Morse Potential on a Quantum Computer and Supersymmetric Quantum Mechanics

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Abstract

The Morse potential describes diatomic molecules and has a finite number of bound states which can be measured through spectroscopy. It is an example of an exactly soluble potential using supersymmetric quantum mechanics. Using the supersymmetric quantum mechanics formalism, researchers can derive a hierarchy of Hamiltonians such that the ground state of the next rung on the hierarchy yields the first excited state of the Hamiltonian below it. This method can determine all the states of the Morse potential by calculating the ground state of each Hamiltonian in the hierarchy. We use the Variational Quantum Eigensolver (VQE) algorithm to calculate the energies of the Hamiltonians and find agreement with the exact expression for the bound state energies of the Morse Potential. We analyze different variational forms, Hamiltonian mappings, and optimizers to study the numerical effect on the calculations.

Methods

Quantum Computing

While classical bits are powered with transistors via electrical currents, quantum bits are usually quantum objects such as electrons or photons. This enables a superposition of states that greatly increases computing power. N qubits are equivalent to 2^N classical bits, making the computational complexity orders of magnitude less for some calculations.

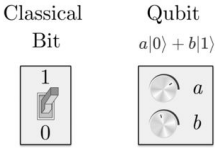

Fig. 1: Classical bit vs. qubit [1].

Variational Quantum Eigensolver

The Variational method is a very powerful approximation in quantum mechanics. It allows researchers to set an upper bound on the ground state of a system by guessing a random wave function and finding the expectation value of the Hamiltonian. Outlined below in equation 1.

$$E_{gs} \leqslant \langle\psi|H|\psi\rangle \equiv \langle H\rangle \quad (1)$$

This avoids having to solve ominous differential equations normally encountered and is very soluble mathematically.

We used IBM's Quantum Information Software Kit (QISKit), to run the VQE algorithm [2] on the Morse potential (eq. 2) [3]. Our goal was to try and calculate with the accuracy and precision the ground state and first excited state for this potential.

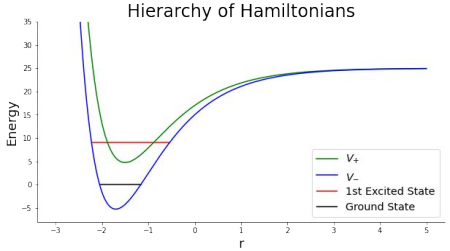

Fig. 2: The Hierarchy of Hamiltonians for the Morse potential.

VQE is limited because it only gives an approximation for the ground state when molecules can have hundreds of excited states that are more interesting. We can use VQE to find excited states by constructing a new Hamiltonian that has a ground state corresponding to an excited state we are interested in (Fig. 2).

$$V_-(x,A) = e^{-2x} - (2A+1)e^{-x} + A^2 \quad (2)$$

$$V_+(x,A) = e^{-2x} - (2A-1)e^{-x} + A^2 \quad (3)$$

Results

Table 1: Results from IBMQ QASM simulator.

Ground State: Exact Energy = 0.88760				
Basis	**# Qubits**	**Optimizer**	**VQE Energy**	**% Error**
Position	3	SPSA	1.06153	19.5962
		COBYLA	12.6171	1321.49
		L_BFGS_B	28.5255	3113.79
		SLSQP	32.6416	3577.53
1st Excited State: Exact Energy = 8.47022				
Basis	**# Qubits**	**Optimizer**	**VQE Energy**	**% Error**
Position	3	SPSA	8.38899	0.958978
		COBYLA	10.4016	22.8024
		L_BFGS_B	71.8171	747.878
		SLSQP	72.0451	750.57

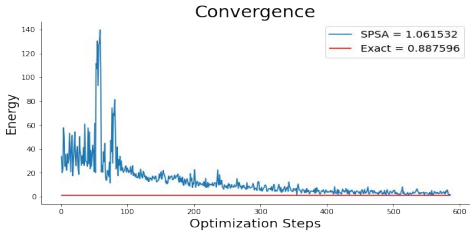

Fig. 3: Convergence for ground state of the Morse Potential.

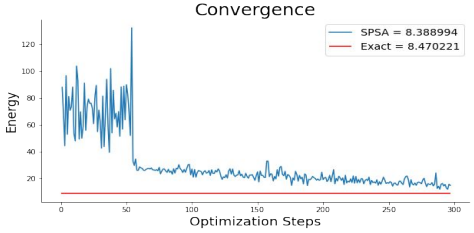

Fig. 4: Convergence for first excited state of the Morse Potential.

Conclusion

We were able to accurately and precisely calculate the ground state and first excited state of the Morse potential. However, a significant trade off between accuracy and precision was prominent. We also ran into run time issues with IBM's public quantum computers as the algorithms are computationally expensive and when extra time for queuing is added the runtime can exceed many days.

Acknowledgements

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References

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