Benchmarking A Variational Quantum Eigensolver for Deuterium Simulation in Qiskit

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Abstract

The variational quantum eigensolver is an iterative algorithm combining classical and quantum computing methods in order to efficiently find the lowest energy state of a physical system. This has application in nuclear physics in the characterisation of heavy, unstable isotopes that are difficult to study empirically or to simulate purely classically. This requires a specific ansatz wavefunction in order to operate, and various ansatz paradigms currently coexist and compete in the literature. This paper investigates the capacity of the open source IBM module Qiskit to simulate a VQE by comparing its output to the exact analytical solutions of a simple Lipkin model nuclear Hamiltonian, with application towards utilising it to develop new and better ansatzes in future.

Introduction

Quantum computers (QCs) provide prospective and exciting solutions to many presently difficult problems. Although still a new field, quantum computing may offer new methodology in a range of scientific and mathematic fields, and has the capacity to revolutionise not only our computing power but also our scientific understanding of the natural world.

On this last note, QCs can more efficiently simulate quantum phenomena than classical computers (CCs). Simulation of quantum many-body phenomena in CCs runs into combinatorial explosion that rapidly overwhelms their computational capacity. A QC completely circumvents this problem by organically replicating the various possible states of a quantum system within its qubits – although moving into this new regime brings problems of its own, both practical and theoretical.

An example of a problem with which CCs struggle but QCs may prove very useful is the simulation of nuclear processes; for a key example, the determination of the ground state energy of a particular nuclide.

This is an important question as a system will tend to relax into its lowest energy state as a point of equilibrium; the behaviour of the nucleus is then affected by what this equilibrium energy eigenstate is. Knowing this ground state energy will allow for an understanding of how that specific isotope should behave in nature, without ever having to manufacture it physically.

Quantum Chromodynamics (QCD) can be used to simulate nuclei from the ground up starting with their constituent quarks – a technique called *ab initio*, 'from the beginning' – but QCD's intricate perturbative aspects make all but very simple calculations infeasible. QCD does allow for constraints to be placed that make it possible to calculate the ground state energy using other methods, however.

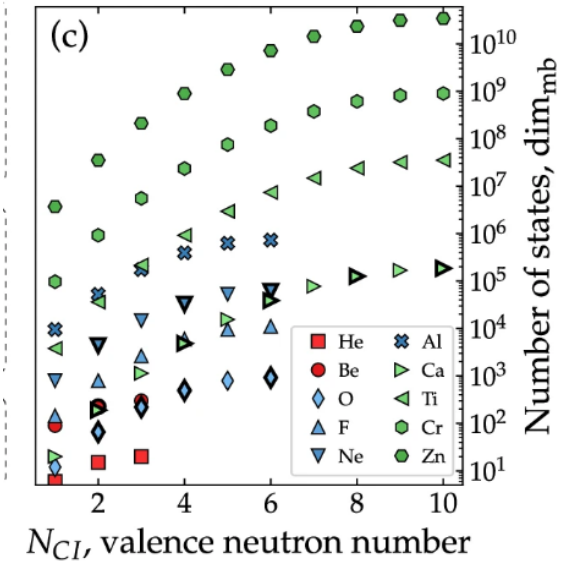
Another method is to use the Nuclear Shell Model (NSM) of the nucleus. This models the nucleons – protons and neutrons – as occupying orbitals of various energies, analogous to the iconic shell orbitals of the electrons. The inner ('inert core') and outer ('highly excited orbitals') nucleon positions are not considered as varying within these calculations; the former never loses particles, the latter never gains them. In practice, only a small number of positions, referred to as the 'valence band', are able to exchange nucleons.

The NSM was developed to explain the phenomenon of 'magic numbers' – isotopes with specific numbers of protons, neutrons, or both tend to be unusually stable. The key insight was to suggest that, in the same way that elements with closed outer shells of electrons are highly stable, isotopes with closed outer shells of protons or neutrons are; nuclides where both the proton and neutron number are magic are called doubly magic and are especially stable.

Simulating the NSM on a CC is not a trivial matter, although easier than an ab initio model. The number of possible positions occupiable within the orbitals by the nucleons undergoes a combinatorial expansion as the size of the nucleus grows, and these have to all be considered within the calculations because of energy minimisation interactions between different nucleons. [1] In mathematical terms the problem of finding the ground state energy of a specific nucleus corresponds to diagonalising a matrix whose dimension grows exponentially with nucleon number.

A CC is unable to simulate the nuclear processes of even relatively light non-magic [2] isotopes because the combinatorial explosion of possible occupation eigenstates – and corresponding exponential explosion of the relevant matrix to be diagonalised - overwhelms their computational capacity.

A QC does not suffer from this same combinatorial problem. It can be nudged into a direct analogue of the nuclear system, its qubits superposing in such a way that they represent the original eigenstates of the nucleus and will output values that correspond to its energies when measured. This means that unstable isotopes that are extremely difficult to create in the lab or to approximate using a CC can be analogised by a QC.



[1] For example an energy minimisation problem is completely trivial if the nucleons falling into the lowest energy orbitals available minimised the total energy – the least excited state for each nucleon corresponds to this energy eigenstate. However, in practice, some unintuitive combination of excitations may have lower energy than this Fermi height state because of the various ways in which orbitals can interact with each other to minimise their energy.

[2] Even relatively large magic isotopes can be fairly trivially simulated on a CC because their shell closure limits the number of possible nucleon positions for the magic nucleon. It as if the entire problem for that specific nucleon is reduced to the 'inert core', with removal of the 'valence band' where all the combinatorial troubles arrive. Indeed, for a 'doubly magic' (both protons and neutrons magic in number) isotope, there is only *one* possible configuration necessary to consider, ignoring excitations above the Fermi height.

Fig 1: The enormous number of possible many-body configurations for different numbers of valence neutrons in various relatively light isotopes. [3]

One especially efficient way that a QC is able to solve for the ground state energy of a given Hamiltonian – for example that describing the wave function of a nucleus - by solving an energy minimisation problem. This can be effectively done by using a Variational Quantum Eigensolver (VQE) – a combination of CC and QC methods. This is a relatively modern technique, developed originally for use in chemistry then more recently implemented in nuclear physics.

The VQE method requires the choice of a specific *ansatz*. This is a mathematical model representing the system that constrains its possible configurations – in this case energy eigenstates - and allows for the energy eigenvalues of these configurations to be found. Once this is chosen, the qubits are prepared in one configuration, and its eigen-energy found. The choice of parameters in the ansatz that correspond to this specific eigenstate are then updated using this eigen-energy to return an eigenstate with a lower eigen-energy. This process continues iteratively until the lowest eigen-energy configuration – the ground state of the Hamiltonian – is found. In this process, the QC holds each configuration, and the CC updates the parameters to feed into the QC at each step to produce a new configuration.

An analogy to the way a VQE works might be the use of Newton's Algorithm to find the roots of a function by iteratively minimising its absolute derivatives. In this case, the CC and QC work together to find a minimum point within a multidimensional space that corresponds to the lowest energy of the modelled nucleus.

The creation of this ansatz is a non-trivial decision. It has to mathematically represent the reduction in state-space associated with the restriction to the valence band, as well as to be able to effectively represent the original physical system being simulated.

The choice of representation of this ansatz in a physical system of qubits is also non-trivial. QCs remain, technologically, in their infancy, and overly elaborate – or 'deep' – quantum systems cannot be well constructed. It is necessary to increase the parsimony of the representation as much as possible to be able to achieve any results on par, let alone surpassing, a CC.

At present, the youth of the field means that many different ansatzes exist, and new ones are being frequently created. Many simulations use an ad-hoc ansatz designed for that specific system, which is then not generalisable. However, universal ansatzes that are applicable to many different systems exist.

An ultimate research goal would be to develop a universal ansatz that is highly efficient and easily constructed, both mathematically and practically, for the simulation of such large, difficult to otherwise study nuclear isotopes.

In this paper, the classical simulation function of the open-source Python module Qiskit is characterised and tested as a tool for this purpose. If this classical simulation of a QC is able to accurately model the behaviour of a VQE algorithm, then it provides an easy-to-use 'sandbox' for the testing of new ansatz ideas without the necessity for any actual quantum computation at the

[3] From *Nuclear shell-model simulation in digital quantum computers*, Pérez-Obiol et al, 2023.

developmental level. It could then join the array of already existing software that can be used in this field.

Methodology

In a recent paper[4], Professor Liang used the Unitary Coupled Cluster (UCC) ansatz to solve for the ground state energy of a simple model of a deuterium nucleus, drawing on earlier work by other researchers[5].

Professor Liang showed that the Lipkin model, a simple two-level model of the nucleus, provides very similar results to the earlier deuterium model when containing only two nucleons. He therefore implemented the Lipkin model for N = 2 using the UCC ansatz, a wavefunction realisation orientated towards a second quantisation [6] description of the physical system, resulting in the creation of a set of qubit circuits. [7]

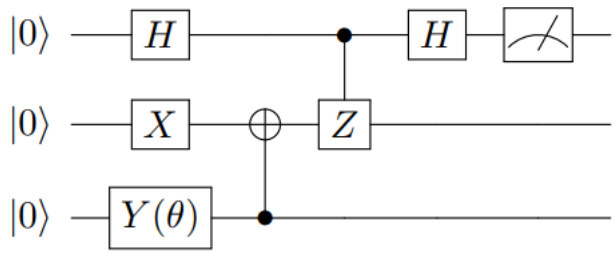
The advantage here is that each circuit has an exact theoretical value, which is a simple function of input parameters to the simulation. Therefore, it provides a useful benchmark of Qiskit; if Qiskit runs the underlying quantum simulation of this VQE correctly – as checked against the exact values – it demonstrates that Qiskit is able to successfully calculate the ground state eigenenergy of a real physical system, and therefore is a useful tool for VQE development.

Results

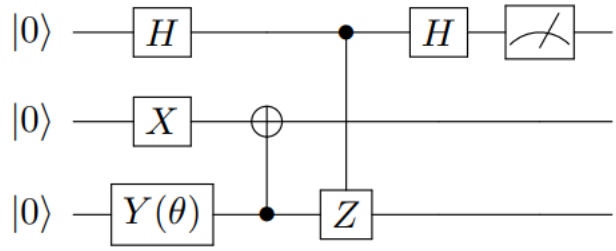
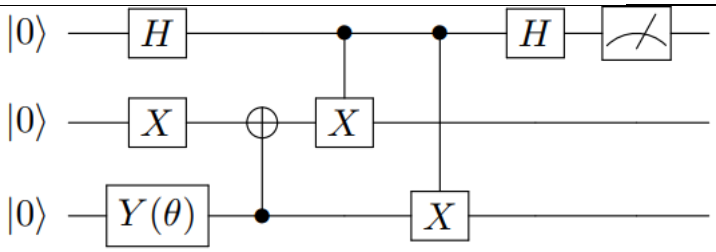
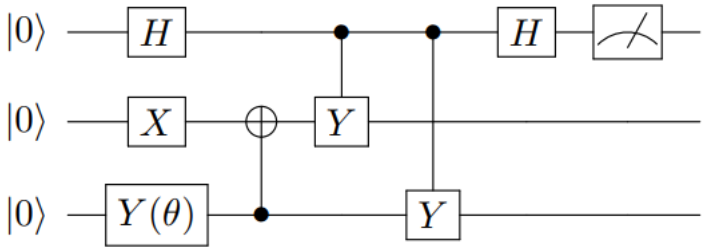
The deuterium Hamiltonian is given:

$$H = 5.906709 + 0.218291Z1 - 6.125Z2 - 2.143304(X + Y).$$

The variables Z1, Z2, X, and Y are given by a set of quantum circuits with outputs that are simple trigonometric functions of certain input angles [8]:

Circuit	Function
	$Z1 = -cos\theta$

[4] *Quantum Computing for Lipkin Model*, Liang, 2019.
[5] *Cloud Quantum Computing of an Atomic Nucleus*, Dumitrescu et al, 2018.
[6] Second quantisation is a mathematical formalisation that uses ladder operators referred to as 'creation and annihilation operators' to track the number of particles and holes (anti-particles) in a given energy level of the system; this can then be used to write the Hamiltonian in terms of created and annihilated particles and holes in all its relevant orbitals.
[7] The representation of a quantum program as a circuit diagram of quantum logic gates is a universal computational model for QCs, analogous to the commonplace use of a Turing Machine to represent a CC.
[8] The angle here is the rotation of the qubit in the Bloch Sphere formalisation, using a unitary Pauli gate.

	$Z2 = cos\theta$
	$X = sin\theta$
	$Y = sin\theta$

The angle for this Lipkin model of the deuterium nucleus is given:

$$\theta = 0.594279 \text{ rads}$$

Which sets the expected values of these variables:

$$Z1 = -0.828552 \text{ MeV}$$

$$Z2 = 0.828552 \text{ MeV}$$

$$X = Y = 0.559912 \text{ MeV}$$

So then the ground state energy is given:

$$H = 5.906709 + 0.218291(-0.828552) - 6.125(0.828552) - 2.143304(2(0.559912))$$

$$H = -1.749161 \text{ MeV}$$

The actual (empirical) ground state energy of a deuterium nucleus is around -2.22 MeV; this result from Professor Liang is, however close to first-order QC approximations produced by Dumitrescu et al (more advanced simulations were able to produce much closer approximations to the real figure).

E from quantum computing				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	$-1.74(3)$	$-2.38(4)$	$-2.18(3)$	
3	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

Fig 2: Dimitrescu et al's table of outputs of the ground energy of the D-2 nucleus on various qubit systems.

These quantum circuits were implemented in Qiskit using a local classical simulation, and their outputs after 1000 shots used to calculate a value of the Hamiltonian.

```
[77]:
1  Bencherz2 = QuantumCircuit(3, 1)
2  Bencherz2.h(0)
3  Bencherz2.rx(np.pi, 1)
4  Bencherz2.ry(ang, 2)
5  Bencherz2.cx(2, 1)
6  Bencherz2.barrier()
7  Bencherz2.cz(0,2)
8  Bencherz2.h(0)
9  Bencherz2.measure(0,0)
10 Bencherz2.draw()
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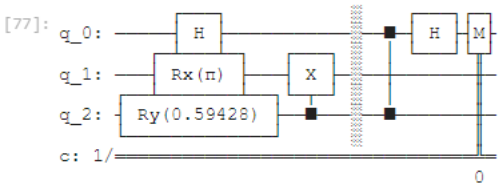

Fig 3: Code implementing and drawing the second circuit of the four.

Value (MeV)	Error
-2.22	0
-1.749161	23.7%
-1.743	24.1%
-1.655363699	29.1%

Fig 4: Comparison of the empirical result, Dimitrescu et al's approximate result, Professor Liang's theoretical result, and Qiskit's classically simulated result.

Discussion and Conclusions

Even using only its classical simulation mode, Qiskit was successfully able to run the UCC ansatz of the Lipkin model deuterium nucleus, producing a result close to both Professor Liang's theoretical Lipkin prediction and the first-order approximation of a qubit simulated D-2 nucleus.

The utility of this is clear by considering both the heavy study of deuterium as an isotope in both astrophysical and nuclear energy research, and also by considering a recent study which implemented the UCC ansatz to study the neutron drip line (NDL) of oxygen. [9]

As isotopes gain more and more neutrons, their behaviour becomes unintuitive. Standard forms of decay accessible by unstable nuclei are alpha, beta, gamma, and fission decay. However, isotopes of

[9] *Prediction of the neutron drip line in oxygen isotopes using quantum computation*, Sarma et al, 2023.

an element with more neutrons than that element's 'neutron drip line' (NDL) access a new form of decay – they directly emit neutrons to decay into lighter isotopes of the same element. The analogy in the name is that the neutrons 'drip' from the overburdened nucleus. This is uncharted territory; it is seen, for example, that very heavy O-isotopes that decay in this way are *more* stable than might otherwise be expected, with much longer half lives.

Isotope	Neutron enrichment	Approximate Half Life (seconds)
Oxygen-16	0	Stable
Oxygen-17	1	Stable
Oxygen-18	2	Stable
Oxygen-19	3	26
Oxygen-20	4	14
Oxygen-21	5	3
Oxygen-22	6	2
Oxygen-23	7	0.097
Oxygen-24	8	0.074
Oxygen-25	9	5.18 * 10^-21
Oxygen-26	10	4.23 * 10^-12

Fig 5: A table of oxygen isotopes, with post NDL nuclides in red. Note the anomalous increase in half life at O-26 compared to O-25.

The presence of the NDL in the isotopic chain of an element and the behaviour of such bizarre neutron decaying isotopes is difficult to experimentally verify – neutron decay isotopes of oxygen, for example, were only experimentally verified *after* my research project completed, in late August 2023 – several months after they were first able to be studied in a QC by Sarma et al. simulation of them in CCs is equally difficult; the heaviest element with a known simulated NDL is neon, atomic number 10.

An QC, which can directly simulate even very heavy isotopes of a nucleus, can be used to model such unexplored areas of the isotopic table, and provide insight into areas of physics that remain completely unassailable by even the most advanced CCs or experimental techniques.

The UCC ansatz clearly has promise to such theoretical modelling, but it can be conceptually difficult to directly implement on a quantum computer. By way of comparison, the Structured Learning (SL) ansatz is far more orientated more towards the parameters fed into a quantum circuit to create the analogue qubits.

As an example of this abstractification, the 'obvious' technique to convert a nuclear model into a set of qubits would be to have each qubit represent a given orbital in the nucleus, with 1 or 0 on that qubit representing whether it is occupied or not. This is, however, often not the most efficient technique; when the whole goal is to improve on CCs' poor efficiency while working with extremely finicky and limited physical qubits, it is more appropriate to produce a qubit configuration with less obvious intuitive relationship to the original situation, but mathematical equivalence to it. However, the outputs of such a module then need be interpreted in the original context to be meaningfully useful for physical predictions.

Drawing on a direct comparison by my supervisor of these ansatzes in a recent paper [10], it may be possible to combine the two techniques to gain the advantages of, and remove the disadvantages of, both. UCC is more orientated to the original system but more complex to work with in a VQE, and SL is more abstract relative to the original system but is easier to iterate. This means UCC results are easier to interpret in the context of the original system but can be more difficult to extract. An ansatz that uses SL for the VQE itself but then 'converts' the results into a second excitation framework to understand in terms of such theoretical predictions – perhaps at the classical iterative level - may be therefore a very useful innovation in this field.

In conclusion, Qiskit has proven itself to be able to effectively implement the UCC ansatz for Lipkin model simulations of the deuterium nucleus, even using only local CC simulation of qubit operations. Future research may focus on use of Qiskit in its remote QC mode, and further use in using Qiskit and the Lipkin approximation as a testbed for the development of new ansatzes, such as the above outlined speculative combination UCC-SL ansatz, in order to aid in the study of isotopes unassailable by present CC or empirical methods.

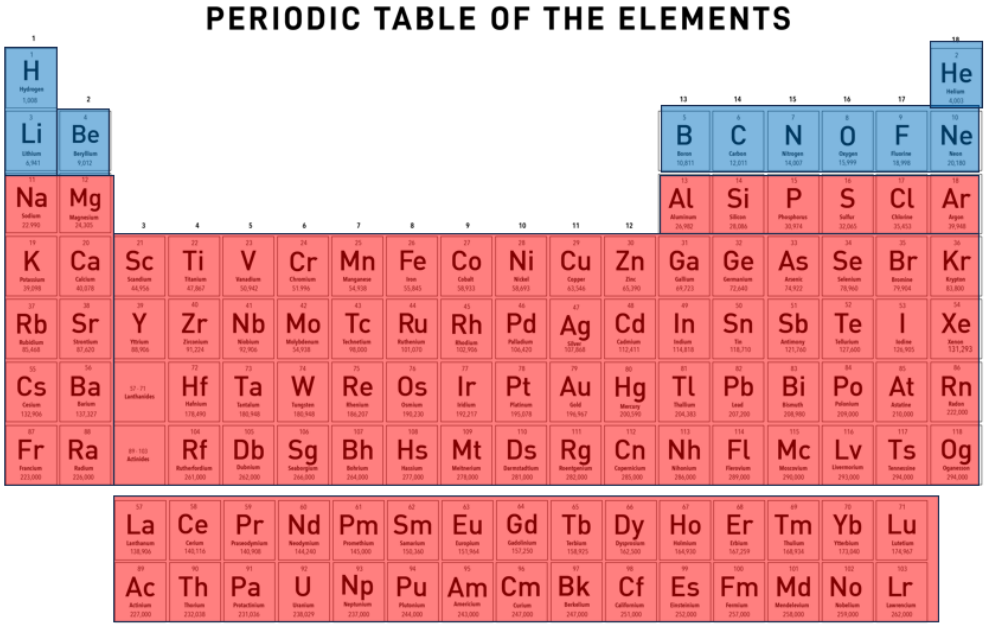

Fig 6: The Periodic Table, with all elements whose NDL, and therefore the behaviour of their heavier isotopes, remains completely uncharacterised.[11]

[10] *Quantum computing for the Lipkin model with unitary coupled cluster and structure learning ansatz*, Liang et al, 2022.

[11] Adapted from The Periodic Table blog, designed by Mia Viljoen.