Fundamental pathologies in Lindblad descriptions of systems weakly coupled to baths

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Introduction

- The microscopically derived quantum master equation up to leading order in system-bath coupling is generally of the Redfield-form, and is known to not preserve complete positivity.
- Here, we show that enforcing complete positivity via any Lindblad form, through any further approximations to Redfield, leads either to a) violatation of thermalization or b) inaccurate coherences leading to violation of local conservation laws.

Accuracy of steady-state

- Take the Hamiltonian of the full setup : $H = \hat{H}_S + \epsilon \hat{H}_{SB} + \hat{H}_B$
- $\hat{\rho}_{\rm NESS} = \sum_{m=0}^{\infty} \epsilon^{2m} \hat{\rho}_{\rm NESS}^{(2m)}$.
- The QME can be written in the so-called TCL form [1]

$$\frac{\partial \hat{\rho}}{\partial t} = \sum_{m=0}^{\infty} \epsilon^{2m} \hat{\mathcal{L}}_{2m}[\hat{\rho}(t)]. \qquad (1)$$

- An order-by-order solution satisfies

$$\left\langle E_\alpha \left| \hat{\mathcal{L}}_2[\hat{\rho}_{\rm SS}^{(0)}] \right| E_\alpha \right\rangle = 0, \qquad (2)$$

$$i(E_\alpha - E_\nu) \left\langle E_\alpha \left| \hat{\rho}_{\rm NESS}^{(2)} \right| E_\nu \right\rangle + \left\langle E_\alpha \left| \hat{\mathcal{L}}_2[\hat{\rho}_{\rm SS}^{(0)}] \right| E_\nu \right\rangle = 0 \quad \forall \ \alpha \neq \nu, \qquad (3)$$

$$\left\langle E_\alpha \left| \hat{\mathcal{L}}_2[\hat{\rho}_{\rm SS}^{(2)}] \right| E_\alpha \right\rangle + \left\langle E_\alpha \left| \hat{\mathcal{L}}_4[\hat{\rho}_{\rm SS}^{(0)}] \right| E_\alpha \right\rangle = 0. \qquad (4)$$

- Usually, the QME is written only upto leading order in system-bath coupling. The NESS obtained from such a QME (like Redfield) satisfies the above equations with $\mathcal{L}_4 = 0$.
- Such a QME predicts diagonal elements with $O(1)$ accuracy, and off-diagonal elements with $O(\epsilon^2)$. The error is $O(\epsilon^2)$. [2].

Imposing Lindblad form by changing $\mathcal{L}_2$

Suppose $\hat{\mathcal{L}}_2$ is changed to $\hat{\mathcal{L}}_2'$ to restore complete positivity while maintaining the same order-of-accuracy. Then, Eqs.(2),(3) become

$$\left\langle E_\alpha \left| \hat{\mathcal{L}}_2'[\hat{\rho}_{\rm SS}'^{(0)}] \right| E_\alpha \right\rangle = 0 \qquad (5)$$

$$i(E_\alpha - E_\nu) \left\langle E_\alpha \left| \hat{\rho}_{\rm SS}'^{(2)} \right| E_\nu \right\rangle + \left\langle E_\alpha \left| \hat{\mathcal{L}}_2'[\hat{\rho}_{\rm SS}'^{(0)}] \right| E_\nu \right\rangle = 0 \quad \forall \ \alpha \neq \nu. \qquad (6)$$

- Same order-of-accuracy implies $\hat{\rho}_{\rm SS}'^{(0)} = \hat{\rho}_{\rm SS}^{(0)}$
- Since $\hat{\mathcal{L}}_2'$ is different from $\hat{\mathcal{L}}_2$, it means the remaining components of $\hat{\mathcal{L}}_2'$, that appear in Eq.(6) are different from the corresponding ones in Eq.(3).
- Coherences are no longer correct upto leading order.
- This inaccuracy of the coherences manifests itself as a violation of local conservation laws.

Numerical Examples

- We numerically test our findings for the following spin-chain setup :

$$\hat{H}_S = \sum_{\ell=1}^{N} \frac{\omega_0^{(\ell)}}{2} \hat{\sigma}_z^\ell - \sum_{\ell=1}^{2} g(\hat{\sigma}_x^\ell \hat{\sigma}_x^{\ell+1} + \hat{\sigma}_y^\ell \hat{\sigma}_y^{\ell+1} + \Delta \hat{\sigma}_z^\ell \hat{\sigma}_z^{\ell+1})$$

$$\hat{H}_{SB} = \sum_{\ell=1,N} \sum_{r=1}^{\infty} (\kappa_{\ell r} \hat{B}_r^{(\ell)\dagger} \hat{\sigma}_-^\ell + \kappa_{lr}^* \hat{B}_r^{(\ell)} \hat{\sigma}_+^\ell),$$

$$\hat{H}_B = \sum_{\ell=1,N} \sum_{r=1}^{\infty} \Omega_r^\ell \hat{B}_r^{(\ell)\dagger} \hat{B}_r^{(\ell)},$$

- We study the local-lindblad equation (LLE), the eigen-basis Lindblad equation (ELE), the Redfield equation (RE), the recently derived universal lindblad equation (ULE).
- The ULE equation [3] is specifically designed to have the same order-of-magnitude of errors as RE ($O(\epsilon^2)$), and is therefore an excellent test-bed for our ideas.

Numerical Results

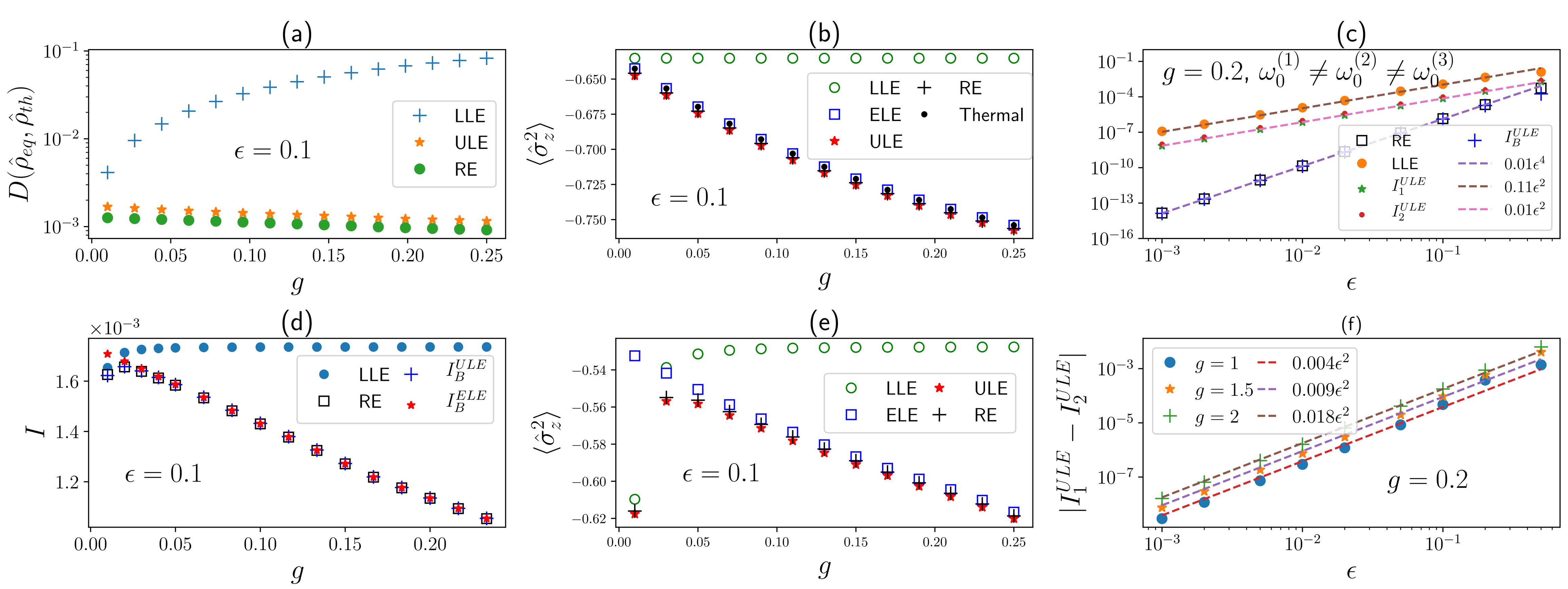

Figure: The top row is for the equilibrium case ($\beta_L = 1$, $\beta_R = 1$) and the bottom row is for the non-equilibrium case ($\beta_L = 5$, $\beta_R = 0.5$). (a) The trace distance between the expected thermal state $\hat{\rho}_{\rm th}$ and the equilibrium steady-state $\hat{\rho}_{\rm eq}$ as a function of g. (b) The local magnetization in equilibrium steady state as a function of g. (c) The scaling of spin currents in equilibrium as a function of system-bath coupling strength ϵ, for the case where $\omega_0^{(1)} = 1, \omega_0^{(2)} = 1.5, \omega_0^{(3)} = 2$. (d) Spin currents and bounday currents in NESS (e) The local magnetization in NESS as a function of g. (f) The scaling of difference between the two bond currents at NESS from ULE as a function of system-bath coupling strength ϵ. Apart from (c), in all other cases, $\omega_0^{(1)} = \omega_0^{(2)} = \omega_0^{(3)} = 1$.

Conclusion

- In weak system-bath coupling, it is impossible to enforce a Lindblad form via additional approximations that simultaneously satisfies thermalization, obeys local conservation laws and gives accurate coherences in energy eigenbasis.
- While generically violating complete positivity, the Redfield equation shows thermalization in equilibrium, always gives correct coherences to leading order and preserves local conservation laws.

Additional Information

- Arxiv link : https://arxiv.org/abs/2105.12091
- Email : djtupkar@uwaterloo.ca

References

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