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Quantum Thermodynamics beyond the weak coupling limit

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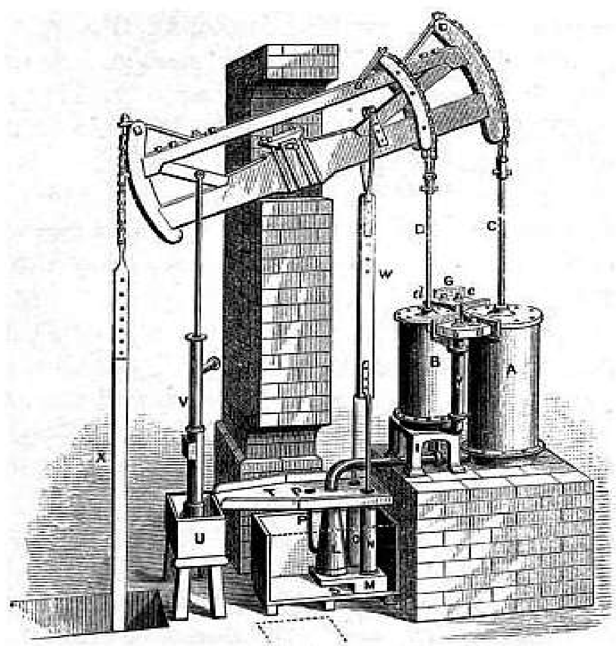
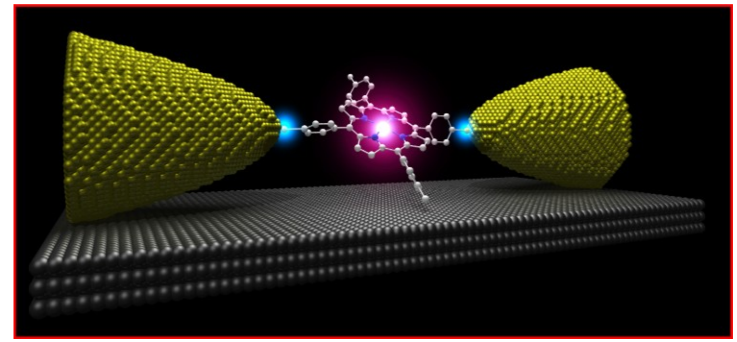
Kyoto, July 29, 2015

Introduction

Thermodynamics in the 19th century:

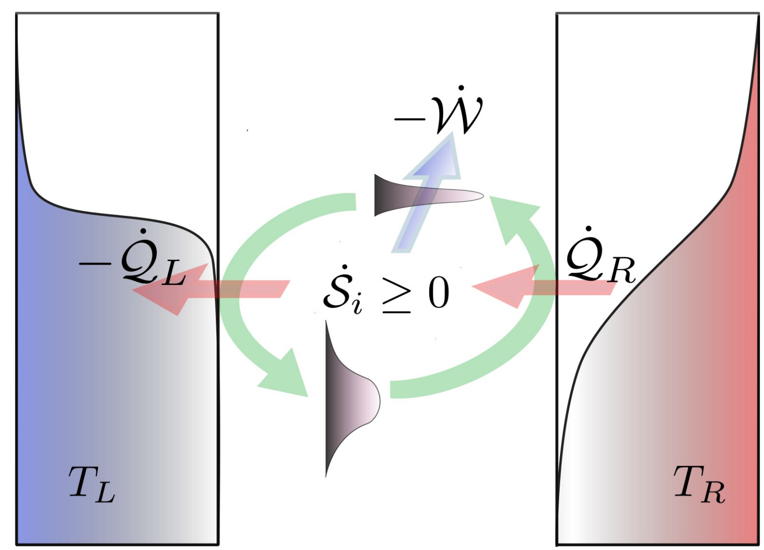


Thermodynamics in the 21th century:



http://www.scm.com/

$$\frac{d}{dt}\mathcal{E} = \sum_\nu \dot{\mathcal{Q}}_\nu + \dot{\mathcal{W}}$$

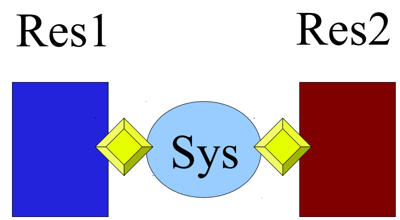


$$\frac{d}{dt}\mathcal{S} = \sum_\nu \frac{\dot{\mathcal{Q}}_\nu}{T_\nu} + \dot{\mathcal{S}}_i$$

Outline

- I) Nonequilibrium Thermodynamics: Phenomenology
- II) Weak coupling: Stochastic Thermodynamics
- III) Strong coupling: An exact identity as the second law
- IV) Strong coupling with NEGF:
    - A) Model and dynamics
    - B) Problems with conventional heat definitions
    - C) A new approach to Quantum Thermodynamics
- Open questions

I) Nonequilibrium Thermodynamics: Phenomenology



- Zeroth law: Existence of equilibrium with a well defined temperature
- First law: $$d_t U(t) = \dot{W}(t) + \sum_\nu \dot{Q}_\nu(t)$$
- Second law: $$\dot{S}_i(t) = d_t S(t) - \sum_\nu \beta_\nu \dot{Q}_\nu(t) \geq 0$$
- Third law: $S^{eq} \to 0$, $d_t S^{eq} \to 0$ when $T \to 0$

Reversible transformation:
(slow trsf. in contact
with one reservoir)

$$\dot{S}_i(t) = 0 \quad , \quad T d_t S^{eq}(t) = \dot{Q}^{eq}(t)$$

Fundamental relation of equilibrium thermodynamics

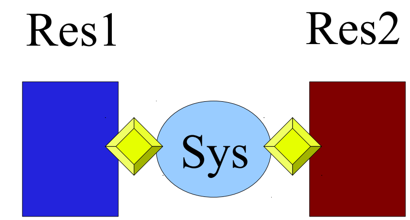
$$T d_t S^{eq}(t) = d_t E^{eq}(t) - \dot{W}^{eq}(t)$$

II) Stochastic Thermodynamics (weak coupling)

Esposito, *Stochastic thermodynamics under coarse-graining*, PRE **85**, 041125 (2012)

Van den Broeck and Esposito, *Ensemble and Trajectory Thermodynamics: A Brief Introduction*, Physica A **418**, 6 (2015)

Microscopically derived
Markovian Quantum Master Equation
+ rotating wave approx



i are the eigenenergies of the system

$$\dot{p}_i = \sum_j w_{ij} p_j = \sum_j \left(w_{ij} p_j - w_{ji} p_i \right)$$

$$w_{ij} = \sum_\nu w_{ij}^{(\nu)}$$

Different reservoirs $T^{(\nu)}$ $\mu^{(\nu)}$

Local detailed balance: $$\frac{w_{ij}^{(\nu)}}{w_{ji}^{(\nu)}} = \exp\left(- \frac{(\epsilon_i - \epsilon_j) - \mu^{(\nu)}(n_i - n_j)}{k_b T^{(\nu)}} \right)$$

Energy, Particle number, Shannon entropy

$$E = \sum_i \epsilon_i p_i \quad , \quad N = \sum_i n_i p_i \quad , \quad S = \sum_i [-k_b \ln p_i] p_i$$

Matter conservation

$$d_t N = \sum_\nu I_N^{(\nu)}$$

Energy and Matter currents

$$I_E^{(\nu)} = \sum_{i,j} w_{ij}^{(\nu)} p_j (\epsilon_i - \epsilon_j)$$

$$I_M^{(\nu)} = \sum_{i,j} w_{ij}^{(\nu)} p_j (n_i - n_j)$$

<u>1st law</u>: (energy conservation)

- $$d_t E = \dot{W} + \dot{W}_c + \sum_\nu \dot{Q}^{(\nu)}$$

Heat $\quad \dot{Q}^{(\nu)} = I_E^{(\nu)} - \mu^{(\nu)} I_M^{(\nu)}$

Mechanical work $\quad \dot{W} = \sum_i p_i d_t \epsilon_i$

Chemical work $\quad \dot{W}_c = \sum_\nu \mu^{(\nu)} I_M^{(\nu)}$

<u>2nd law</u>: (non-conservation of entropy)

- $$\dot{S}_{\mathbf{i}} = d_t S - \sum_\nu \frac{\dot{Q}_\nu}{T_\nu} \geq 0$$

$$\boxed{\dot{S}_{\mathbf{i}} = \frac{k_b}{2} \sum_{\nu,i,j} \left(w_{ij}^{(\nu)} p_j - w_{ji}^{(\nu)} p_i\right) \ln \frac{w_{ij}^{(\nu)} p_j}{w_{ji}^{(\nu)} p_i} \geq 0}$$

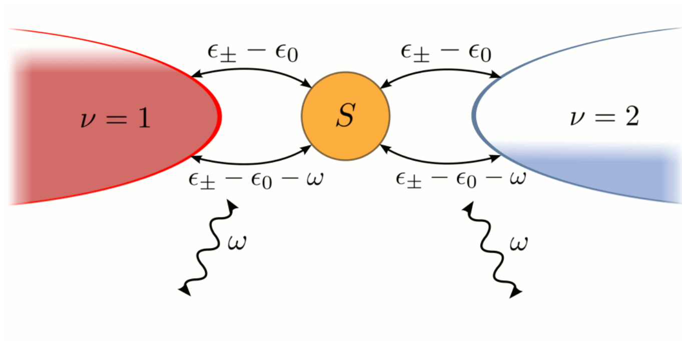
- <u>0th law</u>: $\dot{S}_{\mathbf{i}} = 0$ iff $w_{ij}^{(\nu)} p_j = w_{ji}^{(\nu)} p_i$ (detailed balance = equilibrium)

$$p_i^{eq} = \exp\{-\frac{\epsilon_i - \mu n_i - \Omega^{eq}}{k_b T}\}$$

- <u>3rd law</u>: $T \to 0 \qquad S^{eq} \to 0$

Stochastic thermodynamics for open quantum systems also works for:

- Rapid periodic driving (Floquet theory + weak coupling)



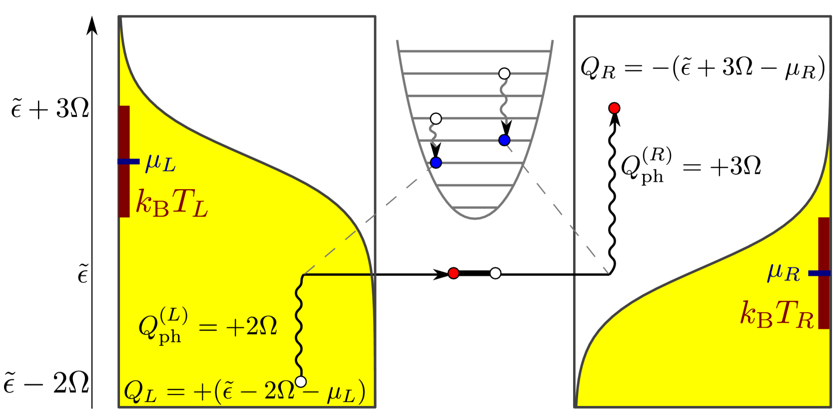
$$\frac{w_{ij}^{(\nu,l)}}{w_{ji}^{(\nu,l)}} = \exp\left(- \frac{(\epsilon_i - \epsilon_j) - \mu^{(\nu)}(n_i - n_j) \boxed{- l\omega}}{k_b T^{(\nu)}} \right)$$

i : quasienergies of the system   Mech. work due to driving

"Stochastic thermodynamics of rapidly driven systems",
Bulnes Cuetara, Engel & Esposito, New J. Phys. **17**, 055002 (2015)

- "Strong couping" with polaron transformation

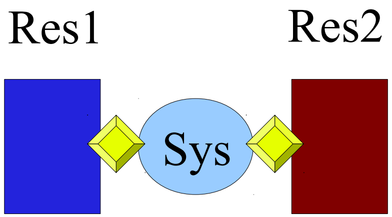
Non-additive in the reservoirs



$$\frac{\gamma_{12,+n_\alpha}^{\alpha}(-\omega)}{\gamma_{21,-n_\alpha}^{\alpha}(+\omega)} = e^{-\beta_\alpha(\omega - \mu_\alpha + n_\alpha \cdot \Omega)} e^{\beta_{\rm ph} n_\alpha \cdot \Omega}$$

"Single electron transistor strongly coupled to vibration:
counting statistics and fluctuation theorem",
Schaller, Krause, Brandes & Esposito,
New J. Phys. **15**, 033032 (2013)

"Thermodynamics of the polaron master equation at finite bias",
Krause, Brandes, Esposito & Schaller,
J. Chem. Phys. **142**, 134106 (2015)



III) An exact identity (strong coupling)

Entropy production as correlation between system and reservoir

Esposito, Lindenberg, Van Den Broeck, New J. Phys. **12**, 013013 (2010)

$$H(t) = H_s(t) + \sum_\nu (H_\nu + V_\nu(t))$$

Single assumption: $\left\{ \begin{array}{l} \rho(0) = \rho_s(0) \prod_\nu \rho_\nu^{\mathrm{eq}} \\ \rho_\nu^{\mathrm{eq}} = \exp\big(-\beta_\nu H_\nu\big)/Z_\nu \end{array} \right.$

- 1st law:

$$\Delta U(t) = W(t) + \sum_\nu Q_\nu(t)$$

- 2nd law:

$$\boxed{\begin{aligned} \Delta_i S(t) &= \Delta S(t) - \sum_\nu \beta_\nu Q_\nu(t) \\ &= D[\rho(t)||\rho_s(t) \prod_\nu \rho_\nu^{\mathrm{eq}}] \geq 0 \end{aligned}}$$

$D[\rho||\rho'] \equiv \mathrm{Tr}\rho \ln \rho - \mathrm{Tr}\rho \ln \rho'$

Energy: $U(t) = \langle \big(H_s(t) + \sum_\nu V_\nu(t)\big) \rangle_t$

Entropy: $S(t) = -\mathrm{Tr}_s \rho_s(t) \ln \rho_s(t)$

Heat: $Q_\nu(t) = \langle H_\nu \rangle_0 - \langle H_\nu \rangle_t = \int_0^t d\tau \mathrm{Tr}\big(H_s(t) + V_\nu(t)\big)\dot{\rho}(t)$

Work: $W = \langle H(t) \rangle_t - \langle H(0) \rangle_0 = \int_0^t d\tau \mathrm{Tr}\big(\dot{H}_s(t) + \sum_\nu \dot{V}_\nu(t)\big)\rho(t)$

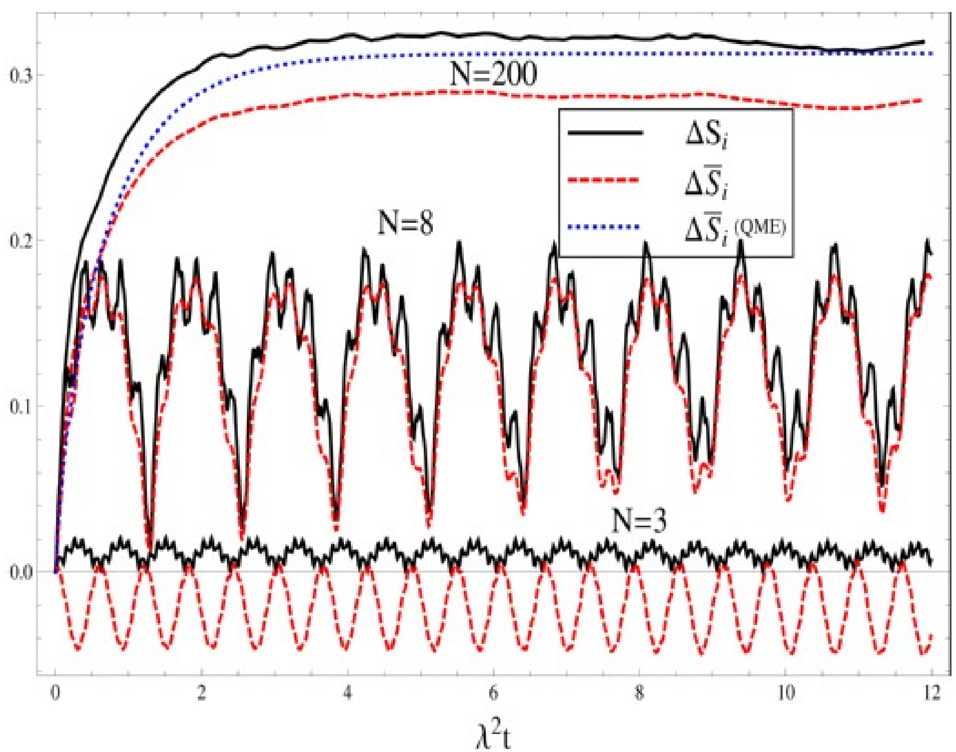
See also Reeb & Wolf, New J. Phys. **16**, 103011 (2014)

Problems

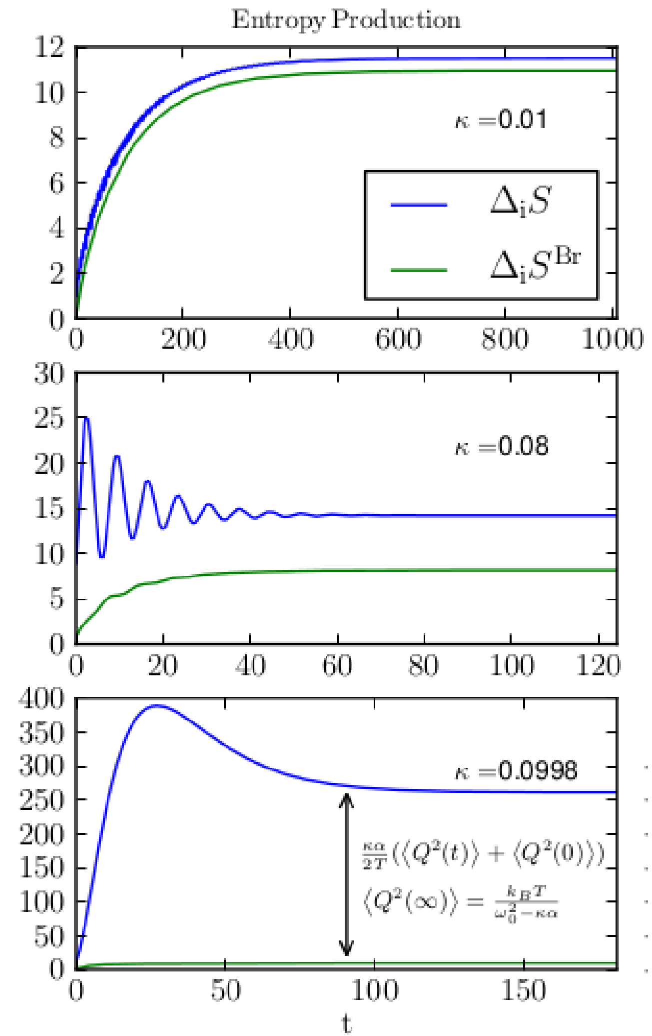
- $$\frac{d}{dt}\Delta_i S \equiv \dot{S}_i(t) = d_t S(t) - \sum_\nu \beta_\nu \dot{Q}_\nu(t)$$ can be negative at finite N as well as at infinite N!
- No zeroth law "build in" the dynamics
- No third law because no equilibrium entropy

Entropy production as correlation between system and reservoir, Esposito, Lindenberg, Van Den Broeck, New J. Phys. **12**, 013013 (2010)

$$H = \frac{\Delta}{2}\sigma_z + H_r + \lambda\sigma_x R$$



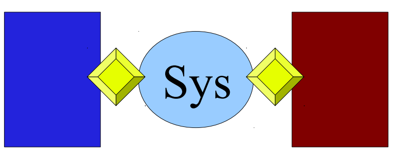
Entropy Production in Quantum Brownian Motion, Pucci, Esposito, Peliti, J. Stat. Mech. (2013) P04005

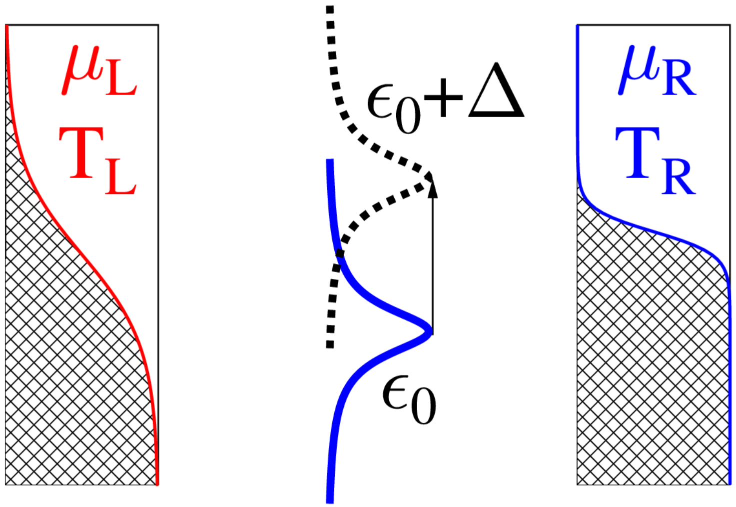


IV) NEGF (strong coupling)

A) Model and dynamics

Externally driven single level quantum dot strongly coupled to Fermionic reservoirs





$$\hat{H}(t) = \hat{H}_S(t) + \sum_\nu \hat{H}_\nu + \sum_\nu \hat{V}_\nu(t)$$

$$\hat{H}_S(t) = \boxed{\varepsilon(t)}\hat{d}^\dagger \hat{d} \qquad \hat{H}_\nu = \sum_{k\in\nu} \varepsilon_k \hat{c}_k^\dagger \hat{c}_k \qquad \hat{V}_\nu(t) = \sum_{k\in\nu} \Big(V_k^\nu(t) \hat{d}^\dagger \hat{c}_k + \text{H.c.} \Big)$$

$$\boxed{u_\nu(t)}\, V_k$$

Contour System Green's functions:

$$G(\tau_1,\tau_2) = -i\left\langle T_c\, \hat{d}(\tau_1)\, \hat{d}^\dagger(\tau_2)\right\rangle \longrightarrow \begin{array}{l} t = (t_1+t_2)/2 \\ s = t_1 - t_2 \end{array} \xrightarrow[\text{trsf}]{\text{Fourier}} \begin{array}{l} t \\ E \end{array}$$

Equations of motion

$$\left(i\frac{\overrightarrow{\partial}}{\partial t_1} - H_S(t_1)\right) G^{s_1 s_2}(t_1,t_2) = \sigma^z_{s_1 s_2}\delta(t_1-t_2) + \sum_{s_3}\int dt_3\, \Sigma^{s_1 s_3}(t_1,t_3)\, s_3\, G^{s_3 s_2}(t_3,t_2)$$

$$G^{s_1 s_2}(t_1,t_2)\left(-i\frac{\overleftarrow{\partial}}{\partial t_2} - H_S(t_2)\right) = \sigma^z_{s_1 s_2}\delta(t_1-t_2) + \sum_{s_3}\int dt_3\, G^{s_1 s_3}(t_1,t_3)\, s_3\, \Sigma^{s_3 s_2}(t_3,t_2)$$

Self-energies (effect of the reservoirs)

$$[\Sigma_\nu(\tau,\tau')]_{mm'} = \sum_{k\in\nu} V_{mk}(t)\, g_k(\tau,\tau')\, V_{km'}(t'), \qquad g_k(\tau,\tau') \equiv -i\langle T_c\, \hat{c}_k(\tau)\, \hat{c}_k^\dagger(\tau')\rangle$$

$$F(t_1,t_2) = \int dt_3\, F_1(t_1,t_3)\, F_2(t_3,t_2) \longrightarrow F(t,E) = F_1(t,E)\underbrace{\exp\left(\frac{1}{2i}\left[\overleftarrow{\partial}_t\,\overrightarrow{\partial}_E - \overleftarrow{\partial}_E\,\overrightarrow{\partial}_t\right]\right)}_{\text{expanded to second order}} F_2(t,E)$$

Slow driving: expanded to second order

"Gradient expansion"

B) Problems with conventional heat definitions

Esposito, Ochoa, Galperin, *On the nature of heat in strongly coupled open quantum systems,*
arXiv:1408.3608 to be replaced soon

$$\dot{Q}_{\nu,\alpha} = J_{\nu,\alpha} - \mu_\nu I_\nu \qquad I_\nu = -\mathrm{Tr}\{\hat{N}_\nu\, d_t\hat{\rho}\}$$

$$J_{\nu,\alpha} = -\mathrm{Tr}\{\big(\hat{H}_\nu + \alpha\hat{V}_\nu\big) d_t\hat{\rho}\}$$

$\alpha = 0$ the interaction is part of the system $\longrightarrow$ this is the standard definition

$\alpha = 1/2$ equal sharing of the interaction between reservoir and system

$\alpha = 1$ the interaction is part of the reservoir

Reversible heat: $$\dot{Q}^{(1)}_\alpha = \frac{d}{dt}\left(\int \frac{dE}{2\pi} f\, A^{(0)}\big[(E-\mu) + (1-2\alpha)(E-\varepsilon)\big]\right) - \int \frac{dE}{2\pi} f\left(A^{(0)}\, d_t\varepsilon + (1-\alpha)\Big[\mathrm{Re}G^{r(0)}\,\partial_t\Gamma + A^{(0)}\,\partial_t\Lambda\Big]\right)$$

f : Fermi distribution

Retarded GF: $G^{r(0)}(t,E) = [E - \varepsilon(t) - \Sigma^r(t,E)]^{-1}$ $\longrightarrow$ Lamb shift

$\longrightarrow$ Broadening

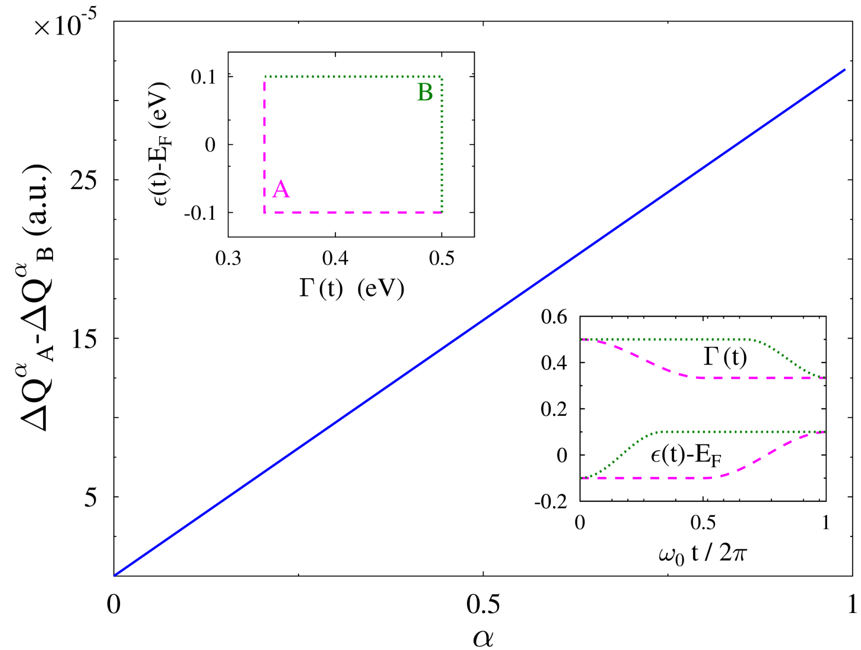
Retarded self-energy: $\Sigma^r(t,E) = \Lambda(t,E) - i\Gamma(t,E)/2$

Spectral function: $$A^{(0)}(t,E) = -2\,\mathrm{Im}\,G^{r(0)}(t,E) = \frac{\Gamma(t,E)}{\big(E-\varepsilon(t)-\Lambda(t,E)\big)^2 + \big(\Gamma(t,E)/2\big)^2}$$

Reversible heat has to be an exact differential:

$$\frac{\partial^2 Q^{(1)}_\alpha}{\partial\varepsilon\,\partial u} = \frac{\partial^2 Q^{(1)}_\alpha}{\partial u\,\partial\varepsilon}$$

This is only true if $\alpha = 0$!



We can obtain entropy by integrating: $d_t S^{eq} = \dot{Q}^{(1)}_0 / T$

$$S^{eq} = \int \frac{dE}{2\pi} A\big(- f \ln f - [1-f]\ln[1-f]\big) \longrightarrow \text{Energy resolved Shannon form}$$

$$+ \underbrace{\int \frac{dE}{2\pi} A f \frac{(E-\varepsilon)}{T}}_{\frac{\langle \hat{V}_\nu(t)\rangle_{eq}}{2T}} + \int \frac{dE}{2\pi} A \ln[1-f]\big(\partial_E \Lambda + \frac{E-\varepsilon-\Lambda}{\Gamma}\partial_E \Gamma\big)$$

Zero in wide band approx.

Problems with third law: When $T \to 0$ $\Rightarrow$ $S^{eq} \to \infty$

C) A new approach to quantum thermodynamics

Quantum thermodynamics: A nonequilibrium Green's function approach
Esposito, Ochoa & Galperin, Phys. Rev. Lett. **114**, 080602 (2015).

Equation of motion for the population of the level $\phi(t,E)$:

$$\boxed{\{E-\varepsilon(t)-\Lambda(t,E);A(t,E)\,\phi(t,E)\}+\{\mathrm{Re}\,G^r(t,E);\Gamma(t,E)\,\phi(t,E)\}=\mathcal{C}(t,E)}$$

$$\{f_1;f_2\}\equiv\partial_E f_1\partial_t f_2-\partial_t f_1\partial_E f_2$$

Retarded Green's functions: $G^r(t,E)=[E-\varepsilon(t)-\Sigma^r(t,E)]^{-1}$

Self-energy:

$$\Sigma^r(t,E)=\underbrace{\Lambda(t,E)}_{\text{Lamb shift}}-\underbrace{i\Gamma(t,E)/2}_{\text{Broadening}}$$

$$\Sigma^r(t_1,t_2)=-i\sum_{\nu=L,R}\sum_{k\in\nu}V_k^\nu(t_1)\,\overset{*}{V}{}_k^\nu(t_2)\,\theta(t_1-t_2)e^{-i\varepsilon_k(t_1-t_2)}$$

Spectral function: $A(t,E)=-2\,\mathrm{Im}\,G^r(t,E)=\dfrac{\Gamma(t,E)}{(E-\varepsilon(t)-\Lambda(t,E))^2+(\Gamma(t,E)/2)^2}$

Energy resolved particle current:

$$\mathcal{C}_\nu(t,E)=\mathcal{C}_\nu^+(t,E)-\mathcal{C}_\nu^-(t,E)\quad\left\{\begin{aligned}\mathcal{C}_\nu^+(t,E)&=A(t,E)\Gamma_\nu(t,E)f_\nu(E)\,[1-\phi(t,E)]\\ \mathcal{C}_\nu^-(t,E)&=A(t,E)\Gamma_\nu(t,E)\phi(t,E)\,[1-f_\nu(E)]\end{aligned}\right.$$

Renormalized spectral function: $\mathcal{A}(t,E) = A(1-\partial_E\Lambda) + \Gamma\partial_E \mathrm{Re}G^r \geq 0$

is positive and normalized

Energy resolved quantities!

$$\left\{ \begin{aligned} \mathcal{N}(t) &= \int \frac{dE}{2\pi}\, \mathcal{A}(t,E)\, \phi(t,E) \\ \mathcal{E}(t) &= \int \frac{dE}{2\pi}\, \mathcal{A}(t,E)\, E\, \phi(t,E) \\ \mathcal{S}(t) &= \int \frac{dE}{2\pi}\, \mathcal{A}(t,E)\, \sigma(t,E) \end{aligned} \right.$$

where $\sigma(t,E) = -\phi(t,E)\ln\phi(t,E) - [1-\phi(t,E)]\ln[1-\phi(t,E)]$

Introduced in the context of the quantum Boltzmann equation by
Ivanov, Knoll, and Voskresensky, Nuclear Physics A 672, 313 (2000)

Balance equations:

$$\begin{cases} d_t\mathcal{N}(t) = \sum_\nu \mathcal{I}_\nu(t) & \\ d_t\mathcal{E}(t) = \sum_\nu \dot{\mathcal{Q}}_\nu(t) + \dot{\mathcal{W}} + \dot{\mathcal{W}}_c & \underline{\text{First law}} \\ d_t\mathcal{S}(t) = \dot{\mathcal{S}}_i(t) + \sum_\nu \frac{\dot{\mathcal{Q}}_\nu(t)}{T_\nu} & \underline{\text{Second law}} \end{cases}$$

Heat $\dot{\mathcal{Q}}_\nu = \mathcal{J}_\nu(t) - \mu_\nu\,\mathcal{I}_\nu(t)$

Particle current $\mathcal{I}_\nu(t) = \int \frac{dE}{2\pi}\,\mathcal{C}_\nu(t,E)$

Chemical work $\dot{\mathcal{W}}_c = \sum_\nu \mu_\nu\,\mathcal{I}_\nu(t)$

Energy current $\mathcal{J}_\nu(t) = \int \frac{dE}{2\pi}\,E\,\mathcal{C}_\nu(t,E)$

Mechanical work $\dot{\mathcal{W}}(t) = \int \frac{dE}{2\pi}\big(- A\,\phi\,\partial_t(E-\varepsilon(t)-\Lambda) - \Gamma\,\phi\,\partial_t \mathrm{Re}\,G^r\big)$

Entropy production

$$\boxed{\dot{\mathcal{S}}_i(t) = \sum_\nu \int \frac{dE}{2\pi}\,\big(\mathcal{C}_\nu^+(t,E) - \mathcal{C}_\nu^-(t,E)\big)\ln\frac{\mathcal{C}_\nu^+(t,E)}{\mathcal{C}_\nu^-(t,E)} \geq 0}$$

Equilibrium:

$\forall\nu : f_\nu(E) = \phi(t,E)$

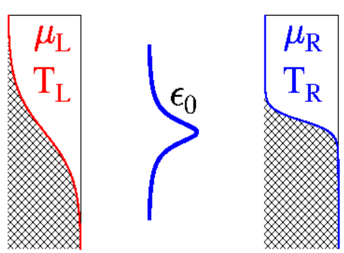
- Weak coupling limit $\xrightarrow[\Lambda \to 0]{\Gamma \to 0}$ we recover stochastic thermodynamics $A, \mathcal{A} \to 2\pi\delta(E-\varepsilon)$

- 0th law: At equilibrium $\phi(t,E) = f(E)$ the Fermi distribution at μ , T

- 3rd law: $T \to 0$ $\sigma^{eq}(E) \to 0$ $\mathcal{S}^{eq} \to 0$

- At nonequilibrium steady state: $\dot{\mathcal{S}}_i(t) = -\sum_\nu \frac{\dot{\mathcal{Q}}_\nu(t)}{T_\nu} \geq 0$

(a)

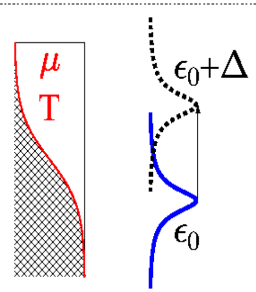


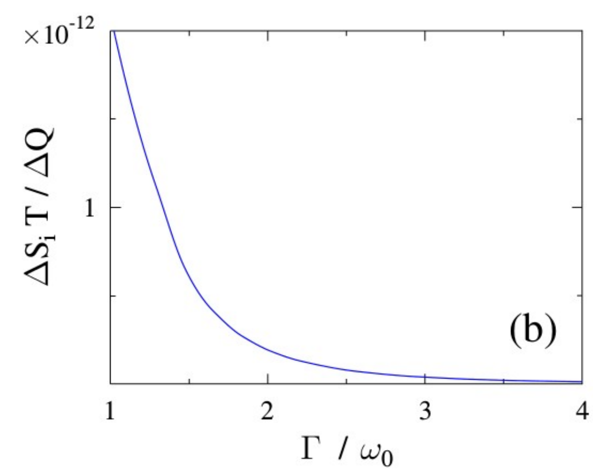
Standard definitions!

$$\dot{\mathcal{Q}}_\nu = \mathcal{J}_\nu(t) - \mu_\nu \mathcal{I}_\nu(t) \quad \begin{cases} \mathcal{I}_\nu(t) = -\mathrm{Tr}\left[\hat{N}_\nu d_t \hat{\rho}(t)\right] \\ \mathcal{J}_\nu(t) = -\mathrm{Tr}\left[\hat{H}_\nu d_t \hat{\rho}(t)\right] \end{cases}$$

- For reversible transformations: $T d_t \mathcal{S}^{eq}(t) = \dot{\mathcal{Q}}(t)$

(b)





Remark

$$\mathcal{C}_\nu(t,E) = C_\nu(t,E) - \{\Lambda_\nu(t,E); A(t,E)\,\phi(t,E)\} - \{\Gamma_\nu(t,E)\,\phi(t,E); \mathrm{Re}\,G^r(t,E)\}$$

$$\mathcal{A}(t,E) = A(1-\partial_E\Lambda) + \Gamma\partial_E \mathrm{Re} G^r \geq 0$$

$$N(t) = \int \frac{dE}{2\pi}\, \boxed{A(t,E)}\, \phi(t,E) \qquad N(t) = \mathrm{Tr}\big[\hat{N}_S\,\hat{\rho}(t)\big]$$

$$E(t) = \int \frac{dE}{2\pi}\, \boxed{A(t,E)}\, E\,\phi(t,E) \qquad E(t) = \mathrm{Tr}\left[\left(\hat{H}_S(t) + \sum_\nu \hat{V}_\nu(t)/2\right)\hat{\rho}(t)\right]$$

$$S(t) = \int \frac{dE}{2\pi}\, \boxed{A(t,E)}\, \sigma(t,E)$$

$$J_\nu(t) = \int \frac{dE}{2\pi}\, E\, \boxed{C_\nu(t,E)} \qquad J_\nu(t) = -\mathrm{Tr}\left[\left(\hat{H}_\nu + \hat{V}_\nu(t)/2\right) d_t\hat{\rho}(t)\right] + \frac{1}{2}\mathrm{Tr}\left[d_t\hat{V}_\nu(t)\hat{\rho}(t)\right]$$

$$I_\nu(t) = \int \frac{dE}{2\pi}\, \boxed{C_\nu(t,E)} \qquad I_\nu(t) = -\mathrm{Tr}\big[N_\nu d_t\hat{\rho}(t)\big]$$

$$d_t E(t) = \sum_\nu \dot{Q}_\nu(t) + \dot{W} + \dot{W}_c \qquad \begin{cases} \dot{W}(t) = \mathrm{Tr}\left[d_t \hat{H}_S(t)\hat{\rho}(t)\right] \\ \dot{Q}_\nu = J_\nu(t) - \mu_\nu\, I_\nu(t) \end{cases}$$

But: $\begin{cases} \dot{Q}^1 \ \text{(reversible heat) is not a state function} \\ \dot{S}_i(t) \equiv d_t S(t) - \sum_\nu \dfrac{\dot{Q}_\nu(t)}{T_\nu} \ \text{can be negative} \end{cases}$

Special case where it works: 1 level, 1 reservoir, wide band, no driving in coupling

Ludovico, Lim, Moskalets, Arrachea, Sanchez, Phys. Rev. B 89, 161306 (2014)

Open questions

Generalization to many orbitals and to interacting systems....

Beyond gradient expansion (for faster driving)....

Fluctuations....

Experiments....

Main references:

Esposito, Lindenberg, Van Den Broeck,
Entropy production as correlation between system and reservoir,
New J. Phys. **12**, 013013 (2010)

Esposito, Ochoa and Galperin,

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Thank you for your attention!