The β-NMR Quantum Annealing Connection

Syd Kreitzman, 03-11-2024, TRIUMF Quantum Strategy Workshop

Short Conclusion:

The utilization of β-NMR Adiabatic Spin Inversion /w Cross Polarization* is a powerful technique to probe and better understand Quantum Annealing. *(βRAIN-CP)

Longer Summary:

- The relevant Hamiltonian for the βRAIN-CP experiment in essentially identical to that used by the quantum annealing computation.
- Controls into the βRAIN spin Hamiltonian are plentiful & flexible.
- The "^{8}Li" polarization function is a measure of the evolution of the spin system into it ground/most-entangled energy/entropy state.
- Modern nano-scale material fabrication technologies will be increasingly able to tailor local nuclear environments to access new classes of relevant Hamiltonians.

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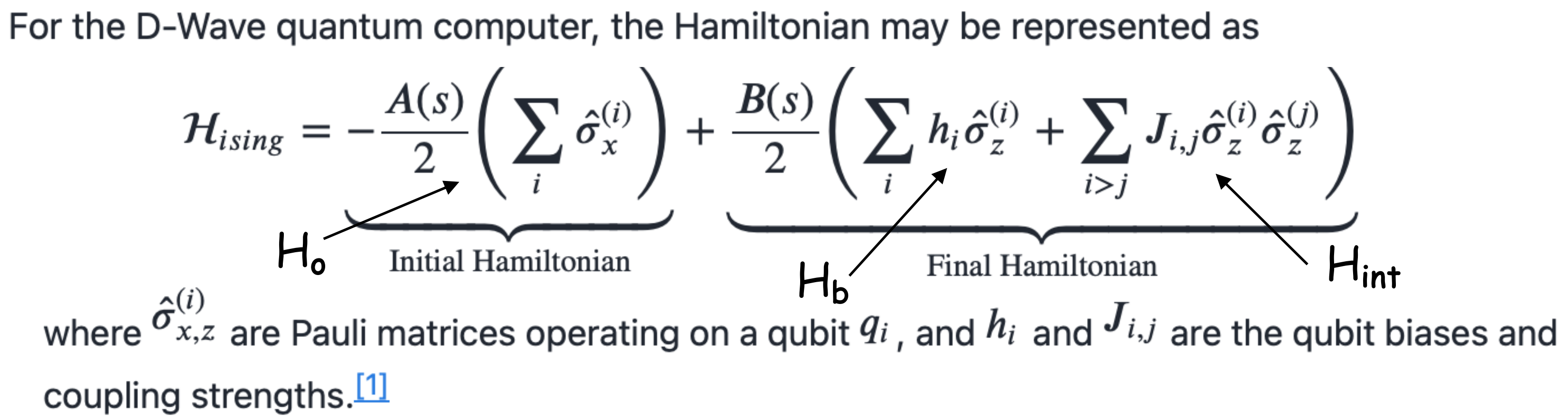
Principles of Quantum Annealing Computation (QAC). … from D-Pace

- map a “hard” optimization problem into:

  “find the ground state of an interacting spin-spin Hamiltonian H_{int}”
- set up a physical quantum spin system that can be “adiabatically” evolved from a know initial state /w initial Hamiltonian H_o into a ground state /w H_{int}.
- Ensure “bias” Hamiltonians H_b are present to adiabatically transform the lowest energy entangled states into a classical measurement.



For the D-Wave quantum computer, the Hamiltonian may be represented as

$$\mathcal{H}_{ising} = \underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2}\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}}$$

where $\hat{\sigma}_{x,z}^{(i)}$ are Pauli matrices operating on a qubit q_i, and h_i and $J_{i,j}$ are the qubit biases and coupling strengths.[1]

Usually A(s) = (1 – t/T), B(s)=t/T … i.e. Ho is reduced from 1 -> 0 as t goes from 0 -> T.
and the initial H_o does not commute with the final (H_b + H_{int})

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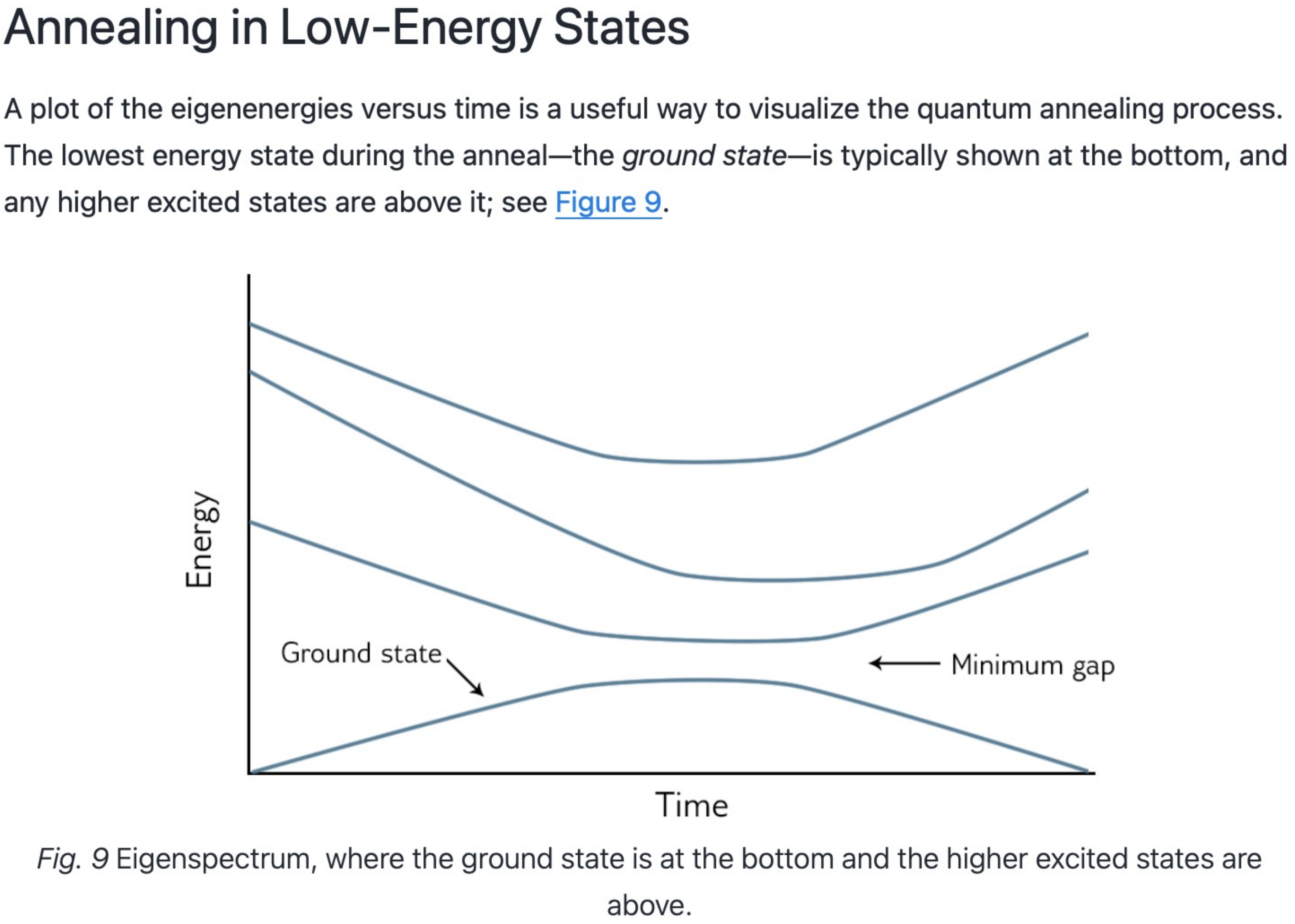


Annealing in Low-Energy States

A plot of the eigenenergies versus time is a useful way to visualize the quantum annealing process. The lowest energy state during the anneal—the *ground state*—is typically shown at the bottom, and any higher excited states are above it; see Figure 9.

Fig. 9 Eigenspectrum, where the ground state is at the bottom and the higher excited states are above.

β-NMR Adiabatic Spin Inversion: Lab Frame Hamiltonians

Lab Frame Hamiltonian:

Circularly polarized Radio Frequency Field
using raising/lowering ops

$$\mathcal{H}(t) = -\omega_\circ^S S^z - \frac{\omega_{rf}^S(t)}{2}[S^+ exp(-i(\omega_\circ^S t+\Delta\phi(t))) + S^- exp(i(\omega_\circ^S t+\Delta\phi(t)))] - \omega_\circ^I I^z$$

$$+ \omega_D[\mathbf{S}\cdot\mathbf{I} - 3(\mathbf{S}\cdot\hat{\mathbf{r}})(\mathbf{I}\cdot\hat{\mathbf{r}})] + \omega_Q[3(\mathbf{S}\cdot\hat{\mathbf{r}}_q)^2 - S(S+1) + \eta((\mathbf{S}\cdot\hat{\mathbf{r}}_{q\dagger})^2 - (\mathbf{S}\cdot\hat{\mathbf{r}}_{q\ddagger})^2)]$$

Neighboring I spin @ $\hat{\mathbf{r}}$

S spin principle quadrupolar axes @ $\hat{\mathbf{r}}_q$ $\hat{\mathbf{r}}_{q\dagger}$ $\hat{\mathbf{r}}_{q\ddagger}$

Assume the “high field case” : ω_o^S, ω_o^I >> ω_D + $|\omega_Q|$; dipole + quadrupole ->

$$+ \omega_D S^z I^z[1 - 3cos^2(\theta)] + \frac{\omega_Q}{2}(3cos^2(\theta) - 1)(3S_z^2 - S(S+1))$$

Define a frequency sweep over a bandwidth $\Delta\Omega$ linear in time during the pulse width t_P.

$$\Delta\omega(t) = \frac{d}{dt}\Delta\phi(t) = \frac{\Delta\Omega}{2}\left(1 - \frac{2t}{t_P}\right) \rightarrow \phi(t) = -\frac{\Delta\Omega}{8t_P}\left(1 - \frac{2t}{t_P}\right)^2$$

Go into doubly rotating frames aligned along the effective fields of the S and I spins respectively

β-NMR Double Resonance & Cross Polarization in the $S \otimes I$ rfs

Assume in the Lab frame an on-resonance rf field on the I-spins was also applied, ie

$$
\begin{aligned}
\mathcal{H}(t) =& -\omega_\circ^S S^z - \frac{\omega_{rf}^S(t)}{2}[S^+ exp(-i(\omega_\circ^S t+\Delta\phi(t))) + S^- exp(i(\omega_\circ^S t+\Delta\phi(t)))] \\
& - \omega_\circ^I I^z - \frac{\omega_{rf}^I}{2}[I^+ \exp(-i\omega_\circ^I t) + I^- \exp(i\omega_\circ^I t)] \\
& + \omega_D[\boldsymbol{S} \cdot \boldsymbol{I} - 3(\boldsymbol{S} \cdot \hat{\boldsymbol{r}})(\boldsymbol{I} \cdot \hat{\boldsymbol{r}})] + \omega_Q[3(\boldsymbol{S} \cdot \hat{\boldsymbol{r}}_{\boldsymbol{q}})^2 - S(S+1) + \eta((\boldsymbol{S} \cdot \hat{\boldsymbol{r}}_{\boldsymbol{q}\dagger})^2 - (\boldsymbol{S} \cdot \hat{\boldsymbol{r}}_{\boldsymbol{q}\ddagger})^2)]
\end{aligned}
$$

I spin rf term

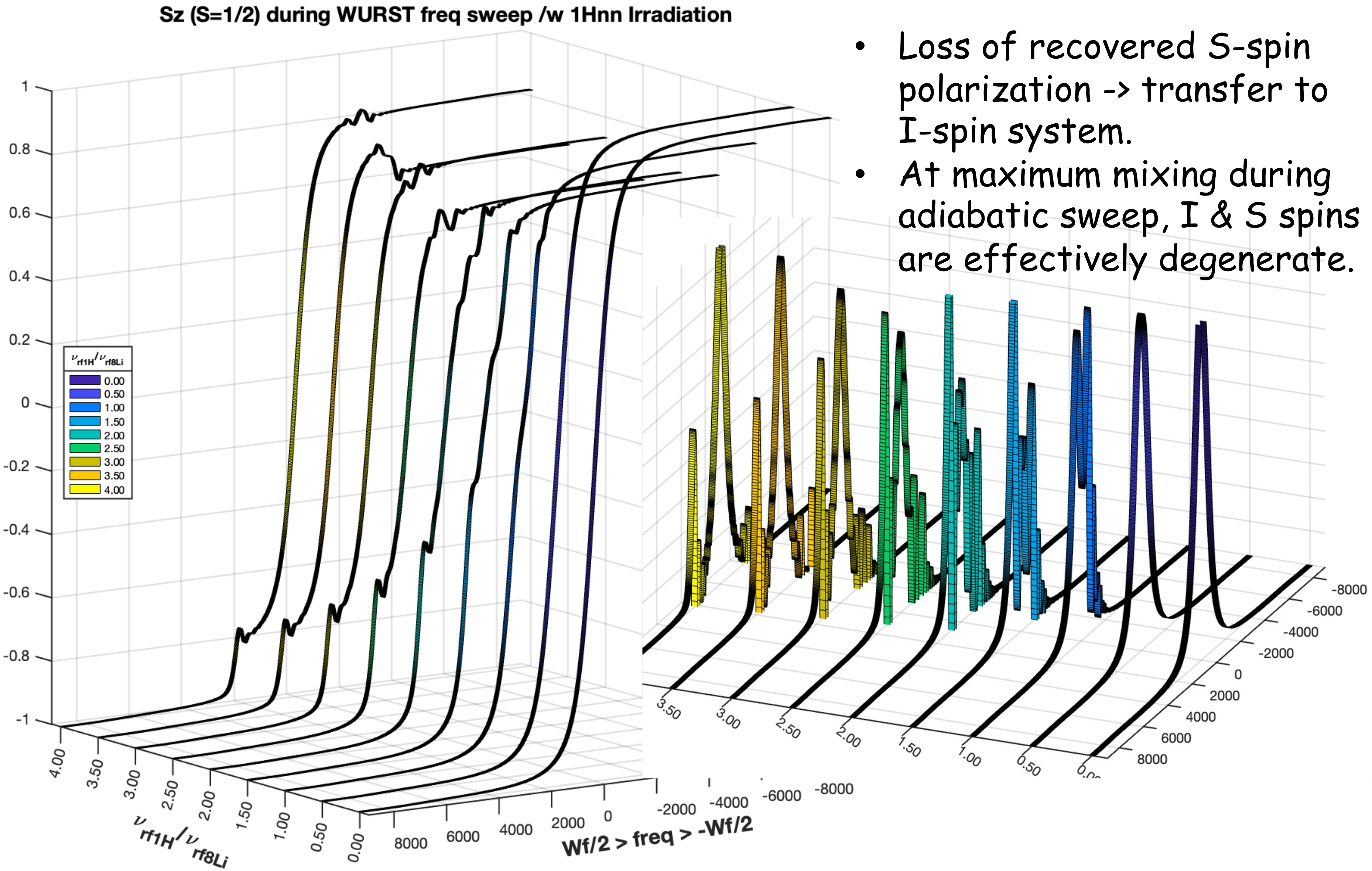
- Following the exact same procedure yields the $\mathcal{H}_m^{ef}$ with the term $-\omega_{rf}^I I^x$
- The I spin initial state is totally unpolarized,

  -> direction of quantization of these spins is arbitrary …
  and it is convenient then to switch I^x and I^z operators to give

$$
\boxed{\mathcal{H}_m^{ef}(t+t_0(\omega_Q, m, \theta)) = -\omega_{ef}^m(t) S_m^{z_{ef}} + \omega_D(\theta)(\cos(\Phi(t)) S_m^{z_{ef}} + \sin(\Phi(t)) S_m^{x_{ef}}) I^x - \omega_{rf}^I I^z}
$$

This effective Hamiltonian is in essence identical to the Quantum Annealing Hamiltonian

Spin ½ ⟨Sz⟩ and d/dt⟨Sz⟩ with I spin RF irrad



- Loss of recovered S-spin polarization -> transfer to I-spin system.
- At maximum mixing during adiabatic sweep, I & S spins are effectively degenerate.

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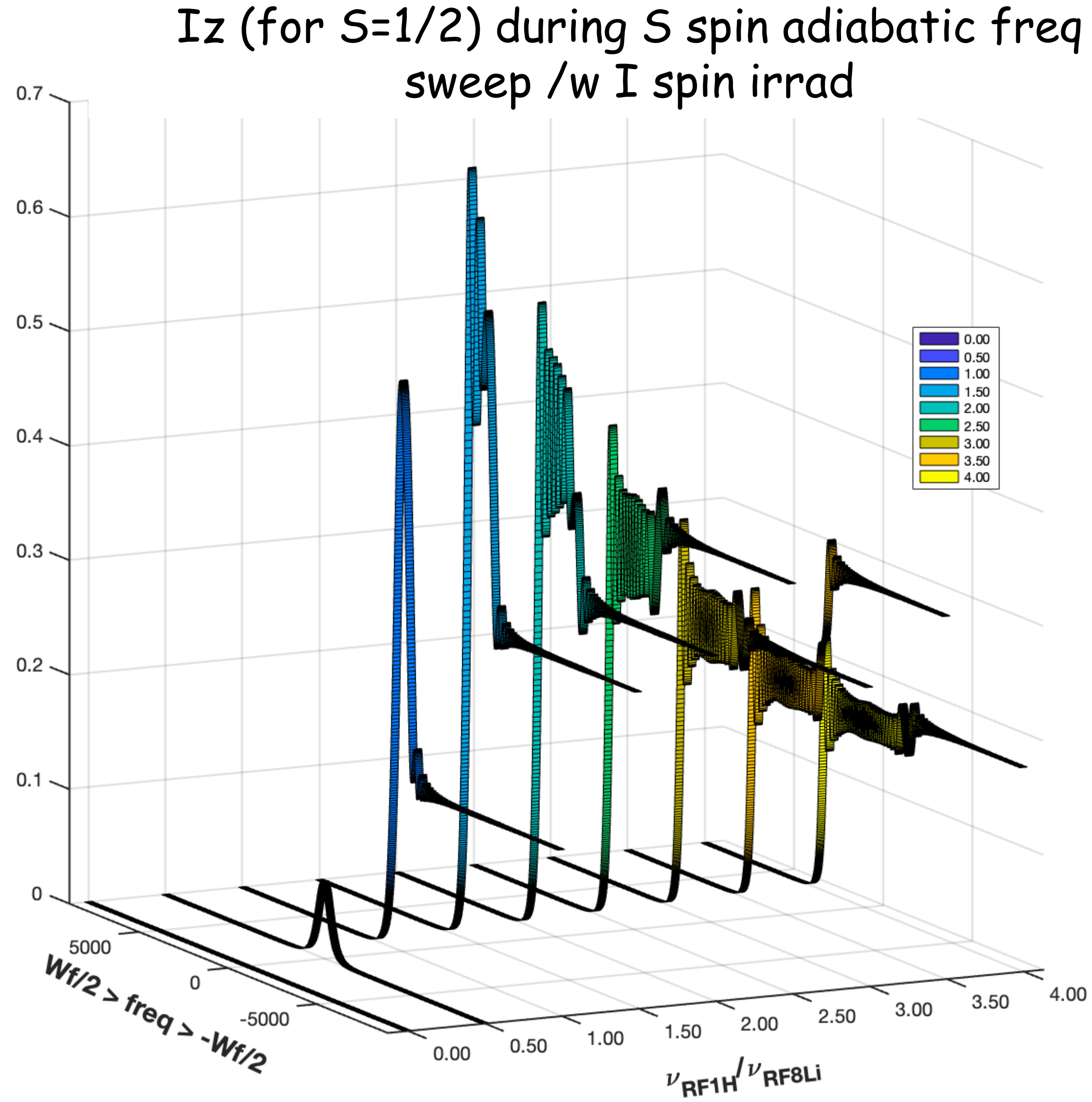
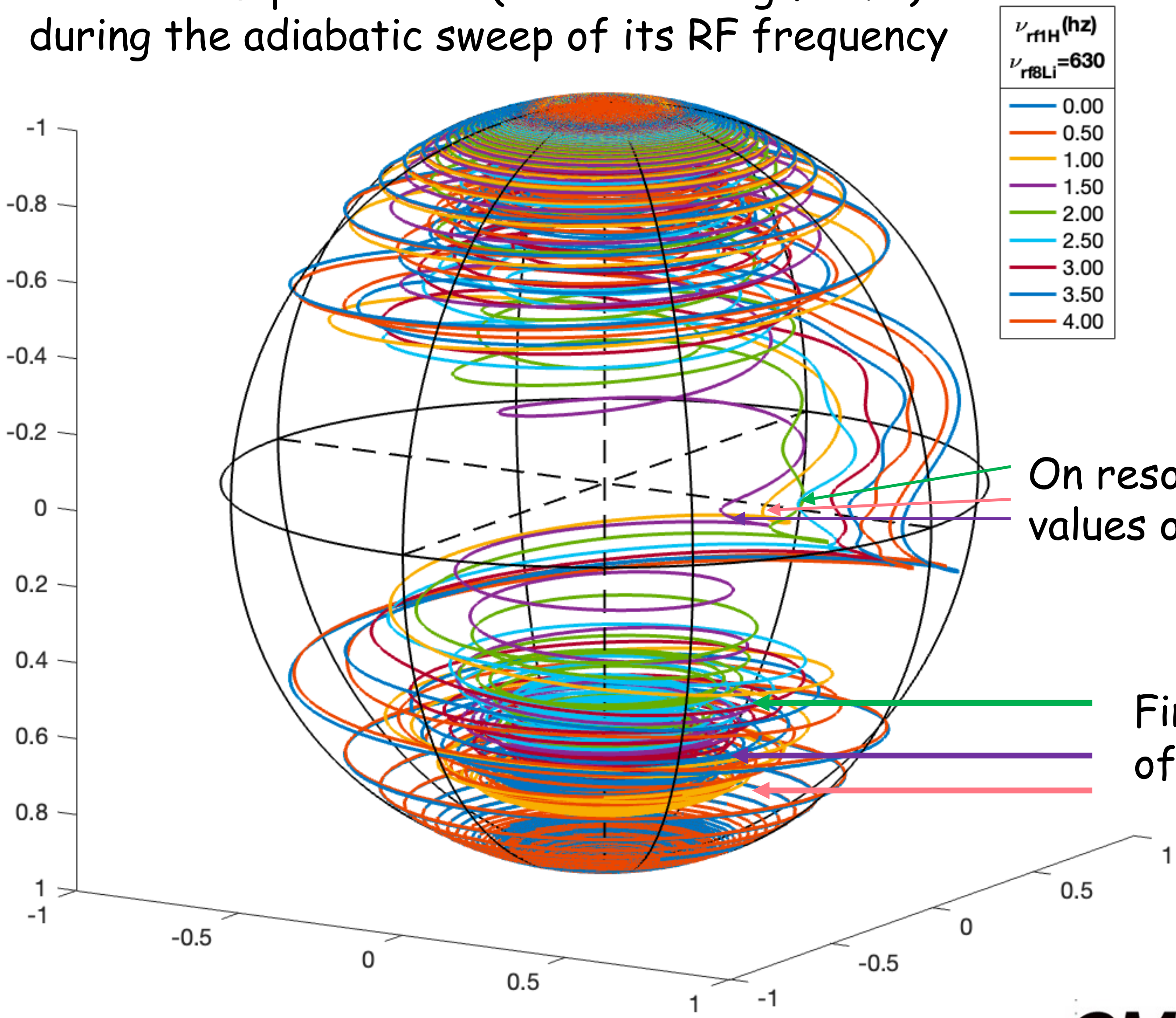
Spin ½ Cross-Polarization <Iz> term /w I Spin irrad



Spin ½ S-polarization evolution during adiabatic pulse /w I Spin irrad

S=1/2 3-D precession (in its rotating frame)
during the adiabatic sweep of its RF frequency



On resonance
values of <Sx>

Final values
of <Sz>

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Conclusion:

The β-NMR Adiabatic Inversion-Cross Polarization Experiment is a window into understanding Quantum Annealer dynamics

nb: The CMMS group will meet with D-Wave at TRIUMF on May 10, to further our mutual understanding.

Thank You !

Merci !

Grazie !

Vielen Dank !

ありがとうございました！

धन्यवाद !

감사합니다 !

Дякую !

Tack !

Bedankt !