Phase Estimation?? Hydrogen?? CHEMISTRY?!?!?!

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The aim of this project was to implement the algorithm for computing the energy of a hydrogen atom as described by Poulin et al. [3]. This algorithm consists of x steps:

1. Create three registers: `counting`, `aux` and `main`.
2. Put the `aux` register in the state $|\beta\rangle$.
3. Put the `main` register in an eigenstate of the Hamiltonian.
4. Estimate phase?
5. ???
6. Profit?

The state $|\beta\rangle$ is given by

$$|\beta\rangle = B\,|0\rangle = \sum_j \beta_j\,|j\rangle\,.$$

The code for phase estimation was adapted from [1], which is in turn based on Nielsen and Chuang [2]. The main complication in this part was that the original code was used 3 counting qubits, instead of 2. Therefore, we adapted it to support any number of qubits. Additionally, the bits had to be adapted to fits the registry structure.

Trouble: unitary B not "normalized" due to inaccuracies of decimal numbers

$$\bar{H} = \frac{H}{\mathcal{N}} = \sum_j |\beta_j|^2 P_j, \tag{1}$$

This is hydrogen Hamiltonian (stolen from [4])

$$\begin{aligned}\hat{H}_{BK} = &- 0.81261I + 0.171201\sigma_0^z + 0.16862325\sigma_1^z - 0.2227965\sigma_2^z + 0.171201\sigma_1^z\sigma_0^z \\ &+ 0.12054625\sigma_2^z\sigma_0^z + 0.17434925\sigma_3^z\sigma_1^z + 0.04532175\sigma_2^x\sigma_1^z\sigma_0^x + 0.04532175\sigma_2^y\sigma_1^z\sigma_0^y \\ &+ 0.165868\sigma_2^z\sigma_1^z\sigma_0^z + 0.12054625\sigma_3^z\sigma_2^z\sigma_0^z - 0.2227965\sigma_3^z\sigma_2^z\sigma_1^z \\ &+ 0.04532175\sigma_3^z\sigma_2^x\sigma_1^z\sigma_0^x + 0.04532175\sigma_3^z\sigma_2^y\sigma_1^z\sigma_0^y + 0.165868\sigma_3^z\sigma_2^z\sigma_1^z\sigma_0^z\end{aligned}$$

where $\beta_j = \sqrt{|\alpha_j|/\mathcal{N}}$. Due to the nature of the scaling factor $\mathcal{N}$, $\sum_j |\beta_j|^2 = 1$.

Poulin et al. [3] define β, B, S and V as following:

$$S = (B(I - 2\left|0\right\rangle\left\langle 0\right|)B^\dagger) \otimes I = (I - 2|\beta\rangle\langle\beta|) \otimes I)$$

$$V = \sum_j \left|j\right\rangle\left\langle j\right| \otimes P_j$$

References

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