

# Study of nuclear magnetic resonance spectra with the multi-modal multi-level quantum complex exponential least squares algorithm

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## Abstract

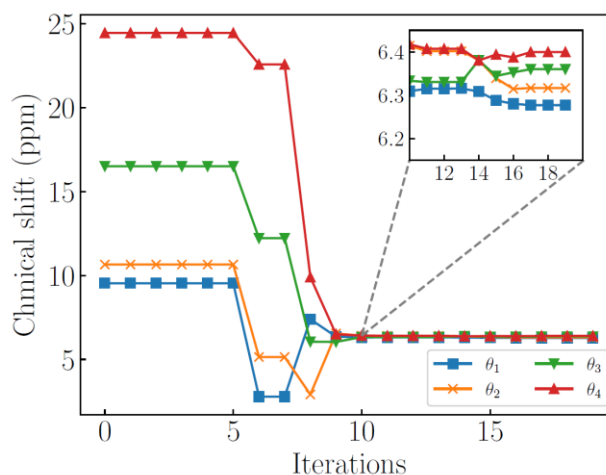
We present a novel application of the multi-modal, multi-level quantum complex exponential least squares (MM-QCELS) algorithm, a state-of-the-art, early fault-tolerant quantum phase estimation (QPE) technique, to the simulation and analysis of nuclear magnetic resonance (NMR) of spin systems [1]. By leveraging the robustness and precision of MM-QCELS [2], we demonstrate enhanced phase resolution in quantum simulations of spin dynamics, also in systems with complex coupling topologies [3]. Our approach enables accurate extraction of spectral features with up to an order of magnitude fewer evaluations of the time series signal in comparison with the conventional Fourier transform, making a significant step toward scalable quantum simulations of NMR Hamiltonians. This work bridges an advanced quantum algorithm design with a practical spectroscopic application, offering a promising new approach for a quantum-based chemical analysis.

## References

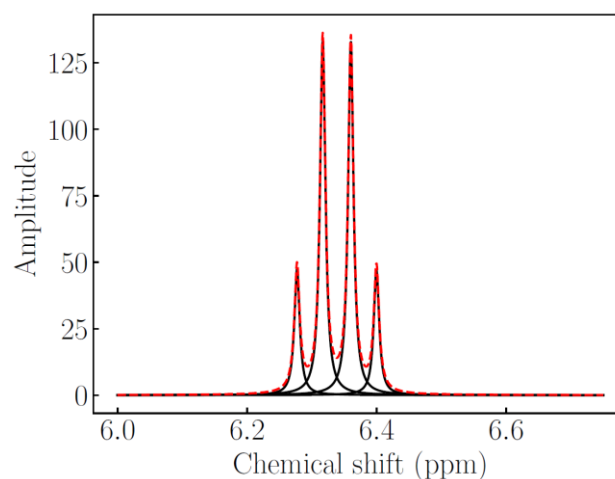
- [1] A.M. Romero, J.M. Kirsopp, G. Buonaiuto, & M. Krompiec, arXiv:2509.24664, (2025)
- [2] Z. Ding and L. Lin, Quantum, (2023), 7, 1136

- [3] A. Khedri, P. Stadler, K. Bark, M. Lodi, R. Reiner, N. Vogt, M. Marthaler and J. Leppäkangas, arXiv:2404.18903, (2024)

## Figures



**Figure 1:** Convergence of the optimal spectral peak positions for cis-3-chloroacrylic acid in the iterative procedure of MM-QCELS



**Figure 2:** NMR spectrum for cis-3-chloroacrylic acid using the optimal parameters obtained from MM-QCELS. The sum of lineshape profiles, which would correspond to a realistically observed NMR spectrum, is also plotted using red dashed lines