Qiskit Advocate Mentorship Program - Final Showcase

https://github.com/qiskit-advocate/qamp-fall-21/issues/28

Qiskit

Variational Quantum Algorithms for Excited States

Qiskit

The Team

- **Mentors**
  - Pauline Ollitrault
  - Steve Wood

- **Mentees**
  - Abhishek Jayachandran
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Aim

Qiskit

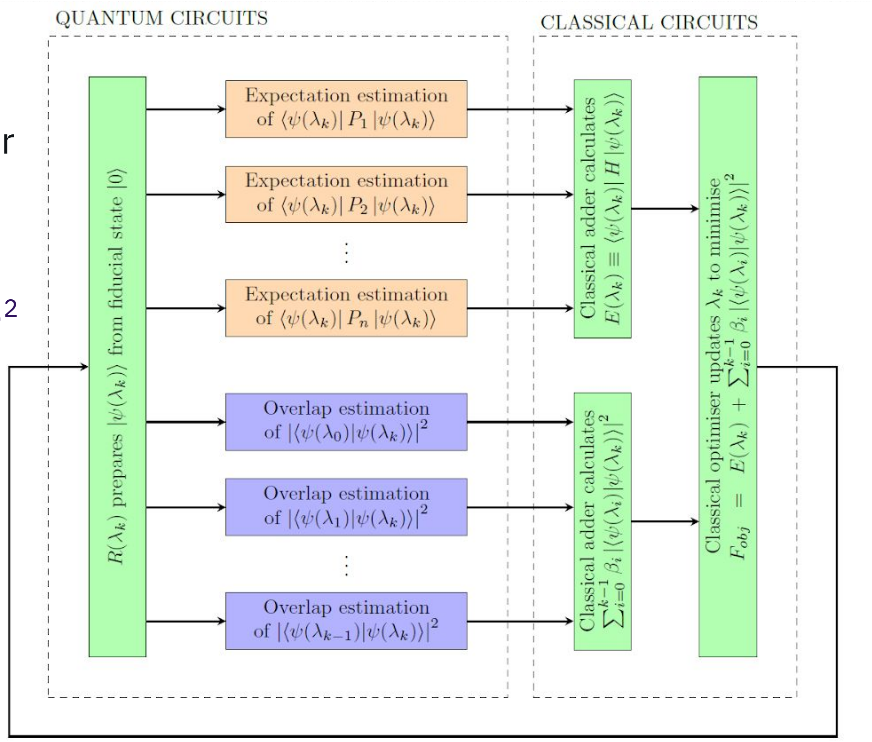
- Implement a generalized variational quantum method for predicting higher energy states of hamiltonians.
- Identify algorithms with reasonable performance for the task
- Add the kstateVQE() algorithm to qiskit terra that implements the EigenSolver() interface.
- Benchmark performance of the methods
- Write a tutorial explaining use of the method

VQD

- The VQD extends the VQE to calculate the k^{th} excited state by optimizing the parameters θ_k for the ansatz state $\langle|\Psi(\theta_k)\rangle$ such that the cost function:

  $$F(\theta_k) := \langle\Psi(\theta_k)|H|\Psi(\theta_k)\rangle + \sum_{i=0}^{k-1}(\beta_i\langle\Psi(\theta_k)|\Psi(\theta_i)\rangle)^2$$

  is minimized.



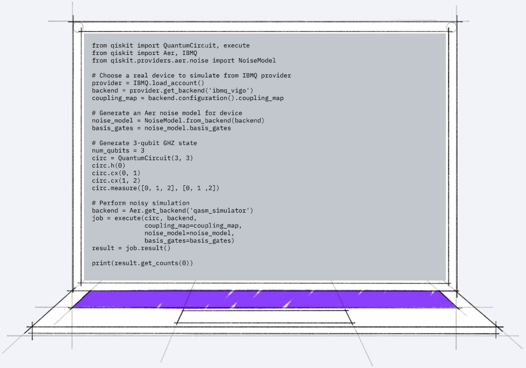
Code Review

```
expect_op, expectation = self.construct_expectation(
    self._ansatz_params, operator, return_expectation=True
)

for state in range(step):

    prev_circ = self.ansatz.bind_parameters(prev_states[state])
    overlap_op.append(~CircuitStateFn(prev_circ)@CircuitStateFn(self.ansatz))


def energy_evaluation(parameters):
    parameter_sets = np.reshape(parameters, (-1, num_parameters))
    # Create dict associating each parameter with the lists of parameterization values for it
    param_bindings = dict(zip(self._ansatz_params, parameter_sets.transpose().tolist()))

    start_time = time()
    sampled_expect_op = self._circuit_sampler.convert(expect_op, params=param_bindings)
    mean = np.real(sampled_expect_op.eval())[0]

    for state in range(step):
        sampled_final_op = self._circuit_sampler.convert(overlap_op[state], params=param_bindings)
        cost = sampled_final_op.eval()
        mean += np.real(self.betas[state] * np.conj(cost) * cost)

    return mean
```

Qiskit

Outcomes

- Learned and understood in detail about variational quantum algorithms and in particular their implementation in Qiskit
- Learned the inner workings of qiskit enough to develop and integrate an algorithm to the terra codebase.
- Implemented the Variational Quantum Deflation Algorithm



Road Ahead

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- Conduct unit tests on code and push to Qiskit Terra
- Write a tutorial explaining use of the kstateVQE and add it to the Qiskit tutorials

Demo