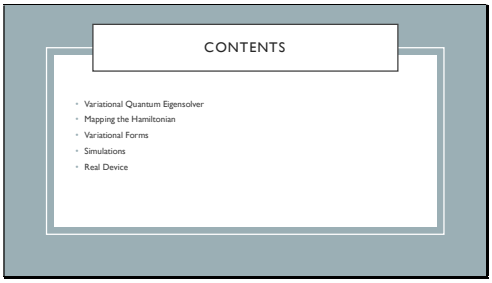
Presentation by Marco Antonio Barroca

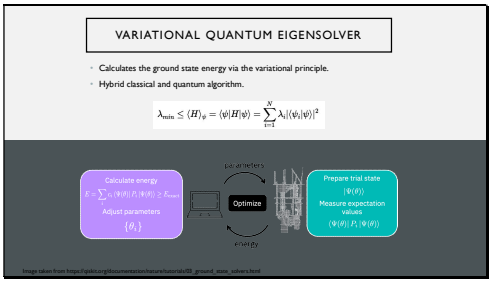
This work was based on a previous project from 2020 that relied on Qiskit as well as Wolfram Mathematica. It was updated to work with the most recent release of Qiskit and expanded to include the study of small perturbations of the harmonic oscillator (anharmonic oscillators).

In this version Mathematica is no longer required.



This is a simple index of what will be discussed in the presentation.

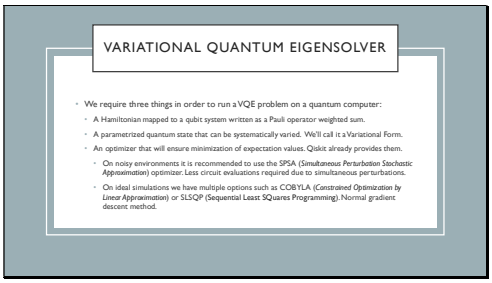
We shall first discuss what the VQE is, then how to build our problem for the algorithm and finally present our results after running the algorithm in simulations and real devices.



The algorithm requires the use of a classical computer.

We provide an initial guess of a parametrized quantum state, the quantum computer prepares the state and calculates the expectation value, the classical computer then updates the wave function to run another iteration based on the calculated expectation value.

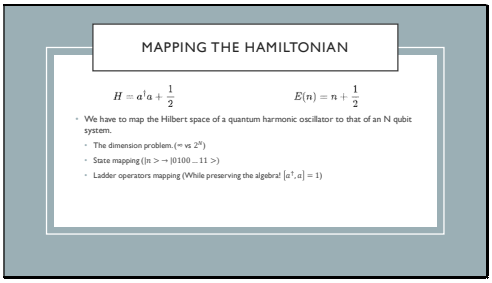
We can reach a lower bound for the expectation values after multiple iterations. This should be the ground state energy.



Optimization works by varying each parameter in the direction which opposes the gradient in order to find a local minimum. This is called gradient descent.

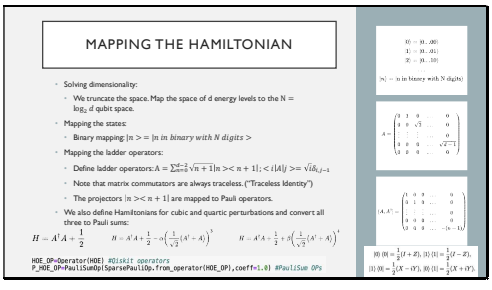
SPSA works by estimating the gradient of the objective function by simultaneously perturbing every parameter randomly and then evaluating the result of the expectation value. The idea is that as every parameter is being shifted, shifts due to noise are less relevant. noise gets "absorbed" into the process. This is also relevant as iterations do not increase with the number of parameters, which means less circuit evaluations.

Other optimizers such SLSQP will only vary one parameter at a time which means an increase in the number of iterations as the number of parameters grow. The exception to this rule is COBYLA making it ideal to reduce the number of iterations on non-noisy environments.



Note that in usual applications of the VQE, molecular Hamiltonians are mapped via Jordan Wigner mapping or alternatives such as parity mapping. Such options are already integrated into Qiskit.

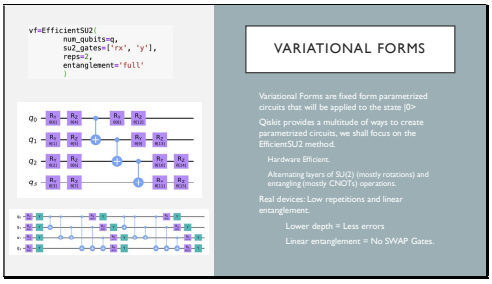
In our problem we must figure out how to realize the mapping of our system.



Converting Qiskit operators to Pauli Sums has become a lot easier recently. In a previous version of this project this had to be done manually on Wolfram Mathematica and imported into Qiskit, presently we can just call Qiskit functions.

It's important to note that these truncated Hamiltonians do not have the same spectrum as the complete ones, fortunately they agree at the ground state which should be enough as we are only interested in the ground state energy. This is only true for small perturbations as well.

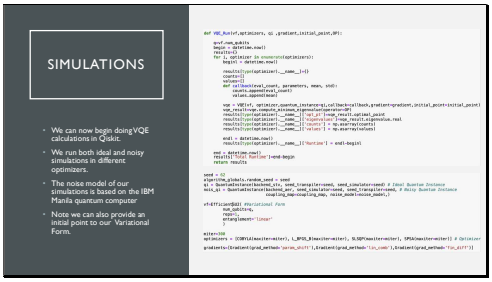
Further information on this can be found in the articles mentioned at the end of the presentation.



Hardware efficient: The recommended way to generate variational forms that will run on noisy environments.

Qiskit allows us to customize the variational form, we can define the number of qubits, which gates to use, the type of entanglement between the qubits, number of repetitions.

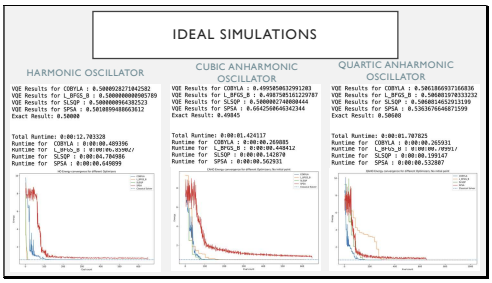
We want low repetitions for lower depth circuits and IBM computers usually prefer linear entanglements. Non-adjacent qubits aren't directly connected, full entanglement would require SWAP gates to entangle non-adjacent qubits increasing depth.



The function on the right executes the VQE algorithm while below we have set the initial parameters for the experiment such as the variational form, optimizer and quantum instance (responsible for simulation parameters such as the noise model)

Being able to provide an initial point to the variational form is interesting because we can use results from similar problems to facilitate the calculations in more complex problems.

In our case we can use the harmonic oscillator results as an initial point for the anharmonic oscillators.

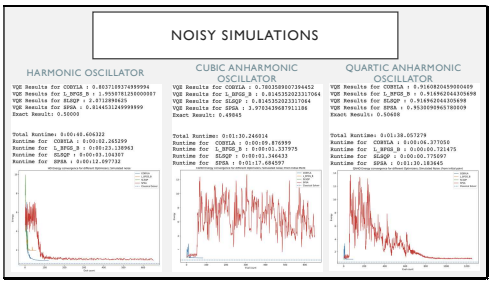


Note that these simulations were done for small perturbations (coupling g=0.2) as we mentioned before our model falls apart for larger perturbations.

SPSA is not the best for ideal simulations, taking longer and providing worse results.

The best optimizer seems to be L_BFGS_B (Limited-memory Broyden-Fletcher-Goldfarb-Shanno Bound) in the case of ideal simulation, although, with exception of SPSA, all the optimizers seem to give satisfactory results.

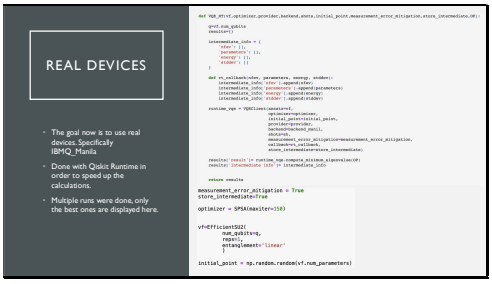
There was no need to provide an optimal initial point for the anharmonic oscillators.



As the noise predictably leads to worse results, we utilize a new strategy. In here we also use the parameters for the best result in the harmonic oscillator as the initial point of the variational form for the anharmonic oscillators.

SPSA results get considerably worse, but as we have improvements with the other three optimizers, we prefer this result. It's also worth noting that computation times decreased for all optimizers.

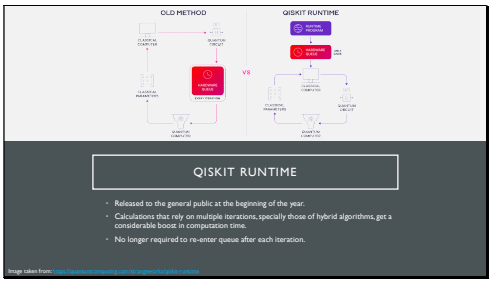
COBYLA now provides us with the best results. We might consider using it on a real device to see if this still holds in reality.



Again, we'll use the results of the harmonic oscillator as an initial point for the other two.

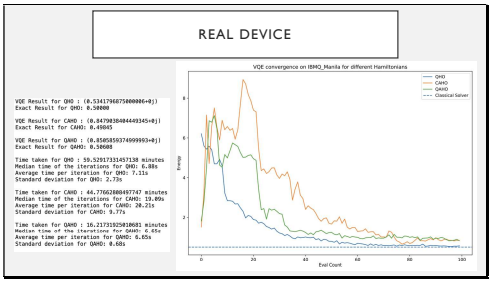
It's worth mentioning Qiskit Runtime before the results as it's recently released and essential to running this on real quantum computers.

Note that we won't display the COBYLA results in this presentation. Suffice to say that they were unsatisfactory.



Previously circuit evaluations would have to re-enter at the back of the queue after every iteration as optimization would take place locally.

With Qiskit runtime this is no longer necessary as the calculation is sent to the cloud as a container so it can be run in a classical computer closer to the quantum computer.



Previously (circa 2020) results would take a lot longer to compute as there was no Qiskit runtime. Running one iteration for the Harmonic oscillator would take the same time for 100 iterations with Qiskit Runtime today.

Note that computation times are inconsistent with more complex tasks taking less time. This is due to how busy the computers were between runs.

These references go deeper on how to work out the mapping of the Harmonic oscillator to a qubit Hamiltonian.