Addendum: Unified framework for open quantum dynamics with memory

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Ruojing Peng, Felix Ivander, Lachlan P. Lindoy & Joonho Lee

This Addendum presents a detailed analysis of the discretization error in time-integration and time-derivative that appear in the Nakajima-Zwanzig equation. This was brought to our attention by Makri et al. [arXiv:2410.08239]. Our analysis in the Addendum shows that the relationship derived in our earlier work [Nat. Commun. 15, 8087 (2024)] is valid within the choice of discretization and is not contaminated by the discretization error.

A recent commentary piece[1] by Makri et al. raised a concern on the discretization error of the discrete-time Nakajima-Zwanzig (NZ) equation employed in our recent work[2]. In light of this, this Addendum provides a detailed analysis on the discretization error in the NZ equation and whether it affects our original analysis.

The continuous-time homogeneous NZ equation[3–5] for the system propagator $U(t)$ is

$$\dot{U}(t) = -iL_sU(t) + \int_0^t d\tau \mathcal{K}(\tau)U(t-\tau) \tag{1}$$

where $L_s = [H_s, \cdot\,]$ and $U(t)$ is defined by $\rho(t) = U(t)\rho(0)$. For the subsequent analysis, it is useful to write its second-order derivative as derived in ref. 6 (see Supplementary Note I for detail)

$$\ddot{U}(t) = (-iL_s)^2U(t) + \mathcal{K}(t) + \int_0^t d\tau \mathcal{F}(\tau)U(t-\tau) \tag{2}$$

where

$$\mathcal{F}(t) = \{\mathcal{K}(t), -iL_s\} + \int_0^t d\tau \mathcal{K}(\tau)\mathcal{K}(t-\tau), \tag{3}$$

and the third-order derivative (see Supplementary Note II for detail)

$$\begin{aligned}\dddot{U}(t) = &\left[(-iL_s)^3 + \{\mathcal{K}_0, -iL_s\} + \dot{\mathcal{K}}_0\right]U(t)\\ &+ \int_0^t d\tau \mathcal{R}(t-\tau)U(\tau)\end{aligned} \tag{4}$$

where

$$\mathcal{R}(t) = \left[\left[(-iL_s)^2 + \mathcal{K}_0\right]\mathcal{K} - iL_s\dot{\mathcal{K}} + \ddot{\mathcal{K}}\right](t). \tag{5}$$

We note that $\mathcal{F}(t) \sim \mathcal{O}(||\mathcal{K}(t)||)$ ($||\cdot||$ denotes Frobenius norm of the matrix) from Young's convolution inequality[7,8]. Furthermore, $\dot{\mathcal{K}}(t)$, $\ddot{\mathcal{K}}(t)$, and hence $\mathcal{R}(t)$ are also $\mathcal{O}(||\mathcal{K}(t)||)$ from the projection of full system-and-bath evolution[9,10].

We now consider the discrete-time version of Eqs. (1), (2) and (4). Following the same convention as our original manuscript, let $t = N\Delta t$, $L = 1 - i\Delta tL_s$, $\rho_N = \rho(N\Delta t)$, $U_N = U(N\Delta t)$, $\mathcal{K}_m = \mathcal{K}(m\Delta t)$ be the continuous-time memory kernel in Eq. (1) evaluated at discrete time steps, and the discrete-time memory kernel, K_m, be defined by discrete time relations

$$U_{N+1} = (I - i\Delta t L_s)U_N + \Delta t^2 \sum_{m=0}^{N} K_{N-m} U_m, \tag{6}$$

from ref. 2 and the discrete-time memory kernel, $\{K_m\}$, is the central quantity used in our original article. Our goal is to demonstrate how the discretization error in the discrete NZ equation propagates into the relationship between $\mathcal{K}_m$ and K_m and whether the time-translational invariance of K_m is, in fact, incorrectly assumed and contaminated by the discretization error.

We begin by considering the time-derivatives of the system propagator at $t = 0$ (i.e., $N = 0$),

$$\ddot{U}_0 = (-iL_s)^2 + \mathcal{K}_0, \tag{7}$$

$$\dddot{U}_0 = (-iL_s)^3 + \{\mathcal{K}_0, -iL_s\} + \dot{\mathcal{K}}_0. \tag{8}$$

The expansion of U_1 at $t = 0$ follows

$$U_1 = I + \Delta t \dot{U}_0 + \frac{\Delta t^2}{2}\ddot{U}_0 + \frac{\Delta t^3}{6}\dddot{U}_0 + \mathcal{O}(\Delta t^4). \tag{9}$$

We can use Eqs. (9) and (6) to obtain

$$K_0 = \frac{1}{2}\left((-iL_s)^2 + \mathcal{K}_0\right) + \frac{\Delta t}{6}\dddot{U}_0 + \mathcal{O}(\Delta t^2). \tag{10}$$

This reveals that our K_0 is related to $\mathcal{K}_0$ up to an additive error $\mathcal{O}(\Delta t)$.

For $N > 0$, we discretize the time-convolution integral in Eqs. (2) and (4) with the left Riemann sum,

$$\ddot{U}_N = (-iL_s)^2 U_N + \mathcal{K}_N + \Delta t \sum_{m=0}^{N-1} \mathcal{F}_{N-m} U_m + \mathcal{O}(N\Delta t^2), \tag{11}$$

$$\dddot{U}_N = \dddot{U}_0 U_N + \Delta t \sum_{m=0}^{N-1} \mathcal{R}_{N-m} U_m + \mathcal{O}(N\Delta t^2). \tag{12}$$

Next, the integral in Eq. (1) is approximated by the trapezoidal rule,

$$\dot{U}_N = -iL_s U_N + \Delta t \left[\frac{1}{2}\mathcal{K}_N + \sum_{m=1}^{N-1} \mathcal{K}_{N-m} U_m + \frac{1}{2}\mathcal{K}_0 U_N\right] + \mathcal{O}(N\Delta t^3). \tag{13}$$

Similarly to Eq. (9), the expansion of U_{N+1} at t = $N\Delta t$ follows (see Supplementary Note III for detail)

$$\begin{aligned} U_{N+1} &= U_N + \Delta t \dot{U}_N + \frac{\Delta t^2}{2}\ddot{U}_N + \frac{\Delta t^3}{6}\dddot{U}_N + \mathcal{O}(\Delta t^4) \\ &= (I - i\Delta t L_S)U_N + \Delta t^2 \left[\sum_{m=0}^{N-1} \mathcal{K}_{N-m} U_m + K_0 U_N\right] \\ &+ \frac{\Delta t^3}{2}\sum_{m=0}^{N-1} \mathcal{F}_{N-m} U_m + \mathcal{O}(N\Delta t^4) \\ &+ \frac{\Delta t^4}{6}\sum_{m=0}^{N-1} \mathcal{R}_{N-m} U_m + \mathcal{O}(N\Delta t^5). \end{aligned} \tag{14}$$

Finally, by comparing Eqs. (6) and (14), we observe

$$K_N = \mathcal{K}_N + \frac{\Delta t}{2}\mathcal{F}_N + \mathcal{O}(\Delta t^2), \tag{15}$$

which reveals how the discretization error used in Eq. (6) propagates into the discrete-time memory kernel. From Eqs. (10) and (15), we see that the discrete-time memory kernel K_N agrees with the continuous-time memory kernel $\mathcal{K}_N$ up to a discretization error of $\mathcal{O}(\Delta t)$ for $N > 0$, and they are related up to an additive error of $\mathcal{O}(\Delta t)$ by L_s at $N = 0$. Furthermore, the discrete-time memory kernel obeys time-translational invariance up to $\mathcal{O}(\Delta t^2)$ since $\mathcal{F}_N$ is time-translationally invariant. Hence, our analysis in the original manuscript is valid up to the discretization error $\mathcal{O}(\Delta t)$, and the discretization error does not change our analysis. We also note that Cao et al. numerically demonstrated the convergence of K_N to $\mathcal{K}_N$ when taking the limit of $\Delta t \to 0$ in ref. 11, which is consistent with our analysis.

Our original work presented a formal, explicit one-to-one mapping between memory kernel and influence functions for various open-quantum system settings including spin, fermionic, and bosonic baths with commuting/non-commuting or diagonalizable/non-diagonalizable system-bath coupling. As mentioned in our original work as well as its supplementary materials and also in ref. 1, there are similarities among our analysis, Cao's transfer tensor method[11], and Makri's small matrix method[12], especially for the simplest setting of a bosonic bath with commuting, diagonalizable system-bath coupling. Our work presents a unified framework for open quantum dynamics for various settings beyond the available analyses and a quantum sensing protocol for a system coupled to Gaussian baths (i.e., learning spectral density from reduced system dynamics).

Data availability

Data generated in this study is fully presented in the main text and Appendices.

Code availability

No code has been used to generate the data.

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Additional information

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