# Notes on the 12 qubit PPS

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Notes about the problems in the 12 qubit PPS preparation, including Matlab codes and Experiments.

#### DEC 12, 2014

Calculating the state to state GRAPE on Ordi2. In pulsefinder folder. paramsfile is 'twqubit\_subS2S.m', and the output file is 'twqubit\_7zto12z'.

```
% Number of timesteps
2
   params.plength = 400;
 3
4
   % Length of each time step
5
   params.timestep = 10e-6;
6
7
   params.subsystem\{1\} = [1 2 3 9 10 11];
8
   params.subsystem\{2\} = [4 5 6 7 8 12];
9
   params.subsys_weight = [6 6];
10
11
   % Input and goal states for state to state
12
   params.rhoin = mkstate('+1ZZZZZZZIIIII',1);
13
   params.rhogoal = mkstate('+1ZZZZZZZZZZZZ',1);
14
15
   % Allow Zfreedom or not
16
   params.Zfreedomflag = 1;
```

The fidelity keeps 0 all the time. Guess the reason is 'Zfreedom'. Set 'params.Zfreedomflag = 0;'. However, still 0.

Annie said maybe due to the length. Her SWAP gate requires 8ms, so I changed 'params.plength = 800;'. But for with or without Zfreedom, fidelity is still 0.

Check if some of my GRAPE settings are wrong. try to repeat Annie's SWAP gate calculation.

```
% Number of timesteps
2
  params.plength = 800;
3
4
  % Length of each time step
5
  params.timestep = 10e-6;
6
7
  params.subsystem\{1\} = [1 2 3 9 10 11];
8
  params.subsystem\{2\} = [4 5 6 7 8 12];
9
  params.subsys_weight = [6 6];
10
11
  \% Input and goal states for state to state
12
  +1IIIIIIIIII;;
13
  14
15
  % Allow Zfreedom or not
  params.Zfreedomflag = 0;
```

The outputfile is 'twqubit\_SWAPC7H5'. And the fidelity is already over 98%. Then I changed 'params.Zfreedomflag = 1;', and the fidelity is over 95% after 30 iterations. Much slower than the no Zfreedom case. Maybe due to different initial guesses.

## **DEC 15, 2014**

Generate all  $\pi/2$  and  $\pi$  pulses for the 7 Carbons, with the Calibration = 25KHz.  $\pi/2$  pulses are 1ms length and 100 steps, and  $\pi$  pulses are 2ms length and 200 steps. Generating Code in 'twqubit\_shape.m'

```
for ii = 1:7
loadfile = ['twqubit_C', num2str(ii), '180', '.mat'];
eval(['load ', loadfile]);
filename1 = ['twqubit_C', num2str(ii), '180_C_25000.txt'];
filename2 = ['twqubit_C', num2str(ii), '180_H_25000.txt'];
make_bruker_shape(pulses{1}, 25000, filename1,1);
make_bruker_shape(pulses{1}, 25000, filename2,2);
end
```

The pulses are saved in Ordi2 '\pulsefinder\12 Qubit\' with the names such as 'twqubit\_C590\_C\_25000.txt'.

I checked all the fidelities of the  $\pi/2$  pulses in the folder '\pulseexam\_12qubit\C\_rotations\check\_grape.m'. The code is in Appendix I.

Unitaries and Fidelities of the pulses will both be saved in 'twqubit\_C590\_Ufid.mat', so they can be called for further calculations in the PPS simulation. Wait for the results.

#### DEC 16, 2014

Combine pulses in the PPS preparation into big shape files, which should be easy for calibrations and pulsefixing.

The code is in the SVN server for Matlab named '\Twqubit\pulse\_combine.m'.

First read all the powers and phases for the  $\pi/2$  and  $\pi$  rotations.

```
for spin_number = 1:7
2
          Name1 = ['twqubit_C', num2str(spin_number), '90_C_25000.txt'];
3
          Name2 = ['twqubit_C', num2str(spin_number), '90_H_25000.txt'];
4
          [power1, phase1] = dataout(Name1, Output1, FirstLine, Length_90);
          [power2, phase2] = dataout(Name2, Output2, FirstLine, Length_90);
5
6
          eval(['power_C', num2str(spin_number), '90_C = power1;']); eval(['phase_C
              ', num2str(spin_number), '90_C = phase1;']);
7
          eval(['power_H', num2str(spin_number), '90_H = power2;']); eval(['phase_H
              ', num2str(spin_number), '90_H = phase2; ']);
8
   end
9
10
   for spin_number = 1:7
          Name1 = ['twqubit_C', num2str(spin_number), '180_C_25000.txt'];
11
12
          Name2 = ['twqubit_C', num2str(spin_number), '180_H_25000.txt'];
13
          [power1, phase1] = dataout(Name1, Output1, FirstLine, Length_180);
14
           [power2, phase2] = dataout(Name2, Output2, FirstLine, Length_180);
15
          eval(['power_C', num2str(spin_number), '180_C = power1;']); eval(['
              phase_C', num2str(spin_number), '180_C = phase1;']);
          eval(['power_H', num2str(spin_number), '180_H = power2;']); eval(['
16
              phase_H', num2str(spin_number), '180_H = phase2;']);
17
   end
```

Then combine them with the free evolutions. Here I set the time step dt = 10us. The code is in Appendix I.

The two output files are 'twqubit\_encoding1\_C' and 'twqubit\_encoding1\_H'. The calibrations are 25000Hz.

## DEC 17, 2014

All fidelities of  $\pi/2$  pulses are done! The folder is '\pulseexam\_12qubit\C\_rotations\'. Use 'check\_power.m' to check the maximal powers for C and H channel.

Rotation	Fidelity	File	MaxPower C	MaxPower H	
$R_x^1(\pi/2)$	0.9838	twqubit_C190_Ufid.mat	56.0%, 14000Hz	22.3%, 5557Hz	
$R_x^2(\pi/2)$	0.9758	twqubit_C290_Ufid.mat	41.7%, 10422Hz	23.5%, 5878Hz	
$R_x^3(\pi/2)$	0.9647	twqubit_C390_Ufid.mat	31.9%, 7979.0Hz	22.3%, 5568Hz	
$R_x^4(\pi/2)$	0.9801	twqubit_C490_Ufid.mat	31.6%, 7892.0Hz	23.8%, 5954Hz	
$R_x^5(\pi/2)$	0.9936	twqubit_C590_Ufid.mat	56.1%, 14033Hz	30.7%, 7678Hz	
$R_x^6(\pi/2)$	0.9683	twqubit_C690_Ufid.mat	57.3%, 14333Hz	34.4%, 8595Hz	
$R_x^7(\pi/2)$	0.9857	twqubit_C790_Ufid.mat	43.7%, 10925Hz	24.8%, 6207Hz	
$R_x^1(\pi)$	0.9699	twqubit_C1180_Ufid.mat	62.6%, 15655Hz	34.9%, 8726Hz	
$R_x^2(\pi)$	0.9537	twqubit_C2180_Ufid.mat	51.1%, 12783Hz	32.4%, 8094Hz	
$R_x^3(\pi)$	0.9330	twqubit_C3180_Ufid.mat	37.4%, 9350.0Hz	24.0%, 5997Hz	
$R_x^4(\pi)$	0.9639	twqubit_C4180_Ufid.mat	45.1%, 11268Hz	20.4%, 5108Hz	
$R_x^5(\pi)$	0.9904	twqubit_C5180_Ufid.mat	67.6%, 16895Hz	31.1%, 7782Hz	
$R_x^6(\pi)$	0.9393	twqubit_C6180_Ufid.mat	71.8%, 17948Hz	33.6%, 8396Hz	
$R_x^7(\pi)$	0.9743	twqubit_C7180_Ufid.mat	51.0%, 12759Hz	32.1%, 8022Hz	

For  $\pi$  pulses, the maximal power of C5 exceeds 100% so it cannot be used. Check if we can generate  $\pi$  pulses by combining two  $\pi/2$  pulses. A potential problem is when calculating the GRAPE, we have considered the 4us free evolutions in the beginning and in the end. If we combine, we will have an unwanted 8us free evolution in the middle of the new  $\pi$  pulse.

Use 'combine90to180' to check the  $\pi$  pulse fidelity. They are very bad actually. All of them are just 0.75 0.76 in fidelity.

So I run 'check\_grape.m' to check the fidelities of the  $\pi$  pulses. Only from C1 to C4, as C5 has exceeds the power limit 25000Hz.

# DEC 22, 2014

Got 4 GRAPE pulses for encoding. The folder is '\pulseexam\_12qubit\C\_rotations\'. The fidelities are in calculation on Ordi2.

Rotation	Fidelity	File	MaxPower C	MaxPower H
$R_x^{5,7}(\pi)$	0.9667	twqubit_C57180_Ufid.mat	32.3%, 8072.5Hz	24.2%, 6049Hz
$R_x^{2,3}(\pi)$	0.8908	twqubit_C23180_Ufid.mat	32.4%, 8101.5Hz	22.8%, 5701Hz
$R_x^{2,3,4,7}(\pi/2)$	0.9156	twqubit_C23180_Ufid.mat twqubit_C234790_Ufid.mat	37.4%, 9358.3Hz	28.9%, 7213Hz
$R_x^{1,5,6}(\pi)$	0.9055	twqubit_C156180_Ufid.mat	32.2%, 8039.7Hz	20.3%, 5086Hz

Have to recalculate many  $\pi$  pulses.

## DEC 23, 2014

Got  $\pi$  pulse on C6. Combine two  $\pi/2$  pulses as the initial guess, with the fidelity 0.75, and then search the optimal  $\pi$  pulse. The convergence speed is very fast, which means initial guess is indeed very important in 12 qubits.

Now C2, C3, C5, C7  $\pi$  pulses are in calculation, with the initial guess.

#### FEB 05, 2015

C2, C3, C5, C7  $\pi$  pulses are all finished, and the update is in the Section Dec 17, 2014.

Also submitted the last pulse for the Encoding. From the PPS.m file in folder 'Twqubit'

```
%Phase Correction
U7 = R(gop(2,X),90)*R(gop(2,-Z),360*(Para(2,2)-20696)*1/2/148.5)*...
R(gop(3,-Y),90)*R(gop(3,-Z),360*(Para(3,3)-20696)*1/2/148.5)*...
R(gop(4,X),90)*R(gop(4,-Z),360*(Para(4,4)-20696)*1/2/148.5)*...
R(gop(7,X),90)*R(gop(7,-Z),360*(Para(7,7)-20696)*1/2/148.5);
```

And the operator is in 'twqubit\_sub\_234790\_and\_phasecorrection.m'

## FEB 06, 2015

The pulse 'twqubit\_sub\_234790\_and\_phasecorrection.m' which is the last piece of the encoding was found!

All  $\pi$  pulses are found. The lowest is 0.9330 for C3 and the highest is 0.9904 for C5. Now is calculating the fidelity of the last piece in Encoding 'twqubit\_C234790withPC\_Ufid.mat'. Will combine all of the pulses in Encoding and check again after this calculation.

The last piece 'twqubit\_C234790withPC\_Ufid.mat' has been checked. The fidelity is 0.9164.

## FEB 12, 2015

When combining all pulses into a large shape file, one has to know how to change a shape for X rotation to Y rotation. It should be a  $\pi/2$  phase difference for every segment in the shape. I am going to check it.

The checking uses 4-qubit Crotonic in the folder 'F:\matlab\pulseexam\_7qubit\4 qubit pulse check'. The target unitary is  $R_x^1(\pi/2)$ , and the pulse is 'Croton\_90x1.txt' with length 1ms, 500 segments and amplitude 6000Hz.

When compared with  $R_x^1(\pi/2)$ , the fidelity is 0.9996. Then I changed the target to  $R_y^1(\pi/2)$  with the GRAPE pulse unchanged. The fidelity goes to 0.4998 which is reasonable.

In order to produce a  $R_y^1(\pi/2)$  from the original X rotation pulse, I added 90 to all phases in all segments. However, the fidelity goes to almost 0. Again all phases are reduced by 90, and this time the fidelity is 0.9996, which is what we want!

Conclusion: If you want to realize a Y rotation based on a X rotation pulse, just change the phase to phase-90 in each segment, and mod by 360 for the spectrometer.

```
phase = phase - 90;
phase = mod(phase, 360);
```

I wrote a program 'grape\_phase' to generate the new phase in the folder 'F:\matlab\pulseexam\_7qubit\'. Used in this manner 'phase\_new = grape\_phase( phase, initial\_phase, end\_phase)', where the initial\_phase and end\_phase can be X, Y, -X, or -Y.

The way to get the new operator is through the equation  $R_z(\theta) = XR_y(\theta)\bar{X}$ . If you know the unitary  $U_x$  of the X rotation pulse, and when you are realizing Y pulse from that one, the new unitary  $U_y$  is thus

$$U_y = R_z(\pi/2)U_x R_z(-\pi/2); (1)$$

Generated the first encoding part, which will evolve Z7 to Z24567. The files 'twqubit\_encoding1\_C' and 'twqubit\_encoding1\_H' are in Ordi2 '\pulseexam\_12qubit'. The total length is 32.98ms. Next I have to check whether the final state after this pulse will be Z24567 or not. So 'check\_encoding.m' is written. The directory is Ordi2 '\pulseexam\_12qubit'. This function will load all necessary .mat files to get the unitaries and calculate the final state based on these unitaries from Z7.

The final fidelity is 0.9832 (the same for with or without gradient) for Z24567. Two files 'U\_encoding1.mat' and 'rho\_encoding1.mat'. Now go on to the second Encoding part.

The fidelity for the second Encoding part is -0.9692 (the same for with or without gradient) for Z1234567. Two files 'twqubit\_encoding2\_C' and 'twqubit\_encoding2\_H' are in Ordi2 '\pulseexam\_12qubit'. The total length is 21.29ms. Then the last piece in Encoding!

The fidelity for the third Encoding part is -0.9160 (the same for with or without gradient) for Z123456789101112. Two files 'twqubit\_encoding3\_C' and 'twqubit\_encoding3\_H' are in Ordi2 '\pulseexam\_12qubit'. The total length is 7.36ms.

**Update on Mar 04**: In the last code, the free evolution time is not the integer times of 10us, but it should be. So the function 'F.m' is modified as

```
function F=F(Hamiltonian, time)
F=diag(exp(diag(-i*Hamiltonian*10e-6*round(time/10e-6))),0);
```

And all the fidelities are recalculated. They are 0.9831 for Encoding 1, -0.9717 for Encoding 2, -0.9124 for Encoding 3.

# FEB 18, 2015

Running the two pulses. One is 'twqubit\_all90.m' which is used for phase cycling, and the other one is 'twqubit\_all90butC7.m' used for the polarization crush in the beginning. The fidelities are obtained!

	0	Fidelity		MaxPower C	MaxPower H
$R_x^{1-12}(\pi/2)$				27.8%, 6956.6Hz	
$R_x^{1-6,8-12}(\pi/2)$	1ms	0.9977	twqubit_all90butC7_Ufid.mat	24.5%, 6134.9Hz	25.0%, 6239Hz

# MAR 3, 2015

All 6 pulses in decoding have been checked.

	Length	Fidelity	File	MaxPower C	MaxPower H
$R_x^{2,3,4,7-12}(\pi)$	2ms	0.9988	twqubit_C2347andH180_Ufid.mat	61.6%, 15400Hz	52.2%, 13039Hz
$R_x^{1,3,4,6}(\pi/2)R_{-y}^{8-12}(\pi/2)$	1ms	0.9974	twqubit_C134690andH90_Ufid.mat	24.8%, 6203.2Hz	22.1%, 5529Hz
$R_x^{2,3,4,5,6}(\pi)$	2ms	0.9984	twqubit_C23456180_Ufid.mat	37.8%, 9438.2Hz	23.0%, 5746Hz
$R_{-y}^{4,6}R_y^{1,3}(\pi/2)R_x^2(\pi/2)R_{-z}^1(6.6\text{ms})$	1ms	0.9982	twqubit_C1234690withPC_Ufid.mat	28.3%, 7070.8Hz	26.9%, 6717Hz
$R_x^{2,7}(\pi)$	2ms	0.9979		29.1%, 7285.3Hz	
$R_y^2(\pi/2)R_x^5(\pi/2)$	1ms	0.9975	twqubit_C2Y5X90_Ufid.mat	28.9%, 7233.9Hz	29.2%, 7292Hz

#### MAR 4, 2015: RE-CHECK THE PPS CIRCUIT IN SIMULATION

I found the decoding part can be simplified. Check it in Matlab.

All the files are saved in Ordi2 '\twqubit\'. For the encoding which consists of three parts, the fidelities have been checked before.

TABLE I. Encoding in 12-qubit PPS

Target State	State Fidelity	Density Matrix	Unitary Operator
IZIZZZXIIIII	1.0000	rho_encoding1.mat	U_encoding1.mat
ZXZZZZIIIII	-1.0000	rho_encoding2.mat	U_encoding2.mat
ZZZZZZZZZZZ	-0.9500	rho_encoding3.mat	U_encoding3.mat

For the phase cycling it has been done too.

TABLE II. Phase Cycling in 12-qubit PPS

Target State	State Fidelity	Density Matrix	Unitary Operator
$ 000\rangle\langle 000  +  111\rangle\langle 111 $	0.9511	rho_phasecycling.mat	NAN

For the decoding part, the simulation is as follows.

TABLE III. Decoding in 12-qubit PPS

Target State	State Fidelity	Density Matrix	Unitary Operator
$A_1 A_5 A_6   +++-00000\rangle + A_1' A_5' A_6'   -++++00000\rangle$	0.8717	rho_decoding1.mat	U_decoding1.mat
$A_1 A_5 A_6 A_7   0 + 00 - 0 - 00000 \rangle + A_1' A_5' A_6' A_7'   0 - 00 + 0 + 00000 \rangle$	0.8570	rho_decoding2.mat	U_decoding2.mat
$A_1 A_5 A_6 A_7 A_5^{new}  000000 - 00000\rangle + A_1' A_5' A_6' A_7' A_5^{new'}  000000 + 00000\rangle$	0.8570	rho_decoding3.mat	U_decoding3.mat

 $A_1$ ,  $A_5$  and  $A_6$  are phases produced by the chemical shift evolutions of C1, C5 and C6 during  $1/2J_{C7H5}$ .  $A_7$  is the phase by the chemical shift evolution of C7 (**Note: C7 is x-iy so the phase is the conjugate**) during  $1/2J_{C2C3}$ , and the coupling evolutions between C7 and all protons.  $A_5^{new}$  is the phase of C5 again in  $1/2J_{27}$ , including the chemical shift evolution and coupling evolutions (J25 and J57 are switched off). So the phases are

$$\begin{split} A_{1} &= \cos(2\pi(\omega_{1} - O_{1})/2\mathsf{J}_{\mathsf{C7H5}}) - isin(2\pi(\omega_{1} - O_{1})/2\mathsf{J}_{\mathsf{C7H5}}), \\ A_{5} &= \cos(2\pi(\omega_{5} - O_{1})/2\mathsf{J}_{\mathsf{C7H5}}) - isin(2\pi(\omega_{5} - O_{1})/2\mathsf{J}_{\mathsf{C7H5}}), \\ A_{6} &= \cos(2\pi(\omega_{6} - O_{1})/2\mathsf{J}_{\mathsf{C7H5}}) - isin(2\pi(\omega_{6} - O_{1})/2\mathsf{J}_{\mathsf{C7H5}}), \\ A_{7} &= \cos(2\pi(\omega_{7} - O_{1})/2\mathsf{J}_{23}) + isin(2\pi(\omega_{7} - O_{1})/2\mathsf{J}_{23}) * \\ \prod_{k=8}^{12} (\cos(\pi\mathsf{J}_{7k}/\mathsf{J}_{23}) + isin(\pi\mathsf{J}_{7k}/\mathsf{J}_{23})), \\ A_{5}^{new} &= \cos(2\pi(\omega_{5} - O_{1})/2\mathsf{J}_{27}) + isin(2\pi(\omega_{5} - O_{1})/2\mathsf{J}_{27}) * \\ \prod_{k\neq 2,5,7} (\cos(\pi\mathsf{J}_{5k}/\mathsf{J}_{27}) + isin(\pi\mathsf{J}_{5k}/\mathsf{J}_{27})) \end{split}$$

When calculating the evolutions in the Decoding part, using the following equations (the evolution is 1/2J with two  $\pi$  pulses inserted in the middle. **Note: without**  $\pi$  **in the end**)

$$(X + iY) \otimes (X + iZ) \longrightarrow (X - iY) \otimes (I + Z),$$

$$(X - iY) \otimes (X + iZ) \longrightarrow (X + iY) \otimes (I - Z),$$

$$(X + iY) \otimes (X - iZ) \longrightarrow (X + iY) \otimes (I - Z),$$

$$(X - iY) \otimes (X - iZ) \longrightarrow (X + iY) \otimes (I + Z).$$

$$(3)$$

#### MAR 10, 2015: CHECK THE SIMULATED SPECTRA FOR THE 12 QUBIT PPS CIRCUIT

The final state 'rho\_decoding3.mat' includes a phase on C7. 'rho\_decoding3(1,33) = 0.1979 + 0.5728i', and I used a Z rotation  $R_z^7(\theta)$  to rotate it into X. The rotating angle  $\theta$  is 1.2381, and the element becomes 0.6060 after the rotation. Note 0.6060/0.7071 (the ideal value) = 0.8570 which is exactly the fidelity for the final state 'rho\_decoding3'. The new state is named 'rho\_12pps\_circuit', and is saved in Ordi2 '\twqubit\rho\_12pps\_circuit.mat'.

The simulation is implemented in Ordi2 '\NMR\Experiments\twqubit'. The main file is 'sim\_twqubit.m'.

Some settings:  $o1_C = 20696$ ,  $o1_H = 2894$ , td = 281684, swh = 30030.

The decoherence time is set in '\SRC\simulator\spectrumfast.m' and the value for C7 is chosen as 450ms.

- 1) For thermal, the spectrum file is saved in 'F:\matlab\_full\IQC\_simulation\PPS 12 qubit\sim\_thermal\_450ms.mat'.
- 2) For PPS of the circuit, copy 'rho\_12pps\_circuit.mat' to the folder '\SRC\simulator\' and change the function 'mkstate.m'. The spectrum file is saved in 'F:\matlab\_full\IQC\_simulation\PPS 12 qubit\sim\_pps\_obC7\_phasefixed.mat' (phase fixed means the final coherence is on X axis by applying a Z rotation).

The comparison (Note the PPS data should be divided by 24) is shown in the following Fig. 1.

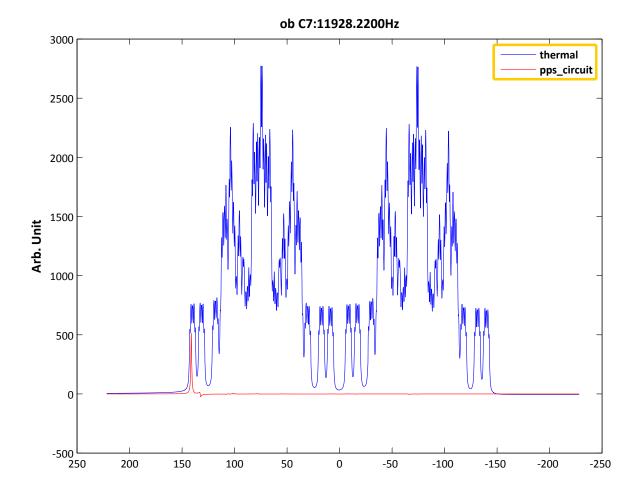


FIG. 1. Comparison of the thermal and PPS produced by the circuit.

#### MAR 10, 2015: CHECK THE SIMULATED SPECTRA FOR THE 12 QUBIT PPS GRAPE

The unitaries for all rotations have been saved in Ordi2. So I only combined them with the free evolutions. Note the time step is 10us, which means the free evolutions are integer times of 10us with the unwanted chemical shift refocusing (important!!!).

Evolution times for every part.

Encoding1:

Name	Total	$1/4J_{27}$	$1/4J_{67} - 1/4J_{27}$	$1/4J_{47} - 1/4J_{67}$	$1/4J_{57} - 1/4J_{47}$	$1/4J_{57}$
Encoding1	32.98ms	6670us	560us	1380us	2880us	11490us

Encoding2:

Name			$1/4J_{23} - 1/4J_{12}$	$1/4J_{23}$
Encoding2	21.28ms	4340us	3300us	7640us

Encoding3:

Name			
Encoding3	7.36ms	1680us	1680us

Decoding1:

	Total		
Decoding1	6.36ms	1680us	1680us

Decoding2:

Name			$1/4J_{23} - 1/4J_{12}$	$1/4J_{23}$
Decoding2	20.28ms	4340us	3300us	7640us

Decoding3:

	Total				
Decoding3	42.32ms	6670us	6670us	11490us	11490us

Updated on April 6: Please ignore the following sentences as Annie found a mistake in check\_grape.m. The unitary of the GRAPE pulse should be U(4us)\*Ugrape\*U(4us), but I wrote Ugrape\*U(8us) by mistake! This will introduce a serious phase error and trigger the following problem. I have fixed it. It is surprising that after applying phase cycling, the state will introduce a phase. The ideal state after phase cycling will have two elements 0.7071 at the top off-diagonal positions, but these two numbers change to 0.5018-0.4057i and 0.5018+0.4057i after GRAPE phase cycling pulse. The absolute value is 0.6453, which is reasonable. Moreover, the state in the decoding part will also involve an unexpected phase in every step. I guess the reason is the imperfections of the GRAPE pulses (some of them are pretty low like 80% fidelity), and the 90 or 180 pulse cannot rotate or refocus the state to the desired axis completely. Anyway, in the following table, I will write both fidelities, with and without this phase correction.

All fidelities  $tr(\rho_{ideal}\rho_{real})$  calculated by the circuit itself and by the GRAPE pulses.

Part	Length	Circuit Fidelity	GRAPE Fidelity
Encoding1	32.98ms	1.0000	0.9831
Encoding2	21.28ms	1.0000	0.9717
Encoding3	7.36ms	0.9500	0.9124
Phase Cycling	1ms	0.9511	0.9126
Decoding1	6.36ms	0.8717	0.8693
Decoding2	20.28ms	0.8570	0.8430
Decoding3	43.32ms	0.8570	0.8234

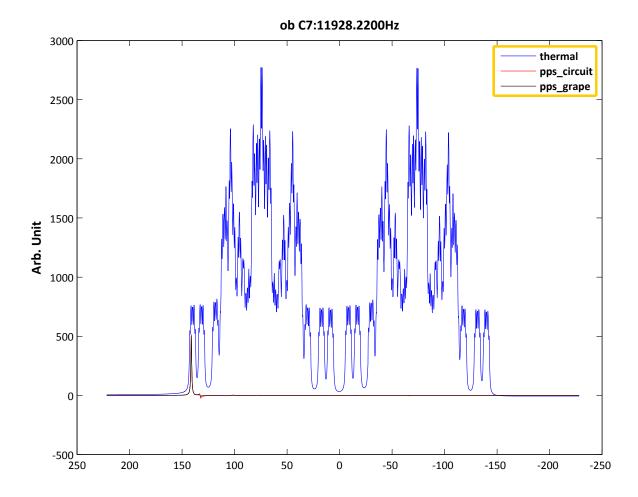


FIG. 2. Comparison of the thermal and PPS produced by the circuit and GRAPE.

## APR 16, 2015: 12-QUBIT CALIBRATION IN EXPERIMENT

The calibration is used for getting the dB of  $\pi/2$  and  $2\pi$  pulses for a fixed length. The au program is written by Annie, including 3 files 'calib.m', 'calibrate.m' and 'getspec.m'. First upload all the three files to Ordi2. Note 'calib.m' is for redirection and it should be in the root folder when opening Matlab in Ordi2. The path is thus '\d29lu\fixpulse\' because Matlab will go to this folder to show the last result of pulse fixing.

The calibration folder is 'twqubit\_calib'. Then select the experiment you want to calibrate, and run 'edau twqubit\_calib'. You have to edit Line 6 'host\_resultpath', Line 24 'TIMES' which means number of loops, the following 'p1', 'd1' and 'pl3', and the starting power. Then in 'calibrate.m', change the targetfolder, ob\_min, ob\_max and figure\_name.

The experiments for calibrating C is titled 'twqubit\_calib\_C', and for calibrating H is 'twqubit\_calib\_H'. For H, I calibrated through the C channel as in experiment we only observe the C channel. The way is to transfer the H signal to C via XZ terms, so I can only calibrate the  $\pi/2$  and  $3\pi/2$  pulses. The results are summarized in the following table

Rotation	Length	Frequency	Exp. No	dB (Apr 16)	dB (Apr 17)	dB (June 25)
C360	40us	25000Hz	11-23 (-3.5dB to -5.9dB)	-4.51dB	-4.38dB	-1.18dB
C360	80us	12500Hz	51-63 (3.0dB to 0.6dB)	1.82dB	1.74dB	
C90	20us	12500Hz	101-113 (3.0dB to 0.6dB)	_	1.00dB	
H270 (by C)	30us	25000Hz	XXXX	_	6.20dB	6.20dB
H360 (by H)	40us	25000Hz	XXXX	_	5.40dB	

Actually only C360 and H270 are usable. The two powers are -4.38dB and 6.2dB for 25KHz.

## APR 18, 2015: ALL PULSES TEST IN 12-QUBIT PPS EXPERIMENT

The folder is 'twqubit\_pps'. Exp 1 and 2 are thermal spectra.

For every pulse I have 4 observations. For C channel, for H channel, pulse-gradient-pulse for C channel, and pulse-gradient-pulse for H channel. Refer to the Appendix to see what the pulses are.

Polarization Crush 11-14: all90butC7

Phase Cycling 21-24: all 90

Encoding

101-104: C57180 105-108: C23180 109-112: C234790 113-116: C156180

117-120: C234790withPC

## Decoding

201-204: C2347andH180 205-208: C134690andH90 209-212: C23456180 213-216: C1234690withPC

217-220: C27180 221-224: C2Y5X90

Single  $\pi/2$  rotations

301-314: C1 to C7 90 rotation (two experiments for one pulse)

Single  $\pi/2$  rotations

315-342: C1 to C7 180 rotation (four experiments for one pulse)

## APR 23, 2015: 12-QUBIT PPS EXPERIMENT

Exp 1000: zg for the thermal without H decoupled

Exp 1001: observe C7 after crushing all the other 6 carbons and a gradient

Exp 1002: the same as 1001 but decoupled H before observing C7

Exp 1003: Encoding 1. observe C7 and decouple H. Almost the same as the 7-qubit experiment.

Exp 1004: Encoding 2. observe C7 and decouple H. Almost the same as the 7-qubit experiment.

Exp 1005: PPS, gradient and observe C7 but no signal...

Exp 1006: PPS, without gradient and observe C7, no signal either...

There is a problem when I calculated the GRAPE. There is a default 4us pre-delay and post-delay on the target unitary, as in experiment when applying the GRAPE pulse these two delays are required (not the minimal value but since GRAPE has considered that it has no effect). However, we do not have enough slots (only SP0 to SP31) for GRAPE pulses so we have to combine them to a big shape. The problem is the time step in the big shape is chosen as 10us, which cannot absorb the 4us delay. If we get rid of the 4us delays during the big shape, the experimental result is totally different.

I tried to use 2us time step size in the big shape instead of 10us, so I can write the 4us delay. Then for every 5 steps (2us\*5=10us) the amplitude and the phase should be the same. In principal it is fine, but when I am fixing the pulse on the H channel, the random noise is so serious that we have to use a low-pass filter to remove the noise. As in the big shape the shape is not smooth any more, some wanted points will be removed by the filter too. I guess no way to solve this except the pulse is smooth.

So maybe need recalculation with Ous pre-delay and post-delay.

#### MAY 9, 2015: RECALCULATION OF GRAPE PULSES WITH OUS BUFFER

According to the fact that 4us cannot be absorbed into a 10us shape pulse, I decided to delete the buffer delay in the GRAPE calculation. An AU program called 'GRAPE\_recal\_nobuffer.m' was written to do it. The directory in Ordi2 is '\pulseexam\_12qubit\C\_rotations\GRAPE\_nobuffer\' or in the SVN '\Matlab\Twqubit\Pulse\_NoBuffer\'.

There are 18 pulses required for recalculation with 8  $\pi/2$  rotations and 10  $\pi$  rotations. In the program, I first regenerate Bx and By from the shaped pulses, and use them as the initial guess, saved in files titled like 'twqubit\_C190\_InitialGuess.mat'. Then generate the params setting file with 0us buffer. **Note the power limit of C channel is set as 12.5KHz instead of 25KHz.** Both the initial guess file and params setting file are transferred to Feynman and Ordi2 by the scp command. A cluster sample is also written and saved in Ordi2 pulsefinder folder.

In calculation on Feynman in the weekend. All the 18 pulses

```
Pulse_Name{1} = 'twqubit_C790';
1
   Pulse_Name{2} = 'twqubit_C290';
3
   Pulse_Name{3} = 'twqubit_C234790';
   Pulse_Name{4} = 'twqubit_C234790withPC';
   Pulse_Name{5} = 'twqubit_C134690andH90';
5
   Pulse_Name{6} = 'twqubit_C1234690withPC';
7
   Pulse_Name{7} = 'twqubit_C2Y5X90';
8
   Pulse_Name{8} = 'twqubit_C590';
9
   Pulse_Name{9} = 'twqubit_C2180';
   Pulse_Name{10} = 'twqubit_C6180';
10
   Pulse_Name{11} = 'twqubit_C4180';
11
   Pulse_Name{12} = 'twqubit_C57180';
12
   Pulse_Name{13} = 'twqubit_C1180';
13
14
   Pulse_Name{14} = 'twqubit_C23180';
   Pulse_Name{15} = 'twqubit_C156180';
15
16
   Pulse_Name{16} = 'twqubit_C2347andH180';
17
   Pulse_Name {17} = 'twqubit_C23456180';
18 | Pulse_Name{18} = 'twqubit_C27180';
```

## MAY 11, 2015: NO BUFFER GRAPE PULSES

Got almost all pulses with fidelity over 0.995. The exception is pulse Number 10, C6180. The reason should be the power limit 12.5KHz is not enough. So change it to 25KHz again and recalculate this GRAPE. All the GRAPE .mat files are transferred to '\Matlab\Twqubit\Pulse\_NoBuffer\'.

An AU program 'make\_shape\_12qubit.m' for making the Bruker shape is used to generate all Burker files. Then the maximal power is checked using 'check\_power\_NoBuffer.m'. The powers are almost the same as the ones from the initial guess, and are updated in the Appendix.

#### MAY 13, 2015: EXPERIMENTS WITH NO BUFFER PULSES

Tested in experiment with the new no-buffer GRAPE pulses. I can still get the 7 coherence by decoupling H channel. To my surprise, if I fixed all the pulses, the performance with the fixed ones is even worse. I guess the reason is when pulse fixing, the baseline is a little bit below 0 for the free evolution. It does not make sense to fix them but the fixing program is indeed trying to fix it. The solution might be fixing each pulse one by one, and then combine all of them with the 0 points for free evolution. It will be done soon.

Exp 1103: Ob Z24567 with H decoupling and non-fixed No Buffer pulses. Look good.

Exp 1104: Ob Z1234567 with H decoupling and non-fixed No Buffer pulses. Look good.

Exp 2103: Ob Z24567 with H decoupling and fixed No Buffer pulses. Worse than 1103, which is surprising.

Exp 2104: Ob Z1234567 with H decoupling and fixed No Buffer pulses. Worse than 1104, which is surprising.

For PPS, there is still no signal. See Exp 1999 and 2000. Exp 1999: PPS by non-fixed No Buffer pulses. No signal. Exp 2000: PPS by fixed No Buffer pulses. No signal.

I tried 'fp' with about 200 scans to get a signal after one phase cycling step, and 80 scans with 'efp' and 'LB=0.3Hz'. So I divided the PPS into 24 experiments, and 80 scans for each experiment. D1 = 60s, so the total time for trying a PPS now is 34 hours...

Note: Explanations to Exp 2103 and 2104. The No Buffer pulses after fixing are even worse because the fixing program has a problem. The pulses itself is a big shape, with tons of 0 points inside to realize free evolutions. However, the pickup coil will detect slight signals for those 0 points (slightly over or below 0). The fixing program tries to correct these points by modifying these 0 to non-zero, which is not reasonable. One way to solve this problem is by fixing all pulses individually and combine them at last. So I fixed all the 18 pulses either 1ms or 2ms, and then used programs called 'pulse\_combine\_encoding\_nobuffer\_fixed.m' and 'pulse\_combine\_decoding\_nobuffer\_fixed.m' in '\Twqubit\Pulses\_NoBuffer\' to combine all of them with 0 points.

Unfortunately the result is not good. It turns out that the signal is still very low with 80 scans. So maybe improve the number of scans can help a little bit.

## MAY 22, 2015: RE-RUN PPS WITH SCAN=200

As there are three days that we will go to Ray's cottage, I set 200 scans for each phase cycling and the total length is thus 3d10hrs. I used a MAC program to automatically set all 24 experimental parameters. The Matlab program to generate this MAC file is 'Genmultizg.m' in '\Twqubit\'. Put the generated file to '\lists\mac\'. The 24 experiments are from Exp 2001 to Exp 2024.

Unfortunately there is no FID after the multizg. I tried some of the 24 experiments and they cannot do fp or efp. Need to figure out why. Another problem is during a long multizg, the sample will unlock at some time. Xinhua said the reason is gradient field. Because the gradient field is applied in z direction, it will affect the locking signal. But we cannot avoid the many gradient fields in between. Try experiment one by one? Anyway, do simulation now. That is, getting the simulated spectrum of each phase cycling, and then compare.

Re-run the 24 experiments again and now they have spectrum. Almost all 0. The sum is not a single peak. Meanwhile, the simulation is done. The folder is '\Twqubit\_Circuit\_PPS\'. First I ran 'rho\_phasecycling\_24steps.m' to get all MAT files of the 24 states, with each one corresponding to a phase cycling step. Then upload all the 24 MAT files to Ordi2 where the 'mkstate.m' function is. Run 'sim\_12pps\_step.m' in '\NMR\EXPERIMENTS\twqubit' to get all the simulated results and transfer them to my laptop. Plot all the 24 figures with the name such as '24\_step\_7.fig' for each one. Every spectrum out of the 24 figures is oscillating seriously which means if the T2\* is not long enough (the case in experiment), we cannot resolve it.

#### JUNE 09, 2015: WRITE A UNIVERSAL PROGRAM FOR SPECTRUM SIMULATION

## Fast spectrum generating code spec\_plot.m in \subfunction

The previous way to simulate the NMR spectrum by giving the density matrix, Hamiltonian, T2\* is via Fourier transform. The code is written by Colm Ryan and it is powerful. However, for 12 qubits it takes more than 40 minutes to get a spectrum. So I write another program to simulate the spectrum. It is universal, and only takes less than 1 minute for a 12-qubit simulation.

The function is 'spec\_plot.m' saved in the '\subfunction' folder. There are four input parameters: Hamiltonian, density matrix, observed spins and T2\*. By giving the Hamiltonian, we can know the frequencies of all possible peaks. For example, in the 12-qubit sample we would like to observe C7. There should be  $2^{11}$  peaks as 11 spins have interactions with C7. The central frequency is  $\omega(7)$ , which is the chemical shift of C7. So the frequency of all peaks would be

$$\omega(7) + \sum_{i=1, i \neq 7}^{12} \pm J_{i7}/2. \tag{4}$$

By the signs of J, we can also know the state of the other qubits. I define +J/2 is  $|0\rangle$  and -J/2 is  $|1\rangle$  to make the  $|00..0\rangle$  appear at the leftmost side in Bruker (highest frequency). After confirming the state of the other qubits, we can convert this state to decimal number, and then know the locations of it in the density matrix, because the density matrix can be understood through states (row 1 is  $|00..0\rangle$ , row 2 is  $|00..1\rangle$  etc.). The element in that position gives the real part and imaginary part of the related peak. Then a Lorentzian shape is plotted with this element as the amplitude and phase, and T2\* as the half-height width. Sum over all the  $2^{11}$  peaks will give the spectrum of C7. And if you want to save the figure and data points, just input a name after running the code. If you input 0, no data will be saved but the spectrum will be shown in a separate window.

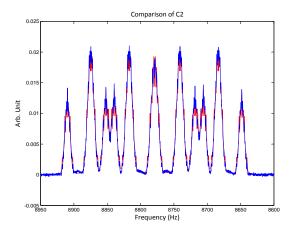
## C2 fitting code fitting\_C2.m in \Twqubit\_Circuit\_PPS\simulation

When I compared the thermal spectrum of C2 and experimental thermal, they do not match at the small J-couplings. This program is written to fit the small J-couplings of C2 by brutal force. I only need to fit the frequency 8900 to 8920 region as all small couplings are involved in it. There are 7 of them: C2C4, C2C5, C2C6, C2H1, C2H2, C2H3, and C2H5. Moreover, C2C4, C2C5, and C2C6 are fixed by the H-decoupled C spectrum. The second assumption is C2H2 and C2H3 have the same couplings to save time. The constraint is the width of this regions equals to the sum over all couplings, that is, only two variables then. C2H2 and C2H1.

The experimental spectrum is saved in 'thermal\_exp\_C\_200.mat' and the scaled factor is defined as the integral (sum) of the region [8900 8920]. There are 13 peaks in total and each peak corresponds to an intensity. In the fitting, we consider the 13 peak frequencies as the target function f, defined as the sum over square error of each peak. If this f is small then 1Hz which means the peak locations are pretty close, go to check the intensities of every peak. The definition of this value g is the same as f. When g is small, it means the peak intensities have the best fit as well as the locations are close too. The T2\*=310ms gives the best match. Refer to the original code for details and the output spectrum is shown below (plotted by 'compared\_C2.m').

Besides, C7 is also compared with T2\*=420ms. The figure plotted by 'compared\_C7.m' is shown below.

Now it is ready to go to check every experimental spectrum of C2 and C7. Indeed, we will just observe these two.





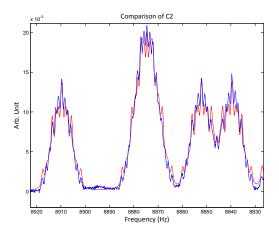


FIG. 4. Detailed comparison.

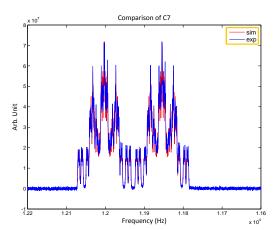


FIG. 5. Comparison of simulated and experimental  ${\bf C7}$  thermal.

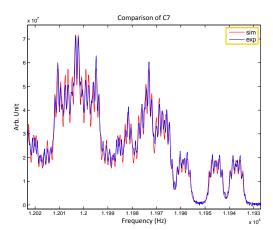


FIG. 6. Detailed comparison.

# JUNE 11, 2015 - AUGUST 17, 2015: IMPLEMENT EVERY ENCODING AND DECODING PART AND COMPARE WITH SIMULATION

Before experiments, I want to find the best setting for 12 qubits.

#### SWH = 30030Hz. DW = 16.65us.

SWH is a fixed value. DW is related to the sampling rate, and reciprocal (inversely proportional) to SWH.

## TD = 65536 and SI = 262144(max).

The real spectrum will have SI points. So if  $SI_iTD$ , it will cut the first SI points from TD when doing FFT. Otherwise, it will add the number of SI-TD points to the tail when doing FFT. Because SWH is very big, we need many many points to keep a high resolution. That is why SI is so big. Meanwhile, if TD is much smaller, we will use a lot of zero points added to the tail of TD, which means the noise is canceled a lot. Small TD gives us a good SNR, but it loses the resolution of small couplings. (For H-decoupled experiments, TD = 281684 for a high resolution.)

## AQ = 1.09s.

AQ is fixed as AQ = DW\*TD.

Then the experiments are (Spectra are shown too)

```
Exp 1398: Observe C7 by Gaussian with H decoupled. NS = 1. TD=281684.
```

Exp 1399: Observe C2 by Gaussian with H decoupled. NS = 1. TD=281684.

Exp 1401: Observe C7 by GRAPE as the reference. NS=10. See Fig. 7

Exp 1402: Observe C2 by GRAPE as the reference. NS=10. To my surprise the phase is different with 1401.

Exp 1403: Observe C7 after encoding1. NS=10. See Fig. 8

Exp 1404: Observe C2 after encoding1. NS=10.

Exp 1405: Observe C7 after encoding1 and decouple H. NS=1. See Fig. 9

Exp 1406: Observe C2 after encoding1 and decouple H. NS=1.

Exp 1407: Observe C7 after encoding2. NS=10. See Fig. 10

Exp 1408: Observe C2 after encoding2. NS=10.

Exp 1409: Observe C7 after encoding2 and decouple H. NS=1. See Fig. 11

Exp 1410: Observe C2 after encoding2 and decouple H. NS=1.

For encoding3 which generates ZZZZZZZZZZZZ, we tested that it cannot be observed. The H channel cannot be decoupled as the state of H is not I. So we directly applied encoding 3 to thermal state, and C-H couplings will evolve.

```
Exp 1411: Observe C7 after encoding3, applied on thermal. NS=1.
```

Exp 1412: Observe C2 after encoding3, applied on thermal. NS=1.

Exp 1413: Observe C3 after encoding3, applied on thermal. NS=1.

Exp 1414: Observe C4 after encoding3, applied on thermal. NS=1.

# AUGUST 12, 2015: CHECK TWO THINGS IN EXPERIMENT

#### APPENDIX I: USEFUL MATLAB CODES

The code to check all the 12-qubit GRAPE fidelities:

```
load Para.mat
 2
   load twpauliX_full.mat
 3
   load twpauliY_full.mat
4
   %% Check all 90 rotations
5
6
   for spin_number = 1:7
7
   Name1 = ['twqubit_C', num2str(spin_number), '90_C_25000.txt'];
8 Name2 = ['twqubit_C', num2str(spin_number), '90_H_25000.txt'];
9
   Amplitude = 25000;
10 | Time = 1e-3;
11 Length = 100;
12 dt = Time/Length;
13 | FirstLine = 19; % the first line which contains power and phase
14
15 | Output1 = 'test1';
16 Output2 = 'test2';
17
18 [power1, phase1] = dataout (Name1, Output1, FirstLine, Length);
19 [power2, phase2] = dataout (Name2, Output2, FirstLine, Length);
20 %% Check
21 \mid X_C = 0; Y_C = 0;
22 | for jj = 1:7
23
       X_C = X_C + KIx{jj};
24
       Y_C = Y_C + KIy{jj};
25
   end
26
27 \mid X_H = 0; Y_H = 0;
28
   for jj = 8:12
29
       X_H = X_H + KIx{jj};
30
       Y_H = Y_H + KIy{jj};
31 end
32
33 U = eye(2^12);
   U = U*expm(-i*H*4e-6);
35 | for ii = 1:Length
36
       Hext = 2*pi*(Amplitude*power1(ii)/100)*(X_C*cos(phase1(ii)/360*2*pi)-Y_C*sin
           (phase1(ii)/360*2*pi))+2*pi*(Amplitude*power2(ii)/100)*(X_H*cos(phase2(ii
           )/360*2*pi)-Y_H*sin(phase2(ii)/360*2*pi));
37
       U = \exp(-i*(Hext+H)*dt)*U;
38
   end
39
   U = U*expm(-i*H*4e-6);
40
   Utar = expm(-i*KIx{spin_number}*pi/2);
41
42
43
   Fidelity = abs(trace(U*Utar'))/2^12
44
45
   savefile = ['twqubit_C', num2str(spin_number), '90_Ufid.mat'];
46
   save (savefile, 'U', 'Fidelity');
47
48
   end
```

The code to combine GRAPE pulses into a big shape file:

```
%% From Z7 to Z24567
1
2
   step_27 = round(1/(4*Para(2,7))/dt);
   step_67_27 = round((1/(4*Para(6,7))-1/(4*Para(2,7)))/dt);
   step_47_67 = round((1/(4*Para(4,7))-1/(4*Para(6,7)))/dt);
4
5
   step_57_47 = round((1/(4*Para(5,7))-1/(4*Para(4,7)))/dt);
6
   step_{57} = round((1/(4*Para(5,7)))/dt);
7
8
   power_encoding1_C = [power_C790_C; zeros(step_27,1);power_C2180_C; zeros(
      step_67_27,1); power_C6180_C; zeros(step_47_67,1); power_C4180_C; zeros(
      step_57_47,1);...
9
                                      power_C5180_C; power_C7180_C; zeros(step_57,1)
                                          ; power_C790_C] * Calibration / Calibration_old;
   phase_encoding1_C = [phase_C790_C; zeros(step_27,1); phase_C2180_C; zeros(
10
      step_67_27,1); phase_C6180_C; zeros(step_47_67,1); phase_C4180_C; zeros(
      step_57_47,1);...
                                      phase_C5180_C; phase_C7180_C; zeros(step_57,1)
11
                                          ; mod((phase_C790_C+90),360)];
12
   power_encoding1_H = [power_H790_H; zeros(step_27,1);power_H2180_H; zeros(
      step_67_27,1); power_H6180_H; zeros(step_47_67,1); power_H4180_H; zeros(
      step_57_47,1);...
13
                                      power_H5180_H; power_H7180_H; zeros(step_57,1)
                                          ; power_H790_H] * Calibration/Calibration_old;
14
   phase_encoding1_H = [phase_H790_H; zeros(step_27,1); phase_H2180_H; zeros(
      step_67_27,1); phase_H6180_H; zeros(step_47_67,1); phase_H4180_H; zeros(
      step_57_47,1);...
15
                                      phase_H5180_H; phase_H7180_H; zeros(step_57,1)
                                          ; mod((phase_H790_H+90),360)];
16
17
   total_time_encoding1 = length(power_encoding1_C)*dt;
18
19
   outputfile = 'twqubit_encoding1_C';
20
   shpfile = fopen(outputfile,'w');
21
       fprintf(shpfile,'##TITLE= %s\n',outputfile);
22
       fprintf(shpfile,'##JCAMP-DX= 5.00 Bruker JCAMP library\n');
23
       fprintf(shpfile,'##DATA TYPE= Shape Data\n');
24
       fprintf(shpfile,'##ORIGIN= Dawei''s GRAPE Pulses \n');
25
       fprintf(shpfile,'##OWNER= Dawei\n');
26
       fprintf(shpfile,'##DATE= %s\n',date);
27
       time = clock;
28
       fprintf(shpfile,'##TIME= %d:%d\n',fix(time(4)),fix(time(5)));
29
       fprintf(shpfile,'##MINX= %7.6e\n',min(power_encoding1_C));
       fprintf(shpfile,'##MAXX= \%7.6e\n',max(power_encoding1_C));
30
31
       fprintf(shpfile,'##MINY= %7.6e\n',min(phase_encoding1_C));
32
       fprintf(shpfile,'##MAXY= %7.6e\n',max(phase_encoding1_C));
33
       fprintf(shpfile,'##$SHAPE_EXMODE= None\n');
       fprintf(shpfile,'##$SHAPE_TOTROT= %7.6e\n',90);
34
35
       fprintf(shpfile,'##$SHAPE_BWFAC= %7.6e\n',1);
36
       fprintf(shpfile, '##$SHAPE_INTEGFAC= %7.6e\n',1);
       fprintf(shpfile,'##$SHAPE_MODE= 1\n');
37
38
       fprintf(shpfile, '##PULSE_WIDTH= %d\n',total_time_encoding1);
39
       fprintf(shpfile, '##Calibration_Power= %d\n',Calibration);
40
       fprintf(shpfile,'##NPOINTS= %d\n',length(power_encoding1_C));
41
       fprintf(shpfile,'##XYPOINTS= (XY..XY)\n');
42
```

```
43 | for ii = 1:length(power_encoding1_C)
44
       fprintf(shpfile, ' %7.6e, %7.6e\n',power_encoding1_C(ii),phase_encoding1_C(
           ii));
45
   end
46
47
       fprintf(shpfile,'##END=\n');
48
49
   outputfile = 'twqubit_encoding1_H';
50
   shpfile = fopen(outputfile,'w');
51
       fprintf(shpfile,'##TITLE= %s\n',outputfile);
52
       fprintf(shpfile,'##JCAMP-DX= 5.00 Bruker JCAMP library\n');
53
       fprintf(shpfile,'##DATA TYPE= Shape Data\n');
54
       fprintf(shpfile, '##ORIGIN = Dawei''s GRAPE Pulses \n');
55
       fprintf(shpfile,'##OWNER= Dawei\n');
       fprintf(shpfile,'##DATE= %s\n',date);
56
57
       time = clock;
58
       fprintf(shpfile,'##TIME= %d:%d\n',fix(time(4)),fix(time(5)));
59
       fprintf(shpfile,'##MINX= %7.6e\n',min(power_encoding1_H));
60
       fprintf(shpfile,'##MAXX= \%7.6e\n',max(power_encoding1_H));
61
       fprintf(shpfile,'##MINY= %7.6e\n',min(phase_encoding1_H));
62
       fprintf(shpfile,'##MAXY= %7.6e\n',max(phase_encoding1_H));
63
       fprintf(shpfile,'##$SHAPE_EXMODE= None\n');
64
       fprintf(shpfile,'##$SHAPE_TOTROT= %7.6e\n',90);
65
       fprintf(shpfile,'##$SHAPE_BWFAC= %7.6e\n',1);
66
       fprintf(shpfile,'##$SHAPE_INTEGFAC= %7.6e\n',1);
67
       fprintf(shpfile,'##$SHAPE_MODE= 1\n');
68
       fprintf(shpfile, '##PULSE_WIDTH= %d\n',total_time_encoding1);
69
       fprintf(shpfile, '##Calibration_Power= %d\n',Calibration);
70
       fprintf(shpfile,'##NPOINTS= %d\n',length(power_encoding1_H));
71
       fprintf(shpfile,'##XYPOINTS= (XY..XY)\n');
72
73
   for ii = 1:length(power_encoding1_H)
       fprintf(shpfile, ' %7.6e, %7.6e\n',power_encoding1_H(ii),phase_encoding1_H(
74
           ii));
75
   end
76
77
       fprintf(shpfile,'##END=\n');
```

## APPENDIX II: IMPORTANT FIGURES AND EXPERIMENTAL SPECTRA

Exp 1401: Observe C7 by GRAPE as the reference. NS=10. Exp 1402: Observe C2 by GRAPE as the reference. NS=10.

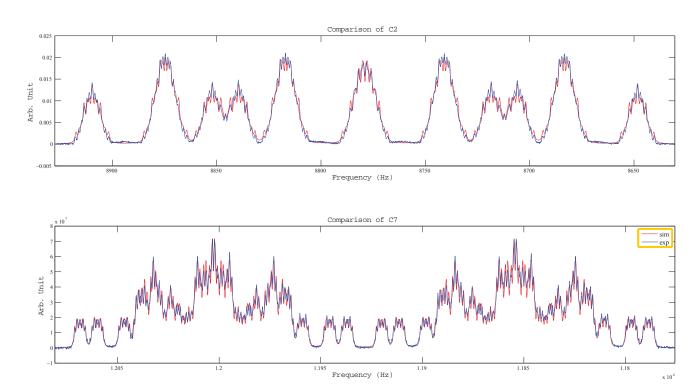


FIG. 7. Comparison of the thermal for C2 and C7. Blue is experiment and Red is the simulation by the fitted Hamiltonian.

Exp 1403: Observe C7 after encoding1. NS=10. Exp 1404: Observe C2 after encoding1. NS=10.

For C2 there is no signal because for Z24567 some couplings are close to 0 and the C2-H couplings broadens the peak. So for 12 qubits, these small couplings cannot be resolved.

For C7 it matches well with the simulation. However, the small couplings are annihilated due to the C7-H couplings too.

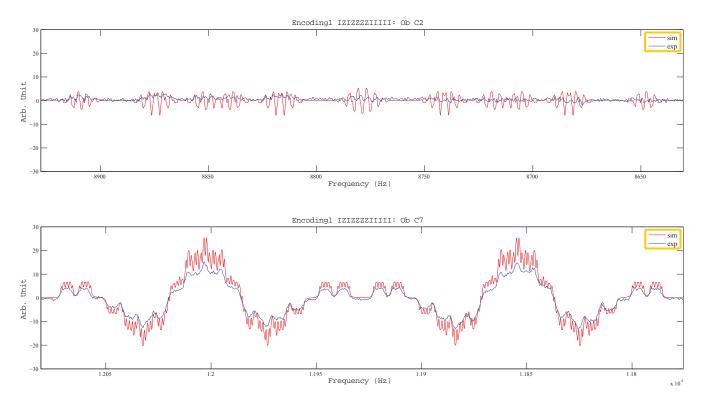


FIG. 8. Encoding 1 for C2 and C7 without H decoupled. 10 scans.

Exp 1405: Observe C7 after encoding1 and decouple H. NS=1.

Exp 1406: Observe C2 after encoding1 and decouple H. NS=1.

Note compare with undecoupled experiments, for decoupling experiments I just used  $1\ scan$ .

For C2 the signal is quite close to the 7-qubit case. Good.

For C7 the same.

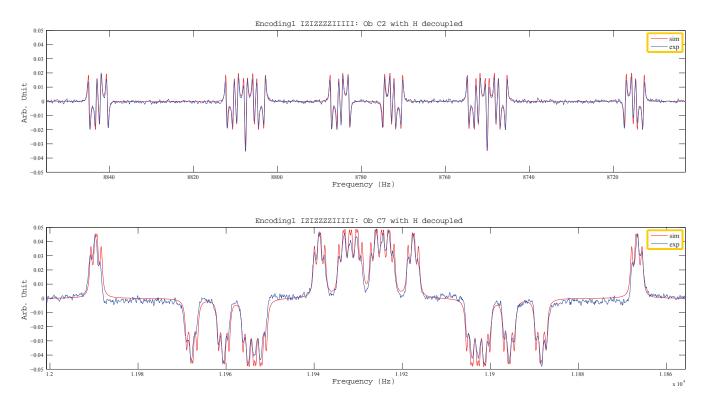


FIG. 9. Encoding 1 for C2 and C7 with H decoupled. 1 scan.

Exp 1407: Observe C7 after encoding 2. NS=10. Exp 1408: Observe C2 after encoding 2. NS=10.

For C2 and C7 there are no signals due to the broaden of the C-H couplings.

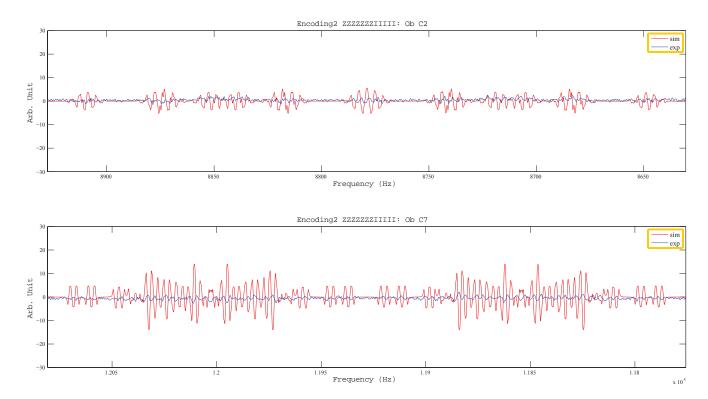


FIG. 10. Encoding 2 for C2 and C7 without H decoupled. 10 scans.

Exp 1409: Observe C7 after encoding2 and decouple H. NS=1.

Exp 1410: Observe C2 after encoding 2 and decouple H. NS=1.

Note compare with undecoupled experiments, for decoupling experiments I just used  $1\ \text{scan}$ .

For C2 and C7 they both look nice.

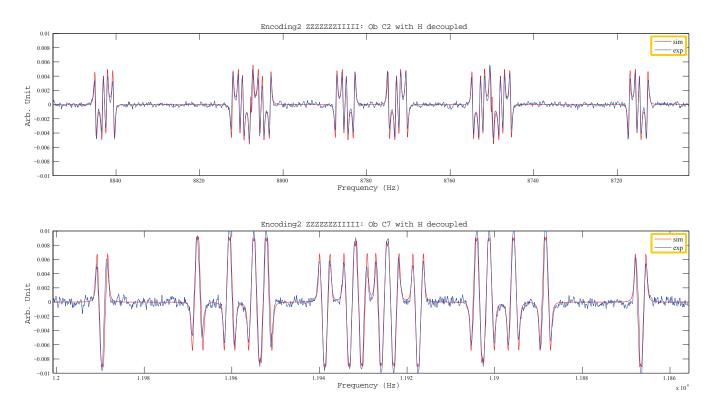


FIG. 11. Encoding 2 for C2 and C7 with H decoupled. 1 scan.

## **APPENDIX III: ALL PULSES FOR 12 QUBITS**

The saving folder is '\pulseexam\_12qubit\C\_rotations\'.

 $\pi/2$  and  $\pi$  rotations on every single spin.

Rotation	Length	Fidelity	File	MaxPower C	MaxPower H
$R_x^1(\pi/2)$	1ms	0.9981	twqubit_C190_Ufid.mat	56.0%, 14000Hz	22.3%, 5557Hz
$R_x^2(\pi/2)$	1ms	0.9986	twqubit_C290_Ufid.mat	41.7%, 10422Hz	23.5%, 5878Hz
$R_x^3(\pi/2)$	1ms	0.9981	twqubit_C390_Ufid.mat	31.9%, 7979.0Hz	22.3%, 5568Hz
$R_x^4(\pi/2)$	1ms	0.9976	twqubit_C490_Ufid.mat	31.6%, 7892.0Hz	23.8%, 5954Hz
$R_x^5(\pi/2)$	1ms	0.9981	twqubit_C590_Ufid.mat	56.1%, 14033Hz	30.7%, 7678Hz
$R_x^6(\pi/2)$	1ms	0.9979	twqubit_C690_Ufid.mat	57.3%, 14333Hz	34.4%, 8595Hz
$R_x^7(\pi/2)$	1ms	0.9986	twqubit_C790_Ufid.mat	43.7%, 10925Hz	24.8%, 6207Hz
$R_x^1(\pi)$	2ms	0.9976	twqubit_C1180_Ufid.mat	62.6%, 15655Hz	34.9%, 8726Hz
$R_x^2(\pi)$	2ms	0.9980	twqubit_C2180_Ufid.mat	51.1%, 12783Hz	32.4%, 8094Hz
$R_x^3(\pi)$	2ms	0.9975	twqubit_C3180_Ufid.mat	37.4%, 9350.0Hz	24.0%, 5997Hz
$R_x^4(\pi)$	2ms	0.9970	twqubit_C4180_Ufid.mat	45.1%, 11268Hz	20.4%, 5108Hz
$R_x^5(\pi)$	2ms	0.9975	twqubit_C5180_Ufid.mat	67.6%, 16895Hz	31.1%, 7782Hz
$R_x^6(\pi)$	2ms	0.9976	twqubit_C6180_Ufid.mat	71.8%, 17948Hz	33.6%, 8396Hz
$R_x^7(\pi)$	2ms	0.9977	twqubit_C7180_Ufid.mat	51.0%, 12759Hz	32.1%, 8022Hz

Pulses for the encoding part of PPS preparation.

Rotation	Length	Fidelity	File	MaxPower C	MaxPower H
$R_x^{5,7}(\pi)$	2ms	0.9980	twqubit_C57180_Ufid.mat	32.3%, 8072.5Hz	24.2%, 6049Hz
$R_x^{2,3}(\pi)$	2ms	0.9978	twqubit_C23180_Ufid.mat	32.4%, 8101.5Hz	22.8%, 5701Hz
$R_x^{2,3,4,7}(\pi/2)$	1ms	0.9970	twqubit_C234790_Ufid.mat	37.4%, 9358.3Hz	28.9%, 7213Hz
$R_x^{1,5,6}(\pi)$	2ms	0.9974	twqubit_C156180_Ufid.mat	32.2%, 8039.7Hz	20.3%, 5086Hz
$R_x^{2,4,7}(\pi/2)R_{-y}^3(\pi/2)R_{-z}^{i=2,3,4,7}((w_i-O_1)*3.36\text{ms})$	1ms	0.9964	twqubit_C234790withPC_Ufid.mat	26.1%, 6514.5Hz	20.2%, 5048Hz

Pulses for polarization crush and phase cycling.

		Fidelity		MaxPower C	MaxPower H
				27.8%, 6956.6Hz	
$R_x^{1-6,8-12}(\pi/2)$	1ms	0.9977	twqubit_all90butC7_Ufid.mat	24.5%, 6134.9Hz	25.0%, 6239Hz

Pulses for the decoding part of PPS preparation.

Rotation	Length	Fidelity	File	MaxPower C	MaxPower H
$R_x^{2,3,4,7-12}(\pi)$	2ms	0.9988	twqubit_C2347andH180_Ufid.mat	61.6%, 15400Hz	52.2%, 13039Hz
$R_x^{1,3,4,6}(\pi/2)R_{-y}^{8-12}(\pi/2)$	1ms	0.9974	twqubit_C134690andH90_Ufid.mat	24.8%, 6203.2Hz	22.1%, 5529Hz
$R_x^{2,3,4,5,6}(\pi)$	2ms	0.9984	twqubit_C23456180_Ufid.mat	37.8%, 9438.2Hz	23.0%, 5746Hz
$R_{-y}^{4,6}R_y^{1,3}(\pi/2)R_x^2(\pi/2)R_{-z}^1(6.6  ext{ms})$	1ms	0.9982	twqubit_C1234690withPC_Ufid.mat	28.3%, 7070.8Hz	26.9%, 6717Hz
$R_x^{2,7}(\pi)$	2ms	0.9979	twqubit_C27180_Ufid.mat	29.1%, 7285.3Hz	21.7%, 5414Hz
$R_y^2(\pi/2)R_x^5(\pi/2)$	1ms	0.9975	twqubit_C2Y5X90_Ufid.mat	28.9%, 7233.9Hz	29.2%, 7292Hz
$R_x^{8,9,10,11,12}(\pi/2)$	1ms	0.9982	twqubit_H90_Ufid.mat	45.6%, 11405Hz	27.5%, 6876Hz

All pulses in the saving folder ' $\pulsee xam_12qubit'$ '. The fidelities in the following table are state fidelities

Files	Length	Target State	State Fidelity
twqubit_encoding1_C, H	32.98ms	IZIZZZZIIIII	0.9831
twqubit_encoding2_C, H	21.28ms	ZZZZZZIIIII	0.9717
twqubit_encoding3_C, H	7.36 ms	ZZZZZZZZZZZZ	0.9124
twqubit_phasecycling_C, H	1 ms	$I_{+}^{\otimes 12} + I_{-}^{\otimes 12}$	0.9125
twqubit_decoding_C, H	68.96 ms	$ Z_7 \otimes  000000000000\rangle$	0.8234

# New Pulses with Ous Buffer Delay

Recalculated 18 pulses with Ous buffer. Here is the information.

Name	Length	MaxPower C	MaxPower H
C790	1ms	46.8%, 11697Hz	27.9%, 6965Hz
C290	1ms	37.8%, 9456Hz	25.8%, 6453Hz
C234790	1ms	39.1%, 9781Hz	29.1%, 7287Hz
C234790withPC	1ms	25.1%, 6286Hz	20.5%, 5130Hz
C134690andH90	1ms	27.2%, 6803Hz	30.3%, 7574Hz
C1234690withPC	1ms	28.9%, 7226Hz	27.3%, 6819Hz
C2Y5X90	1ms	30.5%, 7632Hz	28.8%, 7212Hz
C590	1ms	61.4%, 15348Hz	32.7%, 8171Hz
C2180	2ms	50.9%, 12722Hz	31.4%, 7859Hz
C6180	2ms	75.2%, 18790Hz	33.6%, 8392Hz
C4180	2ms	47.0%, 11760Hz	20.7%, 5173Hz
C57180	2ms	32.4%, 8093Hz	25.4%, 6361Hz
C1180	2ms	63.0%, 15747Hz	35.0%, 8744Hz
C23180	2ms	34.2%, 8540Hz	23.3%, 5827Hz
C156180	2ms	31.6%, 7899Hz	20.7%, 5183Hz
C2347180andH180	2ms	62.2%, 15555Hz	52.0%, 13011Hz
C23456180	2ms	38.0%, 9497Hz	23.2%, 5791Hz
C27180	2ms	28.7%, 7176Hz	21.5%, 5380Hz

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