High-Precision Simulation of Decoherence Phenomena of Qubits

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Decoherence is one of the major obstacles to quantum computation, and extensive numerical studies have been conducted to understand it and contribute to the design of qubits. We provide a method that rigorously describes dynamics of qubits affected by quantum Gaussian noise. Using this method, we show that the conventional numerical methods based on the perturbation, Markov and Born approximation are insufficient to simulate dynamics of qubits. We also demonstrate dynamics of single-qubit gate operations under the effects of quantum noise.

Model and Method

▸ **Model:** system + reservoir model, $\hat{H}_{tot} = \hat{H}_S + \hat{H}_R + \hat{H}_I$.

- $\hat{H}_S \cdots$ system Hamiltonian consisting of qubits
- $\hat{H}_R \cdots$ reservoir Hamiltonian =sources of quantum noise (dielectric loss, quasiparticles, charge fluctuations, two level fluctuators, etc.)
  assuming: Gaussian noise
- $\hat{H}_I \cdots$ System – Reservoir interaction: $\hat{H}_I = -\hat{V} \otimes \hat{X}_b$,
  ($\hat{V} \cdots$ operator acting on the system
  $\hat{X}_b \cdots$ random force operator induced by the reservoir)

⏩ time derivative of the reduced density operator (RDO) in the interaction picture ($\tilde{V}(t) = e^{i\hat{H}_S t/\hbar}\hat{V}e^{-i\hat{H}_S t/\hbar}$, etc.):

$$\dot{\tilde{\rho}}_S(t) = \frac{\partial}{\partial t}\mathrm{tr}_R\left\{\mathcal{T}\left[e^{-i\int dt \tilde{H}_I(t)/\hbar}\hat{\rho}_{tot}(0)e^{i\int dt\tilde{H}_I(t)/\hbar}\right]\right\}$$

(partial trace of the reservoir)

$$= -\frac{1}{\hbar^2}\left[\tilde{V}(t), \mathcal{T}\left\{\int_0^t dt'\left(C(t-t')\underset{\rightarrow}{\tilde{V}}(t')\tilde{\rho}_S(t) - C^*(t-t')\underset{\leftarrow}{\tilde{V}}(t')\tilde{\rho}_S(t)\right)\right\}\right]$$

$$\underset{\rightarrow}{\tilde{V}}(t')\tilde{\rho}_S(t) \equiv \tilde{V}(t')\tilde{\rho}_S(t)$$
$$\underset{\leftarrow}{\tilde{V}}(t')\tilde{\rho}_S(t) \equiv \tilde{\rho}_S(t)\tilde{V}(t')$$

$\cdots$ time-nonlocal equation due to the time-ordering operation $\mathcal{T}\{\bullet\}$

two-time reservoir correlation function:

$$C(t) = \langle \tilde{X}_b(t)\tilde{X}_b(0)\rangle = \int_{-\infty}^{\infty} d\omega S_\beta(\omega)e^{-i\omega t},$$

Spectral noise power $S_\beta(\omega)$ as input

ⓘ Lindblad equation / Redfield approach $\cdots$ ignoring $\mathcal{T}\{\bullet\}$ and changing the interval of the integration; $[0,t] \to (-\infty, t]$

▸ **fp-HEOM:** barycentric representation of $S_\beta(\omega)$

$$\simeq \quad \tilde{S}_\beta(\omega) = \sum_{k=1}^{K}\frac{W_k S_\beta(\Omega_k)}{\omega - \Omega_k}\Bigg/\sum_{k=1}^{K}\frac{W_k}{\omega-\Omega_k},$$

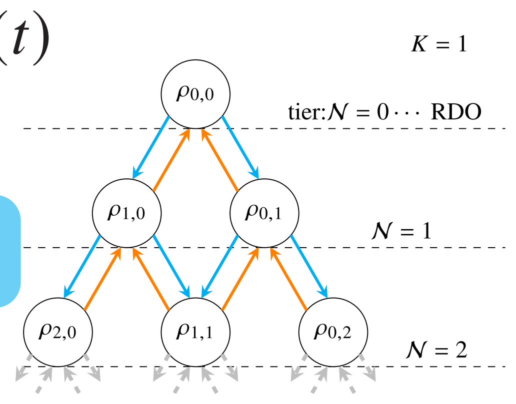
⏩ $C(t) = \sum_{k=1}^{K} d_k e^{-z_k t}, \quad z_k = \gamma_k + i\omega_k, d_k \in \mathbb{C}$,
and introducing auxiliary density operators (ADOs) as

$$\hat{\rho}_{\boldsymbol{m},\boldsymbol{n}}(t) = e^{-i\hat{H}_S t/\hbar}\mathcal{T}\left\{\prod_{k=1}^{K}\left[\left(-i\int_0^t dt' d_k e^{-z_k(t-t')}\underset{\rightarrow}{\tilde{V}}(t')\right)^{m_k} \times \left(i\int_0^t dt' d_k^* e^{-z_k^*(t-t')}\underset{\leftarrow}{\tilde{V}}(t')\right)^{n_k}\right]\tilde{\rho}_S(t)\right\}e^{i\hat{H}_S t/\hbar},$$

where $(\boldsymbol{m},\boldsymbol{n}) = (m_1,\ldots,m_K,n_1,\ldots,n_K)$ and $\hat{\rho}_{\boldsymbol{0},\boldsymbol{0}}(t) = \hat{\rho}_S(t)$

⏩ simultaneous time differential equations
= **free-pole Hierarchical Equations Of Motion (fp-HEOM)**

$$\dot{\hat{\rho}}_{\boldsymbol{m},\boldsymbol{n}}(t) = -i\mathcal{L}_S\hat{\rho}_{\boldsymbol{m},\boldsymbol{n}}(t) - \sum_{k=1}^{K}(m_k z_k + n_k z_k^*)\hat{\rho}_{\boldsymbol{m},\boldsymbol{n}}(t) - i\sum_{k=1}^{K}\mathcal{L}_k^+\hat{\rho}_{\boldsymbol{m},\boldsymbol{n}}(t) - i\sum_{k=1}^{K}\mathcal{L}_k^-\hat{\rho}_{\boldsymbol{m},\boldsymbol{n}}(t)$$

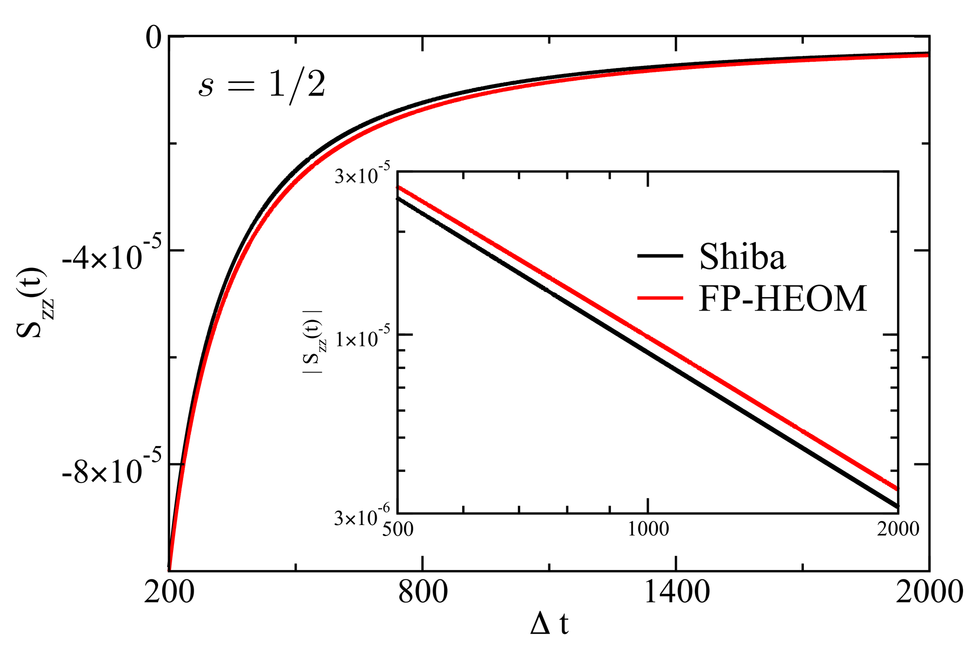


- conventional HEOM: $\omega_k = 0$
  - 👎 restricted profiles of $S_\beta(\omega)$ at elevated temperatures
- **fpHEOM**
  - 👍 arbitrary profiles of $S_\beta(\omega)$ at all temperatures down to $T = 0$
  - 👍 with Matrix Product State (MPS), extremely efficient

Application[1]

"Killer application": Shiba relation for asymptotic times @ $T = 0$, sub-ohmic reservoir $S_\beta(\omega) \propto \omega^s, s < 1$ ($\hat{H}_S = \hbar\Delta\hat{\sigma}_x, \quad \hat{V} = \hbar\hat{\sigma}_z$),

$$S_{zz}(t) = \frac{1}{2}\langle\hat{\sigma}_z(t)\hat{\sigma}_z(0) + \hat{\sigma}_z(0)\hat{\sigma}_z(t)\rangle = \frac{\bar{X}_z^2}{4}\mathrm{Re}\{C(t)\}$$



ⓘ capability of long-time simulation with high accuracy that is challenging for other simulation techniques

[1] M. Xu, Y. Yan, Q. Shi, J. Ankerhold, and J. Stockburger, Phys. Rev. Lett. **129**, 230601 (2022)

Outlook

- study of leakage effects during relaxation process and gate operation
- study of decoherence during application of sequences of pulses
- simulations with real spectral noise powers experimentally obtained
- modeling and simulations of quasiparticle noise
- simulations of qubit arrays
- simulations of optimal control under dissipative conditions

Recent Results

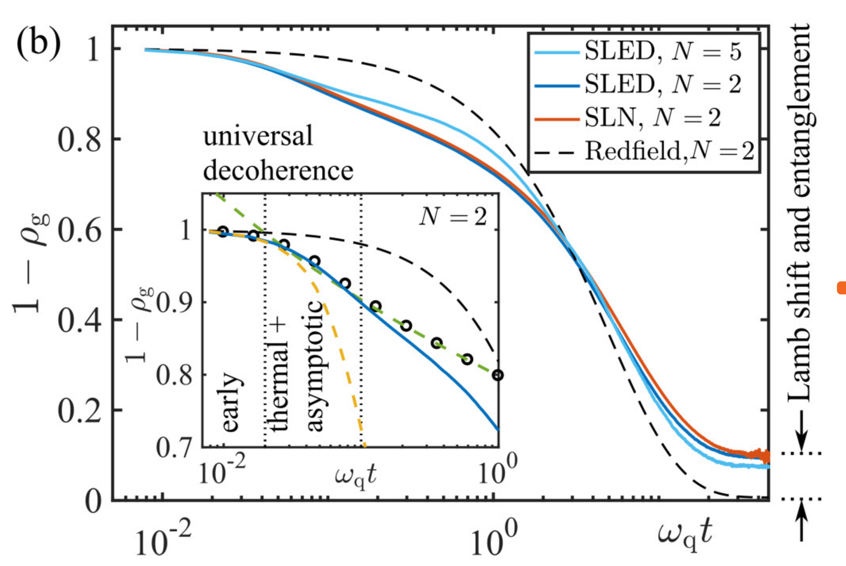
single qubit coupled with reservoir

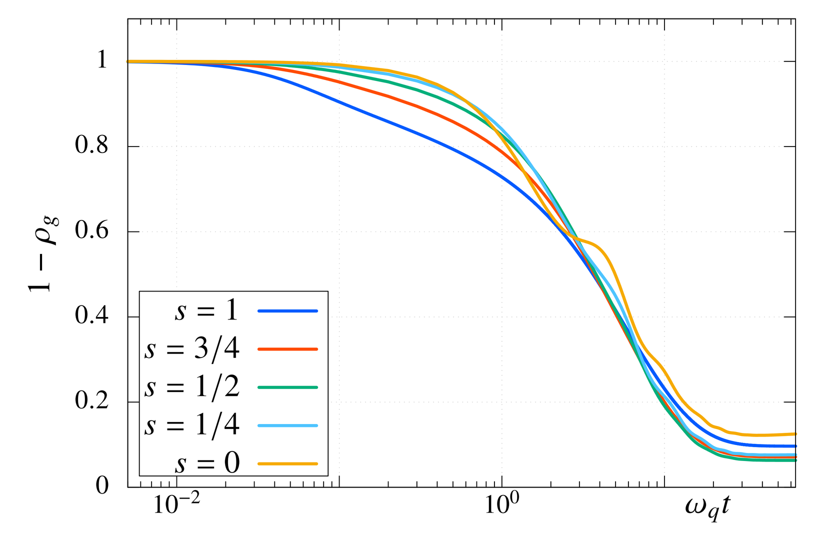
▸ population relaxation($\hat{H}_S = \hbar\omega_q\hat{\sigma}_z/2, \quad \hat{V} = \hbar\hat{\sigma}_x$)

limitation of Redfield approximation [2] ➔ simulating various exponent s of spectral noise power:

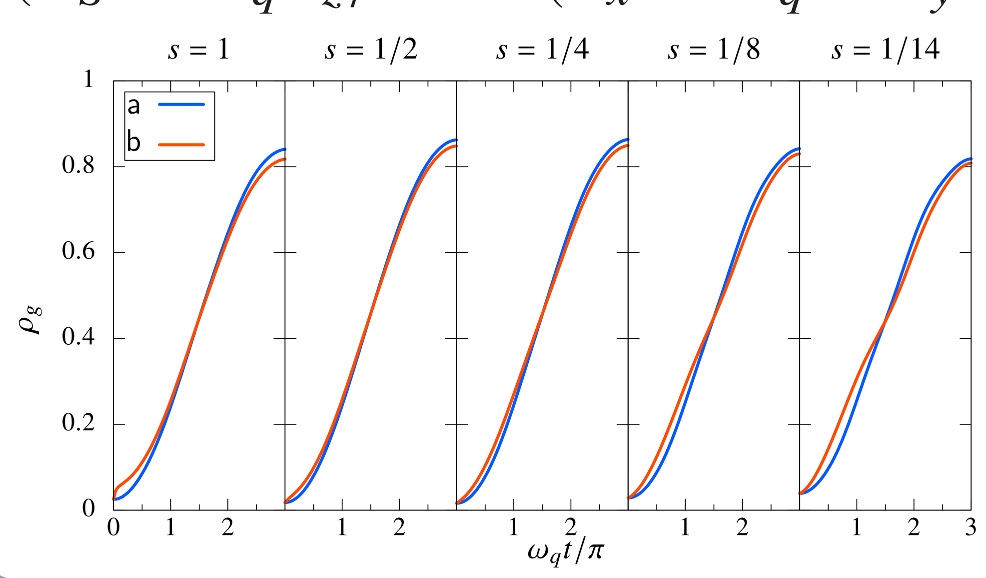
[2] J. Tuorila, J. Stockburger, T. Ala-Nissila, J. Ankerhold, and M. Möttönen, Phys. Rev. Research **1**, 013004 (2019)

$$S_\beta(\omega) = \frac{\hbar\kappa\omega_q^{1-s}\omega^s}{(1+(\omega/\omega_c)^2)^2}\frac{1}{1-e^{-\beta\hbar\omega}} \propto \frac{1}{\beta\hbar\omega^{1-s}} \quad (\omega \to 0)$$





▸ gate operation (single π-pulse about the x axis)
($\hat{H}_S = \hbar\omega_q\hat{\sigma}_z/2 + \hbar\Omega(\hat{\sigma}_x\cos\omega_q t + \hat{\sigma}_y\sin\omega_q t)/2, \quad \hat{V} = \hbar\hat{\sigma}_x$)



different initial states ($\Omega = \omega_q/3$);

a: $\hat{\rho}_a(0) = e^{-\beta\hat{H}_{tot}}/\mathrm{tr}\{e^{-\beta\hat{H}_{tot}}\}$

b: $\hat{\rho}_b(0) = \mathrm{tr}_R\{\hat{\rho}_a(0)\} \otimes \hat{\rho}_R^{eq}$

($\hat{\rho}_R^{eq}$:equilibrium state of the reservoir)