Energetics within autonomous quantum systems: A Schmidt decomposition approach to quantum thermodynamics

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Abstract

During the last decades, the development of a thermodynamic theory for quantum systems has been receiving a great deal of attention, especially from a technological perspective. In this sense, a thermodynamic description applicable to such systems is imperative for designing and developing genuine quantum technologies. Nevertheless, despite the rapid development and rising efforts, there are still subtle and fundamental questions to be answered. Along these lines, it is still unclear how to properly define and establish consistent and general quantum versions of classical thermodynamic concepts and quantities, such as work, heat, entropy and even internal energy. Such a critical lack of consensus intensifies once dealing with open quantum systems in general contexts. In particular, when one analyzes coupling scenarios beyond the approximative regimes and orthodox thermodynamic settings. In this work, we are interested in addressing such fundamental questions. More specifically, we introduce a novel approach for describing the energetic exchange within general autonomous bipartite quantum systems [1]. The formal structure of this proposal is exact and allows the definition of local effective Hamiltonians for characterizing the subsystem's internal energies. This description guarantees symmetrical treatment of the bipartitions and, most importantly, also automatically preserves the thermodynamic notion of energy additivity. In contrast with current methodologies, such a framework does not rely on approximations, particular coupling regimes or additional hypotheses of this kind. Moreover, the obtained expressions also establish a new route for defining other general thermodynamic quantities to the quantum realm, such as work and heat.

Setting the stage

$$|\Psi(t)\rangle \in \mathcal{H}^{(0)} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \longrightarrow i\hbar\tfrac{d}{dt}|\Psi(t)\rangle = \hat{H}^{(0)}|\Psi(t)\rangle$$

- **Pure** $\hat{\rho}^{(0)}(t) \equiv |\Psi(t)\rangle\langle\Psi(t)|$
- **Bipartite** $d^{(1)} \leq d^{(2)}$

Interaction term

$$\hat{H}^{(0)} := \hat{H}^{(1)} \otimes \hat{1}^{(2)} + \hat{1}^{(1)} \otimes \hat{H}^{(2)} + \hat{H}_{int}$$

Local bare Hamiltonians

Schmidt decomposition

$$|\Psi(t)\rangle = \sum_{j=1}^{d^{(1)}} \lambda_j(t)|\varphi_j^{(1)}(t)\rangle \otimes |\varphi_j^{(2)}(t)\rangle$$

- Schmidt coefficients $\{\lambda_j(t) \geq 0; j = 1, ..., d^{(1)}\}$
- Schmidt basis $\{|\varphi_j^{(k)}(t)\rangle; j = 1, ..., d^{(1)}\}$

Local states

$$\begin{cases} \hat{\rho}^{(1)}(t) = \sum_{j=1}^{d^{(1)}} \lambda_j^2(t)|\varphi_j^{(1)}(t)\rangle\langle\varphi_j^{(1)}(t)| \\ \hat{\rho}^{(2)}(t) = \sum_{j=1}^{d^{(1)}} \lambda_j^2(t)|\varphi_j^{(2)}(t)\rangle\langle\varphi_j^{(2)}(t)| \end{cases}$$

Local Effective Hamiltonians

$$|\varphi_j^{(k)}(t)\rangle = \tilde{\mathcal{U}}^{(k)}(t,t_0)|\varphi_j^{(k)}(t_0)\rangle \longrightarrow \begin{cases} i\hbar\frac{d}{dt}\tilde{\mathcal{U}}^{(k)}(t,t_0) = \tilde{H}^{(k)}(t)\tilde{\mathcal{U}}^{(k)}(t,t_0) \\ i\hbar\frac{d}{dt}|\varphi_j^{(k)}(t)\rangle = \tilde{H}^{(k)}(t)|\varphi_j^{(k)}(t)\rangle \end{cases}$$

$$\tilde{H}^{(k)}(t) \equiv i\hbar\sum_{j=1}^{d^{(k)}} \frac{d}{dt}|\varphi_j^{(k)}(t)\rangle\langle\varphi_j^{(k)}(t)|$$

bare Hamiltonian

Given $\hat{H}^{(k)} \equiv \sum_{j=1}^{d^{(k)}} b_j^{(k)}|b_j^{(k)}\rangle\langle b_j^{(k)}|, \longrightarrow \tilde{H}^{(k)}(t) = \hat{H}^{(k)} + \hat{H}_{LS}^{(k)}(t) + \hat{H}_X^{(k)}(t)$

$$\begin{cases} \hat{H}_{LS}^{(k)}(t) := i\hbar\sum_{j=1}^{d^{(k)}}\left(\sum_{l=1}^{d^{(k)}}\left(\frac{d}{dt}r_{jl}^{(k)}(t)\right)r_{jl}^{(k)*}(t)\right)|b_j^{(k)}\rangle\langle b_j^{(k)}|, \\ \hat{H}_X^{(k)}(t) := i\hbar\sum_{j=1}^{d^{(k)}}\sum_{m\neq j}^{d^{(k)}}\left(\sum_{l=1}^{d^{(k)}}\frac{d}{dt}r_{jl}^{(k)}(t)r_{ml}^{(k)*}(t)\right)e^{\frac{i}{\hbar}\left(b_m^{(k)}-b_j^{(k)}\right)t}|b_j^{(k)}\rangle\langle b_m^{(k)}| \end{cases}$$

Global and local dynamics

$$i\hbar\frac{d}{dt}\hat{\rho}^{(0)}(t) = [\hat{H}^{(0)}, \hat{\rho}^{(0)}(t)]$$

$$i\hbar\frac{d}{dt}\hat{\rho}^{(k)}(t) = [\tilde{H}^{(k)}(t), \hat{\rho}^{(k)}(t)] + i\hbar\sum_{j=1}^{d^{(1)}}\frac{d}{dt}\lambda_j^2(t)|\varphi_j^{(k)}(t)\rangle\langle\varphi_j^{(k)}(t)|$$

Local internal energies

Universe's energy

$$U^{(0)} \equiv \langle\hat{H}^{(0)}\rangle = \langle\Psi(t)|\hat{H}^{(0)}|\Psi(t)\rangle \quad \& \quad U^{(0)} = \langle\hat{H}^{(1)}\rangle(t) + \langle\hat{H}^{(2)}\rangle(t) + \langle\hat{H}_{int}\rangle(t)$$

We can show $\langle\hat{H}^{(0)}\rangle = \langle\tilde{H}^{(1)}(t)\rangle + \langle\tilde{H}^{(2)}(t)\rangle = U^{(0)}$

$$U^{(k)}(t) := \langle\tilde{H}^{(k)}(t)\rangle$$

Subsystem's energy

$$U^{(k)} = \langle\hat{H}^{(k)}\rangle(t) + \langle\hat{H}_{LS}^{(k)}(t)\rangle + \langle\hat{H}_X^{(k)}(t)\rangle \longrightarrow$$

Energy additivity

$$U^{(0)} = U^{(1)}(t) + U^{(2)}(t)$$

Phase gauge

$$|\varphi_j'^{(k)}(t)\rangle = e^{(-1)^{k-1}i\theta_j(t)}|\varphi_j^{(k)}(t)\rangle \begin{cases} \tilde{H}'^{(k)}(t) = \tilde{H}^{(k)}(t) + (-1)^k\hbar\sum_{j=1}^{d^{(k)}}\left(\frac{d\theta_j(t)}{dt}\right)|\varphi_j^{(k)}(t)\rangle\langle\varphi_j^{(k)}(t)| \\ \langle\tilde{H}'^{(k)}(t)\rangle = \langle\tilde{H}^{(k)}(t)\rangle + (-1)^k\hbar\sum_{j=1}^{d^{(k)}}\lambda_j^2(t)\left(\frac{d\theta_j(t)}{dt}\right) \end{cases}$$

Physical gauges: For any gauge $\rightarrow$ $\tilde{H}'^{(k)}(t) \rightarrow \hat{H}^{(k)} + \alpha\hat{1}^{(k)}$ $\alpha \in \mathbb{R}$ if $\hat{H}_{int} \rightarrow 0$

As long $\left\{\frac{d}{dt}\theta_j(t) = \alpha \in \mathbb{R}\right\}_j \longrightarrow \tilde{H}'^{(k)}(t) = \tilde{H}^{(k)}(t) + (-1)^k\hbar\alpha\hat{1}^{(k)}$ **&** $\langle\tilde{H}'^{(k)}(t)\rangle = \langle\tilde{H}^{(k)}(t)\rangle + (-1)^k\hbar\alpha$

- **Distinct** absolute energy values $U'^{(k)}(t) = U^{(k)}(t) + (-1)^k\hbar\alpha$
- **Unambigous** spectral gaps

Reference

[1] MALAVAZI, A.; BRITO, F. A Schmidt decomposition approach to quantum thermodynamics. May 2022. Available from: https://arxiv.org/pdf/2205.06917.pdf.

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