Karlsruhe Institute of Technology

VIRTUAL MATERIALS DESIGN

HiT-NMR

SFB 1527 HyPERiON

IMT

Defending gradient field spillover in multi-detector NMR by spin locking

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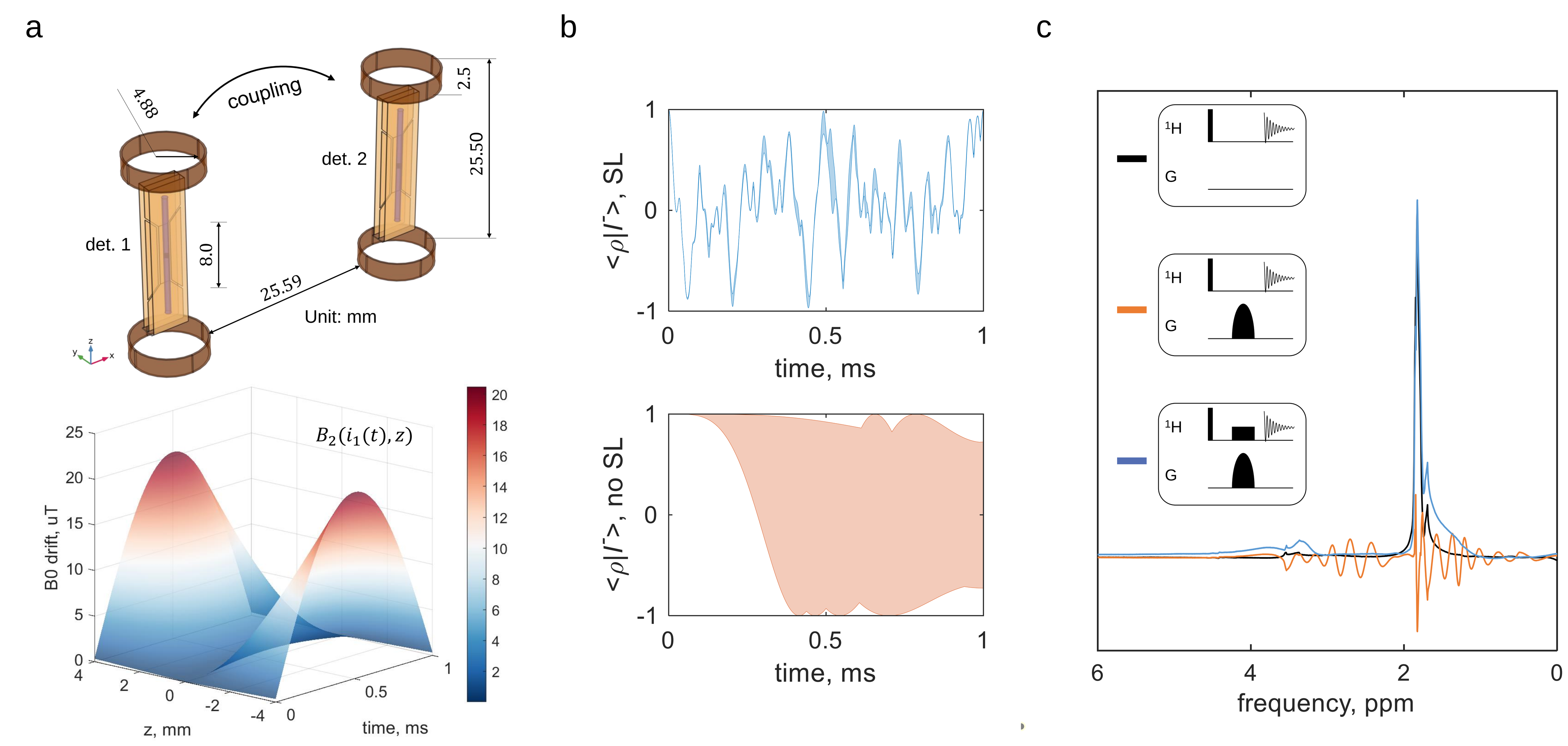
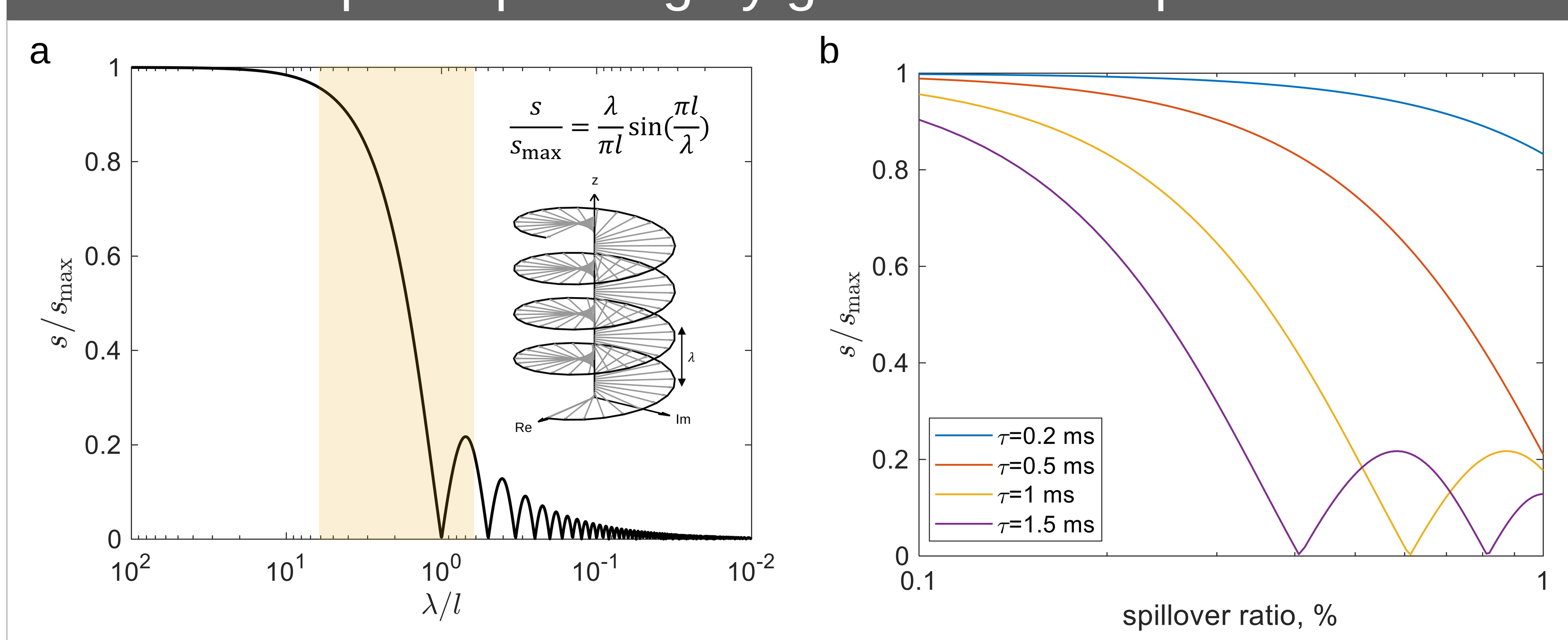
Single spin locking in a 2-detector NMR

- Parallel NMR detectors can enhance the sample throughput.
- Parallel detectors induce radiofrequency coupling and gradient field spillover. While the former has been addressed recently[1], the latter causes unwanted spin dephasing and remains unsolved.
- Spin locking with optimal control pulses[2] can compensate for gradient field spillover.



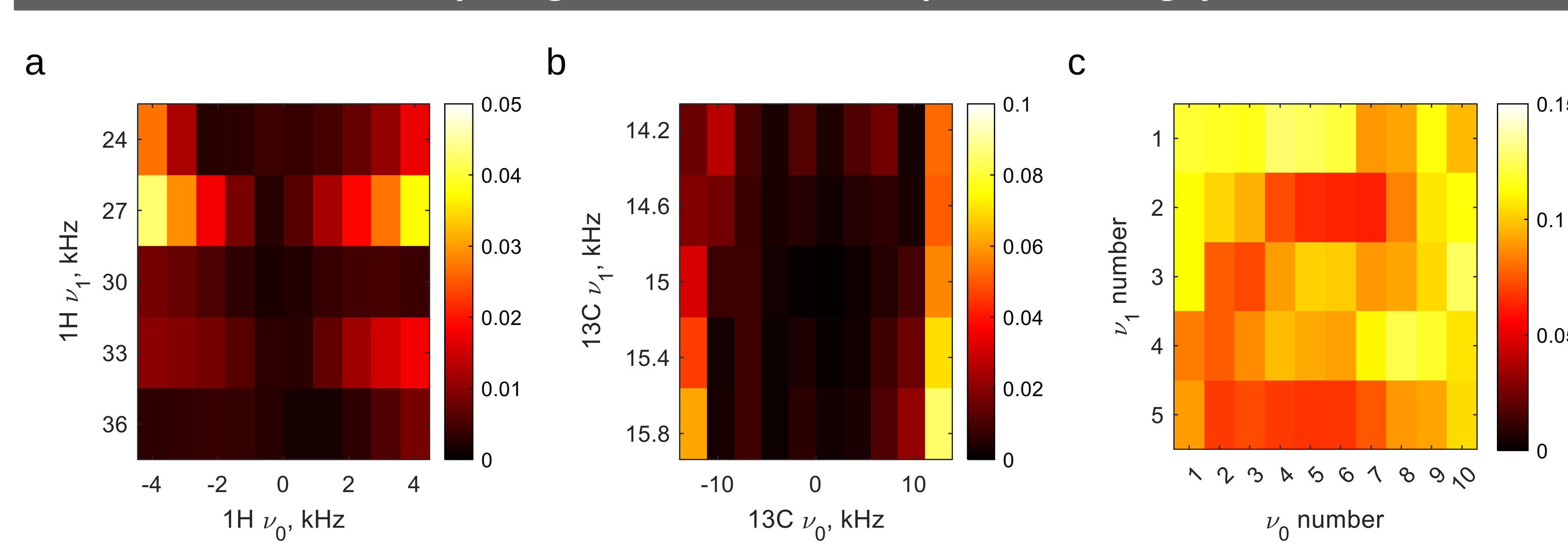
Spin dephasing by gradient field spillover



Signal decay depends on the gradient spillover ratio

Figure 1. Signal intensity under field gradient dephasing. (a) Relative signal intensity plotted against the ratio between helix wavelength and sample length. (b) Relative intensity of the parallel HSQC signal depicted against gradient coupling ratio (see top figure), with varying gradient duration and fixed primary gradient strength (75 Gauss/cm). X-axis is logarithmic. The shaded region in (a) corresponds to τ = 1 ms in (b).

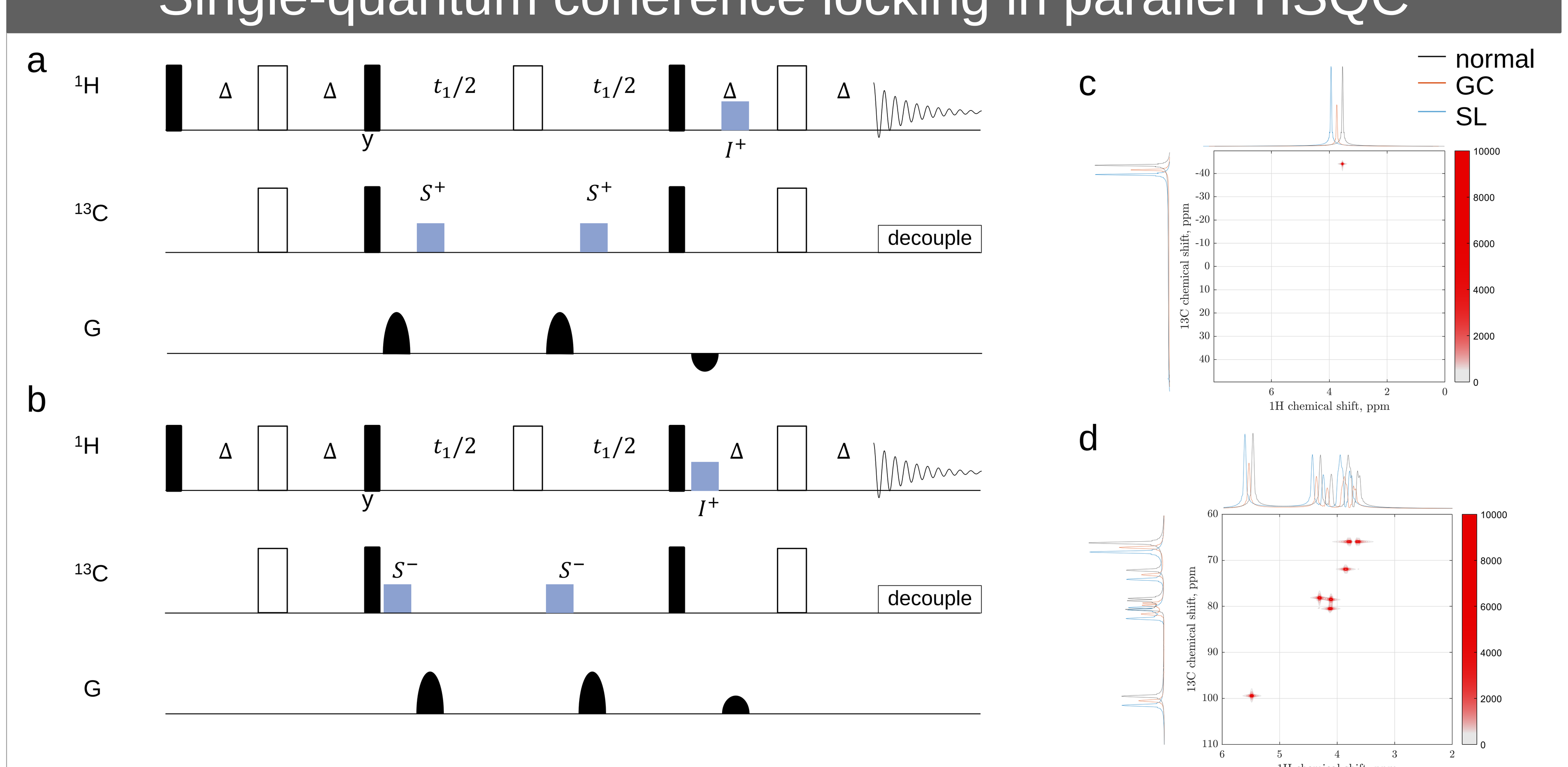
Decoupling effect of the spin locking pulse



***J*-coupling can be neglected during the spin locking**

Figure 2. Scale factor of the J_{HC} coupling as a function of resonance offset and B_1 amplitude. (a) The spin-locking pulse is applied to ^{1}H while ^{13}C is on resonance. (b) The spin-locking pulse is applied to ^{13}C while 1H is on resonance. (c) The spin-locking pulses are applied simultaneously to ^{1}H and ^{13}C, with ν_0 on both channels aligned, and ν_1 on both channels aligned. The spin dynamics calculation was implemented in Spinach[3].

Single-quantum coherence locking in parallel HSQC



Single-quantum coherence was locked using a single-spin locking pulse

Figure 3. (a-b) The scheme for spin locking in a parallel HSQC pulse sequence, blue blocks indicating the spin-locking pulse. (c-d) Simulated parallel HSQC spectra of glycine (c) and glucose (d) respectively. The 'normal' means results without gradient coupling, as a reference, the 'GC' means gradient coupling and the 'SL' means spin locking.

Parallel HSQC experiment

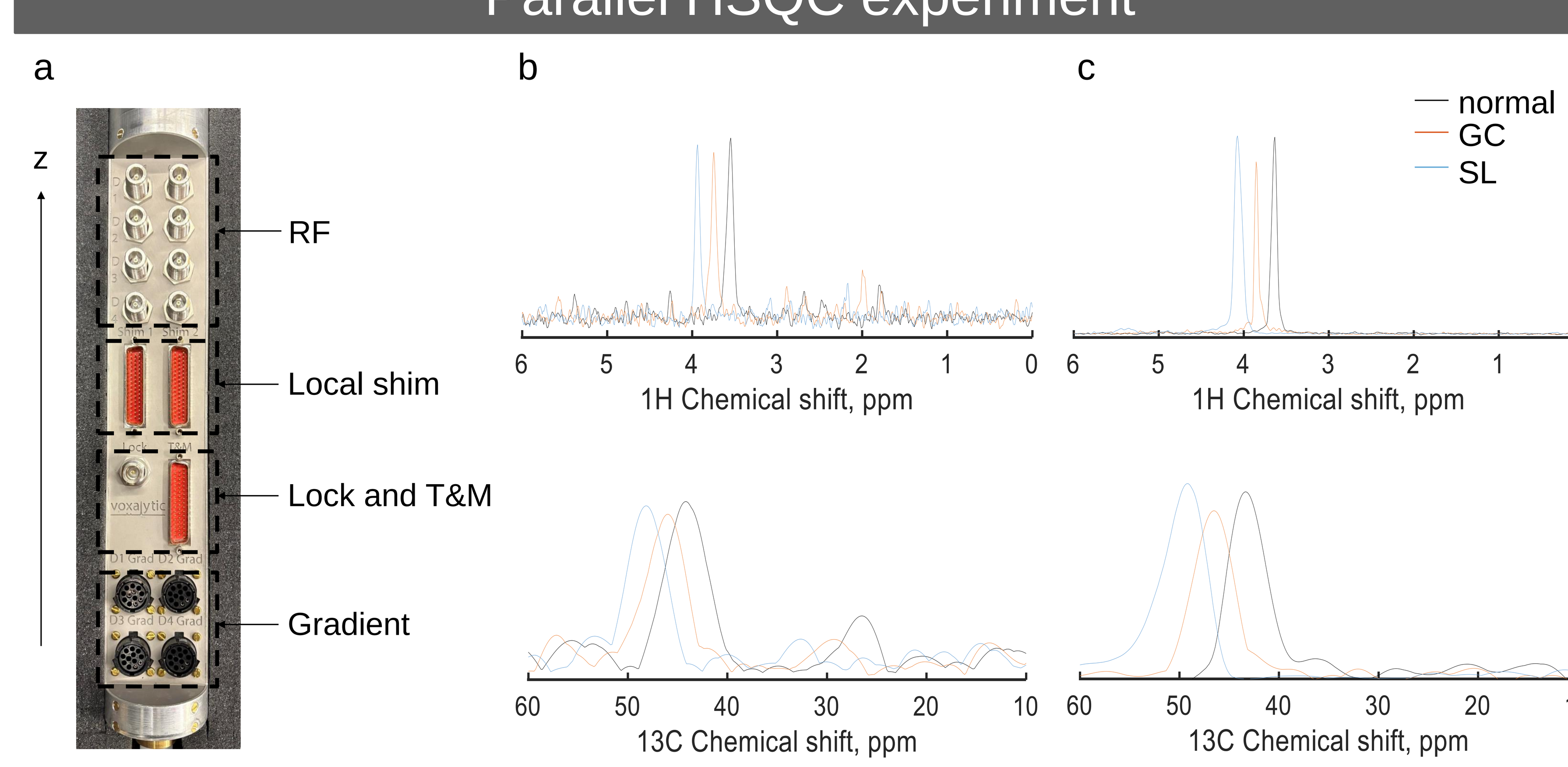


Figure 4. Experimental parallel HSQC spectra obtained using a parallel NMR probe (Voxalytic GmbH) with four detectors, two of which were used, each containing a glycine sample (0.6 M in D_2O). (a) The electrical ports of the probe. (b-c) 1D projections of the spectra from detector 1 (b) and detector 2 (c). The three lines in each plot represent the same data types as described in Figure 3.

References

1. He, Mengjia, et al. "A digital twin for parallel liquid-state nuclear magnetic resonance spectroscopy." Communications Engineering 3.1, 90 (2024).
2. Khaneja, Navin, et al. "Optimal control of coupled spin dynamics: design of NMR pulse sequences by gradient ascent algorithms." Journal of Magnetic Resonance 172.2, 296-305 (2005).
3. Hogben, H. J., et al. "Spinach–a software library for simulation of spin dynamics in large spin systems." Journal of Magnetic Resonance 208.2, 179-194 (2011).

Conclusion & Acknowledgements

- This study proposes a compensation scheme employing optimized pulses to achieve coherence locking during gradient pulse periods. This compensation scheme presents a valuable solution for magnetic resonance probes equipped with parallel gradient coils.
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