

# Open Quantum Systems

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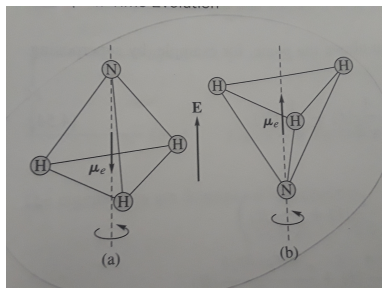
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# Introduction

- ▶ Quantum coherence
- ▶ Ammonia Molecule
- ▶ Spin Chains
- ▶ Spontaneous emission and the Born-Markov Master equation
- ▶ Collisional Decoherence
- ▶ DFS

# The Ammonia Molecule



## Hamiltonian

$$H \rightarrow \begin{pmatrix} E_0 & -\epsilon \\ -\epsilon & E_0 \end{pmatrix} = \begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle \end{pmatrix}$$

Let us solve SE for  $|\psi(0)\rangle = |1\rangle$

- ▶  $i\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle$
- ▶  $|\psi(t)\rangle = U(t)|\psi(0)\rangle$
- ▶  $U(t) = e^{\frac{-iHt}{\hbar}}$ .

# Ammonia Molecule continued

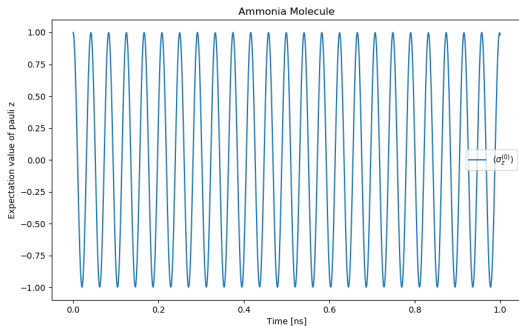
## Solution

$$|\psi(t)\rangle = e^{-\frac{iE_0 t}{\hbar}} \left( \cos\left(\frac{\epsilon t}{\hbar}\right) |1\rangle + i \sin\left(\frac{\epsilon t}{\hbar}\right) |2\rangle \right)$$

## State Matrix

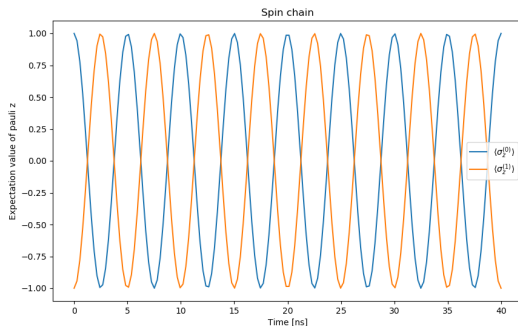
$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| \rightarrow \begin{pmatrix} \cos^2\left(\frac{\epsilon t}{\hbar}\right) & -\cos\left(\frac{\epsilon t}{\hbar}\right) \sin\left(\frac{\epsilon t}{\hbar}\right) \\ i \sin\left(\frac{\epsilon t}{\hbar}\right) \cos\left(\frac{\epsilon t}{\hbar}\right) & \sin^2\left(\frac{\epsilon t}{\hbar}\right) \end{pmatrix}$$

## Time evolution of $\text{Tr}[\rho(t)\sigma_z]$



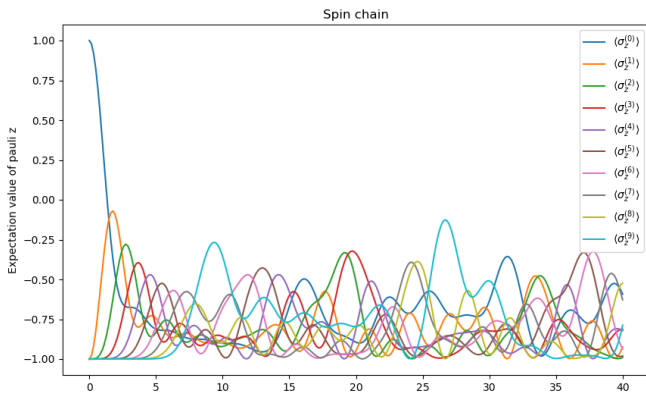
## 2 spin system

- ▶  $H = -\frac{1}{2}[h_0\sigma_z^0 + h_1\sigma_z^1] - \frac{1}{2}[J_x^0\sigma_x^0\sigma_x^1 + J_y^0\sigma_y^0\sigma_y^1 + J_z^0\sigma_z^0\sigma_z^1]$
- ▶  $H \in B(\mathbb{C}^{\otimes 4})$
- ▶ Let  $N = 10$  and  $|\psi(0)\rangle = |10\rangle \in \mathbb{C}^{\otimes 4}$



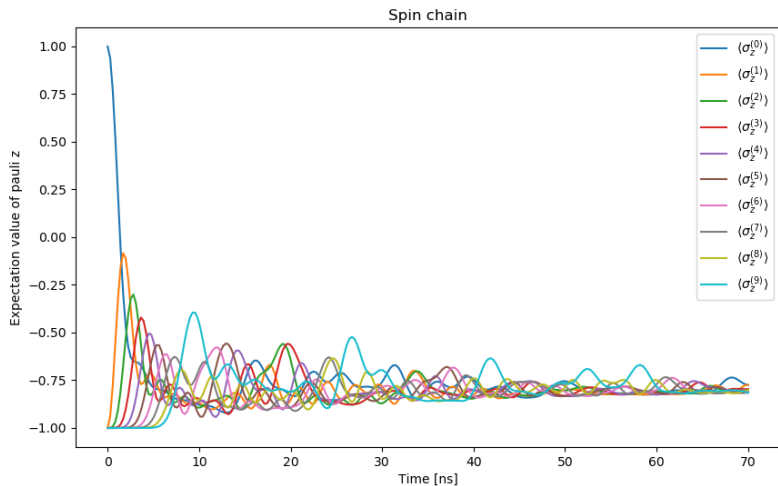
# Spin chains

- ▶  $H = -\frac{1}{2} \sum_n^N h_n \sigma_z^n - \frac{1}{2} \sum_n^{N-1} [J_x^n \sigma_x^n \sigma_x^{n+1} + J_y^n \sigma_y^n \sigma_y^{n+1} + J_z^n \sigma_z^n \sigma_z^{n+1}]$
- ▶  $H \in B(\mathbb{C}^{\otimes 2N})$
- ▶ Solving SE here is hard. Let's use qutip!
- ▶ Let  $N = 10$  and  $|\psi(0)\rangle = |1000000000\rangle \in \mathbb{C}^{\otimes 2N}$



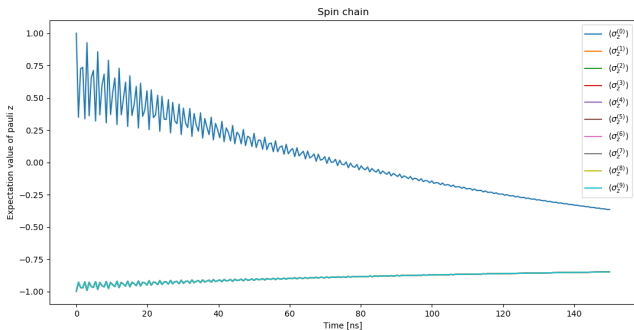
# More on spin chains

## Stronger coupling parameters



# Central spin system

- ▶  $H = -\frac{1}{2} \sum_n^N h_n \sigma_z^n - \frac{1}{2} \sum_n^{N-1} [J_x^n \sigma_x^0 \sigma_x^{n+1} + J_y^n \sigma_y^0 \sigma_y^{n+1} + J_z^n \sigma_z^0 \sigma_z^{n+1}]$
- ▶  $H \in B(\mathbb{C}^{\otimes 2N})$
- ▶ Again, solving SE here is hard. Let's use qutip!
- ▶ Let  $N = 10$  and  $|\psi(0)\rangle = |1000000000\rangle \in \mathbb{C}^{\otimes 2N}$





## Quantum open systems

- ▶ Total system has some *Hilbert* space  $\mathcal{H}_S \otimes \mathcal{H}_E$
- ▶  $|\psi_{SE}\rangle \in \mathcal{H}_S \otimes \mathcal{H}_E$
- ▶ Dynamics provided by Schrödinger's equation.  
 $i\hbar\partial_t|\psi_{SE}(t)\rangle = H|\psi_{SE}(t)\rangle$  where  $H = H_S + H_E + H_I$ .
- ▶  $|\psi_{SE}(t)\rangle = e^{-\frac{it}{\hbar}H}$ . Just like before. We can attain the reduced dynamics by partial tracing over the degrees of freedom pertaining to the environment. i.e.

$$\text{Tr}_E\{|\psi_{SE}(t)\rangle\langle\psi_{SE}(t)|\}$$

# Partial Trace

## Definition

$$\text{Tr}_E\{\cdot\} : T(\mathcal{H}_S \otimes \mathcal{H}_E) \rightarrow T(\mathcal{H}_S)$$

$$\text{Tr}_E\{|\psi_{SE}(t)\rangle\langle\psi_{SE}(t)|\} := \sum_k \langle\phi_k|\psi_{SE}(t)\rangle\langle\psi_{SE}(t)|\phi_k\rangle,$$

where  $\{|\phi_k\rangle\}_k$  is an ONB for  $\mathcal{H}_E$ .

▶ Let us make sure that this map is the correct one.



$$A_S \rightarrow A_S \otimes I_E,$$

$$\langle A_S \otimes I_E \rangle = \text{Tr}\{\rho_{SE}(A_S \otimes I_E)\}.$$

But it can be shown that

$$\text{Tr}\{\rho_{SE}(A_S \otimes I_E)\} = \text{Tr}_S\{\rho_S A_S\}!!!!.$$

## Partial trace

- ▶ There you have it, all we need to do is compute

$$\text{Tr}_E\{|\psi_{SE}(t)\rangle\langle\psi_{SE}(t)|\}.$$

- ▶ This is generally intractable and approximations must be made.
- ▶ Let's switch to the equivalent approach, Von Neumann equation is starting point.

$$\frac{\partial}{\partial t}\rho_{SE}(t) = -\frac{i}{\hbar}[H_{SE}, \rho_{SE}(t)] \quad (1)$$

We can attain the reduced dynamics by partial trace.

$$\frac{\partial}{\partial t}\rho_S(t) = -\frac{i}{\hbar}\text{Tr}_E\{[H_{SE}, \rho_{SE}(t)]\} \quad (2)$$

## Born-Markov approximation

Equivalently.

$$\begin{aligned} \frac{\partial}{\partial t} \rho_S(t) = & -\frac{i}{\hbar} \text{Tr}_E \{ [H_{SE}, \rho_S(0) \otimes \rho_E(0)] \} + \\ & + \frac{i^2}{\hbar^2} \int_0^t dt_1 \text{Tr}_E \{ [H_{SE}, [H_{SE}, \rho_S(t_1) \otimes \rho_E(0)]] \} \end{aligned}$$

- ▶ Here we already begin to make approximations. We have assumed that  $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$ , separable. This is the *Born* approximation.
- ▶ We have also assumed that the environment is unchanged by the system  $S$ . Unfortunately this too is intractable if we are not able to make the approximation  $\rho_S(t_1) \rightarrow \rho_S(t)$ . This makes the integro differential equation above more manageable.

## two-level system in bath

- ▶ Let  $E$  be a large, with respect to the system, bosonic bath and  $S$  be a two-level system. Assuming that the two level system is in the excited state at  $t = 0$  we can use the Born-Markov approximation to arrive at the following equation.



$$\frac{\partial}{\partial t} \rho_S(t) = \frac{-i}{2} (\omega_a + \Delta\omega_a) [\sigma_z, \rho_S(t)] + \gamma D[\sigma_-] \rho_S(t). \quad (3)$$

- ▶  $D[\sigma_-] \rho = \sigma_- \rho \sigma_+ - \frac{1}{2} (\sigma_+ \sigma_- \rho + \rho \sigma_+ \sigma_-)$  This is known as the *Born – Markov* master equation. We now use it to solve for the reduced density matrix.
- ▶ First assume that  $\rho_S(t) = \frac{1}{2} [I_2 + x(t)\sigma_x + y(t)\sigma_y + z(t)\sigma_z]$ , we also constraint the scalar functions to  $\text{Tr}_S\{\rho_S(t)\} = 1$ .

- ▶  $\frac{\partial}{\partial t} z(t) = \text{Tr}\{\sigma_z \frac{\partial}{\partial t} \rho_S(t)\}$
- ▶  $\frac{\partial}{\partial t} y(t) = \text{Tr}\{\sigma_y \frac{\partial}{\partial t} \rho_S(t)\}$
- ▶  $\frac{\partial}{\partial t} x(t) = \text{Tr}\{\sigma_x \frac{\partial}{\partial t} \rho_S(t)\}$

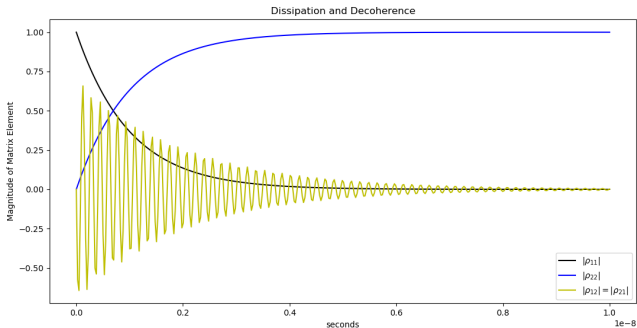
Using the *Lindblad* Master equation to substitute for  $\frac{\partial}{\partial t} \rho_S(t)$  these equations become

- ▶  $\frac{\partial}{\partial t} z(t) = -\gamma(z(t) + 1)$
- ▶  $\frac{\partial}{\partial t} y(t) = (\Delta\omega_a)x(t) - \frac{\gamma}{2}y(t)$
- ▶  $\frac{\partial}{\partial t} x(t) = -(\Delta\omega_a)y(t) - \frac{\gamma}{2}x(t)$

with solutions

- ▶  $z(t) = 2e^{-\gamma t} - 1$
- ▶  $y(t) = -e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta\omega_a)t)$
- ▶  $x(t) = e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta\omega_a)t).$

# Continued



$$\rho_S(t) \rightarrow \begin{bmatrix} e^{-\gamma t} & e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta_a)t) \frac{(1+i)}{2} \\ e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta_a)t) \frac{(1-i)}{2} & 1 - e^{-\gamma t} \end{bmatrix}$$

# Collisional Decoherence



## Set up

Let  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$  be a product *Hilbert* space.

- ▶  $\dim[\mathcal{H}_A] = N$
- ▶  $\dim[\mathcal{H}_B] = M$
- ▶  $\dim[\mathcal{H}] = NM$ .

Take  $H \in \mathcal{B}(\mathcal{H}) = \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$  with the following form.

$$H = \sum_k S_k \otimes E_k \tag{4}$$

- ▶  $S_k \in \mathcal{B}(\mathcal{H}_A)$
- ▶  $E_k \in \mathcal{B}(\mathcal{H}_B)$
- ▶  $S_k = S_k^\dagger$  and  $E_k = E_k^\dagger$ , self adjoint.

Recognize the following equation?  $i\frac{\partial}{\partial t}\psi_t = H\psi_t$ ,  $\psi_t \in \mathcal{H}$ .

## Set Up part 2

The solution to SE in the time independent case is just

$$\psi_t = e^{\frac{-it}{\hbar} \sum_k S_k \otimes E_k} \psi_0 \quad (5)$$

Assuming that  $\psi_0 = [\sum_I c_I \phi_I] \otimes \eta_0$ ,

- ▶  $\{\phi_i\}_i$  form an ONB for  $\mathcal{H}_A$ .
- ▶  $\eta_0 \in \mathcal{H}_B$

$$\psi_t = e^{\frac{-it}{\hbar} \sum_k S_k \otimes E_j} ([\sum_I c_I \phi_I] \otimes \eta_0) \quad (6)$$

Let us move to the state matrix representation.

- ▶  $\rho_t = \psi_t \psi_t^\dagger = e^{\frac{-it}{\hbar} \sum_k S_k \otimes E_k} ([\sum_{l,m} c_l c_m^* \phi_l \phi_m^\dagger] \otimes \eta_0 \eta_0^\dagger) e^{\frac{it}{\hbar} \sum_k S_k \otimes E_k}$

## Decoherence

Partial tracing over the degrees of freedom pertaining to  $\mathcal{H}_B$  we get the  $\mathcal{H}_A$  local non unitary equation.

$$\rho_S(t) = Tr_B[e^{\frac{-it}{\hbar} \sum_k S_k \otimes E_k} ([\sum_{l,m} c_l c_m^* \phi_l \phi_m^\dagger] \otimes \eta_0 \eta_0^\dagger) e^{\frac{it}{\hbar} \sum_k S_k \otimes E_k}] \quad (7)$$

This partial trace in general reduces to some state of the form,

$$\rho_S(t) = \sum_{l,m} a_l(t) a_m^*(t) \phi_l \phi_m^\dagger$$

with  $a_l(t) a_m^*(t) \rightarrow 0$  as  $t \rightarrow \infty$  for  $l \neq m$ .

## Question

From what space  $\mathcal{H}_C \subset \mathcal{H}_A$  may we construct superpositions  $\sum_l c_l \phi_l$  that are immune to decoherence? i.e.

$$\text{Tr}_B [e^{\frac{-it}{\hbar} \sum_k S_k \otimes E_k} ([\sum_{l,m} c_l c_m^* \phi_l \phi_m^\dagger] \otimes \eta_0 \eta_0^\dagger) e^{\frac{it}{\hbar} \sum_k S_k \otimes E_k}] = \sum_{l,m} c_l c_m^* \phi_l \phi_m^\dagger \quad (8)$$

Need  $\{\phi_j\}_i$  ONB, with the exotic property of forming a degenerate eigen space for all  $S_k$ .

$$\psi_t = e^{\frac{-it}{\hbar} \sum_k S_k \otimes E_k} [\sum_l c_l \phi_l] \otimes \eta_0 = \quad (9)$$

$$= [\sum_l c_l e^{\frac{-it}{\hbar} \sum_k \lambda_k I_A \otimes E_k} \phi_l] \otimes \eta_0 = \sum_l c_l \phi_l \otimes [e^{\frac{-it}{\hbar} \sum_k \lambda_k I_A \otimes E_k} \eta_0] \quad (10)$$

## Partial Trace

Let us now partial trace the corresponding density matrix.

$$\rho_S(t) = \sum_{l,m} c_l c_m^* \phi_l \phi_m^\dagger \text{Tr}_B [e^{-\frac{it}{\hbar} \sum_k \lambda_k I_A \otimes E_k} \eta_0 \eta_0^\dagger e^{\frac{it}{\hbar} \sum_k \lambda_k I_A \otimes E_k}]$$

The trace term is just one since density matrices have trace one under unitary evolution.

$$\rho_S(t) = \sum_{l,m} c_l c_m^*$$

. :)

## Example, symmetric dephasing

Consider a system of  $N$  qubits coupled to its environment in the following way.

$$|0\rangle_j \rightarrow |0\rangle_j \quad (11)$$

$$|1\rangle_j \rightarrow e^{i\phi}|1\rangle_j. \quad (12)$$

$j$  indexes over all qubits. Let the initial state be

$$|\psi\rangle_0 = \bigotimes_{j=1}^N (a_j|0\rangle_j + b_j|1\rangle_j).$$

The dephasing process evolves our system into the following state.

$$|\psi\rangle_\phi = \bigotimes_{j=1}^N (a_j|0\rangle_j + b_j e^{i\phi}|1\rangle_j)$$

with a probability  $p_\phi$

## Example continued

The ensemble  $\{|\psi\rangle_\phi, p_\phi\}$  can be expressed equivalently as a mixed state.

$$\rho = \int p_\phi |\psi\rangle_\phi \langle\psi| d\phi$$

$$|\psi\rangle_\phi \langle\psi| \rightarrow \begin{bmatrix} |a_j|^2 & a_j b_j^* e^{-i\phi} \\ a_j^* b_j e^{i\phi} & |b|^2 \end{bmatrix}. \quad (13)$$

For a gaussian distribution  $p_\phi = (4\pi\alpha)^{-\frac{1}{2}} e^{-\frac{\phi^2}{4\alpha}}$  we have

$$\begin{bmatrix} |a_j|^2 & a_j b_j^* e^{-\alpha} \\ a_j^* b_j e^{-\alpha} & |b|^2 \end{bmatrix}. \quad (14)$$

There is indeed decoherence present, lets look for a DFS.

## Example continued

For starters let's consider the case  $N = 2$ . The dephasing for each of the constituents of the corresponding *Hilbert* space  $\mathbb{C}^2 \otimes \mathbb{C}^2$  is summarized by the following.

$$|00\rangle \rightarrow |00\rangle \quad (15)$$

$$|01\rangle \rightarrow e^{i\phi}|01\rangle \quad (16)$$

$$|10\rangle \rightarrow e^{i\phi}|10\rangle \quad (17)$$

$$|11\rangle \rightarrow e^{2i\phi}|11\rangle. \quad (18)$$

$$\text{Span}\{|01\rangle, |10\rangle\}?$$

check...

$$|\psi\rangle = a|01\rangle + b|10\rangle \rightarrow ae^{i\phi}|01\rangle + be^{i\phi}|10\rangle = e^{i\phi}|\psi\rangle$$

It works!!



## Example continued

For  $N = 3$  the largest DFS is  $Span\{|001\rangle, |010\rangle, |100\rangle\}$  or  $Span\{|011\rangle, |101\rangle, |110\rangle\}$

In general  $\max[\dim(DFS)] = \binom{N}{\lfloor \frac{N}{2} \rfloor}$  A textbook application of stirling's formula yields the following.

$$\frac{|\max[\dim(DFS)] - 2^N|}{2^N} \rightarrow 1.$$

The dimension of the optimal DFS becomes relatively close to the dimension of the system for large  $N$ .