Calculating Energy Flows in Strongly Coupled Open Quantum Systems with HOPS

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Premise

- Application of thermodynamic notions to strongly coupled and non-Markovian quantum systems is non-trivial ([1–4] and many more)
- Dynamics of bath and interaction hamiltonians plays an important role → must not be neglected in the strong coupling regime
- The "Hierarchy of Pure States" (HOPS [5, 6]) gives us the ability to simulate non-Markovian and strongly coupled open quantum systems exactly in a scalable way.
- Because HOPS simulates global dynamics → gives access to certain bath dynamics *with no additional effort*

NMQSD/HOPS

Consider the model of a general quantum system ($H_\mathrm{S}(t)$) coupled to N baths

$$H(t) = H_\mathrm{S}(t) + \sum_{n=1}^{N}\left[L_n^\dagger(t)B_n + \mathrm{h.c.}\right] + \sum_{n=1}^{N} H_B^{(n)}, \tag{1}$$

with $B_n = \sum_\lambda g_\lambda^{(n)} a_\lambda^{(n)}$ and $H_B^{(n)} = \sum_\lambda \omega_\lambda^{(n)} \left(b_\lambda^{(n)}\right)^\dagger b_\lambda^{(n)}$. Projecting onto coherent bath states

$$|\psi(t)\rangle = \int \prod_{n=1}^{N}\left(\frac{\mathrm{d}\boldsymbol{z}^{(n)}}{\pi^{N_n}}\mathrm{e}^{-|\boldsymbol{z}|^2}\right)|\psi(t,\underline{\boldsymbol{z}}^*)\rangle\,|\underline{\boldsymbol{z}}\rangle \tag{2}$$

leads to *stochastic* Non-Markovian Quantum State Diffusion (NMQSD)

$$\partial_t\psi_t(\boldsymbol{\eta}_t^*) = -\mathrm{i}H(t)\psi_t(\boldsymbol{\eta}_t^*) + \boldsymbol{L}\cdot\boldsymbol{\eta}_t^*\psi_t(\boldsymbol{\eta}_t^*) - \sum_{n=1}^{N} L(t)_n^\dagger \int_0^t \mathrm{d}s\,\alpha_n(t-s)\frac{\delta\psi_t(\boldsymbol{\eta}_t^*)}{\delta\eta_n^*(s)}, \tag{3}$$

where the $\alpha_n(\tau) = \langle B_n(t)B_n(0)\rangle = \sum_\lambda |g_\lambda|^2\mathrm{e}^{-\mathrm{i}\omega_\lambda t}$ (interaction picture) are the bath correlation functions and the $\eta_n = (\boldsymbol{\eta})_n$ are complex valued Gaussian processes with $\mathcal{M}(\eta_n(t)) = \mathcal{M}(\eta_n(t)\eta_n(s)) = 0$ and $\mathcal{M}(\eta_n(t)\eta_n^*(s)) = \alpha_n(t-s)$. The reduced state of the system is recovered through $\rho = \mathcal{M}(\psi_t(\boldsymbol{\eta}_t^*)\psi_t^\dagger(\boldsymbol{\eta}_t^*))$.

With $\alpha_n(\tau) = \sum_\mu^{M_n} = G_\mu^{(n)}\mathrm{e}^{-W_\mu^{(n)}\tau}$ we define

$$D_\mu^{(n)}(t) \equiv \int_0^t \mathrm{d}s\, G_\mu^{(n)}\mathrm{e}^{-W_\mu^{(n)}(t-s)}\frac{\delta}{\delta\eta_n^*(s)} \quad D^{\underline{\boldsymbol{k}}} \equiv \prod_{n=1}^{N}\prod_{\mu=1}^{M_n}\sqrt{\frac{\underline{\boldsymbol{k}}_{n,\mu}!}{\left(G_\mu^{(n)}\right)^{\underline{\boldsymbol{k}}_{n,\mu}}}}\frac{1}{\mathrm{i}^{\underline{\boldsymbol{k}}_{n,\mu}}}\left(D_\mu^{(n)}\right)^{\underline{\boldsymbol{k}}_{n,\mu}} \tag{4}$$

$$\psi^{\underline{\boldsymbol{k}}} \equiv D^{\underline{\boldsymbol{k}}}\psi \equiv \langle\underline{\boldsymbol{k}}|\Psi\rangle\,. \tag{5}$$

For the Fock-space embedded hierarchy state $|\Psi\rangle$ we find

$$\partial_t|\Psi\rangle = \begin{bmatrix} -\mathrm{i}H_\mathrm{S} + \boldsymbol{L}\cdot\boldsymbol{\eta}^* - \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} b_{n,\mu}^\dagger b_{n,\mu}W_\mu^{(n)} \\ + \mathrm{i}\sum_{n=1}^{N}\sum_{\mu=1}^{M_n}\sqrt{G_{n,\mu}}\left(b_{n,\mu}^\dagger L_n + b_{n,\mu}L_n^\dagger\right)\end{bmatrix}|\Psi\rangle\,. \tag{6}$$

Truncating the hierarchy depth $\underline{\boldsymbol{k}}$ in eq. (6) yields the numeric method.

Finite temperature can be dealt with through substituting $B(t) \to B(t) + \xi(t)$ with

$$\begin{aligned}\mathcal{M}(\xi(t)) &= 0 = \mathcal{M}(\xi(t)\xi(s)) \\ \mathcal{M}\left(\xi(t)\xi^*(s)\right) &= \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega\,\bar{n}(\beta\omega)J(\omega)e^{-\mathrm{i}\omega(t-s)} \\ J(\omega) &= \pi\sum_\lambda |g_\lambda|^2\delta(w-\omega_\lambda).\end{aligned} \tag{7}$$

See [5] for details about finite temperatures and the nonlinear method.

Bath Observables

From eqs. (3) and (4) we find the correspondence $B(t) \leftrightarrow D_t \leftrightarrow \psi^{\underline{\boldsymbol{k}}} \implies$ can calulate observables of type $O_\mathrm{S}\otimes(B^a)^\dagger B^b$ and time derivatives thereof. This grants the hierarchy states a utility beyond the mere simulation of reduced dynamics.

Bath Energy Flow We consider the zero temperature and one-bath case.

$$\begin{aligned} J = -\frac{\mathrm{d}\langle H_\mathrm{B}\rangle}{\mathrm{d}t} &= \left\langle L(t)^\dagger\partial_t B(t) + L(t)\partial_t B^\dagger(t)\right\rangle_\mathrm{I} \\ &= -\mathrm{i}\mathcal{M}_{\eta^*}\langle\psi(\eta,t)|\,L(t)^\dagger\dot{D}_t\,|\psi(\eta^*,t)\rangle + \mathrm{c.c.} \\ &= -\sum_\mu\sqrt{G_\mu}W_\mu\mathcal{M}_{\eta^*}\left\langle\psi^{(0)}(\eta,t)\right|L(t)^\dagger\left|\psi^{\boldsymbol{e}_\mu}(\eta^*,t)\right\rangle + \mathrm{c.c.}\end{aligned} \tag{8}$$

Thus, the expectation value of the bath energy flow is connected to the first hierarchy level states in a transparent and easy to calculate manner.

Interaction Energy A similar expression may be found for the expectation value of the interaction energy

$$\begin{aligned}\langle H_\mathrm{I}\rangle &= -\mathrm{i}\mathcal{M}_{\eta^*}\langle\psi(\eta,t)|\,L(t)^\dagger D_t\,|\psi(\eta^*,t)\rangle + \mathrm{c.c.} \\ &= \sum_\mu\sqrt{G_\mu}\mathcal{M}_{\eta^*}\left\langle\psi^{(0)}(\eta,t)\right|L(t)^\dagger\left|\psi^{\boldsymbol{e}_\mu}(\eta^*,t)\right\rangle + \mathrm{c.c.}.\end{aligned} \tag{9}$$

This result allows us to calculate the energy flow in arbitrarily driven systems.

Possible Applications

- Simulation of Thermal Quantum Machines
- Convergence Criteria: Energy Conservation, Calculating the same observable in multiple ways
- Quantification of Entanglement of System and Bath (Fisher Information of H_I)
- ...

Resources

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