

Pulsed Dynamic Nuclear Polarization: A Comprehensive Floquet Description

Data Collection**Author(s):**

Camenisch, Gian-Marco

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Description of the directories and files contained in this data collection:

G.M. Camenisch, 31.05.2024

All NMR data acquired with the Opencore NMR spectrometer were processed with the scripts located in folder **NMR_process**.

EPR data scripts require functions located in **Functions_EPR_process**.

Scripts used to calculate enhancement factors using operator-based Floquet theory as described in section 2.1 of the main text are located in folder **Numerical_Calculation_Operator_Based_Floquet**.

All data and scripts to generate figures of main text and SI are given in the corresponding folder e.g. all data/scripts for Fig. 4 in main text are contained in folder Fig_4

- Fig_4/Fig_S11/Fig_S12/Fig_S13:

Plotting Script: Paper_Offset_Plots

Experimental results for XiX (blue lines) are in Folder **XiX_exp**. Experimental results for FS-XiX are in folder **FS-XiX_exp**. Experimental raw data generated by Opencore spectrometer are contained in .opd, .opp, .sm2d, .sm2p and ExternalFPGA_Trig_XiX files. .opd file contained the solid echo spectra. Results of all different arrays corresponding to a different microwave frequency during field sweep and are stored in ProcessParameters_lorentz_cosine_square_array_xx.mat where xx is a number ranging from 1 to 561. Overall_Results_lorentz_cosine_square.mat contains experimental enhancements together with frequency sweep axis.

AWG data were saved in the following files:

- Fig_4: XiX_exp: 20220728_0712_dnp_XiX_offset_swp.mat
FS-XiX_exp: 20220729_1400_dnp_FS_XiX_offset_swp.mat
- Fig_S11: XiX_exp: 20220727_2029_dnp_XiX_offset_swp.mat
FS-XiX_exp: 20220727_2029_dnp_XiX_offset_swp
- Fig_S12: XiX_exp: 20220728_2111_dnp_XiX_offset_swp
FS-XiX_exp: 20220802_1357_dnp_FS_XiX_offset_swp
- Fig_S13: XiX_exp: 20220728_1344_dnp_XiX_offset_swp
FS-XiX_exp: 20220802_0726_dnp_FS_XiX_offset_swp

Folders **XiX_sim** and **FS-XiX_sim** contain the files and pdf picture for the calculation of the enhancement factors using operator-based Floquet theory (see section 2.1 in main text or folder **Numerical_Calculation_Operator_Based_Floquet**).

- Fig_6/Fig_S14:

Folder contains matlab script to generate figures Fig. 6 and Fig. S14. Files for enhancement calculated using operator-based Floquet theory are located in subfolder nu1_4.

- Fig_7:

Folder contains matlab script to generate figures Fig. 7. Files for enhancement calculated using operator-based Floquet theory are located in subfolder nu1_4. Experimental enhancements were taken from folder Fig_4/XiX_exp/Overall_Results_lorentz_cosine_square.mat

- Fig_8/Fig_S16/Fig_S17/Fig_S18:

Folder contains matlab script to generate figures Fig. 8, Fig. S16, Fig. S17 and Fig. S18. Files for enhancement calculated using operator-based Floquet theory are located in subfolder tp_15 for case using a constant Rabi frequency of 4 MHz but varying magnetic field and subfolder tp_5 for case where Rabi frequency scales linearly with the magnetic field (see section 3.2.3 for more details).

- Fig_S3:

Folder contains matlab script to generate figures Fig. S3. Matlab script runs only with functions contained in folder Functions_EPR_process. Experimental data are in file 20220725_0932_2pecho_ampswp.mat

- Fig_S4:

Folder contains matlab script to generate figures Fig. S4. Matlab script runs only with functions contained in folder Functions_EPR_process. Experimental data are in file 20220725_0945_2pecho_fs.mat

- Fig_S5:

Folder contains matlab script to generate figures Fig. S5. Matlab script runs only with functions contained in folder Functions_EPR_process. Experimental data are in file 20220725_1027_fstepnut.mat

- Fig_S6:

Folder contains matlab script to generate figures Fig. S6. Matlab script runs only with functions contained in folder Functions_EPR_process. Experimental data are in file 20220725_1136_ampstepnut.mat

- Fig_S7:

Folder contains data for Fig. S7. Experimental raw data generated by Opencore spectrometer are contained in .opd, .opp, .sm2d, .sm2p and Flip_angle files. .opd file contained the solid echo spectra. Results of all different arrays corresponding to a different amplitude on pulses on Opencore during amplitude sweep and are stored in ProcessParameters_lorentz_cosine_square_array_xx.mat where xx is a number ranging from 1 to 31. Overall_Results_lorentz_cosine_square.mat contains experimental enhancements together with amplitude sweep axis.

- Fig_S8:

Folder contains matlab script to generate figures Fig. S8. Matlab script runs only with functions contained in folder Functions_EPR_process. Experimental data are in file 20220725_1359_IRcycled_10shots.mat

- Fig_S9:

Folder contains matlab script to generate figures Fig. S8. Matlab script runs only with functions contained in folder Functions_EPR_process. Experimental data are in file 20220725_1548_2pecho_eseem.mat

- Fig_S10:

Folder contains data for Fig. S10. Experimental raw data generated by Opencore spectrometer are contained in .opd, .opp, .sm2d, .sm2p and SaturationRecovery files. .opd file contained the solid echo spectra. Results of all different arrays corresponding to a different delay in saturation recovery experiment and are stored in ProcessParameters_lorentz_cosine_square_array_xx.mat where xx is a number ranging from 1 to 12. Overall_Results_lorentz_cosine_square.mat contains experimental enhancements together with amplitude sweep axis.

- Fig_S15:

Folder contains matlab script to generate figures Fig. S15. Experimental DNP profile was taken from folder Fig_4/XiX_exp/Overall_Results_lorentz_cosine_square.mat

- Fig_S15:

Folder contains matlab script to generate figures Fig. S15. Experimental DNP profile was taken from folder Fig_4/XiX_exp/Overall_Results_lorentz_cosine_square.mat

- Fig_S19:

Folder contains matlab script to generate figures Fig. S19. Experimental DNP profile was taken from folder Fig_4/XiX_exp/Overall_Results_lorentz_cosine_square.mat