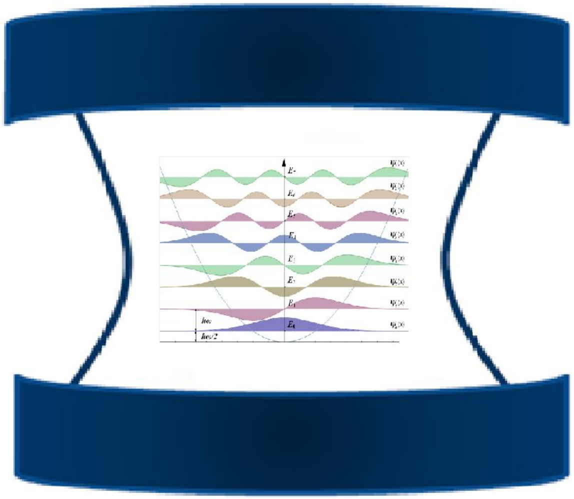
Application to the QBM

- An harmonic oscillator is coupled to an environment consisting of an infinite number of bosonic modes.
- The Hamiltonian is

$$\mathcal{H} = \frac{\omega_0}{2}\left(a^\dagger a + 1/2\right) + \sum_k \omega_k b_k^\dagger b_k + X \otimes B_E$$

$$X = 2^{-1/2}(a + a^\dagger)$$

$$(P = 2^{-1/2} i (a^\dagger - a)) \qquad B_E \equiv \sum_k \left(g_k b_k^\dagger + g_k^* b_k\right)$$



Weak coupling regime

- Analytic Fokker-Planck master equation

$$\frac{d}{dt}\chi^{(\eta)}(q,p,t) = \Big\{\omega_0\left(q\partial_p - p\partial_q\right) - V_1(\eta,t)\left(\partial_{qq}^2 + \partial_{pp}^2\right) - \left(2\Delta(t) + V_1(\eta,t)\right)\frac{q^2+p^2}{4}$$
$$+ \left(V_2(\eta,t) - \gamma(t)\right)\left(q\partial_q + p\partial_p\right) + V_2(\eta,t)\Big\}\,\chi^{(\eta)}(q,p,t)$$

- Analytic solution for the heat flow rate

$$\theta(t) = 2\sigma(0,t)\,\left(\frac{1}{2}D_2(t)\cos(\omega_0 t) + \omega_0\gamma(t)\right.$$
$$\left. + \frac{1}{2}D_1(t)\sin(\omega_0 t) - \omega_0\Delta(t)\right)$$

Strong coupling regime

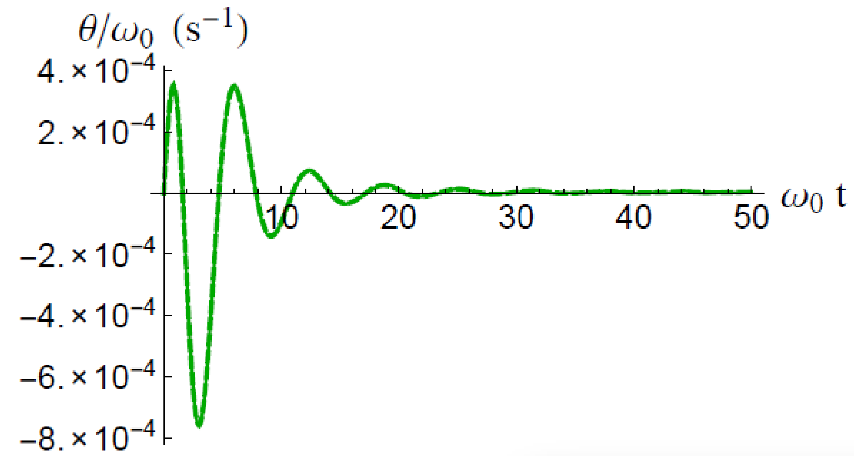
- Fully numerical simulation with finite-number of environmental modes

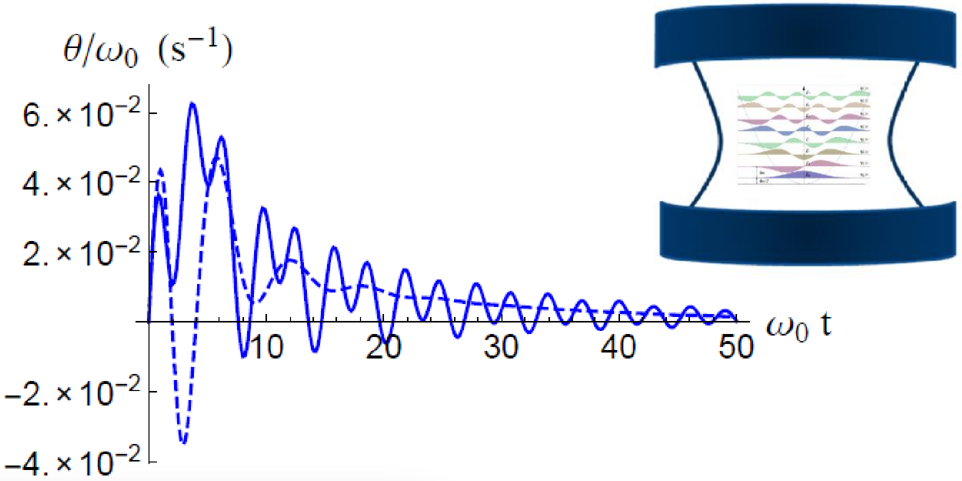
$$\mathcal{H} = \frac{\mathbf{P}^T\mathbf{P}}{2} + \mathbf{X}^T\mathbf{M}\mathbf{X}$$

$$X_i(t) = \sum_{j=1}^{N+1}\left[\mathbf{M}_{ij}^{XX}(t)X_j(0) + \mathbf{M}_{ij}^{XP}(t)P_j(0)\right]$$

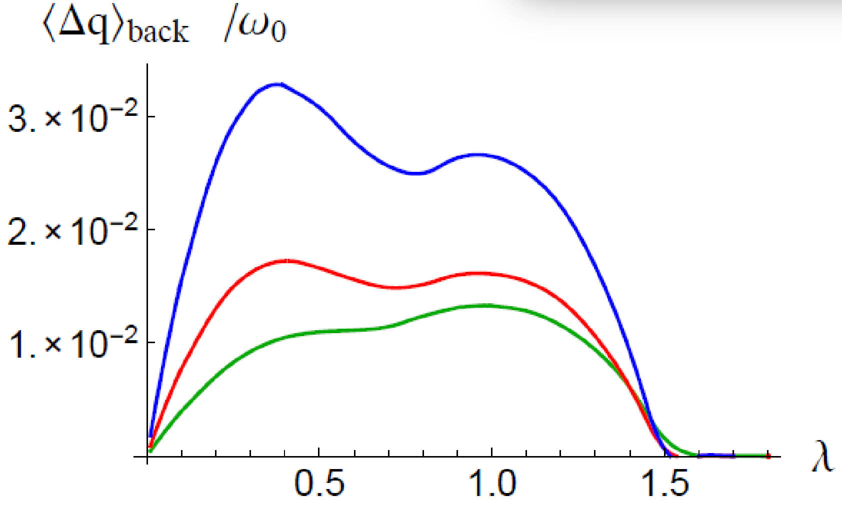
$$P_i(t) = \sum_{j=1}^{N+1}\left[\mathbf{M}_{ij}^{PX}(t)X_j(0) + \mathbf{M}_{ij}^{PP}(t)P_j(0)\right]$$

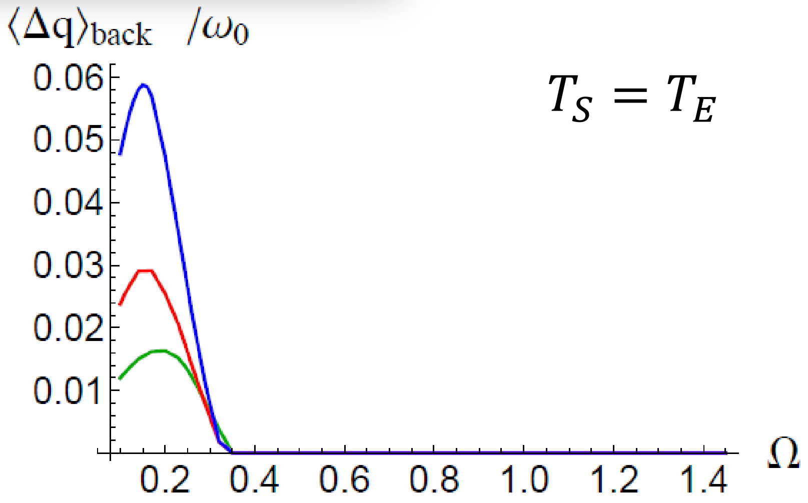
Application to the QBM





$$\langle \Delta q \rangle_{back} = \max_{\rho_S(0)} \frac{1}{2} \int_0^{+\infty} dt \, \left(|\theta(t)| - \theta(t) \right)$$





$T_S = T_E$

G. Guarnieri, J. Nokkala, R. Schmidt, S. Maniscalco, B. Vacchini, PRA 94 (2016)

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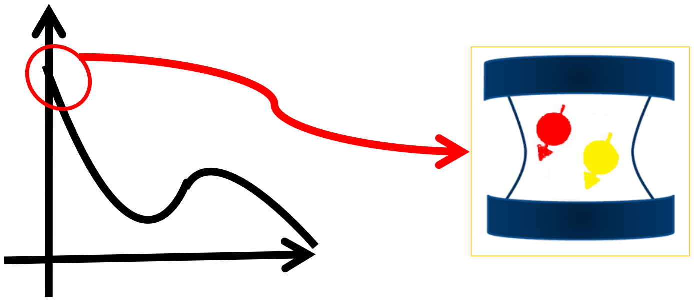
Trace-distance based non-Markovianity measure

$$D(\rho^1,\rho^2) = \frac{1}{2}\|\rho^1 - \rho^2\|_1 = \frac{1}{2}\sum_k |x_k|$$

It is a measure of the distinguishability between quantum states

It is a contraction under the action of PTP maps $D(t,\rho_S^{1,2}) \equiv D\big(\rho_S^1(t),\rho_S^2(t)\big),\quad \rho_S^k(t) = \Lambda(t)\rho_S^k$

Its can be employed to quantify the information flow between S and E



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

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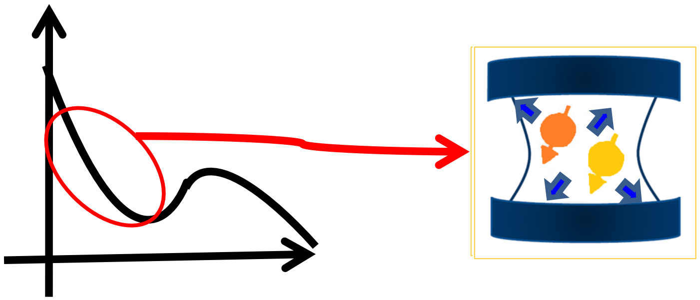

H. – P. Breuer, E. – M. Laine, J- Piilo, PRL **103** 210401 (2009)

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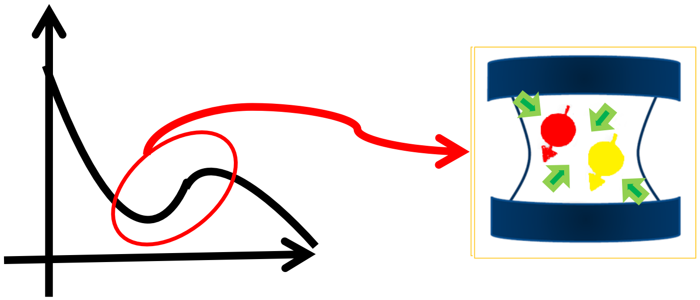


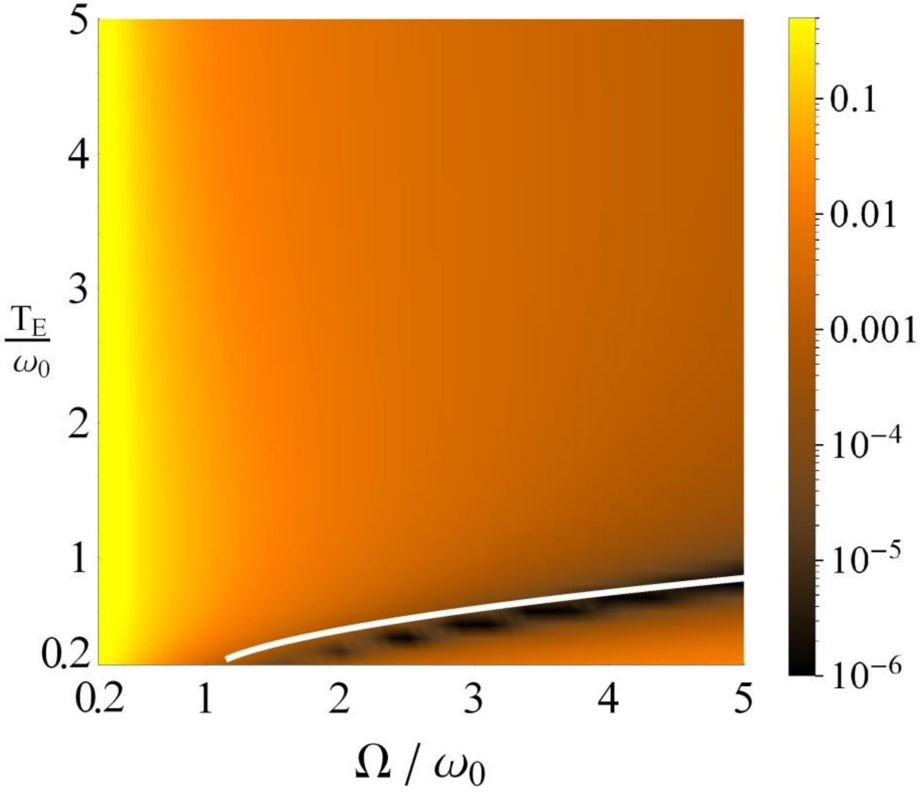
$$\sigma(t,\rho_S^{1,2}) = \frac{d}{dt}D(t,\rho_S^{1,2}) > 0$$

$$\mathcal{N} = \max_{\rho_S^{1,2}(0)} \frac{1}{2}\int_0^{+\infty} dt\ \left(\left|\sigma(t,\rho^{1,2})\right| + \sigma(t,\rho^{1,2})\right)$$

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

Relationship with the non-Markovanity

Spin – boson model



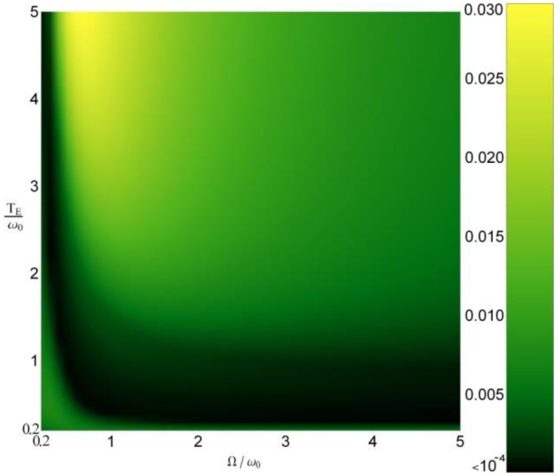
- $\lambda = 0.1$
- The reduced dynamics is always non-Markovian except on the resonance curve, defined by the condition

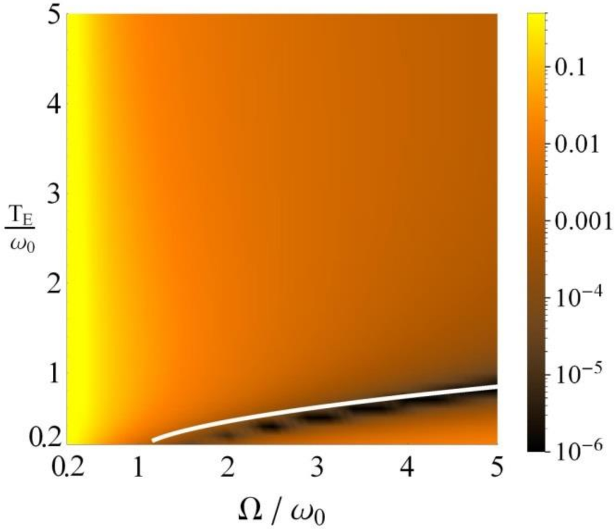
$$\frac{\partial}{\partial \omega} J_{eff}(\omega, \Omega, T_E)_{|\omega=\omega_0} = 0$$

$$J_{eff}(\omega, \Omega, T_E) \equiv J(\omega) \coth\left(\frac{\omega}{2T_E}\right)$$

- Locally white-noise spectrum around the system's transition frequency

Relationship with the non-Markovanity





G. Clos, H. – P. Breuer, PRA **86**, 012115 (2012)

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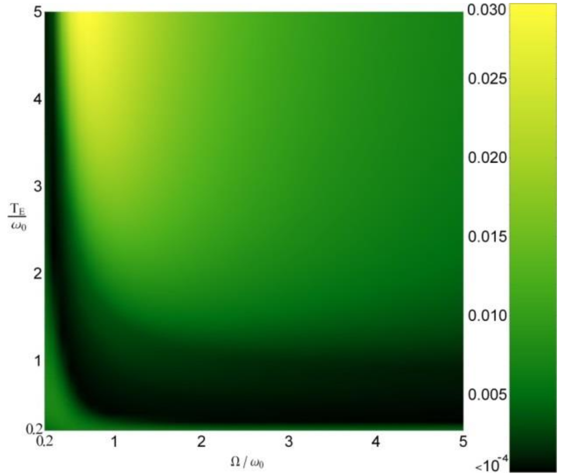
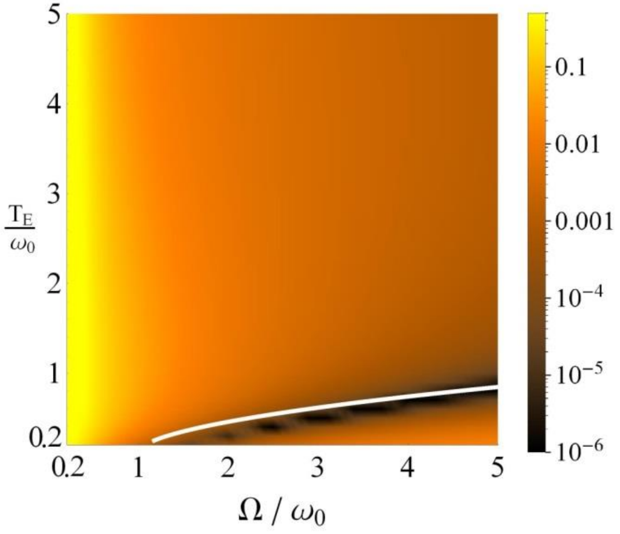
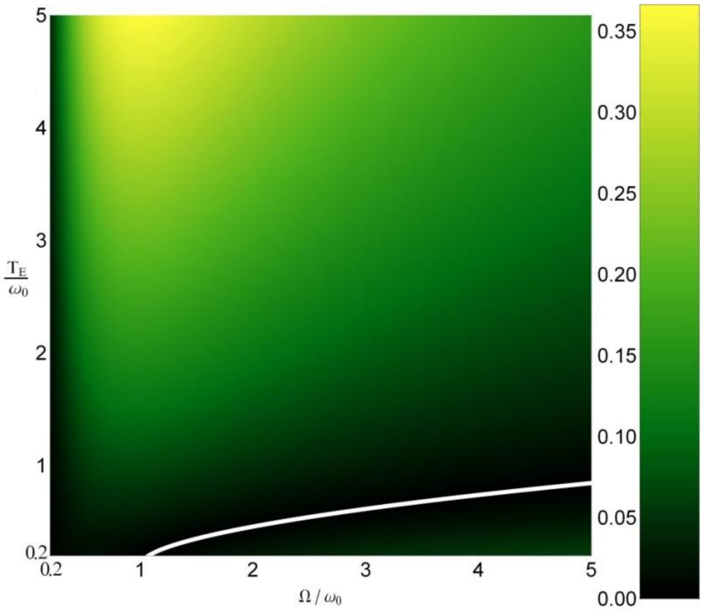




$$\partial_\omega J_{eff}(\omega, \Omega, T_E)_{|\omega=\omega_0}$$



The heat backflow measure is suppressed whenever the resonance condition approximately holds (i.e. on the black region)

The non-Markovianity measure is suppressed whenever the resonance condition strictly holds (i.e. on the white line)

Conclusions

- Heat, in an open quantum systems' scenario, is a delicate concept. One useful way to characterize it is by using the so-called full counting statistics.

- In the framework of non-Markovian open quantum systems we have introduced a condition and a quantitative estimator for the occurrence of **heat backflow** between an open quantum system of interest and its environment

- Explicit applications of this construction is shown for two paradigmatic models, the spin-boson, beyond the Born-Markov and RWA approximations, and the quantum brownian motion, explicitly showing that energy flow from S to E can oscillate in time and can even come back from E to S

- The occurrence of heat backflow represents a stricter condition than non-Markovianity, in the sense that the latter is required in order to witness the former and that, on the contrary, a Markovian dynamics prevents its observation.

THANK YOU FOR YOUR ATTENTION