Introduction to Quantum Thermodynamics: History & Prospects with Ronnie Kosloff

I. (very) Brief History of Q. Thermo.

II Spin-boson model, remarks & warnings

1916 Einstein – stimulated emission v.s. absorption
thermodynamical arguments

1967 Geusic, Scovil, Schultz-Dubios
– maser (laser) as a quantum engine

Quantum Open Systems ~ 1970

- Influence functional (path integrals
- Green functions
- $\boxed{\text{Reduced dynamics} \rightarrow \text{Master Eqs}}$

$$
\begin{tikzcd}
\varrho_{SR}(t_0) \arrow[r, "\mathcal{U}_{SR}(t,t_0)"] \arrow[d, "Tr_B"'] & \varrho_{SR}(t) \arrow[d, "Tr_B"] \\
\varrho_S(t_0) \arrow[r, dashed, "\text{Map ?}"] \arrow[u, bend left, "\Phi"] & \varrho_S(t)
\end{tikzcd}
$$

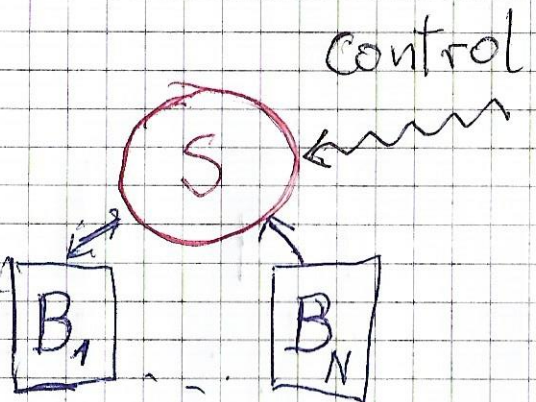
Φ — assignement map

Only product map

$$\Phi(\varrho_S) = \varrho_S \otimes \omega_B \Leftarrow \begin{cases} a) & \text{affine and positive} \\ b) & Tr_B \, \Phi(\varrho_S) = \varrho_S \end{cases}$$

fixed

Reduced dynamics & Master Equations



$$H(t) = H_S^{(0)}(t) + H_B + \lambda H_{SB}$$

$$\frac{d}{dt} U_{SB}(t,t_0) = -i H(t)\, U_{SB}(t,t_0) \qquad (\hbar \equiv 1)$$

Dynamical Map

$$\Lambda \rho_S = \mathrm{Tr}_B\left(U_{SB}(t,t_0)\, \rho_S \otimes \omega_B\, U_{SB}^{\dagger}(t,t_0) \right)$$

Λ – CP trace preserving $\qquad (\Lambda_1 \otimes \Lambda_2$ – CP$)$

$$\Lambda \rho = \sum_{\alpha} W_\alpha \rho W_\alpha^{\dagger}, \qquad \sum_{\alpha} W_\alpha^{\dagger} W_\alpha = 1$$

Time dependency $\quad \Lambda_t \quad (t_0 = 0)$

"Almost always" $\quad \dfrac{d\Lambda_t}{dt} = L_t \Lambda_t \quad \left(L_t = \dfrac{d\Lambda_t}{dt} \Lambda_t^{-1} \right)$

Markovian Dynamics

$$\Lambda_{t+s} = \Lambda_t \Lambda_s \Rightarrow \Lambda_t = e^{tL}$$

$$L\rho = -i[H, \rho] + \frac{1}{2}\sum_\alpha \left([V_\alpha \rho, V_\alpha^\dagger] + [V_\alpha \rho, V_\alpha^\dagger] \right)$$

Lindblad / Gorini-Kossakowski-Sudarshan

Derivations: Weak Coupling Limit, Low Density Limit

validity - separation of time scales, Gaussian (Poisson) properties of baths.

Markovian approximation much better than expected!

(compare to Boltzmann eq.)

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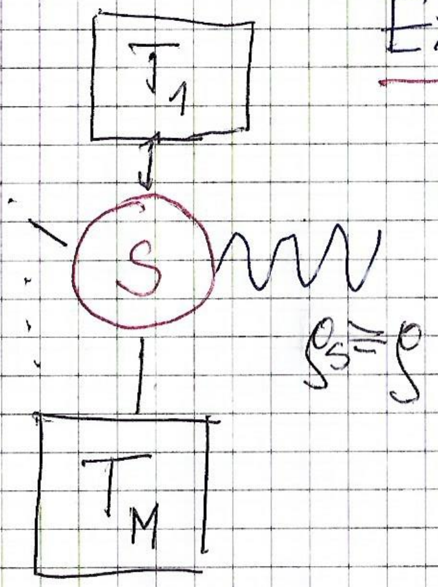
Extension to $H_S(t)$ & Thermodynamics

Ex. 1 $H_S(t)$ – slowly varying (adiabatic approx.)



$$\frac{d\rho}{dt} = -i[H_S(t), \rho] + \sum_{j=1}^{M} \mathcal{L}_j(t)\rho$$

$$\mathcal{L}_j(t)\rho_{\beta_j}(t) = 0 \qquad \rho_{\beta_j} = Z_j^{-1} e^{-\beta_j H_S(t)}$$

I Law
$$\boxed{\frac{dU}{dt} = \frac{dW}{dt} + \frac{dQ}{dt}}$$

$$U = \mathrm{tr}(\rho(t) H_S(t))$$

$$\frac{dW}{dt} = \mathrm{tr}(\rho(t) \dot{H}_S(t))$$

$$\frac{dQ}{dt} = \mathrm{tr}(\dot{\rho}\, H_S(t))$$

II Law
$$\boxed{\frac{dS}{dt} - \sum_{j=1}^{M} \frac{1}{T_j}\frac{dQ_j}{dt} \geq 0}$$

$$S = -k_B \mathrm{Tr}(\rho \ln \rho)$$

$$\frac{dQ_j}{dt} = \mathrm{tr}(H_S(t) \mathcal{L}_j \rho)$$

$$\boxed{\begin{gathered}\mathrm{Tr}(\mathcal{L}\rho(\ln\rho - \ln\bar{\rho})) \leq 0 \\ \mathcal{L}\bar{\rho} = 0 \\ \text{Spohn}\end{gathered}}$$

Applications
Photovoltaic, thermoelectric
fuel cells

Ex 2 Fast periodic $H_S(t)$

Floquet theory + WCL (LDL)

$$\frac{d\rho}{dt} = -i\left[H_S(t), \rho\right] + \underbrace{\mathcal{U}(t)\,\bar{L}\,\mathcal{U}^{+}(t)}_{\text{periodic}}\,\rho$$

I Law – stationary / limit cycle

II Law – based on Spohn inequaliti

Applications (Quantum Optics): external driving by lasers

Reciprocating engines & refigeretors

$$\mathcal{U}_{cyc} = \prod_j \mathcal{U}_j$$

cycles CP maps

$$\mathcal{U}_j = e^{\tau \mathcal{L}_j}$$

GKLS generator

Challenges

- Strongly coupled / correlated systems
- Autonomous machines (fully quantum)
- Basic definitions of work & heat
- "Quantum supremacy" ?
- Information - Thermodynamics Link

⋮

The simplest spin-boson model

$$\sigma_3 |\pm\rangle = \pm |\pm\rangle$$

$$H(t) = \sum_k \omega_k a_k^+ a_k + \lambda(t)\, \sigma_3 \otimes \sum_k (\bar{f}_k a_k + f_k a_k^+)$$

controlled coupling

Ground states

1) $\lambda(t) = 0$

$$|\Psi_\pm^{(0)}\rangle = |\pm\rangle \otimes |vac\rangle, \quad E_g = 0$$

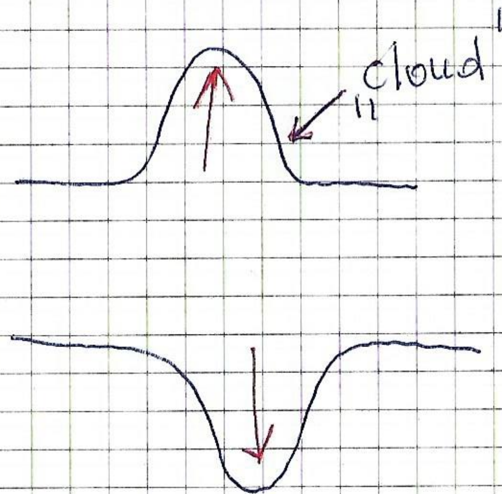
2) $\lambda(t) = 1, \quad |\Psi_\pm\rangle = |\pm\rangle \otimes |[\pm f/\omega]\rangle$

$$\boxed{E_g = -\sum_k \frac{|f_k|^2}{\omega_k}}$$

$$|[\phi]\rangle = \bigotimes_j |[\phi_j]\rangle$$

$$a_j |[\phi_j]\rangle = \phi_j |[\phi_j]\rangle$$

coherent states



$$\langle [+f/\omega] | [-f/\omega] \rangle = \exp\left\{-2 \sum_k \frac{|f_k|^2}{\omega_k^2}\right\}$$

Emerging Superselection Rule

Infinite volume limit

$$\sum_k \frac{|f_k|^2}{\omega_k^2} \to \int_{\omega_{min}}^{\omega_{max}} \frac{|f(k)|^2}{\omega(k)^2}\, dk \xrightarrow{\omega_{min}\to 0} \infty$$

infrared catastrophe!

disjoint states $|[\pm f/\omega]\rangle$, no superpositions („classicality")

phase transition analogy

Dressing transformation (polaron)

$\lambda = 1$, $\sum_k \frac{|f_k|^2}{\omega_k^2} < \infty$ → unitary

$$\begin{cases} a_k \longrightarrow b_k = a_k + \frac{f_k}{\omega_k} \\ \sigma_3 \longrightarrow \tau_3 = \sigma_3 \\ \boxed{\sigma_1 \longrightarrow \tau_1 = U\otimes\sigma^+ + U^+\otimes\sigma^-} \end{cases}$$

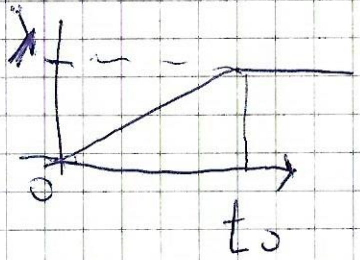
$$H = \sum \omega_k b_k^+ b_k - E_g$$

$$U = \exp 2 \sum_k (\bar{f}_k a_k - f_k a_k^+)$$

suppressed tunneling, decoherence rate $\sim \sum_k \frac{|f_k|^2}{\omega_k^2}$

Thermodynamics of switching process

Zero-temperature case

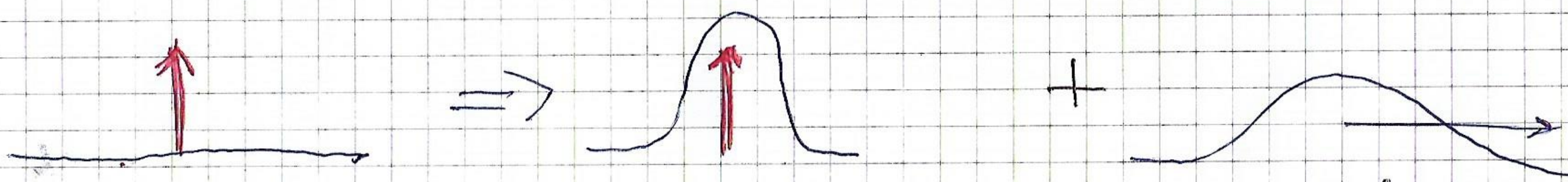


$$|\Psi_\pm(t)\rangle = |\pm\rangle \otimes |[\pm\chi(t)]\rangle$$

for $t > t_0$

$$\chi_k(t) = \underbrace{\frac{\lambda f_k}{\omega_k}}_{\text{„cloud"}} + \underbrace{\left(\frac{\lambda f_k}{\omega_k}\xi_k\right) e^{-i\omega_k t}}_{\text{„traveling wave"}}$$

$|\xi_k| < 1$

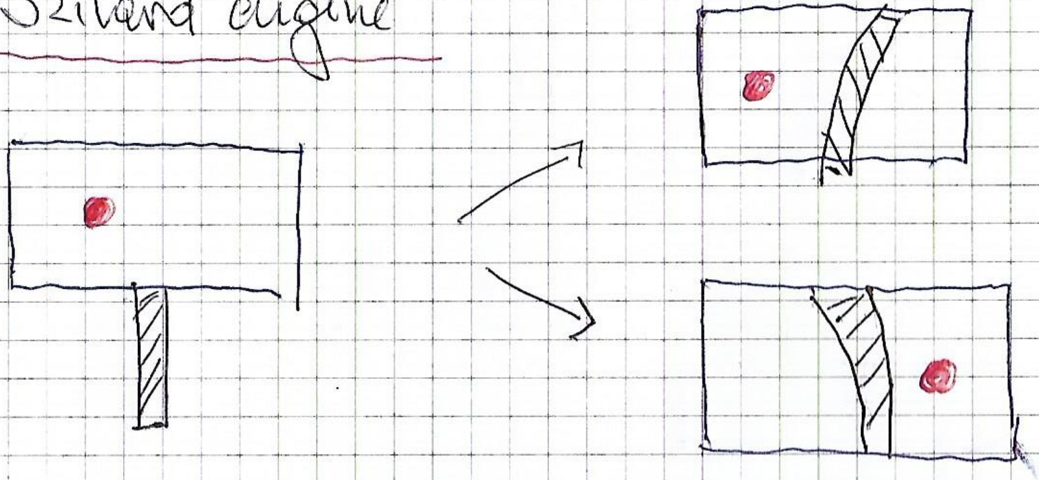


bare spin ⟹ dressed spin + traveling wave (dissipation, heat)

work $W = E_g + \lambda^2 \sum_k |\xi_k|^2 \frac{|f_k|^2}{\omega_k} < 0$

Information – Thermodynamics Link

Ex. Szilard engine



disjoint states, lower free energy

no need for measurement

General case of superselection rule

$$\mathcal{H} = \bigoplus_j \mathcal{H}_j \qquad \mathcal{H}_j \Longleftrightarrow \text{„ergodic component"}$$

mixed states $\qquad \rho = \bigoplus p_j \, \rho_j$

subjective lack of knowledge

Physical entropy

$$S_{phys} = k_B \sum_j p_j \, S_{vN}(\rho_j) = k_B \, S_{vN}(\rho) - k_B \underbrace{\sum p_j \ln \frac{1}{p_j}}_{\text{information}}$$

von Neumann

Cost of a single gate

Landauer $\overline{W}_1 \simeq k_B T \ln 2$ (irreversible)

Brillouin, Kish, R. A

$$\boxed{\overline{W}_1 = \Theta \ln \frac{1}{\epsilon}}$$

$\theta = k_B T$ + quantum corrections

$\epsilon \ll 1$ probability of error

Life time of encoded information

$$\tau \simeq \frac{\tau_0}{\epsilon}$$

$\tau_0 \leftrightarrow$ unprotected