Exercise 1: Wide open systems

We can define the **delocalization entropy** of a system wave function in terms of the coefficients of that wave function

$$S(\psi) = -\sum_k |c_k|^2 \ln(|c_k|^2). \tag{1}$$

Note that this sense of entropy is not defined on the ensemble but on a single wave function.

(a) Demonstrate that the entropy is 0 when the exciton is fully localized on 1 site.

Solution:

Without loss of generality, let $|\psi\rangle = c_1|1\rangle$, where $|c_1|^2 = 1$ to preserve normalization. Then

$$S(\psi) = -|c_1|^2 \ln\left(|c_1|^2\right) = -1 \ln(1) = 0.$$

(b) Calculate the entropy for the fully delocalized state

$$|\psi\rangle = \frac{1}{\sqrt{4}}(|1\rangle + |2\rangle + |3\rangle + |4\rangle). \tag{2}$$

Is the entropy higher in the localized or delocalized state?

Solution:

For this case,

$$S(\psi) = -4\left|\frac{1}{\sqrt{4}}\right|^2 \ln\left(\left|\frac{1}{\sqrt{4}}\right|^2\right) = -4\left(\frac{1}{4}\right)\ln\left(\frac{1}{4}\right) = \ln 4$$

Comparing the 2 entropies, $\ln 4 > 0$, so the delocalized state has a greater entropy.

(c) The dispersion entropy theorem for quantum state diffusion states that for a wide open system

$$\frac{d}{dt}\left(\mathcal{M}_z[S(|\psi_z(t)\rangle)]\right) = -\sum_k \frac{1-|c_k|^2}{|c_k|^2}\langle\psi_z|\hat{L}_k|\psi_z\rangle \leq 0. \tag{3}$$

What does this mean for the average delocalization of the wave function as a function of time? Imagine you start the system in a fully delocalized state, what should happen? On the other hand, if the wave function starts in the totally localized state, what should happen?

Solution:

The mean entropy of an ensemble of trajectories can never increase, but can decrease over time. This means that for a wide open system, an initially localized state will remain localized, whereas a delocalized initial state will be able to localize over time.

(d) Returning to our original formulation of the problem, recognizing that $|\Psi\rangle$ is the total wave function for the system and bath. Explain what your result for part (c) means in terms of this total wave function. What does the dispersion entropy theorem say in terms of the total wave function?

Solution:

Based on the original formulation, in which

$$|\Psi_{\text{tot}}\rangle = \int \frac{d\mathbf{z}}{\pi^N} e^{-|\mathbf{z}|^2} |\psi_{\mathbf{z}^*}(t)\rangle \otimes |\mathbf{z}\rangle,$$

the dispersion entropy theorem implies that the entropy of the system tends to disperse into the large number of bath states, leading to decreased entropy in system wavefunction realizations.

Exercise 2: Limitations of the method

Looking back over this method, what are the major limitations of the method presented? We spoke at the very beginning about the long timescale of method development, so there have been a lot of developments since this method was first developed - what are the key developments you would want to go look for in the literature if you were interested in this method?

Solution:

Limitations of NMQSD include:

- Infeasibility of calculating functional derivative term.
- Requires initial state to be pure.
- Does not preserve normalization.

Future methods would need to evaluate the functional derivative and preserve normalization for physical consistency. Additionally, the method should be capable of treating more complex initial states for applications like spectroscopy.