

USEQIP NMR Laboratory 2

1 Pseudo-pure State Preparation

The thermal equilibrium state in liquid-state NMR is usually highly mixed. For a system with 2 spins, (which can easily be generalized), we say during the lecture that the initial state is given by

$$\rho_{th} \propto e^{-\hat{H}/k_B T} \quad (1)$$

$$\propto \mathbb{1} + \epsilon(\omega_0^1 \hat{Z}_1 + \omega_0^2 \hat{Z}_2) \quad (2)$$

$$\sim \omega_0^1 \hat{Z}_1 + \omega_0^2 \hat{Z}_2 \quad (3)$$

Since the identity component of the state is unobservable in NMR (we can only see population differences), we want to transform the initial thermal state to one where there is an identity component and a deviation density matrix which is a pure state:

$$\rho_{p.p.} = \mathbb{1} + \epsilon \rho_{pure} \quad (4)$$

$$\sim \rho_{pure} \quad (5)$$

This sort of state is generation referred to as “pseudopure state”. Recall in the case of chloroform, we use the hydrogen as spin 1 and the carbon as spin 2. Also, recall that $\omega_0^H/\omega_0^C \approx 4$, therefore

$$\rho_{th} \sim \hat{Z}_1 + \frac{1}{4} \hat{Z}_2 \quad (6)$$

Transforming the thermal state in this manner is not a unitary process, i.e. convince yourself that there exist no unitary transformation \hat{U} such that

$$\rho_{p.p.} = \hat{U} \rho_{th} \hat{U}^\dagger \quad (7)$$

In order to create the needed pseudo pure state, we can implement a non-unitary operation through temporal averaging: summing up the results of different scans with different initial state in each

scan. To be more concrete, let's say we want to implement quantum algorithm \hat{V} on initial state $\rho_0 = |00\rangle\langle 00|$. If we can find n pulse sequences implementing initial states $\rho_1 \dots \rho_n$, such that

$$\sum_{k=1}^n \rho_k = |00\rangle\langle 00|. \quad (8)$$

Then implementing the algorithm \hat{V} on each of these initial states and adding the spectrum of each experiments together will give the same results as if we had performed a single experiment with initial state $|00\rangle\langle 00|$. This is because of the linearity of quantum mechanics, that is

$$\sum_{k=1}^n \hat{V} \rho_k \hat{V}^\dagger = \hat{V} \left(\sum_{k=1}^n \rho_k \right) \hat{V}^\dagger \quad (9)$$

$$= \hat{V} |00\rangle\langle 00| \hat{V}^\dagger \quad (10)$$

The Bruker pulse program language is not particularly flexible so we do this by jumping to different parts of the pulse program depending on which scan we are in.

```
if "l1==1" goto scan1
if "l1==2" goto scan2
if "l1==3" goto scan3

scan1, 1u
;;Pulse program for first scan
1u iu1
goto restofpp

scan2, 1u
;;Pulse program for second scan
1u iu1
goto restofpp

scan3, 1u
;;Pulse program for third scan
1u iu1
goto restofpp

restofpp,1u
;;insert pulse program of desired quantum algorithm here

;;Proton readout pulse
( H90 ph1 ):f2
```

```

go=2 ph31
30m mc #0 to 2 F0(zd)
exit

```

We use the loop counter `l1` to keep track of which scan we are in. The initial value of the loop counter is set in `Topspin`. The command `iu1` increments the loop counter.

1. You should confirm that summing the density matrices from applying the following three unitaries to the thermal state gives a deviation density matrix proportional to $|00\rangle\langle 00|$.

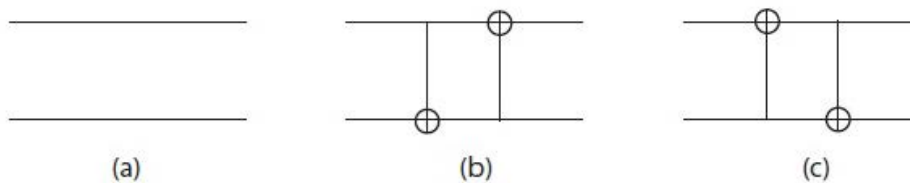


Figure 1: Three circuits for creating a pseudo-pure state on two qubits.

2. Using what you learned in class and the the pre-lab questions on how to implement a CNOT, put together pulse sequences for each of the three scans. Try to compress the sequence as much as possible. You should need only four pulses and two delays. You can pulse simultaneously on two channels by putting the two pulses on the same line in the pulse program.
3. Copy the proton template to experiment 30. Pulse program `zg_USEQIP_pp` provides a template for the pseudo-pure experiments. Change the pulse program to `zg_USEQIP_pp` and edit the pulse program. Add your pulses to the appropriate parts. Add a proton readout pulse before acquisition.
4. In `Topspin`, change the number of scans to 3 through the variable `ns`. Ensure `l1` is set to 1.
5. Run the pulse program.
6. Estimate the fidelity of the pseudo-pure by comparing the relative intensity of the two peaks.

2 Extra Information

To help you show that the above pulse sequence give the desired result, check for yourself that

1. $U_{cnot}(Z_1 \mathbb{1}_2)U_{cnot}^\dagger = Z_1 \mathbb{1}_2$
2. $U_{cnot}(\mathbb{1}_1 Z_2)U_{cnot}^\dagger = Z_1 Z_2$
3. $U_{cnot}(Z_1 Z_2)U_{cnot}^\dagger = \mathbb{1} Z_2$