QUANTUM CONTROL AND COMPUTING

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SC 694: Seminar

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SysCon iitb
Systems & Control

PRESENTATION OUTLINE

INTRODUCTION TO NMR SPECTROSCOPY

WHAT IS NMR?

- Nuclear Magnetic Resonance (NMR) Spectroscopy is a powerful analytical technique.
- It exploits the magnetic properties of certain atomic nuclei (those with non-zero spin, like ^{1}H, ^{13}C, ^{15}N, ^{31}P).
- It probes the local electronic environment around these nuclei.
- Essentially, it listens to how nuclei respond when placed in a strong magnetic field and perturbed by radio-frequency waves.

INTRODUCTION TO NMR SPECTROSCOPY

WHY IS IT IMPORTANT?

- **Structure Determination:** Unparalleled ability to determine the 3D structure of molecules (from small organics to large proteins).
- **Chemical Analysis:** Identifies and quantifies components in a mixture.
- **Dynamics:** Studies molecular motion and interactions.
- **Medical Imaging:** The basis for Magnetic Resonance Imaging (MRI).
- **Materials Science:** Characterises materials at the molecular level.
- **Quantum Information Processing:** A testbed for implementing quantum algorithms.

THEORY BEHIND NMR

NUCLEAR SPIN AND MAGNETIC MOMENT

- Nuclei with an odd number of protons or neutrons possess a quantum mechanical property called spin (I).
- Spinning charged particles generate a magnetic dipole moment (μ). Think of these nuclei as tiny bar magnets.
- Normally, nuclear magnetic moments are randomly oriented.
- When placed in a strong, static external magnetic field (B_0, typically along the z-axis), these moments align either with (lower energy, α state or $|0\rangle$) or against (higher energy, β state or $|1\rangle$) the field.
- For spin $I = 1/2$ nuclei (like ^1H), there are $2I + 1 = 2$ possible orientations. These form the basis for qubits.

THEORY BEHIND NMR

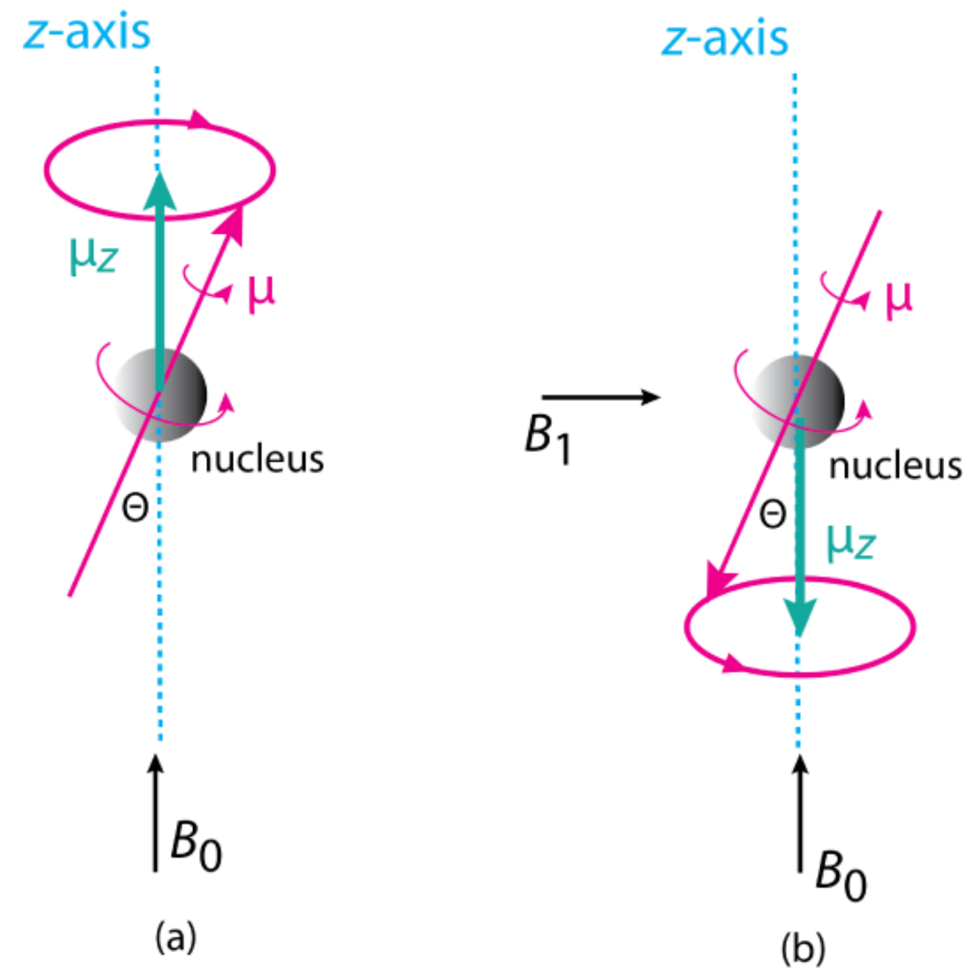
NUCLEAR SPIN AND MAGNETIC MOMENT

- The magnetic moments don't just align; they precess around the axis, like a spinning top tilted in Earth's gravity.
- The frequency of this precession is the **Larmor Frequency (ω_0).**

$$\omega_0 = -\gamma B$$

γ is the **gyromagnetic ratio** (a constant specific to each nucleus type).

- This frequency is directly proportional to the magnetic field strength.



THEORY BEHIND NMR

RESONANCE CONDITION AND RF PULSES

- To manipulate or detect spins, we need to disturb the equilibrium.
- This is done by applying a second, weaker, oscillating magnetic field (B_1) perpendicular to B_0 (e.g., along the x-axis).
- This B_1 field is generated by a **radio-frequency (RF) pulse**.
- **Resonance** occurs when the frequency of the RF pulse matches the Larmor frequency ($\omega_{RF} = \omega_0$) of a specific nucleus.
- At resonance, energy is absorbed, causing **transitions** between the spin states ($|0\rangle \leftrightarrow |1\rangle$). This allows coherent manipulation of the quantum state (e.g., creating superpositions).
- After the RF pulse (B_1) is turned off, the system returns to equilibrium and loses quantum coherence.

THEORY BEHIND NMR

ROTATING FRAME OF REFERENCE

- Analyzing the motion is simpler in a **rotating frame** that rotates around the z-axis at or near the Larmor frequency ($\omega_{rot} \approx \omega_0$).
- In this frame, the strong B_0 effect is largely cancelled out, and the B_1 field appears static.
- The net **magnetisation vector (M)** or the quantum state vector precesses around the effective field in the rotating frame (which is primarily B_1 during the pulse, if on resonance).

THEORY BEHIND NMR

BLOCH EQUATIONS

- A phenomenological description of the behaviour of the net magnetisation vector ($M = (M_x, M_y, M_z)$) under the influence of magnetic fields and relaxation. Useful for **ensemble behaviour.**
- In the rotating frame:

$$dM_x/dt = \Delta\omega M_y - M_x/T_2 + \gamma(M \times B_{eff})_x$$
$$dM_y/dt = \Delta\omega M_x - M_y/T_2 + \gamma(M \times B_{eff})_y$$
$$dM_z/dt = -(M_z - M_0)/T_1 + \gamma(M \times B_{eff})_z$$

Where:

$\Delta\omega = \omega_0 - \omega_{rot}$ (offset frequency)
B_{eff} includes B_1 and offset effects.
M_0 is the equilibrium magnetization (along z).
T_1 and T_2 are relaxation time constants.

NMR AND QUANTUM COMPUTING

QUBITS IN NMR

- **Qubits:** The fundamental unit of quantum information. In NMR, qubits are typically represented by the spin states ($|0\rangle$ and $|1\rangle$) of spin-1/2 nuclei (e.g., ^{1}H, ^{13}C, ^{19}F, ^{31}P) within a molecule dissolved in a solvent.
- **Multi-Qubit Systems:** A single molecule containing multiple, distinct spin-1/2 nuclei acts as a small quantum register. For example, Chloroform ($^{13}CHCl_3$) can be a 2-qubit system (^{1}H and ^{13}C).
- **Addressability:** Different nuclear types (γ) or nuclei in different chemical environments (chemical shift δ) have distinct Larmor frequencies, allowing them to be targeted individually by frequency-selective RF pulses.

NMR AND QUANTUM COMPUTING

CHEMICAL SHIFT AND J-COUPLING

- Nuclei in different chemical environments experience slightly different local magnetic fields due to shielding by surrounding electrons. $B_{local} = B_0(1 - \sigma)$ where σ is the shielding constant. This causes slight variations in their Larmor frequencies: $\omega = \gamma B_0(1 - \sigma)$.
- **Crucial for Quantum Computing:** Allows different nuclei in the same molecule to be addressed individually by RF pulses tuned to their specific resonance frequencies. Each chemically distinct nucleus can serve as a separate qubit.
- The spin state of one nucleus influences the magnetic field experienced by a nearby nucleus through bonding electrons. This leads to splitting of NMR signals into multiplets.
- **Crucial for Quantum Computing:** Provides a natural mechanism for implementing two-qubit gates (like CNOT). The evolution under the J-coupling Hamiltonian for a specific duration allows the state of one qubit to affect the state of another.

ITERATIVE PHASE OPTIMISATION

BROADBAND EXCITATION/INVERSION

- Modern NMR often deals with wide ranges of chemical shifts (e.g., $_{13}$C).
- High magnetic fields exacerbate this spread ($\Delta\nu$ in Hz scales with B_0).
- A simple rectangular RF pulse (*sinc* profile in frequency domain) might not excite or invert spins uniformly across the entire required bandwidth.
- Spins far from the carrier frequency (offset, $\Delta\omega$) experience a different effective field and flip angle.
- **Challenge:** Design RF pulses that achieve a desired effect (e.g., 90° excitation, 180° inversion) uniformly over a large range of frequencies ($\Delta\omega$) using limited RF power (B_1 amplitude).

ITERATIVE PHASE OPTIMISATION

TOPS APPROACH

- TOPS is i**t**erative **op**timisation of pha**s**es. In this approach, the pulse sequence is represented as a sequence of small flip angle pulses with varying phases. The phases are sequentially updated maximising the overlap between initial and target magnetisation over desired bandwidth until a desired fidelity is obtained.
- Method:
  - 1. Start with an initial guess for the phases (e.g., all zero).
  - 2. Iteratively adjust the phase of each segment one by one (sequentially).
  - 3. In each step, choose the phase for the current segment (k) that maximises the performance (fidelity) of the entire pulse sequence.
  - 4. Repeat the sweeps through all phases until convergence.

ITERATIVE PHASE OPTIMISATION

TOPS APPROACH

- We start with the Bloch equation which gives us the magnetisation:

$$\dot{M} = ((\omega_0 + \omega)\Omega_z + A(t)\cos(\omega_0 t + \theta(t))\Omega_x + A(t)\sin(\omega_0 t + \theta(t))\Omega_y)M$$

- In a rotation frame of X = exp(- $\omega_0 t\Omega_z$), the equation transforms to:

$$\dot{X} = (\omega\Omega_z + A(t)\cos\theta(t)\Omega_x + A(t)\sin\theta(t)\Omega_y)X$$

Here ω = [-B,B].

- The evolution of the Bloch vector over total time can be expressed as:

$$X_f(\omega) = U_n(\omega, \theta_n)\cdots U_k(\omega, \theta_k)\cdots U_1(\omega, \theta_1)X_0$$

Where X_f is the final Bloch vector.

ITERATIVE PHASE OPTIMISATION

TOPS APPROACH

- The propagator function U can be expressed as a function of ω and θ as:

$$U_k(\omega, \theta_k) = \exp\left(\Delta t\left(\omega\Omega_z + \cos\theta_k\Omega_x + \sin\theta_k\Omega_y\right)\right)$$

- As the objective is to achieve broadband inversion (or excitation), the θ's are optimised such that X_f reaches equal to or close to Y. ($Y = [0, 0, -1]^T$ for broadband inversion and $Y = [1, 0, 0]^T$ for excitation.)

- Hence the cost function to be maximised is

$$J = \frac{1}{N}\sum_{j=1}^{N} Y' U_n\left(\omega_j, \theta_n\right) \cdots U_k\left(\omega_j, \theta_k\right) \cdots U_1\left(\omega_j, \theta_1\right) X_0$$

TOPS ALGORITHMS

- For TOPS-1, the linear cost function is given by:

$$J(\theta_k) = \frac{1}{N}[\cos\theta_k, \sin\theta_k, 0] \sum_j X_{k-1}(\omega_j) \times Y_{k+1}(\omega_j)$$

- For TOPS-2, the simplified quadratic J is given by:

$$J(\theta_k) = \frac{1}{N}\sum_j^N \{[\cos\theta_k \ \sin\theta_k \ 0].[V_1(\omega_j) + V_2(\omega_j) + V_3(\omega_j)]\}$$

Where

$V_1(\omega_j) = X_{k-1} \times Y_{k+1}$

$V_2(\omega_j) = X_{k-1} \times \omega_j\theta_z' Y_{k+1}$

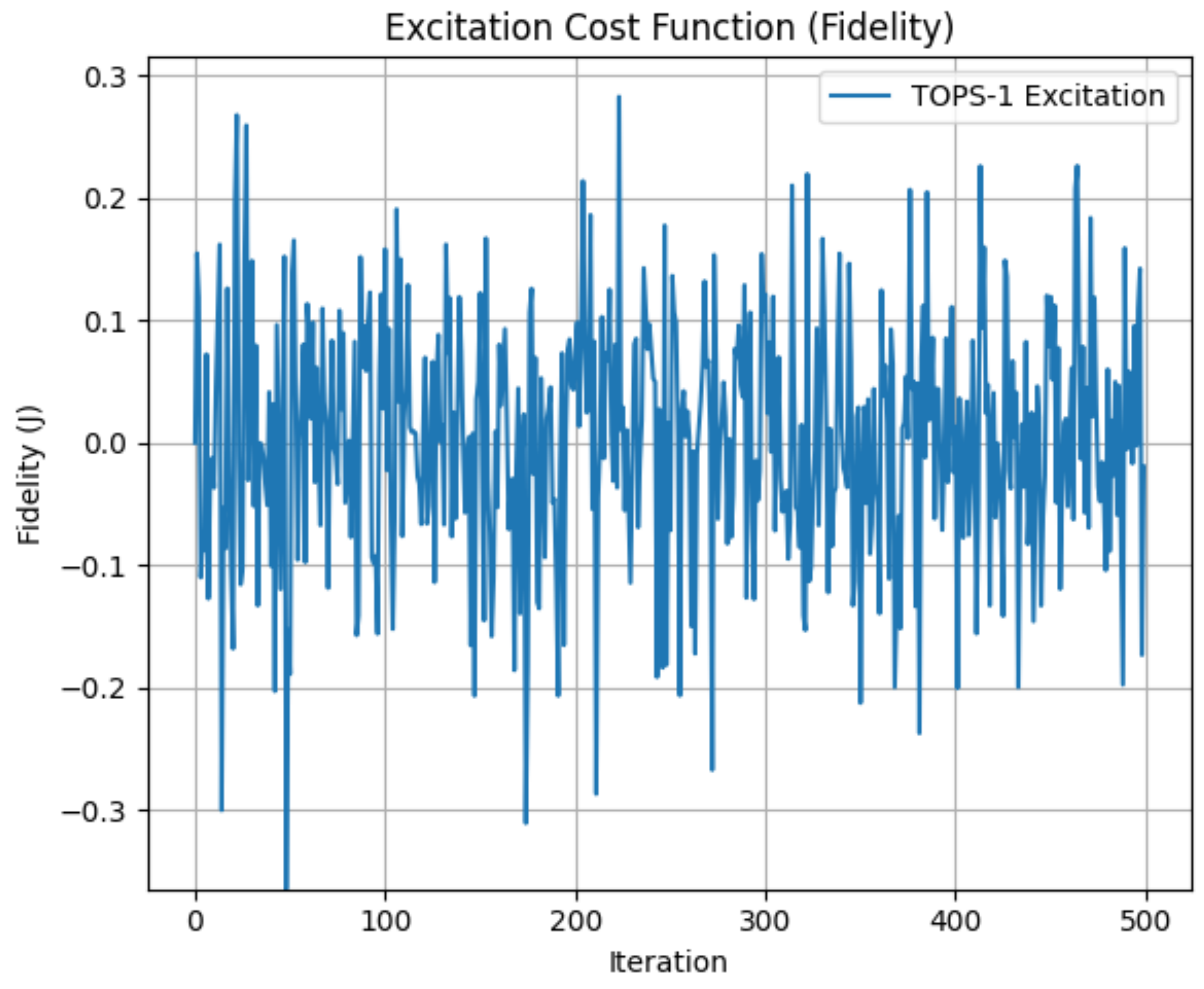
$V_3(\omega_j) = \omega_j\theta_z X_{k-1} \times Y_{k+1}$

CODE IMPLEMENTATION

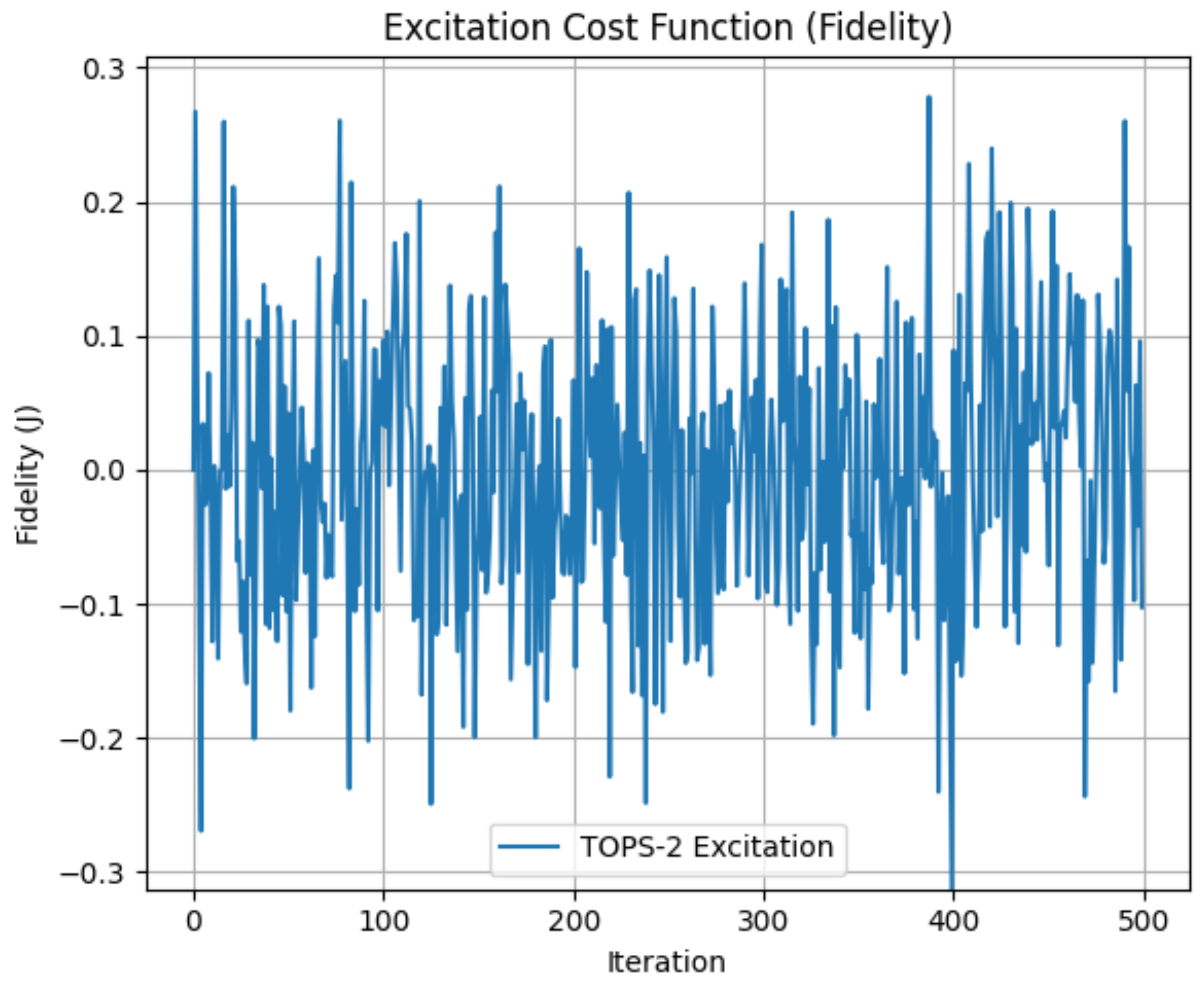
RESULTS

FIDELITY VS ITERATION (INVERSION)

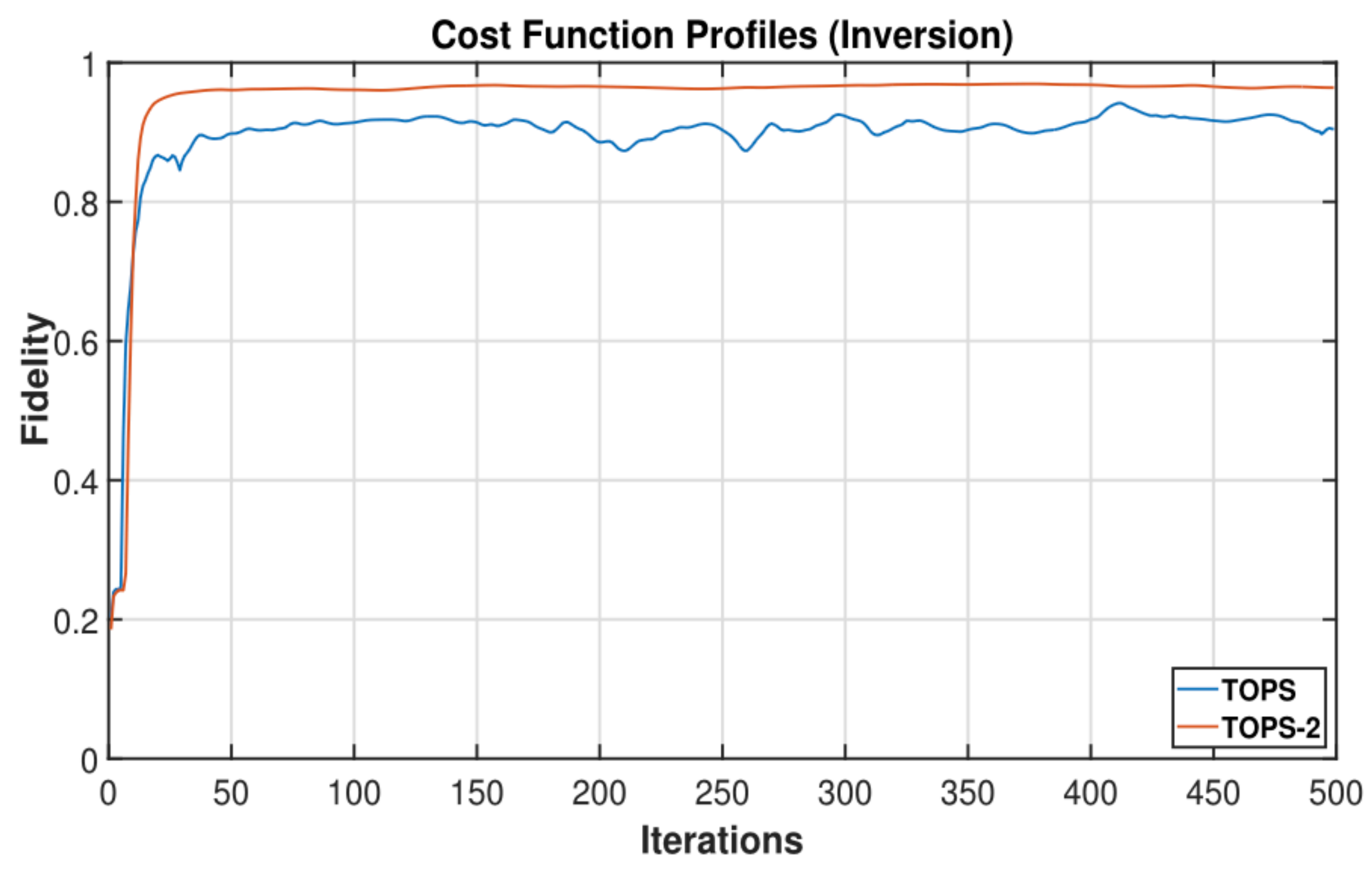
Fidelity (value of the cost function J, which measures how close the final state is to the target state) as a function of the number of Iterations during the optimisation process for the **inversion** pulse.



TOPS-1



TOPS-2

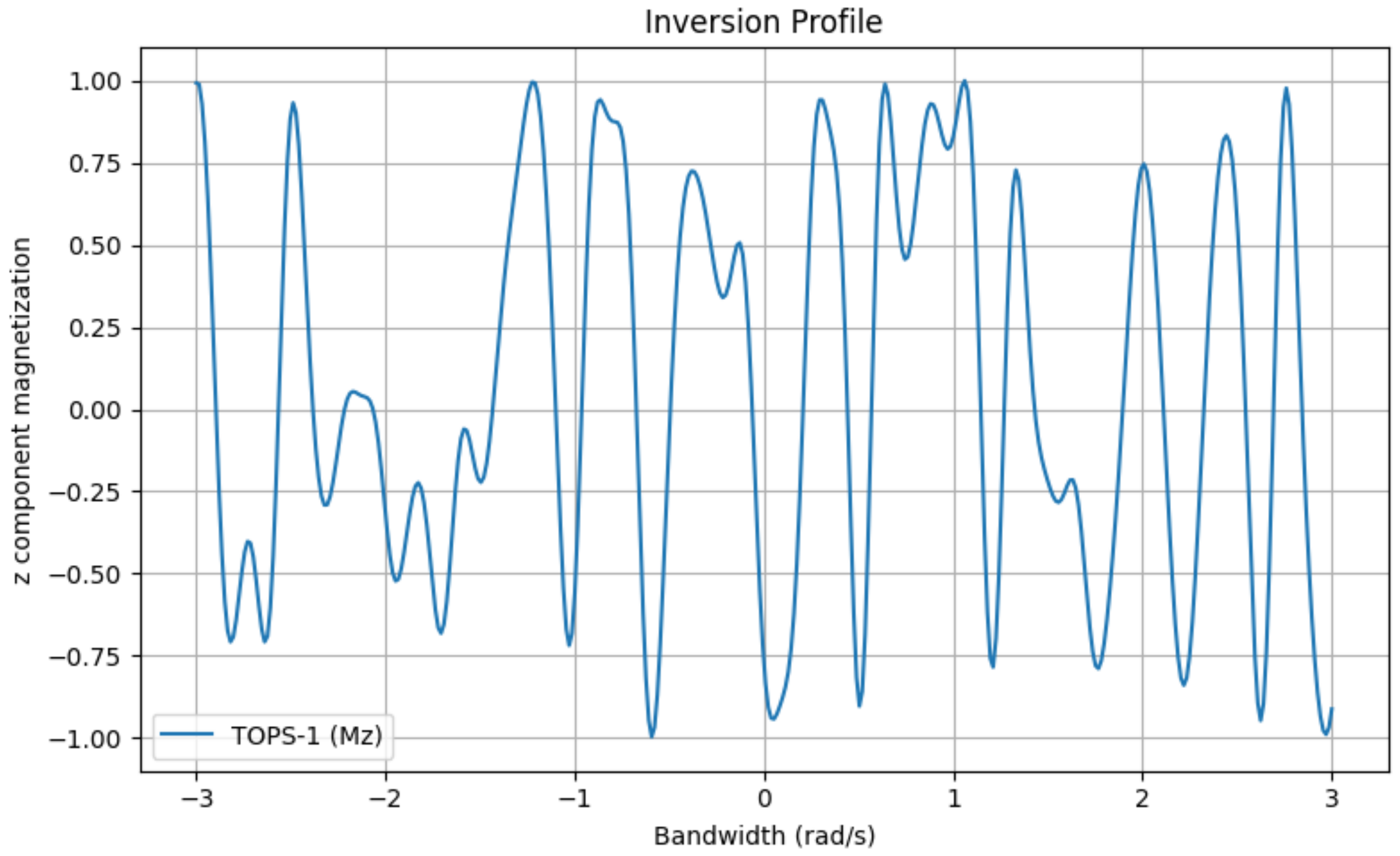


Paper

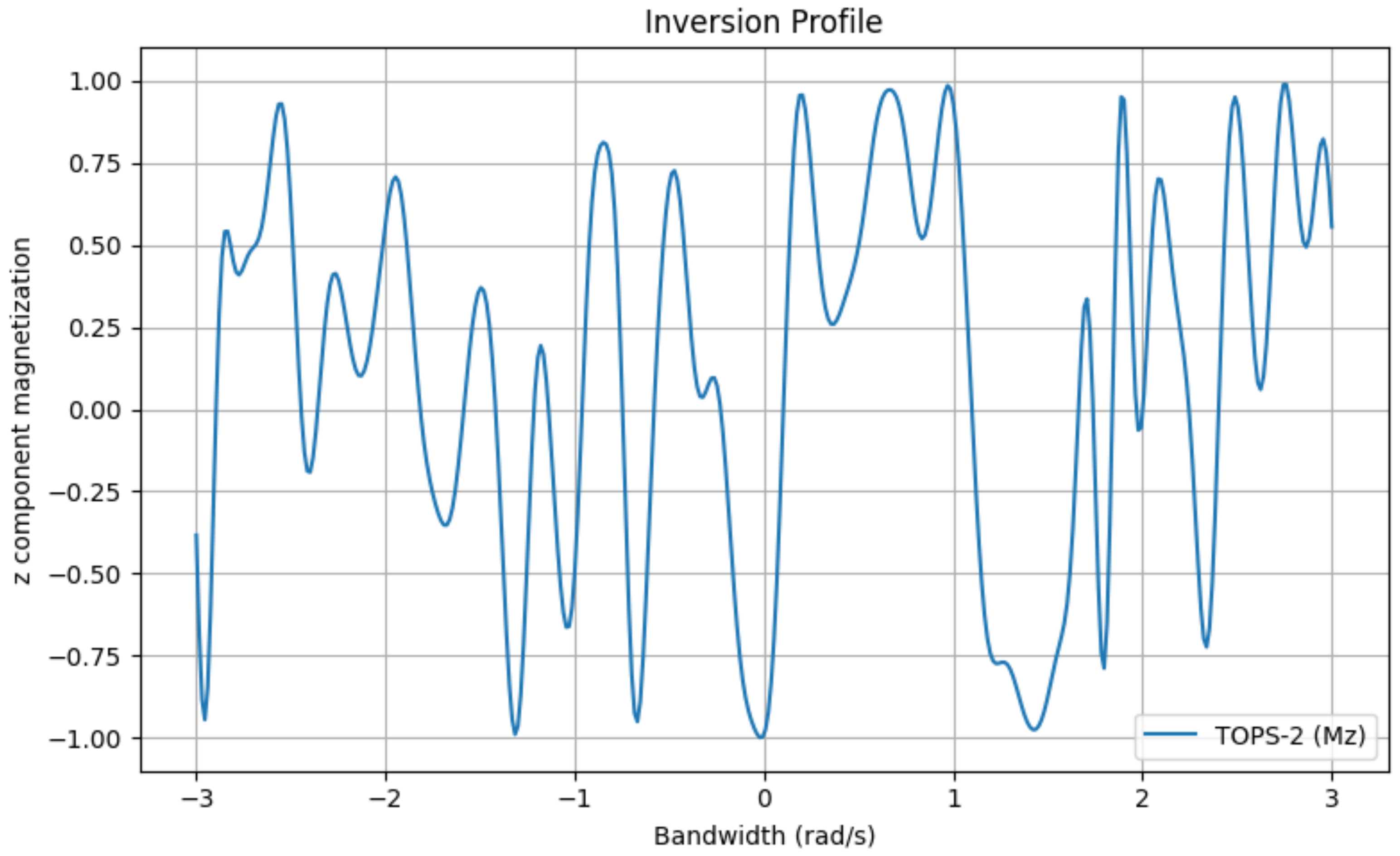
RESULTS

M_Z VS BANDWIDTH (INVERSION)

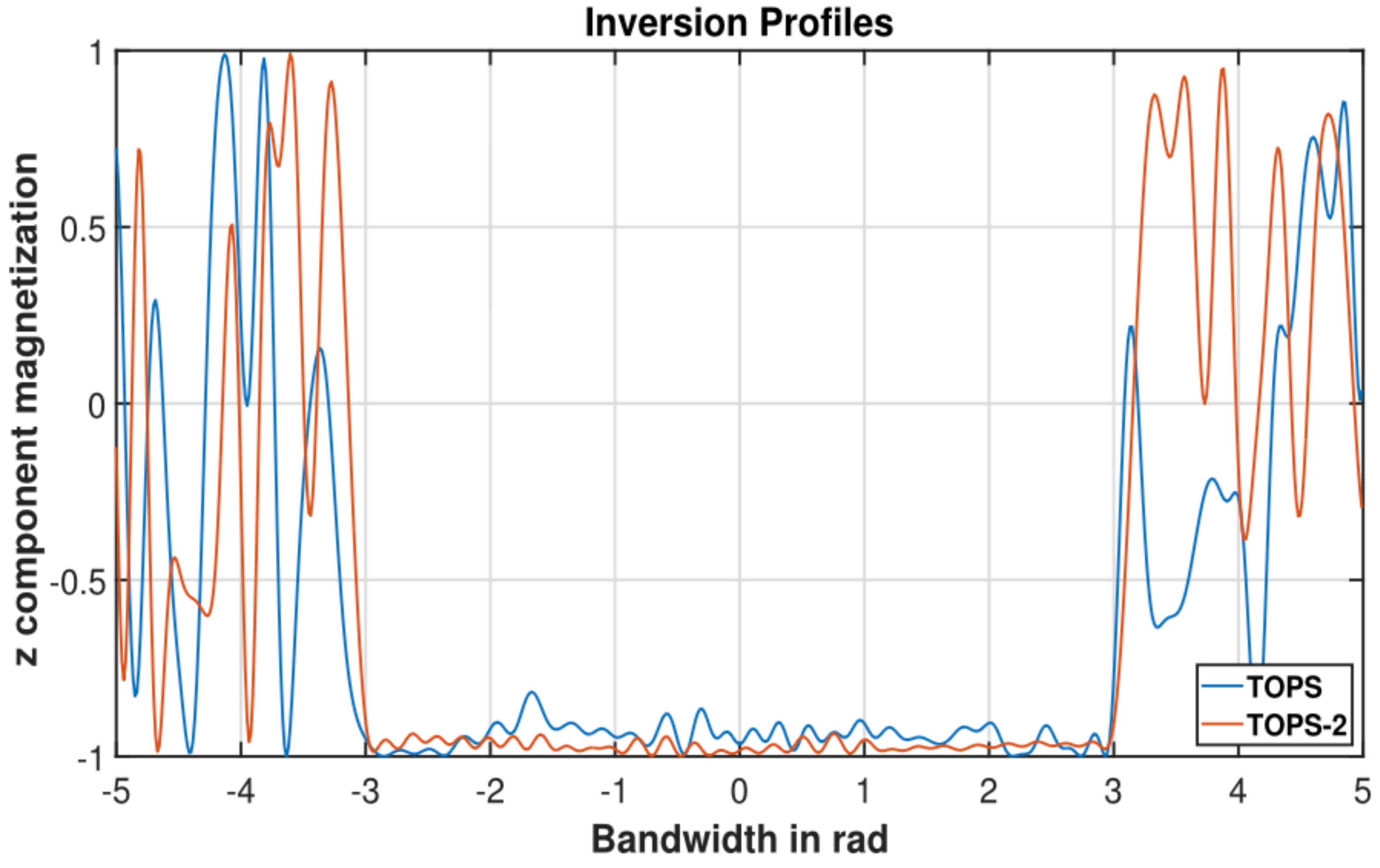
- Z-component of the magnetisation as a function of resonance offset.
- Ideally, for good **inversion**, the z-component should be close to -1 uniformly across the target bandwidth (here, -3 to +3 radians).



TOPS-1



TOPS-2

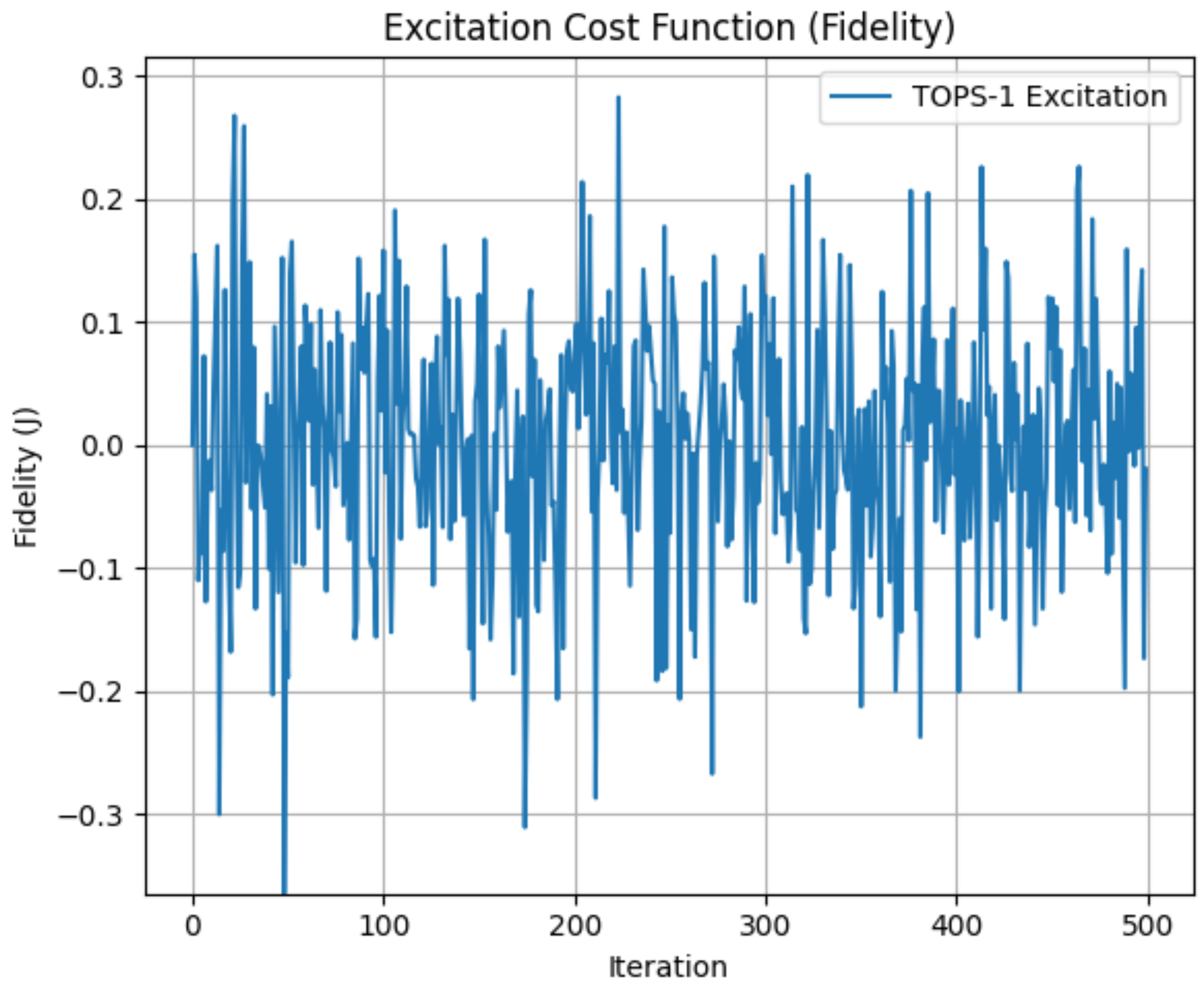


Paper

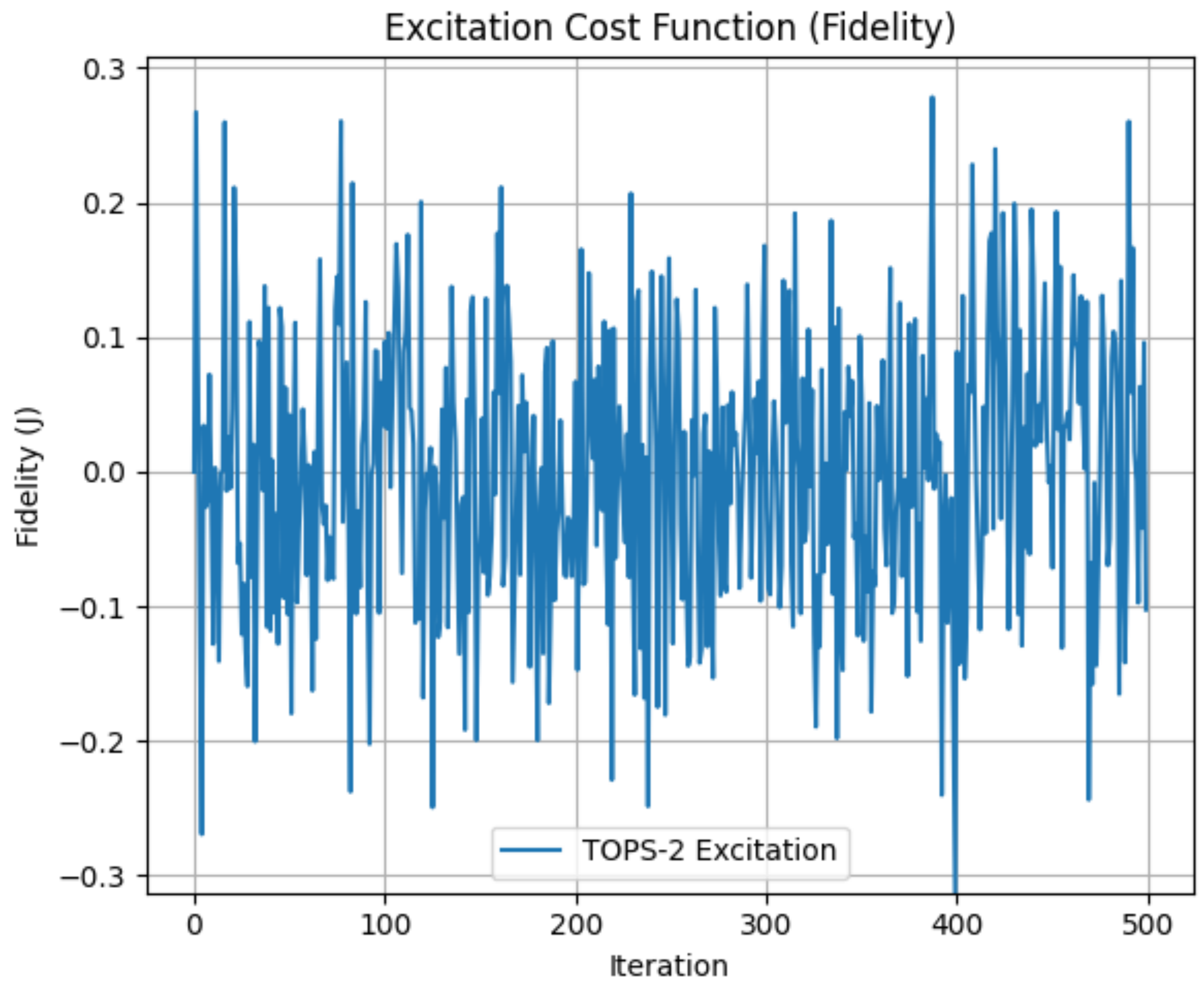
RESULTS

FIDELITY VS ITERATION (EXCITATION)

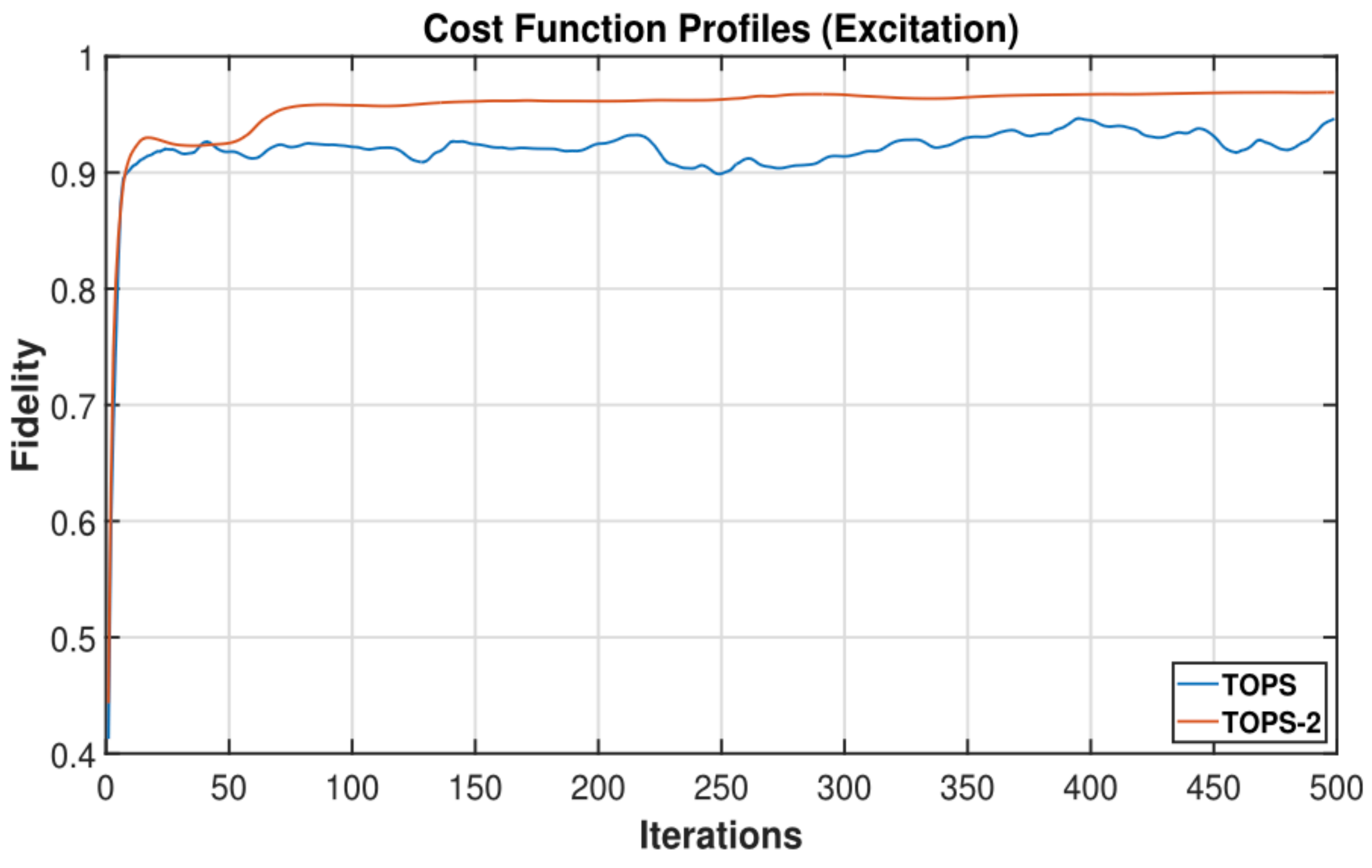
Fidelity (value of the cost function J, which measures how close the final state is to the target state) as a function of the number of Iterations during the optimisation process for the **excitation** pulse.



TOPS-1



TOPS-2

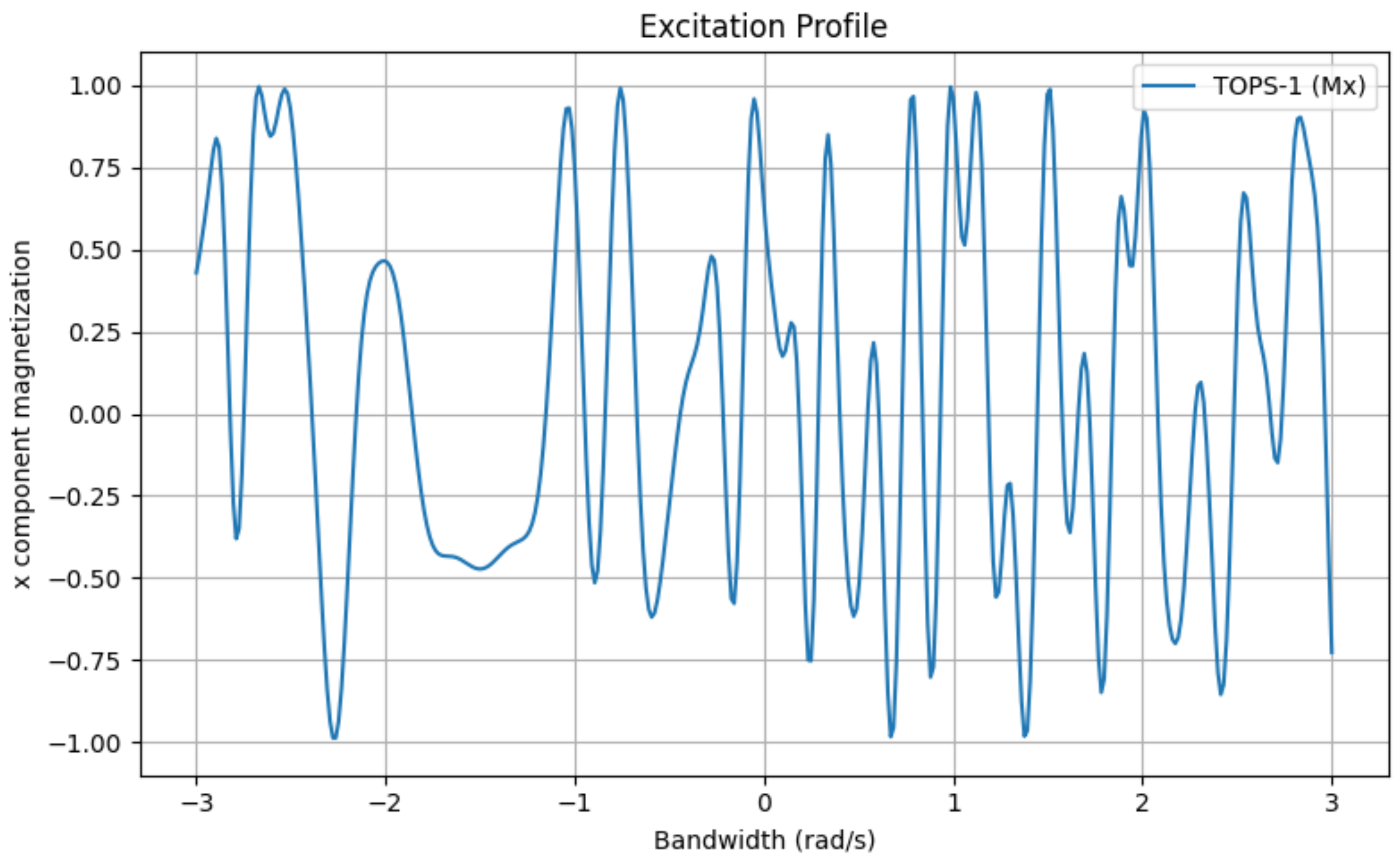


Paper

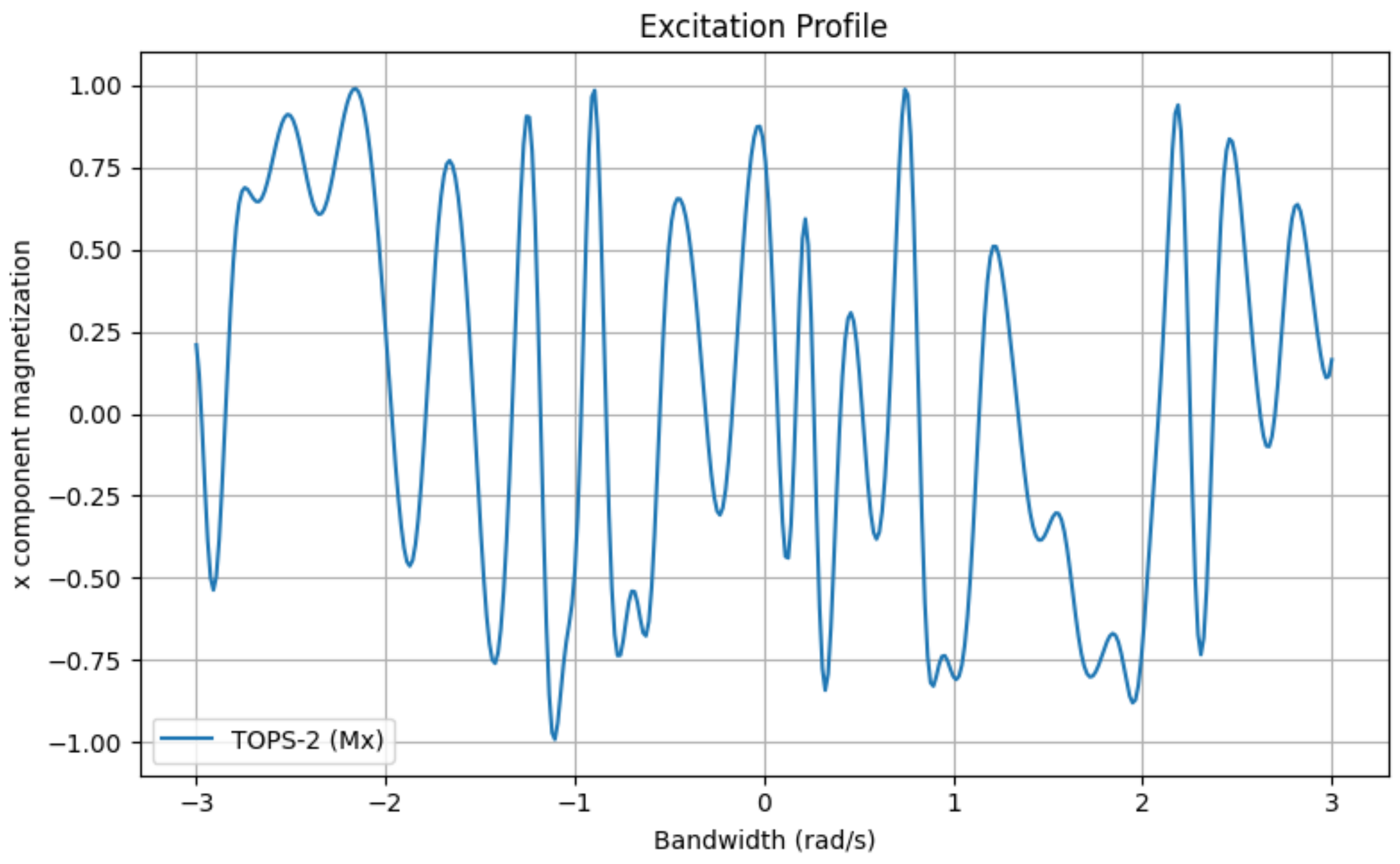
RESULTS

M_X VS BANDWIDTH (EXCITATION)

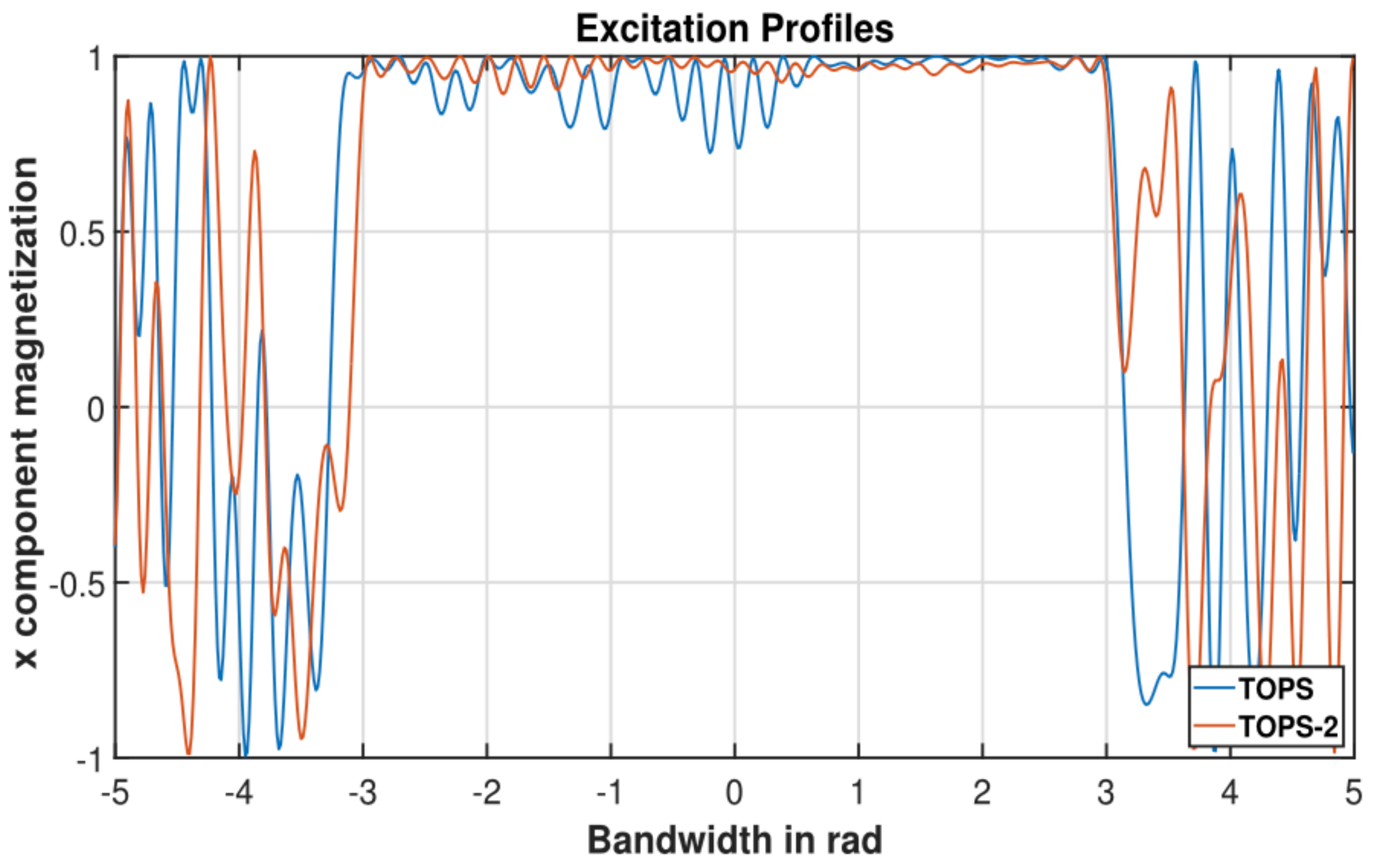
- Z-component of the magnetisation as a function of resonance offset.
- For good **excitation**, the x-component should be close to +1 uniformly across the target bandwidth.



TOPS-1



TOPS-2



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TOPS-1 VS TOPS-2

KEY DIFFERENCES

Feature	TOPS-1	TOPS-2
Primary Goal	Excitation, Inversion	Excitation, Inversion, Mixing (TOCSY)
Propagator Approx.	Linear $(I - iH\Delta t)$	Quadratic $(I - iH\Delta t - 1/2\,(H\Delta t)^2)$
Accuracy	Good for small Δt / low A	Better accuracy, esp. for larger Δt / high A
Phase Update Rule	Closed-form, based on linear approx.	Closed-form, based on quadratic approx.
Complexity	Simpler derivation	More complex derivation, slightly higher computation per step
Performance	Effective	Potentially higher fidelity / broader bandwidth
Application	Broadband Excitation/Inversion	Broadband Excitation/Inversion/Mixing

CONCLUSION

- NMR spectroscopy is a fundamental technique based on the magnetic properties of nuclei.
- Designing RF pulses that perform uniformly over broad frequency ranges (broadband) or selectively target specific frequencies is crucial.
- TOPS algorithms provide an efficient method for designing phase-modulated pulses by iteratively optimising phases in closed form.
- TOPS-2 improves upon TOPS-1 using a quadratic propagator approximation, enhancing accuracy and applicability.
- NMR provides a powerful platform for quantum control, using RF pulses to manipulate nuclear spins (qubits) via single-qubit rotations and J-coupling for multi-qubit gates.
- While facing scalability challenges for large-scale computing, NMR quantum control remains a vital testbed for developing quantum algorithms and high-fidelity control techniques, where pulse design methods like TOPS find relevance.

REFERENCES

- Shetty, T., & Khaneja, N. (2023). Design of NMR Pulses by Iterative Optimization of Phases. Applied Magnetic Resonance, 54, 427–434. https://doi.org/10.1007/s00723-023-01528-9.
- Jacob, J., Shetty, T., & Khaneja, N. (2023). An improved algorithm for design of broadband excitation, inversion, and mixing pulse sequences by iterative optimization of phases: TOPS-2. Journal of Magnetic Resonance, 353, 107501. https://doi.org/10.1016/j.jmr.2023.107501.
- Cavanagh, J., Fairbrother W. J., et al. (2007). Protein NMR Spectroscopy: Principles and Practice. 2nd Edition. Academic Press (Chapters 1 and 2)
- Levitt, M. H., (2006) Spin Dynamics: Basics of Nuclear Magnetic Resonance. John Wiley & Sons. (Chapter 1)
- Vandersypen, L. M. K., & Chuang, I. L. (2005). NMR techniques for quantum control and computation. Reviews of Modern Physics, 76(4), 1037–1069. https://doi.org/10.1103/RevModPhys.76.1037.
- Nielsen, M. A., & Chuang, I. L. (2010). Quantum Computation and Quantum Information: 10th Anniversary Edition. Cambridge University Press. (Chapters on NMR Quantum Computation)

THANK YOU