I. THE BASIC IDEA: QUANTUM PROCESS TOMOGRAPHY

$$\rho(t) = e^{i\mathcal{L}t}\rho(0) \tag{1}$$

It becomes well-known the propagation information of a reduced quantum system could be decoded from the short-time $\rho(t)$, with $t \in [0, t_1]$ (quantum process tomography in quantum computing). The choice of t_1 depends on your requirement of the precision (due to the non-Markovian of the bath). Of course, for isolated system (without bath), $t_1 = dt$ is enough.

Cao14 encoded the dissipative propagation information into the so-called transfer tensors. Here, I try to encode it into the RNN-LSTM networks.

II. MODEL

we consider a quantum system coupled linearly to a harmonic bath, where the total Hamiltonian can be written as

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB} \quad , \tag{2}$$

with

$$\hat{H}_S = \epsilon \hat{\sigma}_z + V \hat{\sigma}_x \quad , \tag{3}$$

$$\hat{H}_B = \sum_{j=1}^{N} \left(\frac{\hat{p}_j^2}{2} + \frac{1}{2} \omega_j^2 \hat{x}_j^2 \right) , \qquad (4)$$

$$\hat{H}_{SB} = f(\hat{q}) \otimes \hat{F} = f(\hat{q}) \otimes \sum_{j=1}^{N} c_j \hat{x}_j . \tag{5}$$

Throughout the calculations, relative units are adopted, with V=1.

In this demon, the Debye spectral density is used,

$$J(\omega) = \frac{\eta \omega \gamma}{\omega^2 + \gamma^2} \ . \tag{6}$$

with $\eta = 2.5, \, \gamma = 0.5.$

The temperature $\beta = 2$ and $\beta = 20$ have been tested. Please see the attached figures.

III. NOTES ON RNN-LSTM

The LSTM has complicated dynamics that allow it to easily memorize information for an extended number of timesteps.

LSTM:
$$h_{t}^{l-1}, h_{t-1}^{l}, c_{t-1}^{l} \to h_{t}^{l}, c_{t}^{l}$$
 (7)

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} T_{2n,4n} \begin{pmatrix} h_t^{l-1} \\ h_{t-1}^{l} \end{pmatrix}$$
(8)

$$c_t^l = f \odot c_{t-1}^l + i \odot g \tag{9}$$

$$h_t^l = o \odot \tanh(c_t^l) \tag{10}$$

Here, $T_{n,m}$ is an affine transform. \odot represents element-wise multiplication.

Please refer to W Zaremba's paper at ICLR 2015 recurrent neural network regularization for details.