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The change in the von Neumann entropy of a bath interacting with a driven quantum system

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IF UJ, Kraków, March 2, 2015

E.A. & Ralf Eichhorn, submitted [arXiv:1412.7029] (2014)
+ what we have found out since

Fluctuation relations

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Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach

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Theoretical Astrophysics, T-6, MS B288, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 18 June 1997)

It has recently been shown that the Helmholtz free-energy difference between two equilibrium configurations of a system may be obtained from an ensemble of *finite-time* (nonequilibrium) measurements of the work performed in switching an external parameter of the system. Here this result is established, as an identity, within the master equation formalism. Examples are discussed and numerical illustrations provided. [S1063-651X(97)10710-3]

$$\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}$$

“The free energy landscape between two equilibrium states is well related to the irreversible work required to drive the system from one state to the other”

Classical fluctuation relations as “trivial identities”

Maes, J. Stat. Phys. **95** 367-392 (1999)
 Gawędzki, arXiv:1308.1518 (2013)

$$\frac{\Pr_B(\text{path})}{\Pr_F(\text{path})} = e^{-\delta S_{env}}$$

as a consequence all the fluctuation relations follow e.g.

$$\left\langle e^{-\delta S_{env}} \right\rangle_{x_i}^{x_f} = \left\langle 1 \right\rangle_{x_f}^{x_i}$$

The physical problem is then to show that this formal mathematical expression really is standard entropy production as given by Clausius’ formula i.e.

$$\delta S_{env} = -\delta Q / T$$

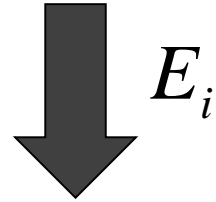
For stochastic kinetics models this is indeed so

Jarzynski, Phys. Rev. E **56** 5018 (1997); Kurchan, J. Phys. A **31** 3719 (1998); Lebowitz & Spohn, J. Stat. Phys. **95** 333 (1999); Gawędzki (2013)

A reminder: fluctuation relations for isolated quantum systems

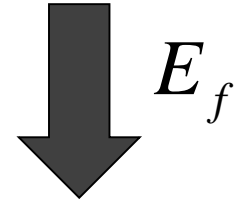
Initial state of the system taken to be in equilibrium

Measurement



external drive state change superoperator Φ

Measurement



$$\rho^{eq} = |n\rangle\langle n| \frac{\exp(-\beta E_n)}{Z^{init}(\beta)} \longrightarrow |i\rangle\langle i| \longrightarrow \rho_f = \Phi(|i\rangle\langle i|) \longrightarrow |f\rangle\langle f|$$

On an isolated system, work done should be: $\delta W[i, f] = E_f - E_i$
 Unitary time development implies: $\Phi(\mathbf{1}) = \mathbf{1}$

$$\langle e^{-\beta \delta W} \rangle_{eq} = \sum_i \frac{e^{-\beta E_i}}{Z^{init}} \sum_f \langle f | \Phi(|i\rangle\langle i|) | f \rangle e^{-\beta(E_f - E_i)} = \frac{Z^{final}}{Z^{init}} = e^{-\beta \Delta F}$$

(i) Kurchan, cond-mat/0007360 (ii) Rastegin & Życzkowski, Phys. Rev. E **89** (2014)

”Quantum δS_{env} ” – is it the change of von Neumann entropy of the bath?

Sounds very reasonable. Proposed and recently investigated in
Esposito, Lindenberg, van den Broeck, New Journal of Physics **12** 013013 (2010)
Pucci, Esposito, Peliti, J. Stat. Mech. P04005 (2013)

Can one compute this? **YES**

Is it the right definition? **NO**

Do we understand why? **PARTLY**

Other uses of computation? **MAYBE**

The Feynman-Vernon theory

$$\rho_{TOT}^{init} = \rho_S^{init} \otimes \rho_B^{eq} \xrightarrow{\rho_{TOT}^{final}} \rho_S^{final} = \text{Tr}_B [\rho_{TOT}^{final}] \longrightarrow |f\rangle\langle f|$$

$$\rho_S^{init} = |i\rangle\langle i|$$

$$P_{if} = \int \psi_i(x_i) \psi_i^*(y_i) \psi_f^*(x_f) \psi_f(y_f) K_{FV}(x_i, y_i, x_f, y_f) dx_i dy_i dx_f dy_f$$

$$K_{FV} = \int dq_i dq'_i dq_f Dq Dq' Dx Dy e^{\frac{i}{\hbar} S_S[x] - \frac{i}{\hbar} S_S[y] + \frac{i}{\hbar} S_I[x, q] - \frac{i}{\hbar} S_I[y, q'] + \frac{i}{\hbar} S_B[q] - \frac{i}{\hbar} S_B[q']} \rho_B^{eq}$$

$$K_{FV} = \int Dx Dy e^{\frac{i}{\hbar} S_S[x] - \frac{i}{\hbar} S_S[y] + i\Phi[x, y]}$$

Integrate out the bath... then assume it is harmonic oscillators and linear coupling...

$$i\Phi[x, y] = \frac{i}{\hbar} S_i[x, y] - \frac{1}{\hbar} S_r[x, y] = \frac{i}{\hbar} \iint_{u \leq s} (x_s - y_s)(x_u + y_u) k_i(s-u) - \frac{1}{\hbar} \iint_{u \leq s} (x_s - y_s)(x_u - y_u) k_r(s-u)$$

A remarkably simple final result...

$$k_i(s-u) = \sum_i \frac{c_i^2}{2m_i \omega_i} \sin \omega(s-u)$$

$$k_r(s-u) = \sum_i \frac{c_i^2}{2m_i \omega_i} \coth \frac{\omega_i \hbar \beta}{2} \cos \omega(s-u)$$

Change of von Neumann entropy

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$$|i\rangle\langle i|$$



$$|f\rangle\langle f| \quad \rho_B^{post} = \frac{1}{P_{if}} \langle f | \rho_{TOT}^{final} | f \rangle$$

$$\rho_{TOT}^{post} = \frac{|f\rangle\langle f| \otimes \langle f | \rho_{TOT}^{final} | f \rangle}{\text{Tr}_B [\langle f | \rho_{TOT}^{final} | f \rangle]}$$

$$\delta \text{Tr} [-\rho_B \log \rho_B] = -\frac{1}{P_{if}} \text{Tr} [\langle f | \rho_{TOT}^{final} | f \rangle \log \rho_B^{eq}] + \text{Tr} [\rho_B^{eq} \log \rho_B^{eq}] + O(\delta\rho^2)$$

$$\log \rho^{eq} = |n\rangle\langle n| (\beta F - \beta E_n) = \beta F |n\rangle\langle n| + \beta \frac{d}{d\varepsilon} \langle n | e^{-\varepsilon H_B} | n' \rangle \Big|_{\varepsilon=0} |n\rangle\langle n'|$$

$$\delta \text{Tr} [-\rho_B \log \rho_B] = -\frac{\beta}{P_{if}} \frac{d}{d\varepsilon} \text{Tr} \left[e^{-\varepsilon H_B} \langle f | \rho_{TOT}^{final} | f \rangle \right] \Big|_{\varepsilon=0} - \beta U_B^{eq}(\beta) + O(\delta\rho^2)$$

For finite ε the integrals over the bath are, as in Feynman-Vernon, Gaussian, and...

$$\delta \text{Tr} [-\rho_B \log \rho_B] = \frac{1}{P_{if}} \text{Tr}_{if} \int \partial_x \partial_y e^{\frac{i}{\hbar} S_S[x] - \frac{i}{\hbar} S_S[y] + \frac{i}{\hbar} S_i[x,y] - \frac{1}{\hbar} S_r[x,y]} (I^{(1)} + I^{(2)} + I^{(3)}) + O(\delta\rho^2)$$

Explicitly...

$$\rho_B^{eq} \otimes |i\rangle\langle i| \xrightarrow{\rho_{TOT}^{final}} \rho_B^{post} = \frac{1}{P_{if}} \langle f | \rho_{TOT}^{final} | f \rangle$$

$$\delta \text{Tr}[-\rho_B \log \rho_B] = \frac{1}{P_{if}} \text{Tr}_{if} \int \rho_x \rho_y e^{\frac{i}{\hbar} S_s[x] - \frac{i}{\hbar} S_s[y] + \frac{i}{\hbar} S_i[x,y] - \frac{i}{\hbar} S_r[x,y]} (I^{(1)} + I^{(2)} + I^{(3)}) + O(\delta\rho^2)$$

$$I^{(1)}[x, y] = \iint_{u \leq s} (x_s - y_s)(x_u - y_u) h^{(1)}(s-u) = -\frac{\beta}{\hbar} \frac{d}{d\beta} S_r$$

$$h^{(1)} = -\sum_i \frac{\beta C_i^2}{4m_i} \sinh^{-2} \frac{\omega_i \hbar \beta}{2} \cos \omega_i (s-u)$$

$$I^{(2)}[x, y] = \iint_{u \leq s} (x_s y_u - x_u y_s) h^{(2)}(s-u)$$

$$h^{(2)} = i \sum_i \frac{\beta C_i^2}{2m_i} \coth \frac{\omega_i \hbar \beta}{2} \sin \omega_i (s-u)$$

$$I^{(3)}[x, y] = \iint_{u \leq s} (x_s y_u + x_u y_s) h^{(3)}(s-u)$$

$$h^{(3)} = \sum_i \frac{\beta C_i^2}{2m_i} \cos \omega_i (s-u)$$

$I^{(1)}, I^{(2)}, I^{(3)}$ are new terms, of similar type but not the same as in Feynman-Vernon.

Caldeira-Leggett model...

$$\sum_i \rightarrow \int_0^\Omega f(\omega) d\omega$$

Ohmic spectral density of the bath oscillators

$$\frac{f(\omega)C^2(\omega)}{m(\omega)} = \frac{2\eta\omega^2}{\pi}$$

First spectral cut-off Ω is taken large. Then a high-temperature limit is taken such that

$$\Omega\hbar\beta \ll 1$$

$$S_i[x, y] = -\frac{\eta}{2} \int (x_s - y_s)(\dot{x}_s - \dot{y}_s) + \text{potential renormalization}$$

$$S_r[x, y] = \frac{\eta}{\hbar\beta} \int (x_s - y_s)^2$$

$$\delta \text{Tr}[-\rho_B \log \rho_B] = \frac{1}{P_{if}} \text{Tr}_{if} \int \mathcal{D}x \mathcal{D}y e^{\frac{i}{\hbar} S_s[x] - \frac{i}{\hbar} S_s[y] + \frac{i}{\hbar} S_i[x, y] - \frac{1}{\hbar} S_r[x, y]} (I^{(1)} + I^{(2)} + I^{(3)}) + O(\delta\rho^2)$$

$$h^{(1)}(s-u) \approx -\frac{2\eta}{\hbar^2\beta} \delta(s-u)$$

$$I^{(1)}[x, y] = -\frac{\eta}{\hbar^2\beta} \int (x_s - y_s)^2 = -\frac{1}{\hbar} S_r[x, y]$$

$$h^{(2)}(s-u) \approx -i\frac{2\eta}{\hbar} \delta'(s-u)$$

$$I^{(2)}[x, y] = \frac{i\eta}{\hbar} \int \dot{x}_s y_s - x_s \dot{y}_s = \frac{2i}{\hbar} S_i[x, y] + \frac{i\eta}{\hbar} \int \dot{x}_s x_s - y_s \dot{y}_s$$

$$h^{(3)}(s-u) \approx -2\eta\beta \delta''(s-u)$$

$$I^{(3)}[x, y] = \beta\eta \int \dot{x}_s \dot{y}_s + \text{boundary terms}$$

Simple (good) consequence

$$\delta \text{Tr}[-\rho_B \log \rho_B] = \frac{1}{P_{if}} \text{Tr}_{if} \int \rho_x \rho_y e^{\frac{i}{\hbar} S_s[x] - \frac{i}{\hbar} S_s[y] + \frac{i}{\hbar} S_i[x,y] - \frac{1}{\hbar} S_r[x,y]} (I^{(1)} + I^{(2)} + I^{(3)}) + O(\delta \rho^2)$$

The highest order term in the functional

$$I^{(3)}[x, y] = \beta \eta \int \dot{x}_s \dot{y}_s$$

This gives a contribution to the entropy change

$$\frac{1}{P_{if}} \left\langle \beta \eta \int \dot{x}_s \dot{y}_s \right\rangle_i^f$$

Compare the work done *on* the system by a friction force (heat transferred *from* a bath)

$$\int (-\eta v) dx = \int -\eta v^2 dt$$

By Clausius' formula the entropy production *in* the bath by reaction to the friction force is then

$$\delta S_{env}^{frict} = \int \beta \eta v^2 dt$$

You get the same by a more involved analysis, which we need for the next term...

Simple (good) consequence

$$\delta \text{Tr}[-\rho_B \log \rho_B] = \frac{1}{P_{if}} \text{Tr}_{if} \int \rho_x \rho_y e^{\frac{i}{\hbar} S_s[x] - \frac{i}{\hbar} S_s[y] + \frac{i}{\hbar} S_i[x,y] - \frac{1}{\hbar} S_r[x,y]} (I^{(1)} + I^{(2)} + I^{(3)}) + O(\delta \rho^2)$$

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$$\delta S_{env}^{frict} = \int \beta \eta v^2 dt$$

You get the same by a more involved analysis, which we need for the next term...

Less simple (good) consequence

$$\delta \text{Tr} \left[-\rho_B \log \rho_B \right] = \frac{1}{P_{if}} \text{Tr}_{if} \int \rho_x \rho_y e^{\frac{i}{\hbar} S_S[x] - \frac{i}{\hbar} S_S[y] + \frac{i}{\hbar} S_i[x,y] - \frac{1}{\hbar} S_r[x,y]} \left(I^{(1)} + I^{(2)} + I^{(3)} \right) + O(\delta \rho^2)$$

The part of $I^{(2)}$ proportional to S_i , and understood in the Stratonovich sense

The Caldeira-Leggett model leads to Kramers-Langevin dynamics for the Wigner function

Therefore, this contribution can be understood as the (classical) expectation value

Compare the work done *on* the system by the fluctuating force (heat transferred *from* a bath)

By Clausius' formula the entropy production *in* the bath by reaction to the fluctuating force is

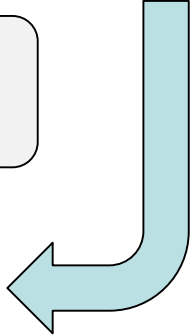
$$\frac{i\eta}{\hbar} \int (y_s - x_s)(\dot{x}_s + \dot{y}_s)$$

$$\frac{i}{\hbar} (y_s - x_s) \rightarrow \frac{\partial}{\partial p} \frac{1}{2} (\dot{x}_s + \dot{y}_s) = \dot{q}_s \rightarrow \frac{p_s}{M}$$

$$\mathbb{E} \left[\int \left(-\beta \frac{p}{M} \right) \circ \sqrt{2k_B T \eta} d\xi \middle| q_i, p_i, q_f, p_f \right]$$

$$\int F_{frict} \circ dx = \int \left(\sqrt{2k_B T \dot{\xi}} \right) v dt$$

$$\delta S_{env}^{fluct} = \int -\beta \left(\sqrt{2k_B T \dot{\xi}} \right) v dt$$



The two remainder terms

$$\delta \text{Tr} \left[-\rho_B \log \rho_B \right] = \frac{1}{P_{if}} \text{Tr}_{if} \int \mathcal{D}x \mathcal{D}y e^{\frac{i}{\hbar} S_S[x] - \frac{i}{\hbar} S_S[y] + \frac{i}{\hbar} S_i[x,y] - \frac{1}{\hbar} S_r[x,y]} \left(I^{(1)} + I^{(2)} + I^{(3)} \right) + O(\delta \rho^2)$$

The part of $I^{(2)}$ which is a complete integral, understood in the Stratonovich sense...

$$\frac{i\eta}{\hbar} \int (x_s \dot{x}_s - y_s \dot{y}_s) = \frac{i\eta}{2\hbar} (x_s^2 - y_s^2)$$

....and the $I^{(1)}$ contribution...

$$-\frac{\eta}{\hbar^2 \beta} \int (x_s - y_s)^2$$

...also understood using Kramers-Langevin dynamics for the Wigner function

$$-\frac{1}{\hbar^2} (x_s - y_s)^2 \rightarrow \frac{\partial^2}{\partial p^2}$$

One can understand these two remainder terms as (classical) expectation values. In the case of the part from $I^{(2)}$ this involves only the (classical) transition probability of the stochastic process over the interval, *see* E.A. & Eichhorn [arXiv:1412.7029].

For this talk we will just note that they give terms beyond the classical $\delta \mathcal{S}_{env}$ of stochastic thermodynamics. So what is wrong?

Back to the change of entropy

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$$\begin{array}{ccc}
 \rho_{TOT}^{init} & \xrightarrow{\quad} & \rho_{TOT}^{final} \\
 \downarrow & & \downarrow \\
 |i\rangle\langle i| & & |f\rangle\langle f|
 \end{array}
 \quad
 \rho_{TOT}^{post} = \frac{|f\rangle\langle f| \otimes \langle f | \rho_{TOT}^{final} | f \rangle}{\text{Tr}_B [\langle f | \rho_{TOT}^{final} | f \rangle]}$$

$$\rho_B^{post} = \frac{1}{P_{if}} \langle f | \rho_{TOT}^{final} | f \rangle$$

$$\delta \text{Tr} [-\rho_B \log \rho_B] = \text{Tr} [\beta H_B \rho_B^{post}] - \text{Tr} [\beta H_B \rho_B^{eq}] + O(\delta \rho^2)$$

Consider this classically, as bath *Shannon* entropy, and without any drive...

$$\delta S(\rho_B) = \beta \int H_B(x_B^f) \rho_B^f(x_B^f) dx_B^f - \beta \int H_B(x_B^i) \rho_B^{eq}(x_B^i) dx_B^i + O(\delta \rho^2)$$

...that is, as here on the left.

Classically the system and the bath is then one big conservative system and total energy is conserved. The Hamiltonian has three terms: the system, the bath and the interaction, and ΔE_S is thus $-(\Delta E_B + \Delta E_I)$. This gives **not** the above, but instead:

$$\delta S_{env} = \beta \int (H_B(x_B^f) + H_I(x_B^f, x_S^f)) \rho_B^f(x_B^f) dx_B^f - \beta \int (H_B(x_B^i) + H_I(x_B^i, x_S^i)) \rho_B^{eq}(x_B^i) dx_B^i$$

Hence, the “very reasonable” starting point is in doubt.

Should we have known better?

Stochastic thermodynamics framework

The system: Of the whole world, a part which is properly cut out is called the system

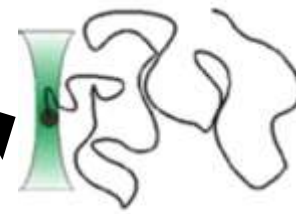
work made **on** the system

δW

$$\Delta U = \delta W + \delta Q$$

δQ

heat given **to** the system



The external system: It is an agent which is capable of controlling macroscopically the system through a parameter a of the potential energy

The thermal environment: The background to which the system is connected...
...keeps no memories of the systems's actions...

The bath is conceptually at equilibrium, not close to equilibrium?

Perhaps however the issue is not so trivial...(work in progress)...

$$\delta S(\rho_B) = \beta \int H_B(x_B^f) \rho_B^f(x_B^f) dx_B^f - \beta \int H_B(x_B^i) \rho_B^{eq}(x_B^i) dx_B^i + O(\delta \rho^2)$$

...the classical quantity.

A bath with a very large number of degrees of freedom is not the same as a second finite-dimensional system. One should compute.

Use the trick of Sasa in “*Collective dynamics from stochastic thermodynamics*” [arXiv:1501.00055]: consider the history of the system as an external variable and integrate out the oscillators. The Shannon entropy change of the bath is then a functional of the system history.

For Caldeira-Leggett model this seems to give the entropy production functional of stochastic thermodynamics. The calculation of the “friction term” is in fact easy.

Maybe a difference between the classical and the quantum bath.

Another use of the calculation?

An initial pure state of system, bath and ancilla

$$|\psi\rangle_{SBA} = |i\rangle_S \otimes \left(\sum_n c_n |i_n\rangle_B |i_n\rangle_A \right)$$

Density matrices $\rho_B^{eq} = \text{Tr}_{SA} [|\psi\rangle\langle\psi|]$ $\rho_A^i = \text{Tr}_{SB} [|\psi\rangle\langle\psi|]$ $S(\rho_B^{eq}) = S(\rho_A^i)$

Disconnect the ancilla, evolve the system and bath up to a measurement, and assume a (big) pure final state

$$|\psi\rangle_{SBAM} = |f\rangle_S \otimes \left(\sum_n d_n |f_n\rangle_{BA} |f_n\rangle_M \right)$$

$$S(\rho_M^f) = S(\rho_{BA}^f) \geq |S(\rho_B^f) - S(\rho_A^f)| = |S(\rho_B^f) - S(\rho_B^{eq})|$$

Absolute value of putative δS_{env} is a lower bound on entanglement between measurement apparatus and system-bath-ancilla.



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