VQE Screening 3

September 18, 2020

1 VQE Screening 3

```
In [1]: scaffold_codeXX = """
        // Ref[2] https://www.asc.ohio-state.edu/perry.6/p5501_sp17/articles/quantum_gates.pdf
        // Ref[3] https://arxiv.org/pdf/1901.00015.pdf
        const double alpha0 = 3.14159265359;
        const double b = 0*3.14159265359, c = 0*3.14159265359, d = 0*3.14159265359;
        // Note that I kept b and c equal to zero and treated d as the parameter of the circuit
       module initialRotations(qbit reg[2]) {
          H(reg[0]);
          Rx(reg[1], alpha0); // Start of creating Psi_in
          CNOT(reg[1], reg[2]);
          H(reg[1]); // End of creating Psi_in
          // Note that Psi_in is entangled
          Rz(reg[1], d); // This is a simple parameterised unitary
          (which is also the exponential of a Pauli matrix)
          // This the controlled version of the parameterised unitary
          Rz(reg[1], (d-b)/2); // Start of Fig. 2.29 of Ref[2]
          with gate parameters b, c, d defined above
          CNOT(reg[0], reg[1]);
          Rz(reg[1], -(d+b)/2);
          Ry(reg[1], -c/2);
          CNOT(reg[0], reg[1]);
          Ry(reg[1], c/2);
          Rz(reg[1], b); // End of Fig. 2.29 of Ref[2]
        }
       module entangler(qbit reg[2]) {
          H(reg[1]);
          CNOT(reg[1], reg[2]);
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H(reg[2]);
          CNOT(reg[2], reg[1]);
        module prepareAnsatz(qbit reg[2]) {
          initialRotations(reg);
          //entangler(reg);
          // I missed out the entangling gates because Psi_in is already entangled
        module measure(qbit reg[2], cbit result[3]) {
          result[0] = MeasX(reg[0]);
          result[1] = MeasX(reg[1]);
          S(reg[0]);
          H(reg[0]);
         result[2] = MeasZ(reg[2]);
        }
        int main() {
          qbit reg[3];
          cbit result[3];
          prepareAnsatz(reg);
          measure(reg, result);
          return 0;
        }
        11 11 11
In [2]: scaffold_codeYY = """
        const double alpha0 = 3.14159265359;
        const double b = 0*3.14159265359, c = 0*3.14159265359, d = 0*3.14159265359;
        // Note that I kept b and c equal to zero and treated d as the parameter of the circuit
        module initialRotations(qbit reg[2]) {
          H(reg[0]);
          Rx(reg[1], alpha0); // Start of creating Psi_in
          CNOT(reg[1], reg[2]);
          H(reg[1]); // End of creating Psi_in
          // Note that Psi_in is entangled
          Rz(reg[1], d); // This is a simple parameterised unitary
```

```
(which is also the exponential of a Pauli matrix)
  // This the controlled version of the parameterised unitary
  Rz(reg[1], (d-b)/2); // Start of Fig. 2.29 of Ref[2]
  with gate parameters b, c, d defined above
  CNOT(reg[0], reg[1]);
  Rz(reg[1], -(d+b)/2);
  Ry(reg[1], -c/2);
  CNOT(reg[0], reg[1]);
  Ry(reg[1], c/2);
  Rz(reg[1], b); // End of Fig. 2.29 of Ref[2]
}
module entangler(qbit reg[2]) {
  H(reg[1]);
  CNOT(reg[1], reg[2]);
  H(reg[2]);
  CNOT(reg[2], reg[1]);
}
module prepareAnsatz(qbit reg[2]) {
  initialRotations(reg);
  //entangler(reg);
 // I missed out the entangling gates because Psi_in is already entangled
}
module measure(qbit reg[2], cbit result[3]) {
  Rx(reg[1], 1.57079632679);
  Rx(reg[2], 1.57079632679);
  result[0] = MeasZ(reg[0]);
  result[1] = MeasZ(reg[1]);
  S(reg[0]);
  H(reg[0]);
  result[2] = MeasZ(reg[2]);
int main() {
  qbit reg[3];
  cbit result[3];
  prepareAnsatz(reg);
  measure(reg, result);
```

```
return 0;
        }
        11 11 11
In [3]: scaffold_codeZZ = """
        const double alpha0 = 3.14159265359;
        const double b = 0*3.14159265359, c = 0*3.14159265359, d = 0*3.14159265359;
        // Note that I kept b and c equal to zero and treated d as the parameter of the circuit
        module initialRotations(qbit reg[2]) {
          H(reg[0]);
          Rx(reg[1], alpha0); // Start of creating Psi_in
          CNOT(reg[1], reg[2]);
          H(reg[1]); // End of creating Psi_in
          // Note that Psi_in is entangled
          Rz(reg[1], d); // This is a simple parameterised unitary
          (which is also the exponential of a Pauli matrix)
          // This the controlled version of the parameterised unitary
          Rz(reg[1], (d-b)/2); // Start of Fig. 2.29 of Ref[2]
          with gate parameters b, c, d defined above
          CNOT(reg[0], reg[1]);
          Rz(reg[1], -(d+b)/2);
          Ry(reg[1], -c/2);
          CNOT(reg[0], reg[1]);
          Ry(reg[1], c/2);
          Rz(reg[1], b); // End of Fig. 2.29 of Ref[2]
        }
        module entangler(qbit reg[2]) {
          H(reg[1]);
          CNOT(reg[1], reg[2]);
          H(reg[2]);
          CNOT(reg[2], reg[1]);
        }
        module prepareAnsatz(qbit reg[2]) {
          initialRotations(reg);
          //entangler(reg);
          // I missed out the entangling gates because Psi_in is already entangled
        module measure(qbit reg[2], cbit result[3]) {
```

```
result[0] = MeasZ(reg[0]);
result[1] = MeasZ(reg[1]);

S(reg[0]);
H(reg[0]);
result[2] = MeasZ(reg[2]);
}

int main() {
  qbit reg[3];
  cbit result[3];

  prepareAnsatz(reg);
  measure(reg, result);

return 0;
}
```

2 Executing it

```
In [4]: from scaffcc_interface import ScaffCC
        openqasmXX = ScaffCC(scaffold_codeXX).get_openqasm()
        openqasmYY = ScaffCC(scaffold_codeYY).get_openqasm()
        openqasmZZ = ScaffCC(scaffold_codeZZ).get_openqasm()
        print(openqasmXX)
        print(openqasmYY)
        print(opengasmZZ)
OPENQASM 2.0;
include "qelib1.inc";
qreg reg[3];
creg result[3];
h reg[0];
rx(3.141593e+00) reg[1];
cx reg[1],reg[2];
h reg[1];
rz(0.000000e+00) reg[1];
rz(0.000000e+00) reg[1];
cx reg[0],reg[1];
rz(-0.000000e+00) reg[1];
ry(-0.000000e+00) reg[1];
cx reg[0],reg[1];
ry(0.000000e+00) reg[1];
```

```
rz(0.000000e+00) reg[1];
h reg[0];
measure reg[0] -> result[0];
h reg[1];
measure reg[1] -> result[1];
s reg[0];
h reg[0];
measure reg[2] -> result[2];
OPENQASM 2.0;
include "qelib1.inc";
qreg reg[3];
creg result[3];
h reg[0];
rx(3.141593e+00) reg[1];
cx reg[1],reg[2];
h reg[1];
rz(0.000000e+00) reg[1];
rz(0.000000e+00) reg[1];
cx reg[0],reg[1];
rz(-0.000000e+00) reg[1];
ry(-0.000000e+00) reg[1];
cx reg[0],reg[1];
ry(0.000000e+00) reg[1];
rz(0.000000e+00) reg[1];
rx(1.570796e+00) reg[1];
rx(1.570796e+00) reg[2];
measure reg[0] -> result[0];
measure reg[1] -> result[1];
s reg[0];
h reg[0];
measure reg[2] -> result[2];
OPENQASM 2.0;
include "qelib1.inc";
qreg reg[3];
creg result[3];
h reg[0];
rx(3.141593e+00) reg[1];
cx reg[1],reg[2];
h reg[1];
rz(0.000000e+00) reg[1];
rz(0.000000e+00) reg[1];
cx reg[0],reg[1];
rz(-0.000000e+00) reg[1];
ry(-0.000000e+00) reg[1];
```

```
cx reg[0],reg[1];
ry(0.000000e+00) reg[1];
rz(0.000000e+00) reg[1];
measure reg[0] -> result[0];
measure reg[1] -> result[1];
s reg[0];
h reg[0];
measure reg[2] -> result[2];
```

2.0.1 Execute on a Simulator

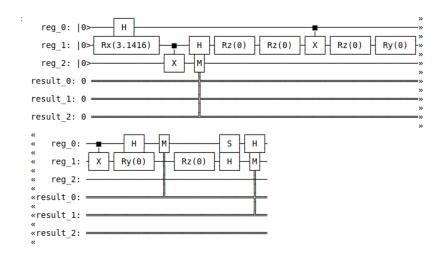
```
In [5]: from qiskit import Aer, Quantum Circuit, execute
        Aer.backends()
Out[5]: [<QasmSimulator('qasm_simulator') from AerProvider()>,
         <StatevectorSimulator('statevector_simulator') from AerProvider()>,
         <UnitarySimulator('unitary_simulator') from AerProvider()>]
In [6]: simulator = Aer.get_backend('qasm_simulator')
        vqe_circXX = QuantumCircuit.from_qasm_str(opengasmXX)
        vqe_circYY = QuantumCircuit.from_qasm_str(openqasmYY)
        vqe_circZZ = QuantumCircuit.from_qasm_str(openqasmZZ)
        num\_shots = 100000
        sim_resultXX = execute(vqe_circXX, simulator, shots=num_shots).result()
        sim_resultYY = execute(vqe_circYY, simulator, shots=num_shots).result()
        sim_resultZZ = execute(vqe_circZZ, simulator, shots=num_shots).result()
        countsXX = sim_resultXX.get_counts()
        countsYY = sim_resultYY.get_counts()
        countsZZ = sim_resultZZ.get_counts()
        expected_valueXX = (countsXX.get('000', 0) - countsXX.get('001', 0)
         - countsXX.get('010', 0) + countsXX.get('011', 0) - countsXX.get('100', 0)
         + countsXX.get('101', 0) + countsXX.get('110', 0) - countsXX.get('111', 0))
          / num_shots
        expected_valueYY = (countsYY.get('000', 0) - countsYY.get('001', 0)
         - countsYY.get('010', 0) + countsYY.get('011', 0) - countsXX.get('100', 0)
         + countsXX.get('101', 0) + countsXX.get('110', 0) - countsXX.get('111', 0))
          / num shots
        expected_valueZZ = (countsZZ.get('000', 0) - countsZZ.get('001', 0)
         - countsZZ.get('010', 0) + countsZZ.get('011', 0) - countsXX.get('100', 0)
          + countsXX.get('101', 0) + countsXX.get('110', 0) - countsXX.get('111', 0))
          / num shots
```

```
expected_value = 0.5 - 0.5 * expected_valueXX - 0.5 * expected_valueYY +
    0.5 * expected_valueZZ
print('The derivative of the lowest eigenvalue with respect to rotation angle, which is:
%s' % expected_value)

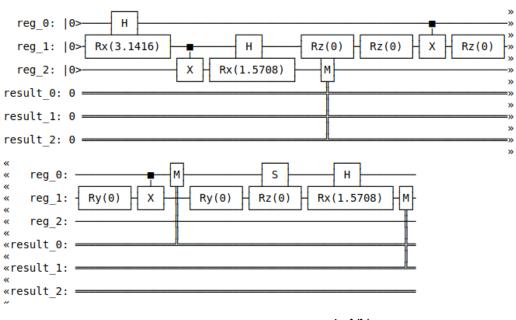
#print(expected_valueXX)
#print(expected_valueYY)
#print(expected_valueZZ)
```

The derivative of the lowest eigenvalue with respect to rotation angle, which is : -0.00041000000000002146

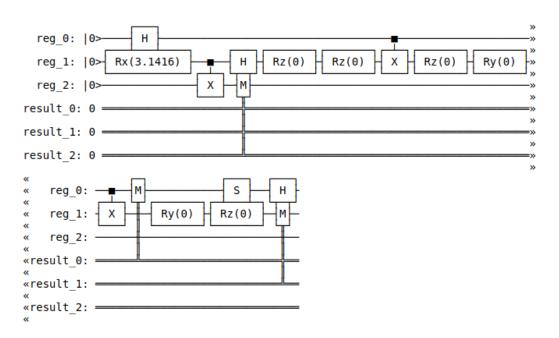
3 Circuit Visualization



vqe_circXX



vqe_circYY



vqe_circZZ