Casting the VQE Unitary Ansatz Operator Into an Equivalent Quantum Circuit

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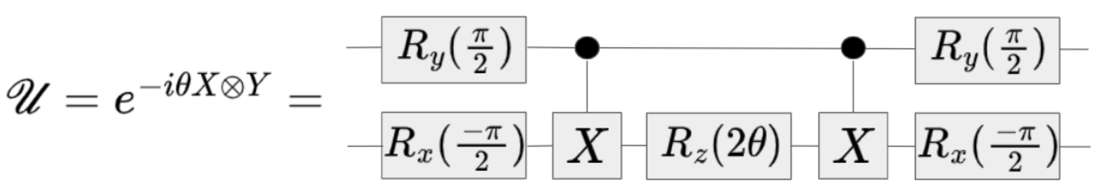
In this notebook, I will mathematically show that we can cast the VQE unitary ansatz $U_{\text{Ansatz}} = e^{-i\,\theta X Y}$ as some equivalent quantum circuit as shown below which we can call U_{circuit}. The objective is to ultimately show that $U_{\text{Ansatz}} = U_{\text{Circuit}}$.



In[•]:=
```
(*Writing out the usual quantum gates*)

(*Identity*)
Iden = IdentityMatrix[2];

(*Pauli Gates*)
X = {{0, 1},
     {1, 0}};
Y = {{0, -ⅈ},
     {ⅈ, 0}};
Z = {{1, 0},
     {0, -1}};

(*Control-NOT*)
CX =  {{1, 0, 0, 0},
       {0, 1, 0, 0},
       {0, 0, 0, 1},
       {0, 0, 1, 0}};

(*Rotation Gates*)
Rx[θ_] := MatrixExp[-ⅈ X θ / 2]
Ry[θ_] := MatrixExp[-ⅈ Y θ / 2]
Rz[θ_] := MatrixExp[-ⅈ Z θ / 2]
```

In[•]:=
```
(*Computing U_Circuit*)
U1 = KroneckerProduct[Ry[π / 2], Rx[-π / 2]];
U2 = CX.KroneckerProduct[Iden, Rz[θ]].CX;
U3 = KroneckerProduct[Ry[-π / 2], Rx[π / 2]];
Ucircuit = U3.U2.U1 // ComplexExpand // Simplify;

U1 = KroneckerProduct[Ry[π / 2], Rx[-π / 2]];
U2 = CX.KroneckerProduct[Iden, Rz[2 θ]].CX;
U3 = KroneckerProduct[Ry[-π / 2], Rx[π / 2]];
Ucircuit = U3.U2.U1 // ComplexExpand // Simplify;

Ucircuit // MatrixForm
```

Out[•]//MatrixForm=

$$\begin{pmatrix} \text{Cos}[\theta] & 0 & 0 & -\text{Sin}[\theta] \\ 0 & \text{Cos}[\theta] & \text{Sin}[\theta] & 0 \\ 0 & -\text{Sin}[\theta] & \text{Cos}[\theta] & 0 \\ \text{Sin}[\theta] & 0 & 0 & \text{Cos}[\theta] \end{pmatrix}$$

In[•]:=
```
(*Now, let's compute and display U_ansatz*)
Uansatz = MatrixExp[-ⅈ θ KroneckerProduct[X, Y]];

Uansatz // MatrixForm
```

Out[•]//MatrixForm=

$$\begin{pmatrix} \text{Cos}[\theta] & 0 & 0 & -\text{Sin}[\theta] \\ 0 & \text{Cos}[\theta] & \text{Sin}[\theta] & 0 \\ 0 & -\text{Sin}[\theta] & \text{Cos}[\theta] & 0 \\ \text{Sin}[\theta] & 0 & 0 & \text{Cos}[\theta] \end{pmatrix}$$

Conclusion

In conclusion, we see that $U_{\text{Circuit}} = U_{\text{Ansatz}}$. Therefore, we really can cast some unitary in terms of other unitary operators (i.e. quantum gates)

In[∘]:=
```
Print["UAnsatz = ", Uansatz // MatrixForm]
Print["UCircuit = ", Ucircuit // MatrixForm]
```

$$U_{\text{Ansatz}} = \begin{pmatrix} \text{Cos}[\theta] & 0 & 0 & -\text{Sin}[\theta] \\ 0 & \text{Cos}[\theta] & \text{Sin}[\theta] & 0 \\ 0 & -\text{Sin}[\theta] & \text{Cos}[\theta] & 0 \\ \text{Sin}[\theta] & 0 & 0 & \text{Cos}[\theta] \end{pmatrix}$$

$$U_{\text{Circuit}} = \begin{pmatrix} \text{Cos}[\theta] & 0 & 0 & -\text{Sin}[\theta] \\ 0 & \text{Cos}[\theta] & \text{Sin}[\theta] & 0 \\ 0 & -\text{Sin}[\theta] & \text{Cos}[\theta] & 0 \\ \text{Sin}[\theta] & 0 & 0 & \text{Cos}[\theta] \end{pmatrix}$$