Qhack Open Hackathon Presentation

1. Introduction

We investigate QAOA and VQE performance for a relatively new class of constrained optimization problems in this open hackathon challenge. In concrete, we consider the supersymmetric (SUSY) quantum mechanic lattice N=2 model introduced by Fendley, Schoutens, and Boer [doi.org/10.1103/PhysRevLett.90.120402]. This model is exciting since determining the supersymmetric ground states of a Hamiltonian with fermion number l is equivalent to finding l-dimensional holes in the corresponding independence complex. The finding of l-dimensional holes in the independence complex is vital in topological data analysis (TDA) - an approach for analyzing data using tools from topology. In general, the SUSY ground states of the lattice N=2 model for graph $G(V,E)$ are connected directly to the cohomology groups of the independence complex $I(G)$. Interested readers might take a look at Chris and Marcos's work for more detail, [arXiv:2107.00011]. Additionally, many systems can be modeled as SUSY quantum mechanics models. The SUSY model could also arise at special points in the phase space of other systems [DOI: 10.1126/science.1248253; doi.org/10.1103/PhysRevB.76.075103]. Nevertheless, there has not been much work in analyzing these models using quantum algorithms.

In $M=m$ model, the Fermions have "hard-core" such that two Fermions must be (m)-distance apart. This results in many of the invalid states having zero energies. These two obstacles usually make VQE not suitable for these problems. One could circumvent this by using post-selection to ensure the state is in the valid subspace; however, this suffers the problem of being unable to control the success probability of sampling. On the technical side, Pennylane is currently not supporting the post-selection circuits. Therefore, we try a new approach by modifying the cost function to penalize when the state is not in the valid subspace. By doing this, the cost function for our VQE is similar to combining the regression problem and classification problem into one cost function.

On the other hand, Grover Mixer-QAOA (GM-QAOA) introduced by Andreas and Stephan at [https://arxiv.org/abs/2006.00354v2] could be suitable for this problem (ignoring the obstacle of creating the simulation blocks) if we could find an efficient unitary operator that initializes states in a superposition of valid states. One way to achieve this is by extending the Grover mixer. This can be done by allowing the initial state to be variational, rather than the equal superposition of all valid states.

2. Fermionic hard-core model

In SUSY quantum mechanics with N=2, the Hamiltonian H is given by

$$H = \{Q, Q^\dagger\}$$

where $Q, Q^\dagger$ are nilpotent operators, i.e. $Q^2 = (Q^\dagger)^2 = 0$. We define the "Fermionic" number operator $F = Q^\dagger Q$. The Hamiltonian commute with the "Fermionic" number operator $[H, F] = 0$. The energy eigenvalues of H are semi-positive definite $E \geq 0$. For $E = 0$, the ground state $|g\rangle$, if exists, is a singlet satisfies $Q^\dagger |g\rangle = Q |g\rangle = 0$. Conversely, if $Q^\dagger |g\rangle = Q |g\rangle = 0$, the state is the ground state with energy $E = 0$. On the other hand, excited states with $E > 0$ are doublet. Let's $H |E\rangle = E |E\rangle$ with $E > 0$ and $Q |E\rangle = 0$, then $Q^\dagger |E\rangle$ is also eigenstate of the Hamiltonian with the same energy.

In the M=1 lattice model, we define the operator Q and $Q^\dagger$ as

$$Q = \sum_i \lambda_i c_i P_i, \quad Q^\dagger = \sum_i \lambda_i c_i^\dagger P_i$$

where $c_i, c_i^\dagger$ are fermionic creation and annihilation operators, the parameters $\lambda_i \in \mathbb{R}$. The operator $P_i = \prod_{\text{j near i}} (1 - c_j^\dagger c_j)$ iterate over the nearest neighbours of site i and enforces the condition that the electrons must be 1-distance apart. The number operator is given by $F = \sum_i c_i^\dagger c_i$ and the Hamiltonian is

$$H = \sum_i \sum_{\text{j next to i}} \lambda_i \lambda_j P_i c_i^\dagger c_j P_j + \sum_i \lambda_i^2 P_i$$

The first term of the Hamiltonian describes the hopping of fermions with hardcore, whereas the second term favours more electrons as long as they are (2)-distance apart. In this sense, the second terms describe a repulsive potential between the fermions. This model can be extended to any $M = m$ by modifying P_i, and for any connected graph. We consider the case $\lambda_i = \lambda = 1$. We

note that by changing λ_i, one could obtain exotic excitations [doi.org/10.1103/PhysRevLett.128.050504]. Nevertheless, our approach is independent on $\{\lambda_i\}$. We map the fermionic system to the qubit system using the Jordan-Wigner transformation for simplicity and for the number symmetry to be the same in both representations.

$$c_i = \prod_{j<i}(-Z_j)\sigma_i^- P_i, \quad c_i^\dagger = \prod_{j<i}(-Z_j)\sigma_i^+ P_i$$

3. Grover Mixer-QAOA (GM-QAOA)

One of the main problems in GM-QAOA is preparing a good initial state $|F\rangle$. Denoting the set of valid states. If we could efficiently prepare an initial state of the form

$$|F\rangle = \sum_{f\in F} c_f \, |f\rangle$$

using a unitary U_S, then we could use the Grover driver

$$U_F(\beta) = e^{-i\beta|F\rangle\langle F|} = U_S[I - (1 - e^{-i\beta}) \, |0\rangle \, \langle 0|]U_S^\dagger,$$

where U_S prepares the initial state $|F\rangle$, i.e. $U_S \, |0\rangle = |F\rangle$. With this expression, the driving block can be efficiently implemented without trotterization.

For the $M = 1$ model, we can construct U_S using generalized multiple control gates (N-Toffoli gate). We define the operator C_i as

$$C_i(\theta_i) = \mathrm{ANTI} - C(\mathrm{j\ near\ i}, i, R_X(\theta_i))$$

where $\mathrm{ANTI\text{-}C}$ is the anti-multi-controlled gate which only activates rotation X on the target qubit if all control qubits are in state $|0\rangle$. The control qubits are identified as site j next to the qubit site i. θ_i is the rotation-angle that rotation X acts on site i qubit. The unitary U_S is defined as a sequence of C_i gates

$$U_S = \prod_i C_i(\theta_i)$$

We can see that the operator U_S creates an unequal weighted superposition of valid states whose amplitudes depend on the angles. One can reduce the depth of U_S by applying C_i, C_j in parallel assuming that sites i, j are not neighbours. Furthermore, for state preparation, we can reduce the number of CNOT gates by keeping track of which node we have applied C_i. For instance, if we have not applied the operator C_i to site j, and we start with $|0\ldots0\rangle$, then we only need to do R_X gate on-site j. We note that the initial states are controlled by the variational parameters $\{\theta_i\}$ such that it is not an equal superposition of all valid states. For equal weight superposition of all valid states, we first create equal weight superposition of all states using Hadamard gates and then post-selection using symmetry syndrome measurement. The symmetry syndrome can be easily implemented using N-Toffoli gates, see figure below.

For the evolutional problem block, we use the above-defined Hamiltonian. However, we can also use

$$U_P(\alpha) = e^{-i\alpha(Q+Q^\dagger)}$$

since

$$H = (Q + Q_\dagger)^2$$

Depending on the underlying graph, the choice of $Q + Q^\dagger$for the problem driving block could result in fewer commuting groups, which leads to better trotterization, as well as lower depth and fewer gates. Nevertheless, in a few experiments that we perform, these two choices lead to relatively the same values. A quick way to estimate the lower bound for the number of ground states is the Witten index, given by

$$W = \mathrm{Tr}[(-1)^F]$$

where the trace is over all valid states.

4. VQE

For VQE, one could simply impose an ansatz, such as Two-local ansatz from Qiskit. Afterwards, we measure the symmetry syndrome (hard-core restriction) of qubit i to auxiliary qubit $\tilde{i}$, and measure it. If the readout of the auxiliary qubits is all zeroes, the qubit state is valid. However, this approach has a problem as we have no control over the success measurement of auxiliary qubits. On the technical side, we cannot find a way to use the PennyLane library to perform post-selection.

As a result, we modify the cost function to include the penalty if the output state is not valid. This can be done by using the symmetry syndrome measurement as above. This problem is extremely similar to combining the regression model and classification model in classical machine learning.

In explicit, we have two measurements $\langle H \rangle, \langle Z \rangle$ where $\langle H \rangle \geq 0$ is the expectation value of the energy and $\langle Z \rangle$ measure how much the state is invalid, reaching $\langle Z \rangle = \pm 1$ for invalid/valid state and somewhere in between for mixture of valid and invalid states. A common approach is to define the cost function f_{cost} as a weighted linear combination of the two

$$f_{cost} = \langle H \rangle + \lambda f_{\text{binary}}(\langle Z \rangle)$$

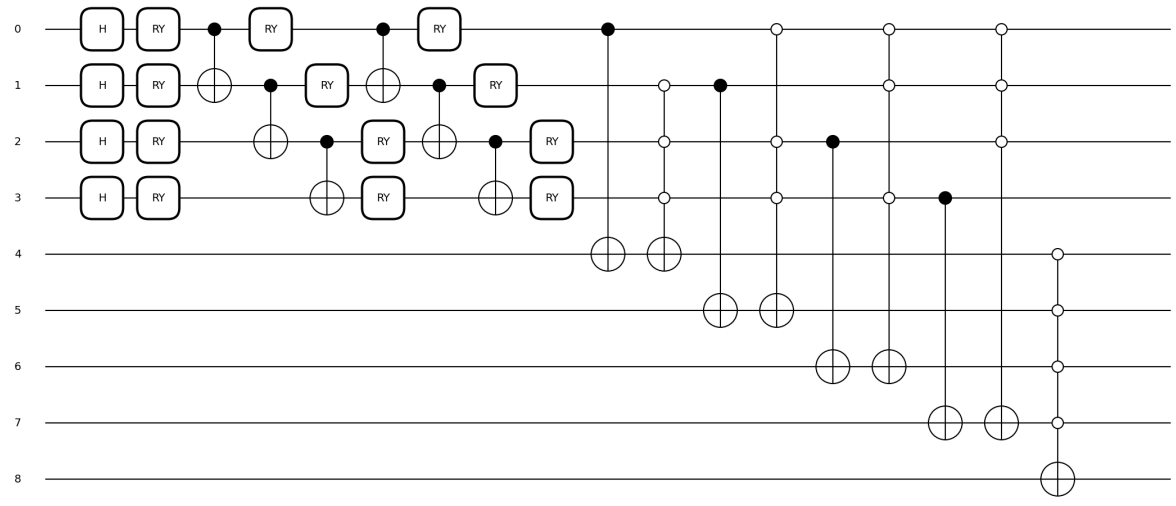
However, this function does not necessarily enforce the state to be valid. We propose another cost function of the form

$$f_{cost} = (\langle H \rangle + E_{\text{off-set}}) \times \left[-\ln\left(\epsilon_{tol} + \frac{1 - \langle Z \rangle}{2}\right) + \alpha \right]$$

with $E_{\text{off-set}}, \epsilon_{tol} > 0, \alpha > \ln(\epsilon_{tol} + 1)$. The terms $E_{\text{off-set}}$and α are used to ensure none of the terms would vanish. The term ϵ_{tol} is used to avoid the singular at 0 of the natural logarithm function. Quantitatively, this is the product of the expected energy and cross-entropy. Due to the exponential steepness of the cross-log functions near $\langle Z \rangle = 1$, we expect that the optimizer would try to ensure the state is valid first, then expand in the variational parameter space to minimize the energy.

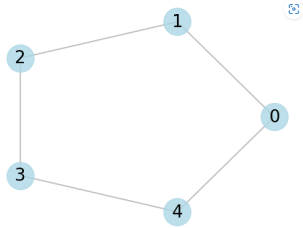
5. Experiment result

Here is what a VQE ansatz looks like, we have the array of Hadamard gates for state preparation followed by the two-local ansatz. Finally, we have the symmetry syndrome measurement using auxiliary qubits. We then measure the computation qubit (1→4 in the below picture) with respect to the Hamiltonian and the last auxilary qubit (8 in the below picture) which respect to Z.

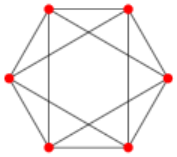


We consider the 5-site chain with periodic boundary condition (5-cycle), tetrahedron, octahedral, and cubical graph (pictures from Wolfram Mathworld) for our experiments. In all these models, we can confirm that there exists ground energy $E = 0$ by evaluating

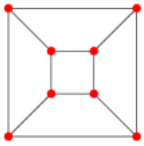
the Witten index of the graph.



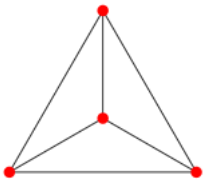
5-cycle



Octahedral



Cubical graph



Tetrahedron

VQE approach with the naive cost function $f_{\text{cost}} = \langle H \rangle + \langle Z \rangle$

Graph G	Ansatz	Layer	$\langle H \rangle$	$\langle Z \rangle$	f_{cost}
Tetrahedron	Two-local	1	0	1	1
Octahedral	Two-local	1	0.012	0.988	≈ 1
Cubical graph	Two-local	1	0	1	1
5-cycle	Two-local	1	0	1	1

We see that for the naive cost function, we can minimize $\langle H \rangle$ to zero. However, the output states are totally invalid This is due to the fact that $P_i \left|\psi\right\rangle = 0$ if site i has an occupied neighbor. This results in many of the invalid states having zero energy and creating a trapping potential in the parameter space. This is why we need a new cost function that can enforce symmetry.

VQE approach with the cost function $f_{cost} = (\langle H \rangle + E_{\text{off-set}}) \times \left[-\ln\left(\epsilon_{tol} + \frac{1-\langle Z \rangle}{2}\right) + \alpha \right]$.

Graph G	Ansatz	Layer	E_{offset}	ϵ_{tol}	α	$\langle H \rangle$	$\langle Z \rangle$
5-cycle	Two-local	1	1	0.01	0.2	0.82	-0.98
5-cycle	Two-local	2	1	0.01	0.2	0.103	-0.95
Tetrahedron	Two-local	1	1	0.01	0.2	0	-1.0
Octahedral	Two-local	1	1	0.01	0.2	2	-1.0
Octahedral	Two-local	2	1	0.01	0.2	2	-1.0
Octahedral	Two-local	3	1	0.01	0.2	2	-1.0
Cubical graph	Two-local	1	1	0.01	0.2	2	-1.0
Cubical graph	Two-local	2	1	0.01	0.2	2	-1.0
Cubical graph	Two-local	3	1	0.01	0.2		

We can observe that all the output states are valid. However, there is a trade-off that the variational energy is not minimized for the more complex circuits. In fact, we see that increasing the number of layers does not resolve this problem (Octahedral and Cubical graph).

GM-QAOA approach with the cost function $f_{QAOA} = \langle H \rangle$, all the result states are valid (or have the probability of being outside the invalid subspace significantly small).

Graph G	QAOA depth	f_{QAOA}
5-cycle	1	0
Tetrahedron	1	0
Octahedral	1	≈ 1
Octahedral	2	≈ 1
Octahedral	3	0

We do not run the cubical graph for GM-QAOA as the Pauli-decomposition of the Hamiltonian is tremendous (this is the issue we have mentioned earlier that we are assuming we can implement the Hamiltonian efficiently). Nevertheless, we can see that for the 5-cycle, tetrahedron, and octahedral graph, the GM-QAOA outperforms the VQE significantly, and increasing the number of layers does increase the accuracy of the estimation.

6. Conclusion

In this open hackathon problem, we have attempted to solve the SUSY quantum mechanic lattice model N=2 using two approaches VQE and GM-QAOA. For the VQE approach, instead of using post-selection, we show that by modifying the cost function appropriately, which is the product of cross-entropy and energy expectation value in our case, one can perform VQE for constraint optimization problems. Nevertheless. it is highly sensitive to the choice of the cost function, and the optimization may be non-optimal since the valid state spaces could be dissociated in the variational parameter spaces (for instance, one may need to cross a large landscape of invalid states when going from one valid state to another). Hence, it would be an interesting future problem to find better classes of cost functions for the symmetry constraint problems. For the GM-QAOA approach, we show that if one could efficiently implement the Hamiltonian on the circuit, then GM-QAOA could potentially outperform VQE for constraint optimization problems. As a trade-off, the GM-QAOA would need better fidelity multi-qubit gates to implement the U_S gate defined above.

On a side note, as we mentioned at the beginning, the SUSY quantum mechanics model could arise in many systems as well as applications. Nevertheless, it has not received much attention from the quantum computation community. Therefore, we hope that our hackathon project could bring it to the spotlight.