# Mestrelab Research

Simulating NMR Spectra with a Quantum Computer

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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.
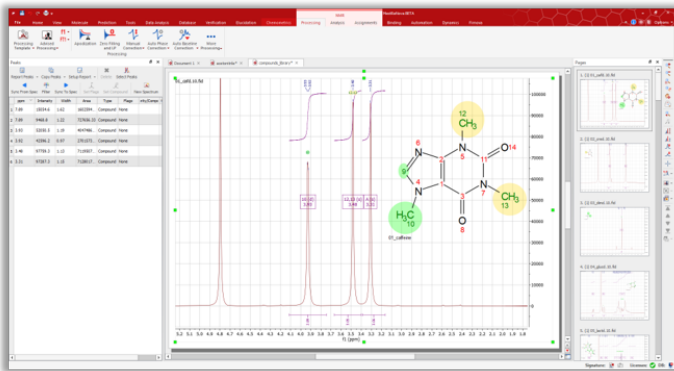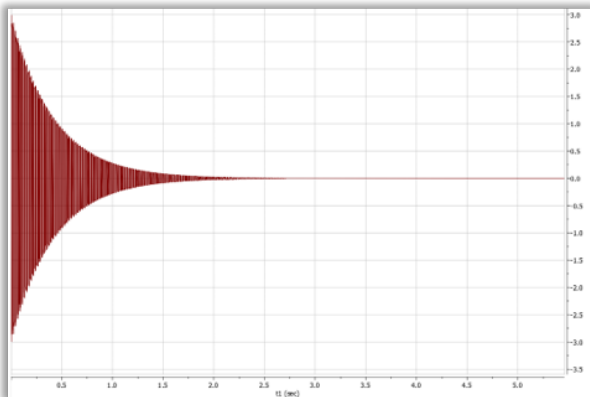
Nuclear Magnetic Resonance Spectroscopy (1/3)

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.
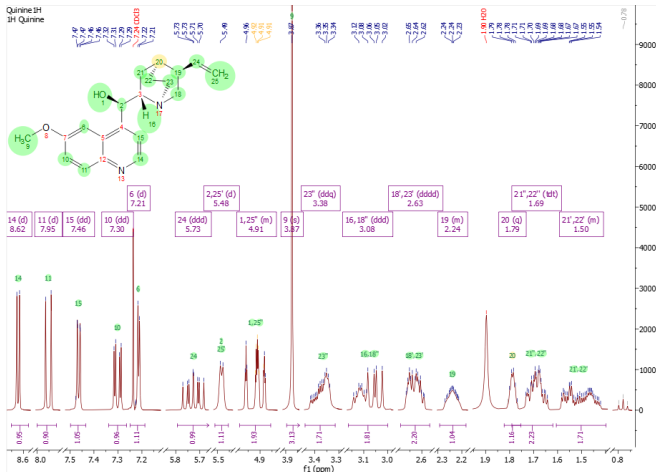
Nuclear Magnetic Resonance Spectroscopy (2/3)

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.

$$H = \sum_k w_k S_{kz} + \sum_{i,j}^{k} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$H = \begin{pmatrix} \frac{w_1+w_2}{2} + \frac{J}{4} & 0 & 0 & 0 \\ 0 & \frac{w_1-w_2}{2} - \frac{J}{4} & \frac{J}{2} & 0 \\ 0 & \frac{J}{2} & \frac{-w_1+w_2}{2} - \frac{J}{4} & 0 \\ 0 & 0 & 0 & \frac{-w_1-w_2}{2} + \frac{J}{4} \end{pmatrix}$$

The first part is called the Zeeman interaction, and is influenced by the chemical shifts of the individual nuclei.

The second part is due to the coupling between the different nuclei. It is proportional to J, the interaction amplitude.

Variational Quantum Eigensolver

VQE is a variational quantum algorithm wich combines both quantum and classical computers, suitable for the current NISQ era.

A parametrized quantum circuit measures the expected value of the Hamiltonian $\langle \Psi_\theta | H | \Psi_\theta \rangle$. The state $|\Psi_\theta\rangle$ is built starting from an initial state and then applying a parametrized ansatz $U(\theta)$. The classical optimizer tries to minimize this value finding the best parameters θ.
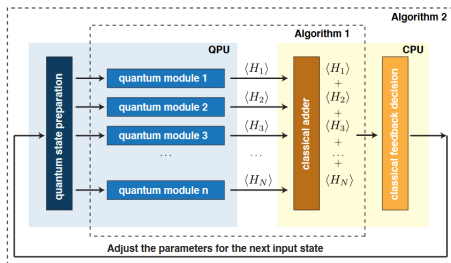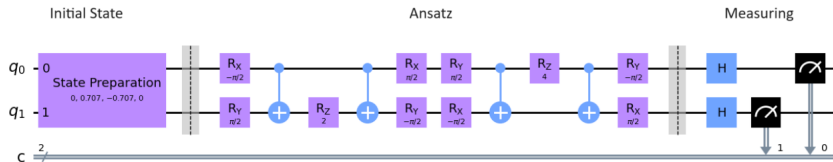

Figure: VQE scheme from *A variational eigenvalue solver on a quantum processor*, Peruzzo

Simulating VQE

Qiskit is an open-source toolkit for simulating quantum circuits.

For each operator a quantum circuit is built. For each iteration of the optimization process the circuit must be ran several times in order to calculate $\langle H \rangle$ with accuracy.

Improving VQE

As originally proposed, the Variational Quantum Eigensolver only finds the ground state of the Hamiltonian. However, we need the complete set of eigenstates and eigenvalues.

Some techniques allow finding the rest of eigenstates: modifying the cost function, orthogonal ansatz, folded spectrum method...

In the Folded Spectrum Method the excited states are found by searching the ground state of the modified hamiltonian $(H - Iw)^2$ where w is close to the corresponding energy.

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.
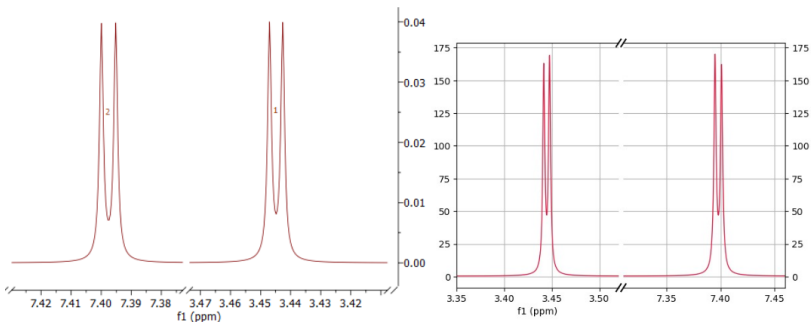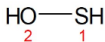
Thank you.

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