Variational Quantum Eigensolver

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Here I define a few symbolic operations:

```
In[ ]:= (*Aesthetic Way to write tensor products. The function MatrixQ decides wether
         we should use the function for matrices, kron[], or for vectors, vkron[]*)
        a_ ⊗ b_ := If[MatrixQ[a] == True, kron[a, b], kronV[a, b]]

        (*This makes an arbitrary number of products define,
        such as |0⟩ ⊗ |0⟩ ⊗ |0⟩ ⊗ |1⟩, etc...*)
        a_ ⊗ b_ ⊗ c__ := (a ⊗ b) ⊗ c
```

Here we define the Hamiltonian from the problem statement

In[ ]:= $H := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

```
In[ ]:= H
Out[ ]= {{1, 0, 0, 0}, {0, 0, -1, 0}, {0, -1, 0, 0}, {0, 0, 0, 1}}
```

And we also define the Pauli Matrices:

In[ ]:=

$\sigma 0 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix};$

$\sigma x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};$

$\sigma y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};$

$\sigma z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$

Below we try to decompose the matrix H using the form given in the hints:

$$H = \alpha + \beta\, \sigma_z \otimes \sigma_z + \gamma\, \sigma_x \otimes \sigma_x + \delta\, \sigma_y \otimes \sigma_y$$

In[ ]:=
```
ClearAll[α,β,γ,δ];
Solution = Solve[H==α σ0 ⊗ σ0 + β σz ⊗ σz + γ σx ⊗ σx + δ σy ⊗ σy,{α,β,γ,δ}]
```

Out[ ]=
$$\left\{\left\{\alpha \to \frac{1}{2},\ \beta \to \frac{1}{2},\ \gamma \to -\frac{1}{2},\ \delta \to -\frac{1}{2}\right\}\right\}$$

And we find that the coefficients should be $\left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right)$ so that the decomposition holds. Just to perform a sanity check we can see that indeed check that when we multiply the basis elements by these coefficients we get the expected result:

In[ ]:=
```
α σ0 ⊗ σ0 + β σz ⊗ σz + γ σx ⊗ σx + δ σy ⊗ σy/.Solution[[1]]//MatrixForm
```

Out[ ]//MatrixForm=
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Below I try to this in a general way, finding all the 16 coefficients for each basis element $\sigma_i \otimes \sigma_j$. We begin by defining an array with the Pauli Basis elements for 2 x 2 matrices and also an array with undetermined coefficients
$(c_0, \ldots, c_{16})$, because we're looking for a decomposition of the type:

$$M = c_0\, I_2 \otimes I_2 + c_1\, I_2 \otimes \sigma_z + \ldots + c_{16} \sigma_y \otimes \sigma_y$$

for any matrix $M_{4\,x\,4}$

In[ ]:=
```
σ:={σ0,σz,σx,σy}
PauliCoefficients:=Array[c,16]
```

Now we build a list with each basis element $\sigma_i \otimes \sigma_j$, given by the variable *PauliCombinations:*

In[ ]:=
```
PauliCombinations=Table[Table[σ[[i]] ⊗ σ[[j]],{i,1,4}],{j,1,4}];
PauliCombinations=Transpose[{Flatten[Transpose[PauliCombinations],1]}];
Transpose[PauliCombinations]//MatrixForm
```

Out[ ]//MatrixForm=
$$\left(\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & - \end{pmatrix}\right.$$

Here we perform the decomposition in this basis, summing each basis element multiplied by its corresponding coefficient, just like in

$$M = c_0\, I_2 \otimes I_2 + c_1\, I_2 \otimes \sigma_z + \ldots + c_{16} \sigma_y \otimes \sigma_y$$

In[ ]:=
```
PauliDecomposition=Table[PauliCoefficients[[i]]*PauliCombinations[[i]],{i,1,Length@PauliCom
PauliDecomposition//MatrixForm;
PauliDecomposition=Total[PauliDecomposition,2];
PauliDecomposition//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} c[1]+c[2]+c[5]+c[6] & c[3]-i\,c[4]+c[7]-i\,c[8] & c[9]+c[10]-i\,c[13]-i\,c[14] & c[11]-i\,c[12] \\ c[3]+i\,c[4]+c[7]+i\,c[8] & c[1]-c[2]+c[5]-c[6] & c[11]+i\,c[12]-i\,c[15]+c[16] & c[9]-c[10]- \\ c[9]+c[10]+i\,c[13]+i\,c[14] & c[11]-i\,c[12]+i\,c[15]+c[16] & c[1]+c[2]-c[5]-c[6] & c[3]-i\,c[4] \\ c[11]+i\,c[12]+i\,c[15]-c[16] & c[9]-c[10]+i\,c[13]-i\,c[14] & c[3]+i\,c[4]-c[7]-i\,c[8] & c[1]-c[2] \end{pmatrix}$$

Now we leave to Mathematica the task of solving this system for 16 variables. We can see that we recover the previous solution for the matrix H:

In[ ]:=
```
Decomposition=Solve[H == PauliDecomposition,PauliCoefficients]
```

Out[ ]=
$$\left\{\left\{c[1]\to\frac{1}{2},\ c[2]\to 0,\ c[3]\to 0,\ c[4]\to 0,\ c[5]\to 0,\ c[6]\to\frac{1}{2},\ c[7]\to 0,\ c[8]\to 0,\ c[9]\to 0,\ c[10]\to 0,\ c[11]\to -\frac{1}{2},\ c[12]\to 0,\ c[13]\to 0,\ c[14]\to 0,\ c[15]\to 0,\ c[16]\to -\frac{1}{2}\right\}\right\}$$

Explicitly performing the operation $c_0\, I_2 \otimes I_2 + c_1\, I_2 \otimes \sigma_z + \ldots + c_{16} \sigma_y \otimes \sigma_y$ we see that this is indeed equal to H:

In[ ]:=
```
Print["H is ",Total[Table[PauliCoefficients[[i ]]*PauliCombinations[[i]],{i,1,Length@PauliCo
```

$$\text{H is } \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The First Example

Now, we will solve the eigenproblem analytically and compare with our numerical results. The eigen-values of this Matrix are:

In[ ]:=
```
Eigenvalues[H]
```

Out[ ]= {-1, 1, 1, 1}

The vector corresponding to the smallest eigenvalue is

In[ ]:=
```
Normalize[Eigenvectors[H][[1]]]//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

Here we define the relevant gates for the circuit, moreover, we also study the action of the circuit on the qubits. It will be given by:

$$\left|\psi\right\rangle = (R_X(\theta) \otimes I)\, \mathrm{CX}\, (H \otimes I) \left|0\right\rangle \left|0\right\rangle$$

This will be equal to:

$$\left|\psi\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{Cos}\left[\frac{\theta}{2}\right] \\ -\mathrm{i}\ \mathrm{Sin}\left[\frac{\theta}{2}\right] \\ -\mathrm{i}\ \mathrm{Sin}\left[\frac{\theta}{2}\right] \\ \mathrm{Cos}\left[\frac{\theta}{2}\right] \end{pmatrix}$$

In[ ]:=

$$\mathrm{CX} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix};\mathrm{HG}=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix};\mathrm{RX}[\theta\_]:=\begin{pmatrix} \mathrm{Cos}\left[\frac{\theta}{2}\right] & -i\ \mathrm{Sin}\left[\frac{\theta}{2}\right] \\ -i\ \mathrm{Sin}\left[\frac{\theta}{2}\right] & \mathrm{Cos}\left[\frac{\theta}{2}\right] \end{pmatrix}$$

```
ClearAll[U,θ]
U[θ_]:=(RX[θ]⊗σ0).CX.(HG ⊗σ0);
U[θ].({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} \frac{\mathrm{Cos}\left[\frac{\theta}{2}\right]}{\sqrt{2}} \\ -\frac{i\ \mathrm{Sin}\left[\frac{\theta}{2}\right]}{\sqrt{2}} \\ -\frac{i\ \mathrm{Sin}\left[\frac{\theta}{2}\right]}{\sqrt{2}} \\ \frac{\mathrm{Cos}\left[\frac{\theta}{2}\right]}{\sqrt{2}} \end{pmatrix}$$

We can verify that this ansatz let us finding the appropriate eigenvector, up to a phase factor of i. We simply have to pick $\theta = \pi$

In[ ]:=
```
I U[π].({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

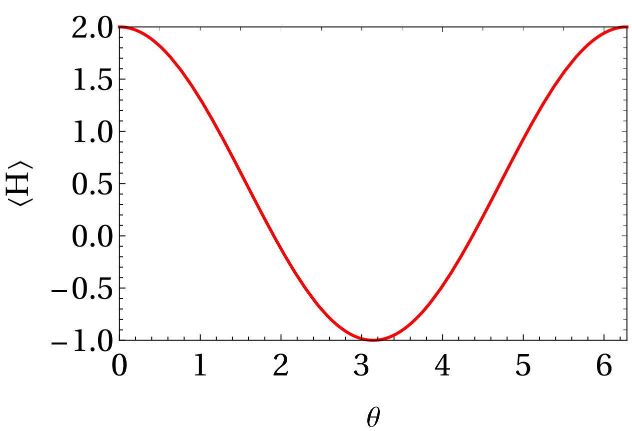
$$\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

Finally, we plot the expected value of the energy for different values of θ:

In[ ]:=
```
⟨O_⟩ψ_ :=Conjugate[ψ].O.ψ
Avgx=-0.5*⟨σy⊗ σy⟩U[θ].({1,0}⊗{1,0});
Avgy=-0.5*⟨σy⊗ σy⟩U[θ].({1,0}⊗{1,0});
Avgz=0.5*⟨σz⊗ σz⟩U[θ].({1,0}⊗{1,0});
```

In[ ]:=
```
Plot[0.5 + Avgx + Avgy + Avgz,{θ,0,2π},PlotStyle→{Red},FrameLabel→ {"θ","⟨H⟩"}]
```

Out[ ]=



The second example

Now we discuss the second example. The decomposition for the matrix from the sample task in the site

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

is:

In[ ]:=
```
H2= (0  0   0  0
     0  -1  1  0
     0  1  -1  0
     0  0   0  0);

Decomposition=Solve[H2 == PauliDecomposition,PauliCoefficients]
```

Out[ ]= $\left\{\left\{c[1]\to-\frac{1}{2},\ c[2]\to0,\ c[3]\to0,\ c[4]\to0,\ c[5]\to0,\ c[6]\to\frac{1}{2},\ c[7]\to0,\ c[8]\to0,\ c[9]\to0,\ c[10]\to0,\ c[11]\to\frac{1}{2},\ c[12]\to0,\ c[13]\to0,\ c[14]\to0,\ c[15]\to0,\ c[16]\to\frac{1}{2}\right\}\right\}$

Thus, we can write this matrix as:

In[ ]:=
```
H2:= 1/2 (- σ0 ⊗ σ0+σz ⊗ σz +  σx ⊗ σx + σy⊗ σy) ;
```

The eigenstuff for this Matrix is:

In[ ]:=
```
Eigenvalues[H2]
Normalize[Eigenvectors[H2][[1]]]//MatrixForm
```

Out[ ]= {−2, 0, 0, 0}

Out[ ]//MatrixForm=

$$\begin{pmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

The ansatz we can use is : (IX) CX (RZ I) (HI) | 00 >, where angle in RZ is our variational paramete

In[ ]:=
```
CX = (1 0 0 0
      0 1 0 0
      0 0 0 1
      0 0 1 0);HG= 1/√2 (1  1
                         1 -1);RZ[θ_]:=(Exp[-ⅈ θ/2]    0
                                        0        Exp[ⅈ θ/2])
ClearAll[U,θ]
U[θ_]:=(σ0 ⊗σx).CX.(RZ[θ]⊗σ0).(HG ⊗σ0);
```

The final state vector will be:

In[ ]:=
```
U[θ].({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} 0 \\ \frac{e^{-\frac{i\theta}{2}}}{\sqrt{2}} \\ \frac{e^{\frac{i\theta}{2}}}{\sqrt{2}} \\ 0 \end{pmatrix}$$

We can verify that we simply have to pick $\theta = \pi$:

In[ ]:=
```
-i U[π].({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

Here we show the intermediate steps, with the wave function after the first gate:

In[ ]:=
```
(HG ⊗σ0).({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

The second gate:

In[ ]:=
```
(RZ[θ]⊗σ0).(HG ⊗σ0).({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} \frac{e^{-\frac{i\theta}{2}}}{\sqrt{2}} \\ 0 \\ \frac{e^{\frac{i\theta}{2}}}{\sqrt{2}} \\ 0 \end{pmatrix}$$

The third gate:

In[ ]:=
```
CX.(RZ[θ]⊗σ0).(HG ⊗σ0).({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} \frac{e^{-\frac{i\theta}{2}}}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{e^{\frac{i\theta}{2}}}{\sqrt{2}} \end{pmatrix}$$

Third Example

Finally, I apply this to one last example

In[ ]:=
```
H3 = σz ⊗ σz +  σx ⊗ σy;
H3//MatrixForm
Eigenvalues[H3]
Eigenvectors[H3]〚1〛// Normalize//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & -i \\ 0 & -1 & i & 0 \\ 0 & -i & -1 & 0 \\ i & 0 & 0 & 1 \end{pmatrix}$$

Out[ ]= {-2, 2, 0, 0}

Out[ ]//MatrixForm=

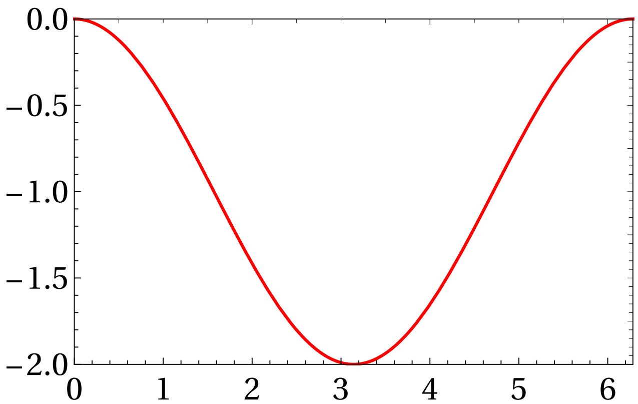
$$\begin{pmatrix} 0 \\ -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

We can simply apply a (RZ[-π/2]⊗I) gate after the first Haddamard Gate.

Plotting this:

In[ ]:=
```
U[θ_]:=(σ0 ⊗σx).CX.(RZ[θ]⊗σ0).(RZ[-π/2]⊗σ0).(HG ⊗σ0);
⟨O_⟩ρψ_ :=If[MatrixQ[ρψ]==True,Tr[ρψ.O],Conjugate[ρψ].O.ρψ]
Avgzz=⟨σz⊗ σz⟩U[θ].({1,0}⊗{1,0});
Avgxy=⟨σx⊗ σy⟩U[θ].({1,0}⊗{1,0});
Plot[Avgzz + Avgxy,{θ,0,2π},PlotStyle→{Red}]
```

Out[ ]=



The final wave function is:

In[ ]:=
```
U[θ].({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} 0 \\ \frac{e^{\frac{i\pi}{4}-\frac{i\theta}{2}}}{\sqrt{2}} \\ \frac{e^{-\frac{i\pi}{4}+\frac{i\theta}{2}}}{\sqrt{2}} \\ 0 \end{pmatrix}$$

we can take $\theta = \pi$ to get the correct eigenvalue :

In[ ]:=
```
Exp[-I π/4]  U[π].({1,0}⊗{1,0})//MatrixForm
```

Out[ ]//MatrixForm=

$$\begin{pmatrix} 0 \\ -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$