Quantum Computations of Dark Energy Models

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***Abstract*—Dark energy is considered the main physical reason for the accelerating expansion of the universe, indirectly observed first in the 1990s through experiments such as the measurements of the luminosity distance of the type Ia supernovae (SN Ia). Different theoretical models for dark energy have been constructed through the years, all unique from the number of needed dimensions, required values of the cosmological constant λ, to the needed parameters to permit such exotic phenomena. Dark energy models simulated in this project include supercritical models as well as modified Einstein-Maxwell theories in six dimensions. Exponentially suppressed models with small values of λ, models with modified Einstein-Maxwell landscape equations and Einstein-Born-Infield flux compactification models will also be discussed, though not simulated in code. Potentials for each of the models will be used to construct the Hamiltonian and calculate their ground state energies. Python-based quantum computing software development kit Qiskit and Mathematica are the main tools used in the construction of the hamiltonians for the different models. The main quantum algorithm used throughout the experiment is the Variational Quantum Eigensolver (VQE), an algorithm developed by IBM for obtaining the minimum eigenvalue of a system. Analyses and computations of the hamiltonians and ground state energies of the models have been completed, with comparisons made between both the classical results calculated in Mathematica and the VQE results using different combinations of simulators and optimizers.**

I. Introduction

Quantum computing brings many advantages over classical computational methods, having greater processing power and speed. It is still a budding field, as only the framework for it is in place and the likelihood of commercial quantum computers is still in the distant future. However, that isn't to say it does not have its' uses at the moment. There are various applications of its' techniques now in day, allowing an increased precision of analysis in chemical systems to a greater sense of cybersecurity due to the entangled nature of quantum bits, qubits. It's as Richard Feynman once said, "... if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.", referring to the complicated certainty of the difficulty of modeling natural systems via classical computational methods.

This leads us to the systems of interest in the scope of this experiment - cosmological models with different interpretations of dark energy. Dark energy studies is a new field, stemming from astronomical observations made recently in the 1990s'. Seen as the reason as to why the universe expands at an accelerating rate, it is one of the most busy fields in cosmology right now, as understanding what exactly it is and its' behavior may allow us to uncover more about the past state of the universe, as well as predict how the universe may evolve in the future. String theory, quantum loop gravity, supersymmetry - all of these are exotic theories all include the mathematics of dark energy into it, introducing new particles such as the dilaton and radion to be able to back the mathematical and scientific reasoning of their theories.

Given the possibilities of various mathematical and theoretical explanations trying to give the existence of dark energy justification, it stands to reason that we as scientists want to use all types of tools to better understand these models. This sort of quantum computing application to cosmological models isn't the norm, as there have been few experiments which uses the power of quantum computing to study these types of models [7]. For this experiment, we will be looking to apply quantum computational methods, specifically the application of a quantum algorithm, onto some different cosmological dark energy models and calculate the ground state energies, E_{gs}, of every one of the models' potentials. We will compare our quantum computational results to ones made through classical computational means, and identify any possible advantages in using the quantum techniques.

Section II will cover quantum computing aspects needed for this project, discussing some of the basics as well as IBM's' quantum library QISkit and the specific quantum algorithm used throughout. We will then move onto dark energy in Section III, where we'll review what dark energy models are being examined in this project. Results of the exact ground state energies for each of the models will be analyzed in Section IV along with other values and plots, with discussions and conclusions made from the results discussed in Section V.

II. Quantum Computing

For the aim of this experiment, dealing with complicated equations of advanced theoretical systems, it is important to use tools such as quantum computing as alternativew and perhaps more efficient instruments of calculations and visualizations. The computational basis which quantum computing is built upon, dependent on the state of data rather than discrete values, allows for more computing power and processing speeds. Superposition and entanglement of the qubits, along with the usage of quantum circuits to manipulate the state of the qubit, allows for more advanced computing capabilities.

An important component of this experiment in regards to quantum computing is the implementation of a quantum algorithm to our models in calculating the ground state energy,

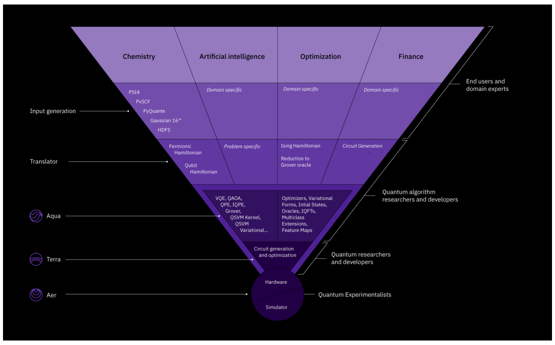


Fig. 1: Qiskit Software Stack

E_{gs}, for each one. Quantum algorithms differ from their classical counterparts from the concept of data now being encoded into the state of a set of input quantum bits, referred to as qubits, to the quantum circuits which interact with the generalized state of the qubit as it passes through [2].

A. Variational Quantum Eigensolver

Qiskit is an open source software development kit released by IBM which allows users to simulate and work with quantum computers in constructing circuits, algorithms, and much more. Qiskit is composed of four different elements - Terra, Aer, Ignis, Aqua - all of which serve different functions and consist of various modules which allow the user to utilize different quantum computing structures, as depicted in Fig. 1. The quantum algorithm which we use on the models is from this SDK, within the aqua element, and is called the variational quantum eigensolver (VQE) algorithm.

The VQE is based off the variational principle of quantum mechanics, which claims that

$$E_{gs} \leq \langle\psi|H|\psi\rangle \equiv \langle H\rangle \tag{1}$$

where Eq. 1 states that the expectation value of the H in the state ψ is bound to overestimate the expected value of the ground state energy. But as the trial state ψ is changed to a form which is much more accurate to the correct expression, the expectation value for H begins to represent a closer estimation of the ground state energy. So what the VQE essentially does is fine-tune the form of the ansatz wave function until a close approximation of the expected value is reached. A representation of the VQE process is illustrated in 2. There are many parameters which the VQE takes into account, but two important ones that are truly defined by the user are the optimizers and simulators being used.

For this experiment, the two simulators being used in the VQE include the statevector simulator and qasm simulator. Statevector simply executes a single shot of a Qiskit quantum circuit and then returns the final quantum statevector of the simulation. On the other hand, the qasm simulator actually mimics a actual quantum device, executing multiple shots of a quantum circuit.

Local optimizers are used in the algorithm, which seek to find the optimal value for a problem within the neighboring set of a candidate solution, as opposed to global optimizers which look at larger sets of solutions. Optimizers used for this experiment are limited to the Limited-memory BFGS Bound optimizer (L_BFGS_B), Constrained Optimization By Linear Approximation optimizer (COBYLA) and Sequential Least SQuares Programming optimizer (SLSPQ). These were used by past interns for other projects, so we decided to utilize these in this case as well.

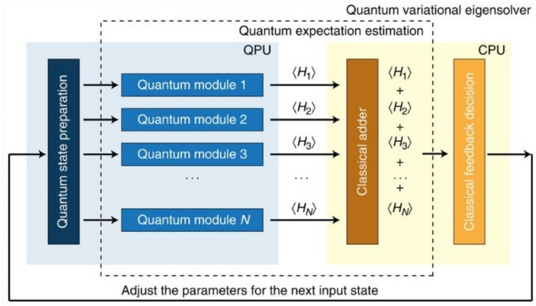


Fig. 2: Variational Quantum Eigensolver Flowchart

III. Dark Energy

A large number of recent observational data strongly suggest that we live in a flat, accelerating Universe composed of $\sim$1/3 of matter and $\sim$2/3 of an exotic component with large negative pressure, referred to as dark energy [19]. It is now recognized as the physical reason for which the universe expands at an accelerating rate, an observation made in the 90's which went against our decades long belief that we had been living in a static universe. But with experiments such as the spectral and photometric observation of the Type Ia supernovae, limitations were put on cosmological parameters and showed this accelerating expansion [16].

If looking at the total observed energy-density of the universe, there have been experiments which already led us to know certain components' values. When it came to the total atomic matter density (baryonic and dark) in the universe, that came out to only around 30% of the total energy-density. So it was hypothesized that around 70% would have to be composed of some unknown energy, which has been labeled as the dark energy. This partition of the energy-density of the universe is illustrated in Fig. 3.

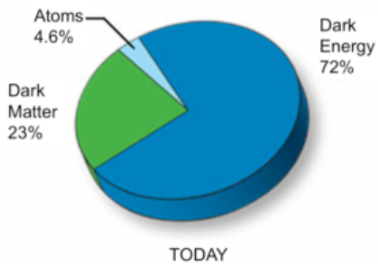


Fig. 3: Energy-density distribution of the universe

An important physical term which has been measured over the past years is the cosmological constant λ, also known as the vacuum energy density, Ω_λ [17]. First introduced by Einstein in an effort to explain his theory of a static universe, it was re-implemented after the observations of dark energy so it is theoretically possible to explain the accelerated expansion of the universe. Calculating an acceptable value for λ requires one of the highest level of fine-tuning in physics, with the order of magnitude being on the scale of 10^{18} and precision to a large degree of magnitude. That leads to the biggest discrepancy that physicists face with the cosmological constant, as our measured value for λ is smaller than the theorized value by an order of 120 magnitudes. There have been calculations which better the observed values, such as ones by Weinberg [18] and Alexander Vilenkin, but this cosmological constant problem remains as a hotbed of discussion within the scientific community.

With the different interpretations of λ, and other parameters and concepts that deal with dark energy, there are many different models that arise to explain dark energy and how it may fit into other theories. In this experiment, we will just focus on simulating two - a dilaton potential describing a supercritical model and the Einstein-Maxwell theories modified to apply to six dimensions.

A. Dilaton Potential

The first model being simulated is one based on supercritical string theories in more than 10 higher extra dimensions, described by an Einstein frame dilaton potential [12]. When speaking of a dilaton potential in the context of this model, it takes the form

$$V(\phi) = e^{\frac{4}{d-2}\phi}(a - be^{\phi} + ce^{2\phi}) \tag{2}$$

where the parameters a, b, c, and d are all set constants - in the case of this experiment and normalization sake set to 50, 100, 50, and 4, respectively. It's also seen in Eq. 2 that the potential is dependent on a variable ϕ, known as the dilaton. The dilaton is a type of particle theorized by string theory and quantum gravity, and depending on the value for it, the potential of these types of models will also change. This model, the modified Einstein-Maxwell models talked about in the section and sample potential introduced later in the paper are all dependent on the dilaton.

Illustrated in Fig. 4, the potential has a local minimum at x = 0, in which the dilaton has no value. The quantum tunneling behavior of the wave functions is also apparent, as it is shown how they decay while within the peak and oscillate on either side of it, and how those wave functions whose energies are above the peaks oscillate normally as they are not affected. Just for simplicity sake, the modified EM theory discussed in Section III.B is of the same shape and wave function behavior and is not shown for that reason.

There are interest in these types of models as they are an example of models in which cosmological constant reduction by flux relaxation can be explored, leading to another route of understanding the value of λ.

B. Modified Einstein-Maxwell Theories in Six Dimensions

In this second model, physicists were able to extend the Hartle-Hawking proposal, which states that the quantum state

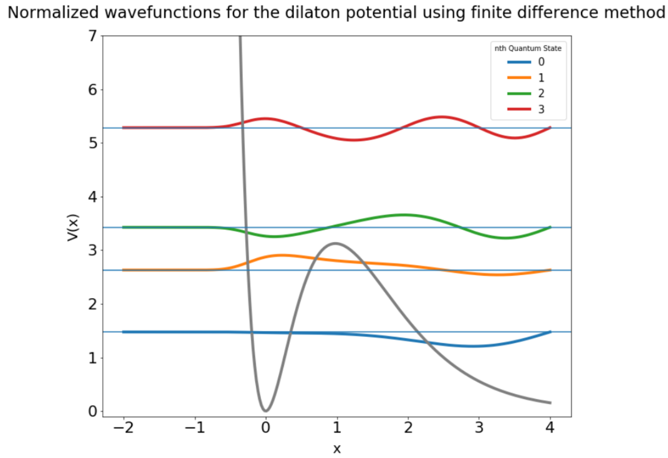


Fig. 4: Dilaton potential plotted along its' first four wave functions at their corresponding energy levels

of the universe is defined by a path integral over compact 4-metrics and regular matter fields, to higher dimensional models [9]. This extended HH proposal is then used to construct a cosmological wave function for the Einstein-Maxwell theory in six dimensions. The canonical formalism of the Einstein-Maxwell (EM) theories may easily be extended to higher dimensions, in this specific case six, so the application of the extended HH proposal is allowable in this particular case.

The potential equation for this model is in the form of

$$V(\phi) = \frac{1}{3}[\epsilon e^{-3\sqrt{6}\phi} - 2e^{-2\sqrt{6}\phi} + e^{-\sqrt{6}\phi}] \tag{3}$$

where the constant ϵ is dependent on values of the cosmological constant and gravitational constant, G.

It is important that we note the form of the Hamiltonian for these models, which will be the same for all of them. It is simply

$$H = \frac{p^2}{2} + V(\phi) \tag{4}$$

where the p is the canonical momentum of the system, which it then added with the desired potential, a function of the dilaton. Another note to make is in regards to units of the potential energies of the models discussed in this paper. All of the potentials will be described in the same units used in [9], which is reduced planck mass, M_P. The relation between planck mass and the reduced form is

$$M_P = \sqrt{\frac{\hbar c}{8\pi G}} = \frac{m_P}{\sqrt{8\pi}} \tag{5}$$

where m_P is the Planck mass, G is the gravitational constant, c is the speed of light and $\hbar$ is reduced Planck constant.

C. Additional Models

Additional dark energy models, though were not simulated as part of this experiment, are worth noting. The first of which is those involving flux compactifications, which is a generalization of the Kaluza-Klein models and deals in the manner in which extra dimensions are compactified and if the compactifications allow fluxes to pass through [4]. An example of this is the flux compactification with respect to the Einstein-Born-Infield theory [15], where the EBI theory is considered and the flux vacua after spontaneous flux compactification is studied. Another theories include those which deal with the landscape equations of Einstein-Maxwell [3], and compactifications within de-Sitter space [5] and dynamic extra dimensions [4]. There are also models which steer away from flux compactifications, and deal with exponentially suppressed models [11], even including some cases where the cosmological constant may have a negative value.

IV. Results

The hamiltonians for all of the models were created through the finite difference method, in which the potential and kinetic matrices are made and then added up to construct the hamiltonian matrix. The H matrix is then diagonalized to obtain the eigenvalues (energies) and eigenfunctions (wave functions). The lowest eigenvalue is then singled out, and recorded as ground state energy for that hamiltonian.

The two potentials run through the VQE include the aforementioned dilaton potential as well as a constructed sample potential. This potential

$$V(\phi) = e^{-0.25\phi}(e^{-2\phi} - 2e^{-2\phi} + 1) \tag{6}$$

was formulated and chosen as a comparison to the models due it's similar shape and behavior of wave functions, as is illustrated in Fig. 5.

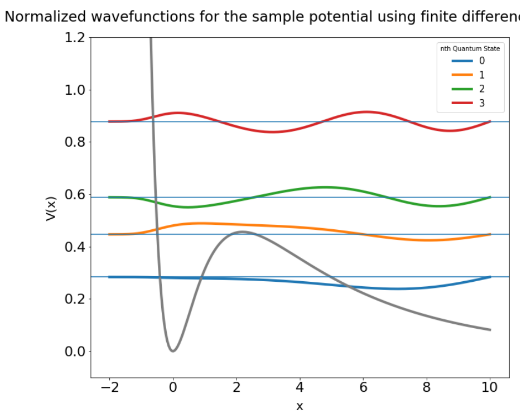
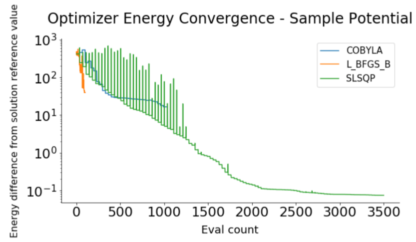


Fig. 5: The sample potential plotted alongside its' first four wave functions at their corresponding energy levels

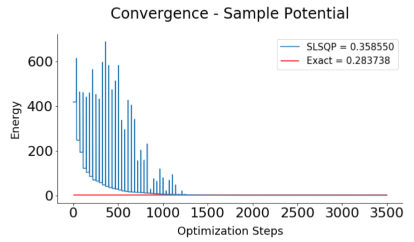
Mathematica Results	
Model	Ground State Energy
Sample	0.159456
Dilaton	0.0287246
Modified EM	0.0174982

TABLE I: Mathematica results for the ground state energies of the sample, dilaton, and modified Einstein-Maxwell potentials

Before discussing the results calculated through the VQE algorithm, there are some classically obtained values calculated through Mathematica that should be considered. Presented in Table I, the three potentials - dilaton, modified Einstein-Maxwell, and sample - were plug into Mathematica and manipulated in the finite difference basis to classically retrieve their ground state energies. All values for the ground state energies from Mathematica were acceptable results, due to their closeness to the minimum of the potential and their respective wave functions behaving similar to the potentials depcited in Fig. 4 and Fig. 5.



(a) Energy convergence for the different optimizer used on the sample potential



(b) Number of optimization steps for the most efficient optimizer to near the exact energy

Fig. 6: Optimizer and Energy Convergence plots for the sample potential while using the statevector simulator

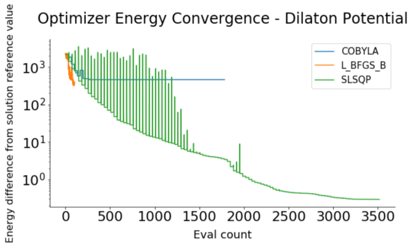
A. VQE

So with the dilaton and sample potential run through the VQE algorithm, different values were calculated for the ground state energies of the models. These values, six different ones for each model due to the various combinations of optimizers and simulators, are illustrated in Table II.

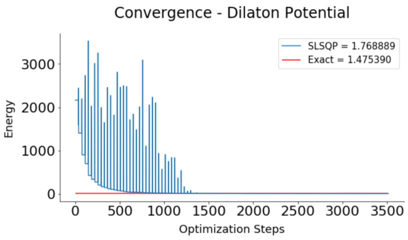
Sample Potential VQE Results			
Optimizer	Statevector Simulator	QASM Simulator	Exact Energy
SLSQP	0.358550	1.183140	0.28373794
L_BFGS_B	16.869957	3.368392	
COBYLA	39.830447	142.121231	
Dilaton Potential VQE Results			
SLSQP	1.768889	4.641707	1.47538977
L_BFGS_B	461.631826	47.301525	
COBYLA	317.526316	257.750962	

TABLE II: VQE results for both the sample and dilaton potential

Basing off the results in Table II, we were able to write up code in the pythons script which plotted the different optimizers and evaluation counts it took for them to reach their ground state energy values. After doing that, it became evident that the SLSQP resulted in energy values that were within statistical significance to the exact, so another plot showing



(a) Energy convergence for the different optimizer used on the dilaton potential



(b) Number of optimization steps for the most efficient optimizer to near the exact energy

Fig. 7: Optimizer and Energy Convergence plots for the dilaton potential while using the statevector simulator

the number of optimization steps it took for SLSQP to reach its' minimum energy value was created for both models.

It's important to note that these plot, illustrated in Fig. 6 and Fig. 7, only plotted and considered the optimizers while being used with the statevector simulators. This is based on the observations that results from the qasm simulator, depicted in Table II, had too great of percent errors from the exact values to be considered as acceptable values. As such, the optimization steps in these cases were deemed not relevant enough to make these plots.

Comparing the Mathematica and VQE values in Tables I and II, we are able to calculate the percent error shown in Table III to be able to visualize the level of accuracy of these results to the expected values. For the calculated percent errors, that only ones shown are those which calculated values are at least under 100% away from the exact ground state energy value. So no percent errors for results from the Qasm simulator, or as well as the COBYLA and L_BFGS_B, are shown and indicates that that simulator and optimizers did not result in allowable results and should be disregarded for future analyses on these models.

Potential Percent Error Values (%)			
	Einstein-Maxwell	Dilaton	Sample
SLSQP with Statevector	N/A	19.89297	26.36672
Mathematica	17.49820	93.83297	43.80166

TABLE III: Percent errors for both VQE and Mathematica results, where percents below 100% away from the expected are shown

V. Conclusion

We used quantum computing to simulate dark energy models and explore features such as stability and tunneling in the potential. Analyzing the results from both Mathematica and the VQE listed in Tables I and II, it is clear that there are accurate results in some cases, and others not. It is clear that in terms of percent errors and magnitude of difference between computed and expected values for E_{gs} that the best VQE results stemmed from using the combination of the statevector simulator and SLSQP optimizers, producing percent errors from the expected of 19.89297% and 26.36672% for the dilaton and sample potential, respectively. But it is also important to note that the values for the energy levels through our python scripts were not accurate to the true value of the potentials' minimum of 0, instead calculating the ground state energy to be at levels of either 0.28373794 or 1.47538977 for the sample and dilaton potential. In this regard, the Mathematica results for the ground state energy are more accurate as they are closer to the minimum values of the potentials. This discrepancy in the python script and VQE should be looked at in future experiments and fixed, as to knowing why we get ground state energy values that are not as close to the minimum as they should be will be beneficial.

In the future we wish to work in other basis, like the position and oscillation ones, as to allow more freedom in manipulating and visualizing the wave functions of the potentials and perhaps to get more precise results with the ground state energy values. These models and potentials should also be modeled using different quantum algorithms, such as finite temperature or quantum tunneling algorithms, in order to see how the results differ and if there is any algorithms which produce more precise and accurate results.
We would also like to couple these models to gravity, to see how they would effect the early and late Universe. Additionally we'll also like to simulate the other dark energy models, see how they behave and how the VQE applies to them. Models such as those theorized by Randall on the compactification with respect to de Sitter space [5], or those involving exponentially suppressed cosmological constants looked at by Itoyama [11] are of interest.

This experiment showed the capabilities of quantum computing applications to these models, while also demonstrating its' faults. With many more models and potentials to explore, different combinations of simulators and optimizers to use, and much more parameters to change, there is a lot of potential to improve upon these results and expand upon this experiment to model various different types of dark energy and cosmological models through the power of quantum computing.

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