Task 4

Question 2

We apply the analysis to the H2 molecule example considered in Task 5, and in the notebook, “S5_circuit_qec.ipynb”

first group quantities

Here are the terms from the first measurement group of the Hamiltonian

In[56]:=
```
Clear[z0, z1, z2, z3]
```

In[57]:=
```
firstgroup = -.5339 + 0.0673 (z0 + z1) + .0067 (z2 + z3) +
  .1274 z0 z1 + .0650 (z0 z2 + z2 z3) + .1298 (z0 z3 + z1 z2) + .1337 z2 z3
```

Out[57]=
```
-0.5339 + 0.1274 z0 z1 + 0.0673 (z0 + z1) + 0.1337 z2 z3 +
 0.0067 (z2 + z3) + 0.1298 (z1 z2 + z0 z3) + 0.065 (z0 z2 + z2 z3)
```

For this group, there are only two measured outcomes, i.e. |a> = |1100> and |b> = |0011>.
For these two outcomes, the expectation values of the first-group operator Ahat are as follows.

Start with the first state, |1100>

In[58]:=
```
z0 = -1; z1 = -1; z2 = 1; z3 = 1;
```

In[59]:=
```
aAa = firstgroup
```

Out[59]=
```
-0.6536
```

<a|Ahat|a> = -0.6536

On to the second state, |0011>

In[60]:=
```
z0 = 1; z1 = 1; z2 = -1; z3 = -1;
```

In[61]:=
```
bAb = firstgroup
```

Out[61]=
```
-0.4112
```

<b|Ahat|b> = -0.4112

The probabilities for the two states are

In[62]:=
```
pa = .71163; pb = .28837 ;
```

The energy expectation value from the first measurement group is thus:

In[63]:=
```
EA = pa aAa + pb bAb
```

Out[63]=
```
-0.583699
```

Next we need to compute variances. First, we compute the expectation value for the Hamiltonian squared, by squaring the eigenvalues:

In[64]:=
```
EA2 = pa aAa^2 + pb bAb^2
```

Out[64]=
```
0.352762
```

then the standard deviation becomes

In[65]:=
```
sigA = Sqrt[EA2 - EA^2]
```

Out[65]=
```
0.109808
```

second group quantities

Here are the terms from the second measurement group of the Hamiltonian

In[31]:=
```
secondgroup = .0648 (-x0 x1 y2 y3 + x0 y1 y2 x3 + y0 x1 x2 y3 - y0 y1 x2 x3)
```

Out[31]=
```
0.0648 (-x2 x3 y0 y1 + x0 x3 y1 y2 + x1 x2 y0 y3 - x0 x1 y2 y3)
```

Unfortunately, as discussed in Task 5, we are not privy to the precise transformation that converts all of the above into z operators. This means, we cannot apply the correct procedure, as we could for the first group, since we don't know the meaning of the two basis functions that emerge in this case, i.e.

$|a\rangle = |1101\rangle$ and $|b\rangle = |1100\rangle$.

Nevertheless we can make some estimates, because the probability distribution in this case is extremely lopsided:

In[66]:=
```
pa = .95291; pb = .04709 ;
```

Assuming an energy difference between the two levels that is equal to that of the first group, ie.

In[67]:=
```
dltE = bAb - aAa
```

Out[67]=
```
0.2424
```

and knowing from the other notebook that the second-group energy estimate is

In[68]:=
```
EB = -0.2347328133167589
```

Out[68]=
```
-0.234733
```

we can estimate the two second-group eigenenergies as follows:

In[70]:=
```
Clear[aBa, bBb]
```

In[71]:=
```
NSolve[{dltE == bBb - aBa, EB == pa aBa + pb bBb}, {aBa, bBb}]
```

Out[71]=
```
{{aBa → -0.246147, bBb → -0.00374743}}
```

In[73]:=
```
aBa = -0.2461474293167589`; bBb = -0.0037474293167590023`;
```

and now we can compute the standard deviation which should be small.

In[74]:=
```
EB2 = pa aBa^2 + pb bBb^2
```

Out[74]=
```
0.0577361
```

In[76]:=
```
sigB = Sqrt[EB2 - EB^2]
```

Out[76]=
```
0.0513479
```

Number of measurements needed for fully commuting (FC) partitioning

Of course, all of the above analysis refers to the FC partitioning case. Using Eq. 3 from the instructions, and setting the error on the left hand side equal to .001, we find

In[77]:=
```
err = .001;
```

In[79]:=
```
Solve[err == (sigA + sigB) / Sqrt[NT], NT]
```

Out[79]=
```
{{NT → 25971.3}}
```

About 26,000 measurements are needed. Good thing we did 100,000 measurements!

second group quantities: qubit-wise commuting (QWC) partitioning

Here, we can clearly keep the old FC first grouping as one of our QWC groupings. However, NONE of the four contributions to the old FC second grouping can be combined together. So we need to treat each of the four terms as a separate group.

Expectation values for each term are easy to work out for individual transformed basis functions, as are the transformations (from x or y to z) in each case. However, we did not do the calculation that would have provided amplitudes for the solution Psi across each of these basis functions. Thus, it is not possible to estimate the number of measurements that would be required in the QWC
case.