Mestrelab Research

Simulating NMR Spectra with a Quantum Computer

Joaquín Ossorio Castillo

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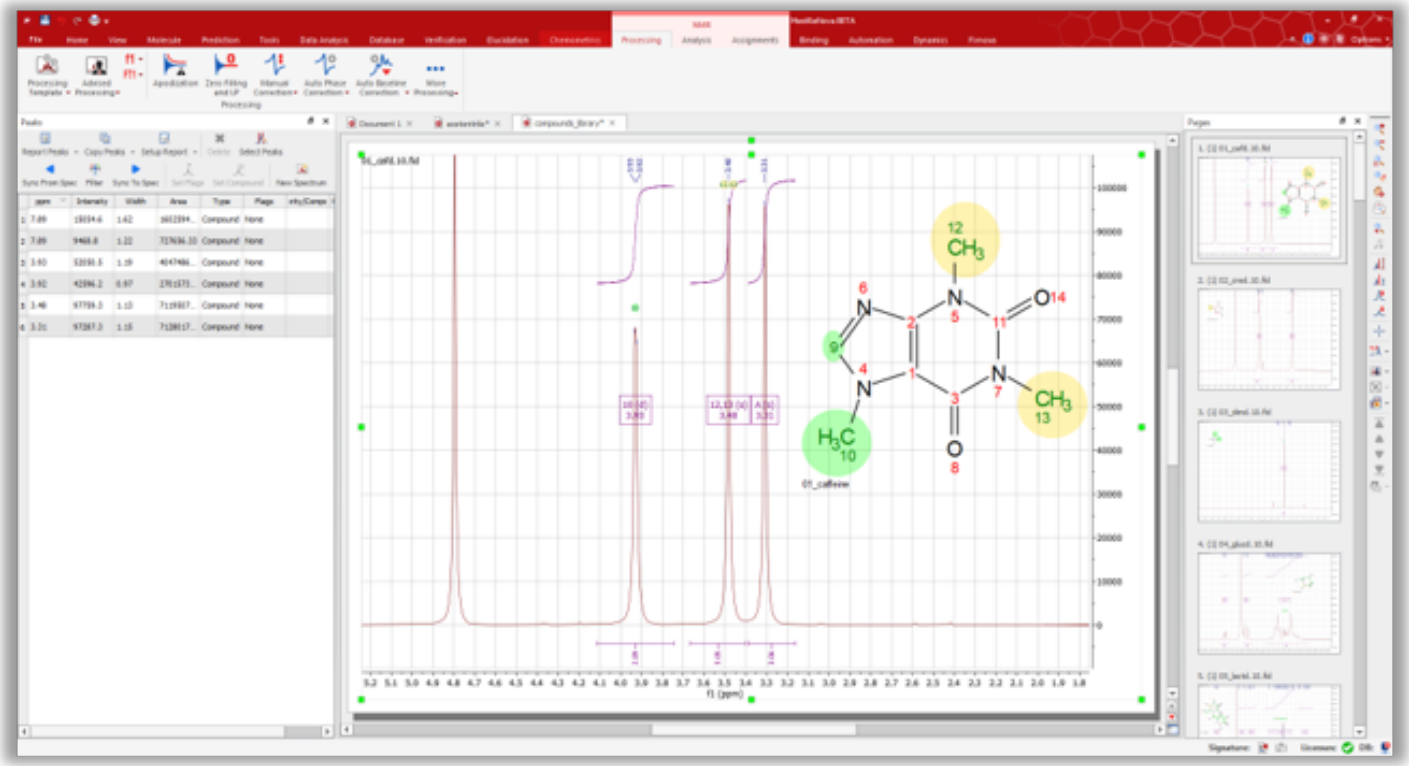
Mnova and Mestrelab Research

MestReNova or Mnova is a multi-vendor software suite developed by Mestrelab Research and designed for combined techniques of NMR, LC/GC/MS, and Electronic and Vibrational Spectroscopy. It has grown from an academic research project to provide quality scientific software to thousands of customers.

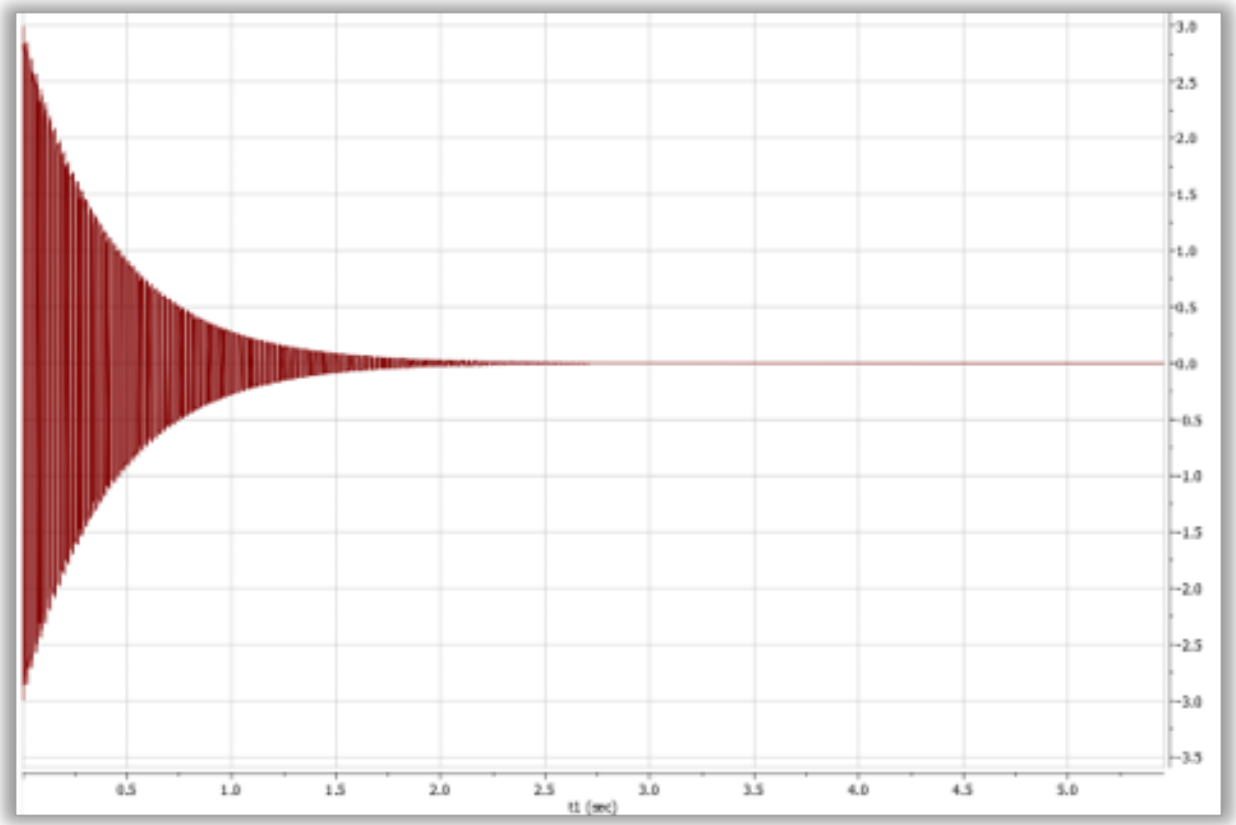


Nuclear Magnetic Resonance Spectroscopy (1/3)

Nuclear magnetic resonance spectroscopy (NMR) is a non-destructive analytical technique used, among other applications, to study the structure and chemical composition of molecules in solution and solid state. The technique is based on the interaction of atomic nuclei with a magnetic field and a radiofrequency field.

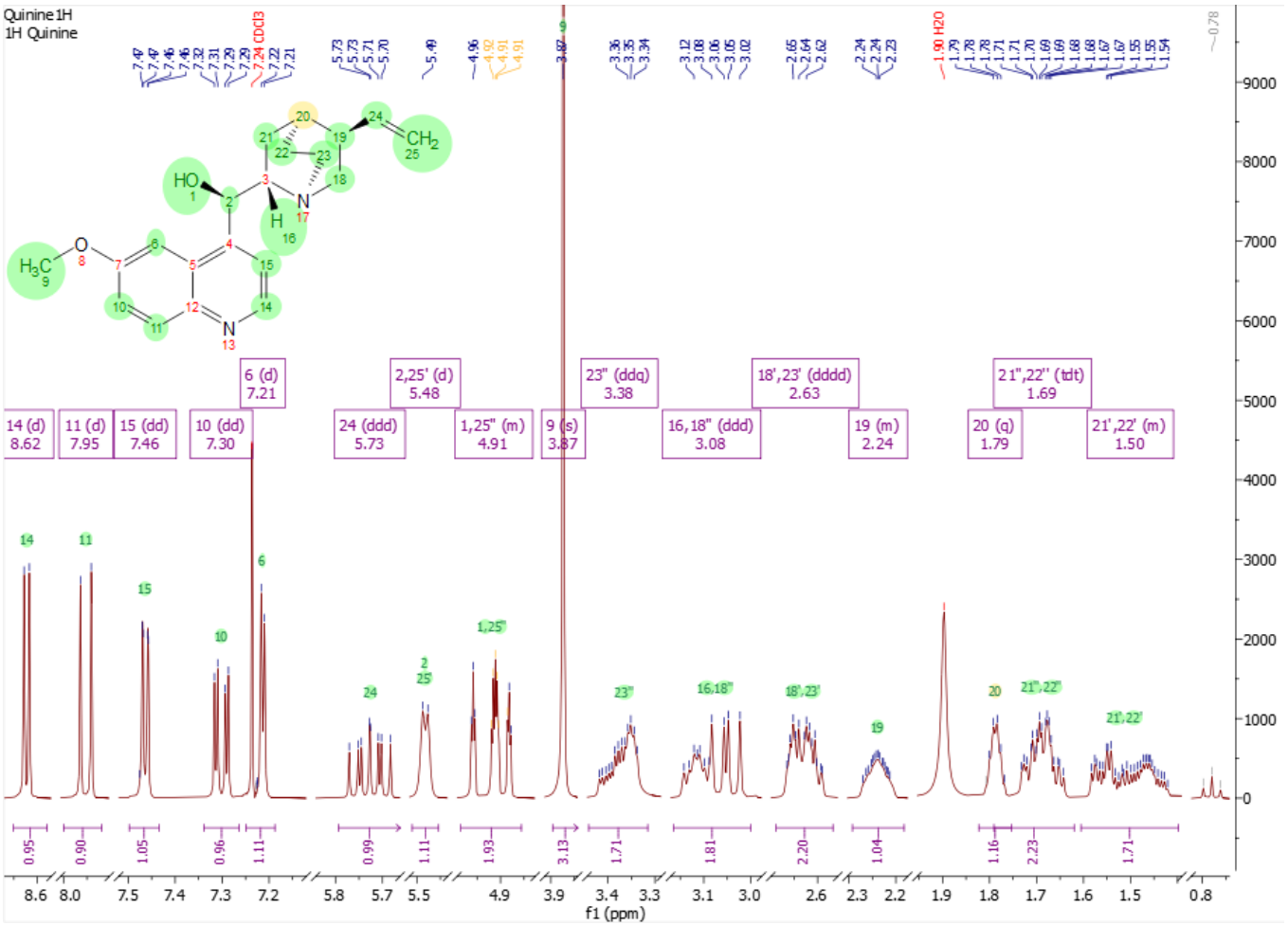
Nuclear Magnetic Resonance Spectroscopy (2/3)

The output of NMR spectrometers is known as the 'Free Induction Decay' signal, or FID for short.



Nuclear Magnetic Resonance Spectroscopy (3/3)

The Fourier transform of the FID, which converts the signal from the time domain to the frequency domain, is what is referred to as the 'NMR spectrum'.



The problem: Simulating NMR Spectra

Accurate and efficient simulation of NMR spectra from a molecule's spin system requires constructing the Hamiltonian matrix of said spin system, whose dimensions increase exponentially with respect to the number of corresponding atoms in the molecule.

Subsequently, this Hamiltonian matrix is diagonalized to calculate its eigenvalues and eigenvectors. It is precisely the calculation of the eigenvalues and eigenvectors of the Hamiltonian matrix that poses a bottleneck in the current algorithm.

The FID of the spin system is calculated from those eigenvalues and eigenvectors according to a certain resolution and magnetic field.

Currently, this simulation is carried out quickly enough for molecules up to 12 or 13 nuclei. For larger molecules, fragmentation occurs to prevent undesirably long computational times, but losing accuracy in the process.

The Hamiltonian Matrix of a Spin System

A spin system is a collection of quantum particles possessing spin, undergoing interaction. The Hamiltonian of this type of system under an external magnetic field is described by the quantum Heisenberg model.

$$H = \sum_{k} w_k S_{kz} + \sum_{i,j}^{k} J_{ij} \vec{S_i} \cdot \vec{S_j}$$

The first part is called the Zeeman interaction, and is influenced by the chemical shifts of the individual nuclei. As each particle possesses an intrinsic magnetic moment (the nuclear spin), the applied field will excite each individual particle. We can assume that the magnetic field is oriented along the Z-axis.

The second part is due to the coupling between the different nuclei (the spin of each nucleus interacts with the spins of the surrounding nuclei). It is proportional to the product of both magnetic moments, being J the interaction amplitude. In this case we cannot assume the magnetic field to be oriented along the Z-axis.

Quantum Phase Estimation

Given a unitary operator U acting on m qubits (i.e., a unitary matrix of dimension $2^m \times 2^m$), then all its eigenvalues have unit modulus. Thus, if φ is an eigenvector of U, then $U\varphi = e^{2\pi i\theta}\varphi$ for some $\theta \in \mathbb{R}$ (we can assume that $0 \leq \theta < 1$). The idea of the algorithm is to obtain θ with high probability, thus obtaining the eigenvalue associated with the eigenvector φ.

This approach requires fully coherent evolution, which has not been reached yet in current quantum computers.

It is mandatory to verify on each step that the value obtained is in fact an eigenvalue.

Does not inherently provide information about eigenstates.

Variational Quantum Eigensolver

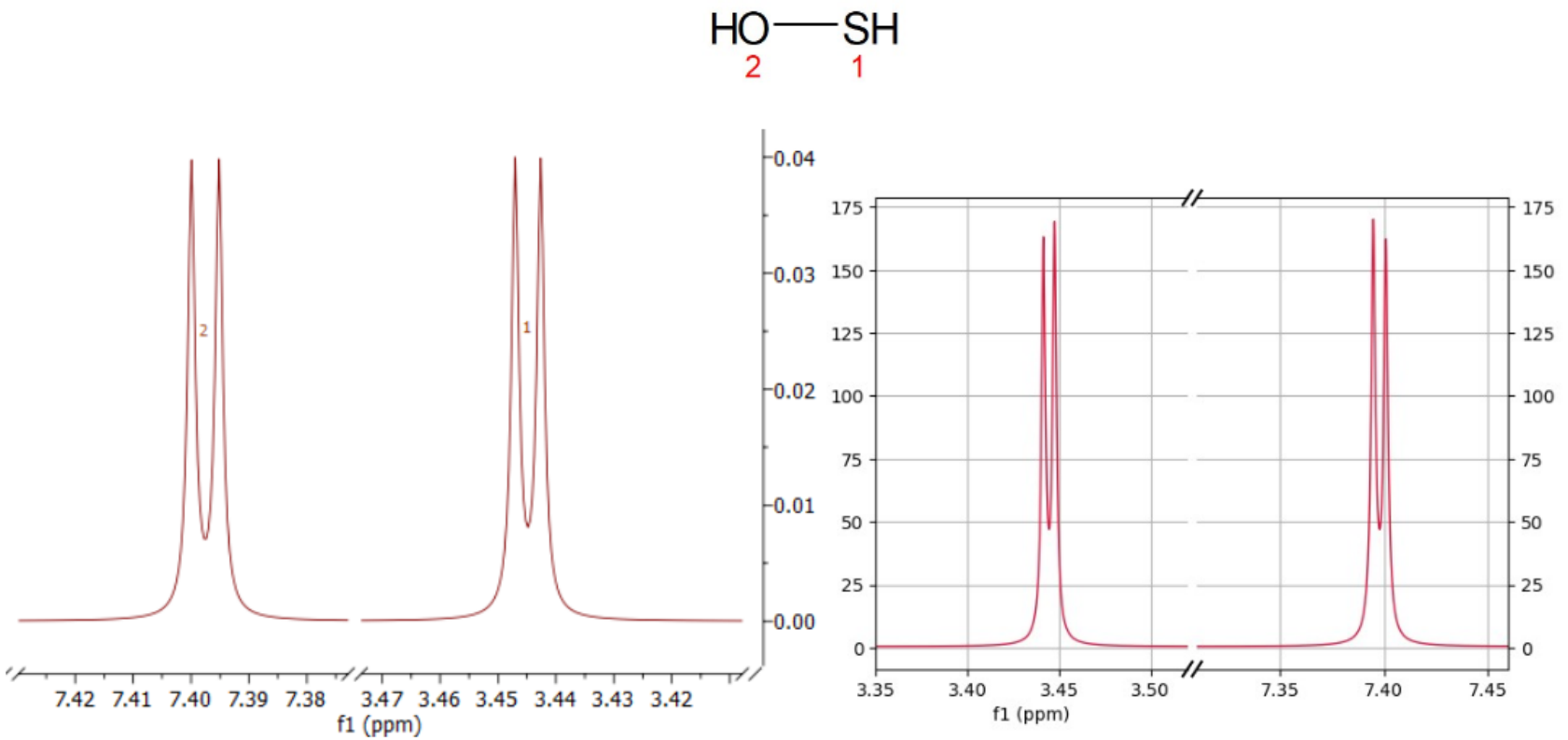
VQE belongs to a family of algorithms called VQAs (short for variational quantum algorithms), which make use of classical optimization to optimize the parameters of the quantum circuit involved in the process. Thus, it requires combining a quantum processor with a classical computer.

Its main advantage is that the requirements of such quantum processor can already be found in the current state of quantum computing, usually referred to as the noisy intermediate-scale quantum —NISQ— era.

The chosen ansatz plays a critical role in the success of VQE, along with a good estimation of ground states for the spin system.

Current Results with VQE

By combining the VQE algorithm and the folded spectrum method with suitable estimations of our Hamiltonian eigenstates, we were able to obtain the information needed to reconstruct the sulfanol molecule ^{1}H-NMR spectrum. Future research should focus on studying its viability for larger spin systems.



Thank you.

joaquin@mestrelab.com

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