Quantum Systems Coupled to Thermal Reservoirs

with H. Spohn, Adv. Chem. Phys. (1978)
L. Pastur, J. Phys. A (2004)

Question: How do we get an equation for the density matrix of system coupled to reservoirs which is analogous to classical case, i.e.

$$\frac{\partial \hat{\mu}}{\partial t} = \frac{1}{i}[H, \hat{\mu}] + \hat{\mathcal{K}}\hat{\mu}$$

In addition to obvious requirements of $\hat{\mathcal{K}}$ preserving normalization and positivity of $\hat{\mu}$ there is the "Lindblad complete positivity" condition $\hat{\mu}_t = \Phi_t \hat{\mu}_0$

Quantum Stochastic Maps

$$\hat{\mathcal{K}}\hat{\mu} = \frac{1}{2}\sum_{\alpha,\beta} c_{\alpha\beta}\{[F_\alpha, \rho F_\beta^+] + [F_\alpha \rho, F_\beta^+]\}$$

$\hat{\mu}$ is density matrix of system with finite N-dimensional Hilbert space, F_β are system operators

$tr(F_\beta^+ F_\beta) = \delta_{\alpha\beta}$, $\{c_{\alpha\beta}\}$ positive matrix

How do we get such a $\hat{\mathcal{K}}$?

$$H_\lambda = H_S \otimes 1^R + 1 \otimes H^R + \lambda H^{SR}$$

$$U_t^\lambda W = e^{-iH_\lambda t} W e^{iH_\lambda t}$$

$H^R = H_1^R + \cdots + H_n^R$, infinite reservoirs

$\omega^R = \omega^1 \otimes \cdots \otimes \omega^n$

$\omega^{(i)}$ KMS (Gibbs) states at β_i

At $t=0$, joint $\hat{\mu}_0 \otimes \omega^R$

$$\hat{\mu}_t = Tr_R[U_t^\lambda(\hat{\mu}_0 \times \omega^R)] = \Lambda_t^\lambda \hat{\mu}$$

$$\hat{\mathcal{K}}\hat{\mu}_t = \lambda^2 \int_0^t ds\, \hat{K}(t-s)\hat{\mu}_s$$

$$\rho_{st}^\lambda = \lim_{t\to\infty} \Lambda_t^\lambda \hat{\mu}_0 \quad \text{if it exists}$$

Proven: Fröhlich et al, Jakšić-Pillet for single (free) reservoir and small λ (other technicalities)

$$\rho_{st}^\lambda = Tr[\exp -\beta(H_0 + H^R + H^{SR})]/Z$$

van Hove limit, $\lambda\to 0, t\to\infty, \lambda^2 t\to\tau$

then (basically)

$$\frac{\partial\hat{\mu}}{\partial t} = \frac{i}{\hbar}[H,\hat{\mu}] + \underbrace{\left(\lambda^2 \int_0^\infty ds\, K(s)\right)}_{\mathcal{K}}\hat{\mu}$$

Entropy Production

$$\sigma = -\frac{d}{dt} \mathrm{Tr}\, \hat{\mu}_t \log \hat{\mu}_t + \Sigma \beta_k J_k$$

$$\geq 0$$

For a single reservoir; β

$$\sigma = -\frac{d}{dt} \mathrm{tr}(\hat{\mu}_t \log \hat{\mu}_t) + \frac{d}{dt} \mathrm{tr}(\hat{\mu}_t \log \hat{\mu}^\beta)$$

$$= -\frac{d}{dt} S_G(\hat{\mu}_t | \hat{\mu}^\beta) \geq 0$$

relative entropy.

I dont know if generally

$-\frac{d}{dt} S_G(\hat{\mu}_t | \hat{\rho}_{st})$ is positive?

Dedicated to
Bob Dorfman
and to all those who
search for a peace which
recognizes the rights and
humanity of all and the
superiority of none.