ENERGY COUNTING STATISTICS IN OPEN QUANTUM SYSTEMS

A microscopic approach to thermodynamic consistency

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ENERGY COUNTING STATISTICS IN OPEN QUANTUM SYSTEMS

A microscopic approach to thermodynamic consistency

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OUTLINE

Open Quantum Dynamics and Master Equations

1. Thermodynamic consistency: first and second law
2. Beyond secular quantum master equations
3. Thermodynamics of QMEs starting from a microscopic description

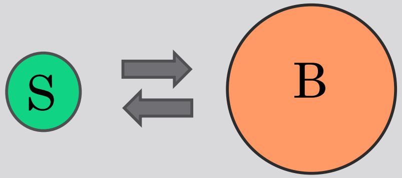
Anton S. Trushechkin
"Derivation of the Bloch-Redfield quantum master equation by Bogoliubov's method and generalization of the Born approximation"

Juzar Thingna
"Beyond weak-coupling quantum master equations"

Marco Merkli
"Correlation Decay and Markovianity in Open Systems"

THERMODYNAMIC CONSISTENCY

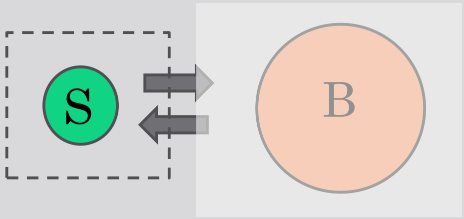
System + Bath dynamics



$$\dot{\rho}_{\mathrm{SB}}(t) = -i[H(t), \rho_{\mathrm{SB}}(t)]$$

Trace B

Reduced System dynamics



$$\rho_{\mathrm{S}}(t) = \mathcal{V}(t,0)[\rho_{\mathrm{S}}(0)]$$

WORK W, HEAT Q, ENERGY VARIATION ΔE, SYSTEM ENTROPY ΔS

Average Consistency:

AVERAGE FIRST LAW

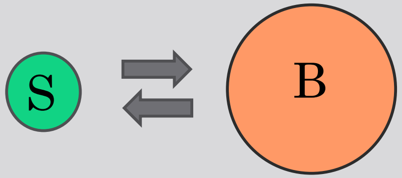
$$\langle W \rangle = \langle Q \rangle + \langle \Delta E \rangle$$ ✓

AVERAGE 2nd LAW

$$\langle \Delta S \rangle \geq -\langle Q \rangle / T$$ ✓

THERMODYNAMIC CONSISTENCY

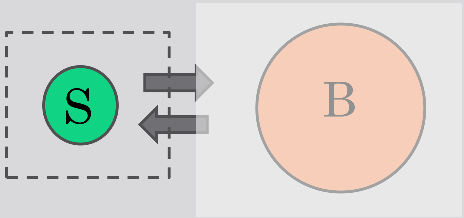
System + Bath dynamics



$$\dot{\rho}_{SB}(t) = -i[H(t), \rho_{SB}(t)]$$

Trace B

Reduced System dynamics



$$\rho_S(t) = \mathcal{V}(t,0)[\rho_S(0)]$$

WORK W, HEAT Q, ENERGY VARIATION ΔE, SYSTEM ENTROPY ΔS

Full Consistency:

FIRST LAW

$$W = \Delta E + Q$$ ✓

FLUCTUATING 2nd LAW

FLUCTUATION THEOREM ✓

THERMODYNAMIC (IN)CONSISTENCY

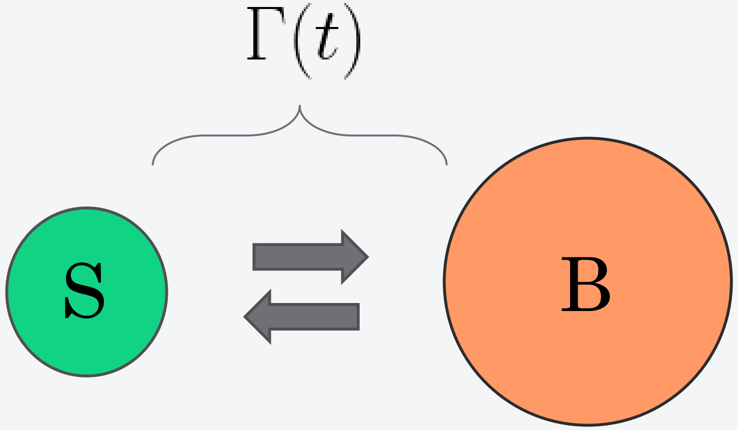
Ohmic Bath in time-dependent strong coupling

$$m\ddot{x} = -V'(x) - \left[\Gamma(s)\dot{x} + \frac{1}{2}\dot{\Gamma}(s)x\right] + \sqrt{2D(s)}\,\xi(s)$$

DISSIPATION

SEKIMOTO FORCE

NOISE



$$Q = -\int_0^t ds\,\dot{x}(s)\left[\underbrace{-\Gamma(s)\dot{x}(s) + \sqrt{2D(s)}\,\xi(s)}_{\text{FORCE}}\right]$$

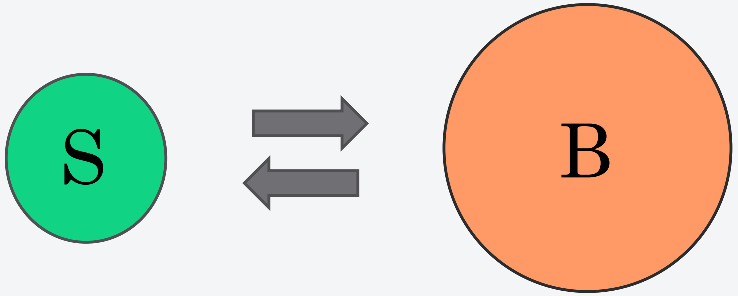
AVERAGE FIRST LAW

Not satisfied

E. Aurell, Entropy, 19 595 (2017)

FLUCTUATION THEOREM

Gibbs state: $$\rho(0) = \frac{e^{-\beta H_B}}{Z_B} \otimes \frac{e^{-\beta H_S}}{Z_S}$$



Work generating function: $$G(t,\lambda) = \int dW\, P(t,W) e^{\lambda W}$$

FLUCTUATION THEOREM

$$G_{\mathrm{R}}(t, -\lambda - \beta) = G(t,\lambda) e^{\beta \Delta F_{eq}}$$

- **Jorge Kurchan, *J. Phys. A: Math. Gen.* 31 3719 (1998)**
- **G.N. Bochkov, and Y. E. Kuzovlev, *Zh. Eksp. Teor. Fiz.* 72, 238 (1977)**
- **G. Gallavotti and E. G. D. Cohen, *Phys. Rev. Lett.* 74, (1995)**
- **J. L. Lebowitz and H. Spohn, *J. Stat. Phys.* 95, pages 333 (1999)**

FLUCTUATION THEOREM

FLUCTUATION THEOREM

$$G_{\mathrm{R}}(t,-\lambda-\beta)=G(t,\lambda)e^{\beta\Delta F_{eq}}$$

$\lambda=-\beta$

JARZYNSKI EQUALITY

$$G(t,-\beta)=\langle e^{-\beta W}\rangle=e^{-\beta\Delta F_{eq}}$$

C. Jarzynski, *Phys. Rev. Lett.* 78, 2690 (1997)

Jensen's inequality

AVERAGE 2ND LAW

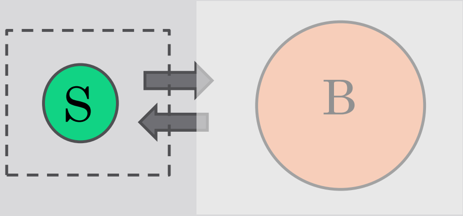
$$\langle W\rangle\geq-\beta\Delta F_{eq}$$

Beyond secular QMEs

Consistency of (beyond secular) master equations

- **D. Farina, and V. Giovannetti, *Phys. Rev. A* 100, 012107 (2019)**
- **D. Davidović, *Quantum* 4, 326 (2020)**
- **F. Nathan and M. S. Rudner, *Phys. Rev. B* 104, 119901 (2021)**
- **A. Trushechkin, *Phys. Rev. A* 106, 042209 (2022)**

Reduced System dynamics



$$\rho_S(t) = \mathcal{V}(t,0)[\rho_S(0)]$$

- **G. McCauley, et Al., *Npj Quantum Inf.* 6, 74 (2020)**
- **K. Ptaszyński and M. Esposito *Phys. Rev. Lett.* 123, 200603 (2019)**

Bloch-Redfield equation

Reduced dynamics of an open quantum system under the Born-Markov approximation:

$$\frac{d\widetilde{\rho}_{\mathrm{s}}(t)}{dt} = \sum_{\alpha,\beta} \int_0^t d\tau\, c_{\alpha\beta}(\tau)[\widetilde{A}_\beta(t-\tau)\widetilde{\rho}_{\mathrm{s}}(t), \widetilde{A}_\alpha^\dagger(t)] + \mathrm{H.c.},$$

- **F. Bloch, *Phys. Rev.* 105, 1206 (1957)**
- **A. G. Redfield, *Advances in Magnetic and Optical Resonance* 1, 1-32 (1965)**

Apply second Markov approximation and project on an operatorial basis

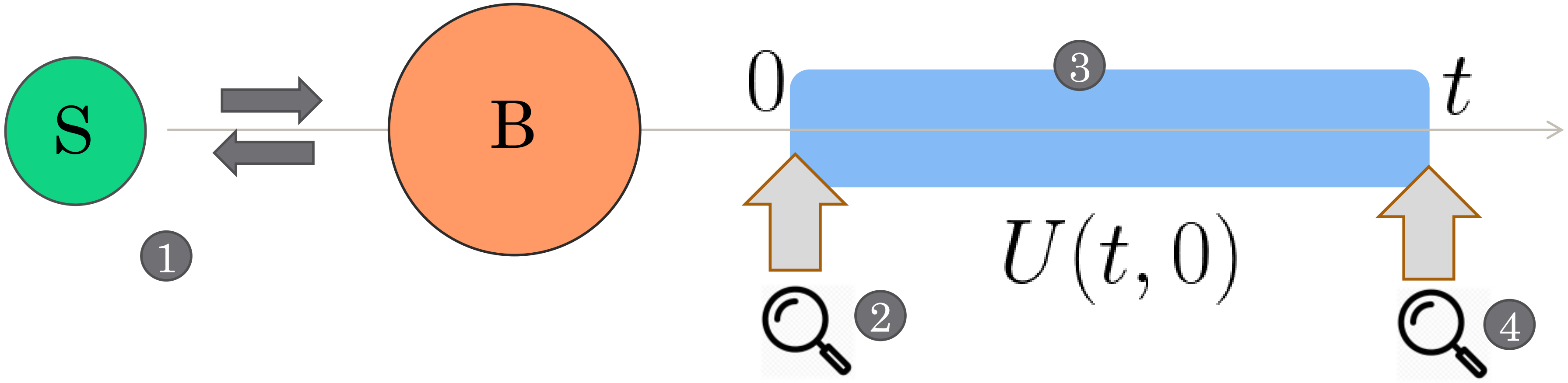
$$\mathcal{L}^{\mathrm{Red}}[\rho_{\mathrm{S}}] = -i[H', \rho_{\mathrm{S}}] + \sum_{i,j=1}^{N^2} \chi_{ij} \left[F_i \rho_{\mathrm{S}} F_j^\dagger - \frac{1}{2}\{F_j^\dagger F_i, \rho_{\mathrm{S}}\} \right]$$

Kossakowski matrix

In general

$$\chi \ngeq 0$$

Thermodynamics of QMEs



① System preparation

$\rho(0)$

② First measurement of $A = \sum_a a|a\rangle\langle a|$

Collapse to: $|a_0\rangle\langle a_0|$

③ Unitary evolution

$U(t,0)|a_0\rangle\langle a_0|U^\dagger(t,0)$

④ Second measurement

Collapse to: $|a_1\rangle\langle a_1|$

Preliminary: two-point measurements

1) We look at the outcomes difference : $a_1 - a_0$

2) There is an associated probability: $P(a_1 - a_0)$

3) We compute the moment generating function: $G(\lambda) = \sum_{\delta} P(\delta) e^{\lambda \delta}$

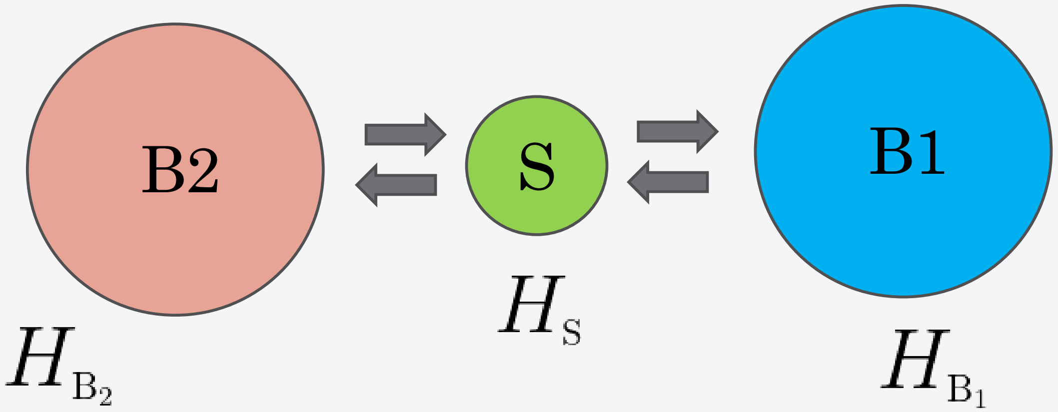
The MGF can be easily expressed as:

$$G(\lambda, t) = Tr[\hat{U}(t,0)\hat{\rho}(0)e^{-\lambda \hat{A}}\hat{U}^{\dagger}(t,0)e^{\lambda \hat{A}}]$$

M. Esposito, U. Harbola, and S. Mukamel, *Rev. Mod. Phys.* 81, 1665 (2009)

Internal energy, heat and entropy

- System coupled to many baths:



- Apply two point measurement to:
- And you have….

H_S	$H_{B_{1/2}}$	$-\log \rho_S$
INT. ENERGY	HEAT	ENTROPY
ΔE	$Q_{1/2}$	ΔS

Internal energy, heat and entropy

- And you have….

INT. ENERGY	HEAT
ΔE	Q_ν

$$\boldsymbol{\lambda}_{\mathrm{B}} \cdot \boldsymbol{Q} = \sum_\nu \lambda_\nu Q_\nu$$

- Joint probability density: $P(t, \Delta E, Q_\nu)$
- Joint MGF $G(t, \lambda_{\mathrm{S}}, \lambda_\nu) = \langle P(t, \Delta E, Q_\nu) e^{\lambda_{\mathrm{S}} \Delta E} e^{\boldsymbol{\lambda}_{\mathrm{B}} \cdot \boldsymbol{Q}} \rangle$

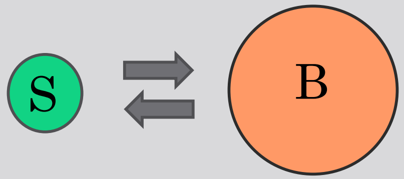
FLUCTUATION THEOREM

$$G(t, \lambda_{\mathrm{S}}, \boldsymbol{\lambda}_{\mathrm{B}}) e^{\beta_{\mathrm{S}} \Delta F_{eq}} = G_{\mathrm{R}}(t, -\lambda_{\mathrm{S}} - \beta_{\mathrm{S}}, -\boldsymbol{\lambda}_{\mathrm{B}} - \boldsymbol{\beta}_{\mathrm{B}})$$

Consistency at unitary level

- Unitary evolution of system + thermal baths

System + Bath dynamics



$$\dot{\rho}_{\text{SB}}(t) = -i[H(t), \rho_{\text{SB}}(t)]$$

FIRST LAW

$$W = \Delta E + Q$$ ✓

AVERAGE FIRST LAW ✓

FLUCTUATING 2nd LAW

FLUCTUATION THEOREM ✓

AVERAGE 2nd LAW ✓

Tilted evolution

We can write the MGF of heat and energy using tilted evolution

$$G = Tr[U(t,0)\rho(0)e^{-\lambda_{\mathrm{S}} H_{\mathrm{S}}(0)} e^{-\boldsymbol{\lambda}_{\mathrm{B}} \cdot \boldsymbol{H}_{\mathrm{B}}} U^{\dagger}(t,0) e^{\lambda_{\mathrm{S}} H_{\mathrm{S}}(t)} e^{\boldsymbol{\lambda}_{\mathrm{B}} \cdot \boldsymbol{H}_{\mathrm{B}}}]$$

$$G = Tr[U_{\lambda_S,\lambda_B}(t,0)\rho(0)U^{\dagger}_{\lambda_S,\lambda_B}(t,0)]$$

Tilted evolution:

$$U_{\lambda_S,\lambda_B}(t,0) = e^{\frac{\lambda_{\mathrm{S}}}{2} H_{\mathrm{S}}(t)} e^{\frac{\boldsymbol{\lambda}_{\mathrm{B}}}{2} \cdot \boldsymbol{H}_{\mathrm{B}}} U(t,0) e^{-\frac{\lambda_{\mathrm{S}}}{2} H_{\mathrm{S}}(0)} e^{-\frac{\boldsymbol{\lambda}_{\mathrm{B}}}{2} \cdot \boldsymbol{H}_{\mathrm{B}}}$$

Thermodynamics: from unitary description to QMEs

Tilted Unitary Ev. $U_{0,\lambda_B}(t,0)\rho_S(0)\otimes\rho_B(0)U^{\dagger}_{0,\lambda_B}(t,0)$

Trace baths

$$\rho_{0,\boldsymbol{\lambda_B}}(t) = \sum_k M_k^{\boldsymbol{\lambda_B}\,\dagger}(t,0)\rho_S(0)M_k^{\boldsymbol{\lambda_B}}(t,0)$$

Semigroup hypothesis

Tilted Master Eq. $\dot{\rho}_{0,\boldsymbol{\lambda_B}}(t) = \mathcal{L}_{0,\boldsymbol{\lambda_B}}\rho_{0,\boldsymbol{\lambda_B}}(t)$

Recover G by tracing the tilted density matrix

$$G = Tr[\rho_{0,\lambda_B}(t))]$$

Generalized quantum detailed balance (GQDB)

Tilted Master Eq: $$\dot{\rho}_{0,\boldsymbol{\lambda_B}}(t) = \mathcal{L}_{0,\boldsymbol{\lambda_B}}\rho_{0,\boldsymbol{\lambda_B}}(t)$$

The FT derived in the unitary case, after tracing the baths and introducing the tilted generator, can be written as

$$\mathcal{L}^{\mathrm{R}}_{0,\boldsymbol{\lambda_B}}[\ldots] = \mathcal{L}^{\dagger}_{0,-\boldsymbol{\lambda_B}-\boldsymbol{\beta_B}}[\ldots]$$ (GQDB)

$\mathcal{L}^{\dagger}$ Is the adjoint dynamical generator

ADJOINT

$$Tr[\mathcal{L}[B]A] = Tr[B(\mathcal{L}^{\dagger}[A])^{\dagger}]$$

Generalized quantum detailed balance (GQDB)

$$\mathcal{L}^{\mathrm{R}}_{0,\boldsymbol{\lambda_B}}[\ldots] = \mathcal{L}^{\dagger}_{0,-\boldsymbol{\lambda_B}-\boldsymbol{\beta_B}}[\ldots] \qquad \text{(GQDB)}$$

1. Obtained combining the semigroup hypothesis with the fluctuation theorem
2. Can be used to check if microscopic derivations of QMEs are consistent
3. We have to understand its connections with usual DB

Consistency of microscopic derivations: results

Redfield equation violates GQDB:

$$\mathcal{L}^{\mathrm{Red\ R}}_{0,\boldsymbol{\lambda_B}}[\ldots] \neq \mathcal{L}^{\mathrm{Red}\,\dagger}_{0,-\boldsymbol{\lambda_B}-\boldsymbol{\beta_B}}[\ldots]$$

Redfield equation violates positivity

H.P. Breuer, and F. Petruccione.
The theory of open quantum systems,
Oxford University Press on Demand, 2002.

Redfield equation steady state is not a good approx. Of the open system S.S.

C. H. Fleming and N. I. Cummings
***Phys. Rev. E* 83, 031117 (2011)**

J. Thingna, et al. *Phys. Rev. E* 88, 052127 (2013)

Consistency of microscopic derivations: results

Redfield equation violates GQDB:

$$\mathcal{L}^{\mathrm{Red\,R}}_{0,\boldsymbol{\lambda_B}}[\ldots] \neq \mathcal{L}^{\mathrm{Red}\,\dagger}_{0,-\boldsymbol{\lambda_B}-\boldsymbol{\beta_B}}[\ldots]$$

Secular approx. restores GQDB:

$$\mathcal{L}^{\mathrm{Sec\,R}}_{0,\boldsymbol{\lambda_B}}[\ldots] = \mathcal{L}^{\mathrm{Sec}\,\dagger}_{0,-\boldsymbol{\lambda_B}-\boldsymbol{\beta_B}}[\ldots]$$

Secular QMEs

- **E. B. Davies** ***Comm. Math. Phys.*** **39 , 91 (1974)**

Some non-secular schemes Restore GQDB:

$$\mathcal{L}^{\mathrm{Sym\,R}}_{0,\boldsymbol{\lambda_B}}[\ldots] = \mathcal{L}^{\mathrm{Sym}\,\dagger}_{0,-\boldsymbol{\lambda_B}-\boldsymbol{\beta_B}}[\ldots]$$

Consistency of non-secular QMEs

Some non-secular schemes
Restore GQDB:

$$\mathcal{L}^{\text{Sym R}}_{0,\boldsymbol{\lambda_B}}[\ldots] = \mathcal{L}^{\text{Sym}\,\dagger}_{0,-\boldsymbol{\lambda_B}-\boldsymbol{\beta_B}}[\ldots]$$

$\mathcal{L}^{\text{Red}} \Rightarrow \mathcal{L}^{\text{Sym}}$

G. McCauley, et Al., *Npj Quantum Inf.* 6 74 (2020)

When it works: time scales separation

(Nearly degenerate jumps)

$\tau_B \ll \tau_d, \tau_S$

Or

(Secular condition)

$\tau_B, \tau_S \ll \tau_d$

Detailed balance and GQDB

DB and GQDB are different. For a single bath we have

GQDB + Strict Energy cons. = DB

$$\mathcal{L}^{\mathrm{R}}_{0,0}[\dots] = e^{-\frac{\beta}{2}H_{\mathrm{S}}}\mathcal{L}^{\dagger}_{0,0}[e^{\frac{\beta}{2}H_{\mathrm{S}}}\dots e^{\frac{\beta}{2}H_{\mathrm{S}}}]e^{-\frac{\beta}{2}H_{\mathrm{S}}}$$

ADJOINT

$$Tr[\mathcal{L}[B]A] = Tr[B\left(\mathcal{L}^{\dagger}[A]\right)^{\dagger}]$$

- **R. Alicki, *Rep. Math. Phys.* 10, 249 (1976)**
- **W. A. Majewski, *J. Math. Phys.* 25, 614 (1984)**
- **F. Fagnola and V. Umanità, *Mathematical Notes* 8, 108 (2008)**

Summary and discussion

Fluctuation theorem at unitary level (2^{nd} law)

SEMIGROUP

GQDB: consistency for QMEs

Redfield equation	✗
Secular equation	✓
Symmetrized QME	✓

Strict energy conservation

+

=

Detailed Balance

Redfield equation	✗
Secular equation	✓
Symmetrized QME	✗

Conclusions

- We introduced a condition on QMEs, necessary to have Thermodynamic consistency (FTs, 2nd law): the GQDB
- We have shown that Redfield equation is not consistent: breaks GQDB (and then braks FT, 2nd law)
- The secular approximation and beyond secular schemes (symmetrization) restore GQDB.
- DB is more restrictive than GQDB, and can be obtained using GQDB if we assume strict energy conservation.
- (Extra) Symmetrized QMEs don't satisfy DB, but satisfy energy conservation only in average.