Models of Quantum Machines

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Why quantum thermodynamic?

- Applicability of the laws of thermodynamics and related bounds (e.g. Carnot) in the quantum domain.
- New designs of microscopic engines and refrigerators.
- Thermodynamical bounds on (quantum) information processing.
- Technological and biological applications.

A general scheme of QUANTUM MACHINE

- S - a microscopic "small" system - "working fluid"

- $\{B_j; j = 1, .., M\}$ - quantum heat bath at temperatures T_j (e.g. bosonic free field, ideal Fermi/Bose gas)

- $\{f_\alpha(t); \alpha = 1, ..., K\}$ - external control (classical, deterministic) parameters

- Total Hamiltonian

$$H_{tot} = \Big(H_S + \sum_\alpha f_\alpha(t) h_\alpha\Big) + \sum_j H_{B_j} + \sum_j H_{SB_j}$$

Slowly varying external control

Spohn, Lebowitz (1978), Davies, Spohn (1978), RA (1979)(weak coupling + adiabatic limits)

Reduced dynamics of S is approximated by the Markovian Master equation:

$$\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)] + \sum_j \mathcal{L}_j(t)\rho(t), \tag{1}$$

where $\mathcal{L}_j(t)$ is a Lindblad-Gorini-Kossakowski-Sudarshan generator

Zero-th Law of Thermodynamics

$$\mathcal{L}_j(t)\rho_j^{eq}(t) = 0 \ , \ \rho_j^{eq}(t) = \frac{e^{-\beta_j H(t)}}{\mathrm{Tr} e^{-\beta_j H(t)}} \ . \tag{2}$$

$H(t)$ - *total, physical Hamiltonian of* S, $\beta_j = 1/kT_j$

First Law of Thermodynamics

W-work performed on S, Q - heat absorbed by S, E - internal energy of S

$$E(t) = \mathrm{Tr}\big(\rho(t)H(t)\big) \tag{3}$$

$$\frac{d}{dt}W(t) = \mathrm{Tr}\big(\rho(t)\frac{dH(t)}{dt}\big) \ , \tag{4}$$

$$\frac{d}{dt}Q(t) = \mathrm{Tr}\big(\frac{d\rho(t)}{dt}H(t)\big) = \sum_j \mathrm{Tr}\big(H(t)\mathcal{L}_j(t)\rho(t)\big) \equiv \sum_j \frac{d}{dt}Q_j(t) \ . \tag{5}$$

Q_j - heat absorbed by S from B_j.

Second Law of Thermodynamics

Entropy - $S(t) = -k\mathrm{Tr}\big(\rho(t)\ln\rho(t)\big)$

$$\frac{d}{dt}S(t) - \sum_j \frac{1}{T_j}\frac{d}{dt}Q_j(t) = \sum_j \sigma_j(t) \geq 0 \tag{6}$$

$\sigma_j(t)$ - entropy production caused by B_j

$$\sigma_j(t) = k\mathrm{Tr}\big(\mathcal{L}_j(t)\rho(t)[\ln\rho(t) - \ln\rho_j^{eq}(t)]\big) \geq 0 \tag{7}$$

Exercise

Show (7) using Lindblad H-theorem for $S(\rho|\rho') = \mathrm{Tr}(\rho\ln\rho - \rho\ln\rho')$ and CP-dynamical map Λ. Use $\Lambda = \exp\{s\mathcal{L}_j(t)\}$, $\rho' = \rho_j^{eq}(t)$

$$S(\Lambda\rho|\Lambda\rho') \leq S(\rho|\rho') \tag{8}$$

Periodic control

- Weak coupling limit can be combined with Floquet theory to produce Markovian master equations with periodic in time generators (RA, Lidar,Zanardi, (2006))

- With a proper definition of heat currents, II-law is satisfied.

- At the steady state I-law allows to compute stationary power and prove the Carnot bound even for a general non-equilibrium stationary environment.

- New types of microscopic engines and refrigerators can be designed.

See recent and future papers by RA, Gelbwasser, Kolar, Kosloff, Kurizki, Szczygielski.

A model of quantum machine

A qubit with periodic modulation

$$H(t) = \frac{1}{2}\omega(t)\sigma^3 \ , \ \omega(t+\tau) = \omega(t), \ \frac{1}{\tau}\int_0^\tau \omega(s)ds = \omega_0 \geq 0 \qquad (9)$$

weakly coupled to hot and cold baths at T^h, T^c

$$H_{int} = \sigma^1 \otimes (B^h + B^c). \qquad (10)$$

The Markovian master equation (notice time-independence of $\mathcal{L}^{c(h)}$)

$$\frac{d\rho(t)}{dt} = -i\frac{1}{2}\omega(t)[\sigma^3, \rho(t)] + \mathcal{L}^c\rho(t) + \mathcal{L}^h\rho(t). \qquad (11)$$

Sketch of derivation

Unitary propagator (interaction picture) for the total system (μ-small constant)

$$U_\mu(t,0) = \mathcal{T}\exp\Big\{\frac{-i\mu}{\hbar}\int_0^t \sigma^1(s)\otimes R(s)\,ds\Big\} \tag{12}$$

$$\sigma^1(t) = \sum_{q\in\mathbf{Z}}\big(\xi(q)e^{-i(\omega_0+q\Omega)t}\sigma^- + h.c.\big) \tag{13}$$

$$\xi(q) = \frac{1}{\tau}\int_0^\tau e^{i\int_0^t(\omega(s)-\omega_0)ds}e^{-iq\Omega t}dt, \tag{14}$$

$$R(t) = B^h(t) + B^c(t)\ ,\ B^a(t) = e^{iH_{B_a}t}\,B^a\,e^{-iH_{B_a}t} \tag{15}$$

$\{\omega_0 + q\Omega; q\in\mathbf{Z}\}$ - "Bohr's quasi-frequencies"

Reduced dynamics (interaction picture)

$$\rho(t) = \Lambda(t,0)\rho \equiv \mathrm{Tr}_R\big(U_\mu(t,0)\rho \otimes \rho_R U_\mu(t,0)^\dagger\big) \tag{16}$$

Cumulant expansion

$$\Lambda(t,0) = \exp\sum_{n=1}^{\infty}[\mu^n K^{(n)}(t)], \tag{17}$$

Born approximation, WCL, Gaussian approximation:

$$\Lambda(t,0) = \exp[\mu^2 K(t) + O(\lambda^3)]. \tag{18}$$

$$K(t)\rho = \frac{1}{2}\int_0^t ds\int_0^t du\,\mathrm{Tr}(\rho_R R(s)R)\sigma^1(s)\rho\sigma^1(u) + \cdots \tag{19}$$

Markov approximation (in the interaction picture) – $K(t) \simeq t\mathcal{L}$

Generator's structure

For $a = c$, or $a = h$, $\Omega = 2\pi/\tau$ we have

$$\mathcal{L}^a \rho = \sum_{q \in \mathbf{Z}} \mathcal{L}^a_q \rho \tag{20}$$

$$\begin{aligned} \mathcal{L}^a_q \rho &= \frac{P(q)}{2} \Big(G^a(\omega_0 + q\Omega)\big([\sigma^- \rho, \sigma^+] + [\sigma^-, \rho\sigma^+]\big) \\ &+ G^a(-\omega_0 - q\Omega)\big([\sigma^+ \rho, \sigma^-] + [\sigma^+, \rho\sigma^-]\big)\Big) \end{aligned} \tag{21}$$

$$G^a(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} \langle B^a(t) B^a \rangle_{T_a} dt = e^{\omega/k_B T_a} G^a(-\omega), \tag{22}$$

$$P(q) = |\xi(q)|^2 \;, \; \xi(q) = \frac{1}{\tau} \int_0^\tau e^{i \int_0^t (\omega(s) - \omega_0) ds} e^{-iq\Omega t} dt. \tag{23}$$

"Local", cold and hot heat currents

$$\mathcal{J}^a{}_q(t) = \frac{1}{2}(\omega_0 + q\Omega)\mathrm{Tr}\big(\sigma^3\,\mathcal{L}_q^a\rho(t)\big)\ ,\ \mathcal{J}^a(t) = \sum_{q\in\mathbf{Z}}\mathcal{J}^a{}_q(t). \tag{24}$$

The second law of thermodynamics

$$\frac{d}{dt}S(t) \geq \frac{\mathcal{J}^c(t)}{T_c} + \frac{\mathcal{J}^h(t)}{T_h}\ ,\ S(t) = -k_B\mathrm{Tr}\big(\rho(t)\ln\rho(t)\big). \tag{25}$$

Heat currents at the stationary state $\tilde{\rho}$

$$\tilde{\mathcal{J}}^a = \frac{1}{2}\sum_{q\in\mathbf{Z}}(\omega_0 + q\Omega)\mathrm{Tr}\big(\sigma^3\,\mathcal{L}_q^a\tilde{\rho}\big) \tag{26}$$

The II-law

$$\frac{\tilde{\mathcal{J}}^c}{T_c} + \frac{\tilde{\mathcal{J}}^h}{T_h} \leq 0. \tag{27}$$

The I-law and the stationary power

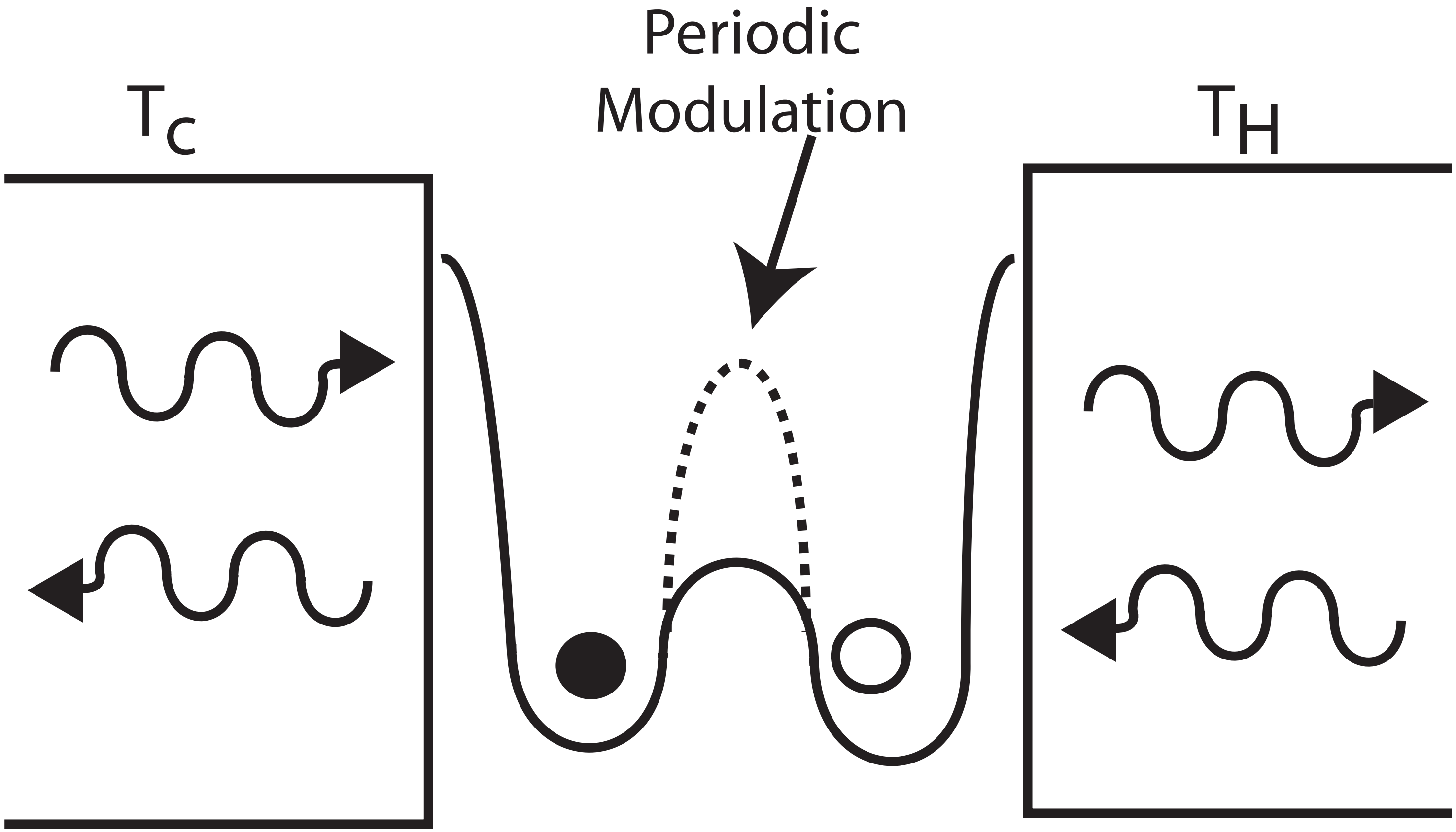
$$\tilde{\mathcal{P}} = -\tilde{\mathcal{J}}^c - \tilde{\mathcal{J}}^h. \tag{28}$$

Carnot bounds on the engine efficiency η and the coefficient of performance (COP) for the refrigerator

$$\eta = \frac{-\tilde{\mathcal{P}}}{\tilde{\mathcal{J}}^h} \leq 1 - \frac{T_c}{T_h},\ COP = \frac{\tilde{\mathcal{J}}^c}{\tilde{\mathcal{P}}} \leq \frac{T_c}{T_h - T_c}. \tag{29}$$

An example of implementation

Charged particle in double-well potential with modulated barrier



Universal machine

Can work as engine or refrigerator and reaches Carnot bounds

Time-dependence of the external field

$$\omega(t) = \omega_0 + \lambda \sin(\Omega t) \tag{30}$$

$$0 \leq \lambda << \Omega \leq \omega_0. \tag{31}$$

$\lambda/\Omega << 1$ implies

$$P(0) \simeq 1 - \frac{1}{2}\Big(\frac{\lambda}{\Omega}\Big)^2 \,,\; P(\pm 1) \simeq \Big(\frac{\lambda}{2\Omega}\Big)^2 \tag{32}$$

are relevant.

Spectral separation condition

$$G^c(\omega) \simeq 0 \text{ for } \omega \geq \omega_0 \text{ and } G^h(\omega) \simeq 0 \text{ for } \omega \leq \omega_0, \tag{33}$$

The formulas for heat currents and power

$$\begin{aligned}\tilde{\mathcal{J}}^h &= N(\omega_0+\Omega)(e^{-(\frac{\omega_0+\Omega}{k_B T_h})} - e^{-(\frac{\omega_0-\Omega}{k_B T_c})}) \\ \tilde{\mathcal{J}}^c &= -N(\omega_0-\Omega)(e^{-(\frac{\omega_0+\Omega}{k_B T_h})} - e^{-(\frac{\omega_0-\Omega}{k_B T_c})}) \\ \tilde{\mathcal{P}} &= -2N\Omega(e^{-(\frac{\omega_0+\Omega}{k_B T_h})} - e^{-(\frac{\omega_0-\Omega}{k_B T_c})})\end{aligned} \tag{34}$$

where

$$0 \le N = (\frac{\lambda}{2\Omega})^2 \frac{G^c(\omega_0-\Omega)G^h(\omega_0+\Omega)}{G^c(\omega_0-\Omega)\left[1+e^{-(\frac{\omega_0-\Omega}{k_B T_c})}\right] + G^h(\omega_0+\Omega)\left[1+e^{-(\frac{\omega_0+\Omega}{k_B T_h})}\right]} \tag{35}$$

A critical value of the modulation frequency

$$\Omega_{cr} = \omega_0 \frac{T_h - T_c}{T_h + T_c} \tag{36}$$

For $\Omega < \Omega_{cr}$ the machine works as an engine with

$$\eta = \frac{2\Omega}{\omega_0 + \Omega} \tag{37}$$

and for $\Omega > \Omega_{cr}$ as a refrigerator with

$$COP = \frac{\omega_0 + \Omega}{2\Omega} \tag{38}$$

At Ω_{cr} the engine/refrigerator reaches its maximal Carnot efficiency/COP, by the vanishing value of power/cold current.

Conclusions:

- The class of periodically driven and weakly coupled to environment quantum systems possess a complete and mathematically sound description in terms of Markovian master equations.
- For this class basic thermodynamical notions are consistently defined and the laws of thermodynamics are derived from first principles.
- No quantum miracles happen. The standard Carnot bounds hold.
- Various promising designs of microscopic quantum machines are obtained as byproducts.