finding the decomposition

start with the defenition of a state as before

$$|\psi\rangle = \sum_{ij} C_{ij} |S_i\rangle |B_j\rangle$$

with energy eigenvalues $\{E_{ij}\}$

but now define the combined states with interactions as

$$|\psi\rangle = \sum_{n} C_n |N_n\rangle$$

with energy eigenvalues $\{E_n\}$

We now need to find the representation of a arbitary bath state in the interaction included basis in order to perform the partial trace.

equating the representations of $|\psi\rangle$, and taking a single bath state existing so $C_{ij} = 0$ unless $i = z$ where z is the index of the desired bath state,

$$\sum_{i} C_{iz} |S_i\rangle |B_z\rangle = \sum_{n} C_n |N_n\rangle$$

we observe

$$|\psi\rangle (|S_i\rangle |B_j\rangle) = |\psi\rangle (|B_j\rangle |S_i\rangle)$$

As $|\psi\rangle$, as the seperated basis allows each element of the system to act only on it's corrosponding element. We use this to remove $|B_j\rangle$ from the bracket.

$$|B_z\rangle \left(\sum_{i} C_{iz} |S_i\rangle \right) = \sum_{n} C_n |N_n\rangle$$

left multiply by $\sum_{i'} C^{\star}_{i'z} \langle S_{i'}|$,

$$\left(\sum_{i'} C^{\star}_{iz} \langle S_{i'}| \right) |B_z\rangle \left(\sum_{i} C_{iz} |S_i\rangle \right) = \left(\sum_{i'} C^{\star}_{i'z} \langle S_{i'}| \right) \sum_{n} C_n |N_n\rangle$$

$$|B_z\rangle \left(\sum_{ii'} C_{iz} C^{\star}_{iz} \langle S_{i'}|S_i\rangle \right) = \left(\sum_{i'} C^{\star}_{i'z} \langle S_{i'}| \right) \sum_{n} C_n |N_n\rangle$$

$$|B_z\rangle \left(\sum_{ii'} C_{iz}C^\star_{iz}\delta_{ii'}\right) = \left(\sum_{i'} C^\star_{i'z}\langle S_{i'}|\right)\sum_n C_n |N_n\rangle$$

$$|B_z\rangle \left(\sum_{i} C_{iz}C^\star_{iz}\right) = \sum_{i'n} C^\star_{i'z}C_n \langle S_{i'}|N_n\rangle$$

$$|B_z\rangle = \frac{\sum_{i'n} C^\star_{i'z}C_n \langle S_{i'}|N_n\rangle}{\sum_i C_{iz}C^\star_{iz}}$$

Density matrix

Introduce $\rho = |\psi\rangle\langle\psi|$

$$\rho = (\sum_q C_q |N_q\rangle)(\sum_{q'} C^\star_{q'}\langle N'_q|)$$

Find the partial trace,

$$\sum_z \langle B_z|\rho|B_z\rangle = \sum_z \left(\frac{\sum_{in} C_{iz}C^\star_n |S_i\rangle\langle N_n|}{\sum_i C^\star_{iz}C_{iz}}\right)\left(\sum_q C_q |N_q\rangle\right)\left(\sum_{q'} C^\star_{q'}\langle N'_q|\right)\left(\frac{\sum_{i'n'} C^\star_{i'z}C_{n'}\langle S_{i'}|N'_n\rangle}{\sum_i C_{iz}C^\star_{iz}}\right)$$

$$\sum_z \langle B_z|\rho|B_z\rangle = \frac{1}{\left(\sum_i C_{iz}C^\star_{iz}\right)^2}\sum_z\sum_{in}\sum_{qq'}\sum_{i'n'} C_{iz}C^\star_n C_q C^\star_{q'}C^\star_{i'z}C_{n'}|S_i\rangle\langle N_n|N_q\rangle\langle N'_q|N'_n\rangle\langle S_{i'}|$$

use orthonormality, $q' = n', q = n$,

$$\sum_z \langle B_z|\rho|B_z\rangle = \frac{1}{\left(\sum_i C_{iz}C^\star_{iz}\right)^2}\sum_z\sum_{in}\sum_{i'n'} C_{iz}C^\star_n C_n C^\star_{n'}C^\star_{i'z}C_{n'}|S_i\rangle\langle S_{i'}|$$

and find the density element $\hat{\rho}^{\text{reduced}}_{S_1,S_2}$, applying orthonormaity we obtain $i = 1, i' = 2$

$$\hat{\rho}^{\text{reduced}}_{S_1,S_2} = \sum_{nn'}\|C_n\|^2\|C_{n'}\|^2\sum_z \frac{C_{1z}C^\star_{2z}}{\left(\sum_i \|C_{iz}\|^2\right)^2}$$

$$\hat{\rho}_{S_1,S_2}^{\text{reduced}} = \sum_n \|C_n\|^2 \sum_{n'} \|C_{n'}\|^2 \sum_z \frac{C_{1z} C_{2z}^\star}{\left(\sum_i \|C_{iz}\|^2\right)^2}$$

$$\hat{\rho}_{S_1,S_2}^{\text{reduced}} = \sum_z \frac{C_{1z} C_{2z}^\star}{\left(\sum_i \|C_{iz}\|^2\right)^2}$$

Both sums over

$$