Note on Quantum Chemistry

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1 Introduction

2 Molecular orbital models

2.1 PEA

2.1.1 Hamiltonian reduction methods

2.1.2 BK-tree

2.2 VQE

2.2.1 Ground state

2.2.2 Excited state

2.2.3 Ansatz

2.2.4 UCC

Calculation check on Appendix B of [https://arxiv.org/pdf/1805.04340.pdf]

$$T_1 = \sigma_{ij}\theta_{ij}(a_i^\dagger a_j - a_j^\dagger a_i) \tag{1}$$
$$T_2 = \sigma_{ijkl}\theta_{ijkl}(a_i^\dagger a_j^\dagger a_k a_l - a_l^\dagger a_k^\dagger a_j a_i) \tag{2}$$

After the Jordan-Wigner transformation for N qubits, which is given by:

$$a_j = 1^{\otimes j} \otimes \frac{1}{2}(X + iY) \otimes Z^{\otimes N-j-1} \tag{3}$$
$$a_j^\dagger = 1^{\otimes j} \otimes \frac{1}{2}(X - iY) \otimes Z^{\otimes N-j-1} \tag{4}$$

then for $i > j$

$$a_i^\dagger = 1^{\otimes j} \otimes 1^{\otimes i-j} \otimes \frac{1}{2}(X + iY) \otimes Z^{\otimes N-i-1} \tag{5}$$
$$a_j = 1^{\otimes j} \otimes \frac{1}{2}(X - iY) \otimes Z^{\otimes i-j} \otimes Z^{\otimes N-i-1} \tag{6}$$

$$
\begin{aligned}
a_i^\dagger a_j &= 1^{\otimes j} \otimes \frac{1}{2}(X - iY) \otimes Z^{\otimes i-j-1} \otimes \frac{1}{2}(X + iY) Z \otimes 1^{\otimes N-i-1} && (7)\\
&= 1^{\otimes j} \otimes \frac{1}{2}(X - iY) \otimes Z^{\otimes i-j-1} \otimes \frac{1}{2}(-Y + iX) \otimes 1^{\otimes N-i-1} && (8)\\
a_j^\dagger a_i &= 1^{\otimes j} \otimes \frac{1}{2}(X + iY) \otimes Z^{\otimes i-j-1} \otimes \frac{1}{2} Z (X - iY) \otimes 1^{\otimes N-i-1} && (9)\\
&= 1^{\otimes j} \otimes \frac{1}{2}(X + iY) \otimes Z^{\otimes i-j-1} \otimes \frac{1}{2}(Y + iX) \otimes 1^{\otimes N-i-1} && (10)
\end{aligned}
$$

Then

$$
\begin{aligned}
a_i^\dagger a_j - a_j^\dagger a_i &= 1^{\otimes j} \otimes \frac{1}{2}\left[X \otimes Z^{\otimes i-j-1} \otimes Y - Y \otimes Z^{\otimes i-j-1} \otimes X\right] \otimes 1^{\otimes N-i-1} && (11)\\
&= \frac{i}{2} \bigotimes_{a=j+1}^{i-1} Z_a \left[Y_j X_i - X_j Y_i\right] && (12)
\end{aligned}
$$

Since

$$
[Y_j X_i, X_j Y_i] = Y_j X_i X_j Y_i - X_j Y_i Y_j X_i = -Z_j Z_i + Z_j Z_i = 0, \tag{13}
$$

Therefore

$$
\begin{aligned}
\prod_{ij} \exp\left[\theta_{ij}(a_i^\dagger a_j - a_j^\dagger a_i)\right] &= \prod_{i>j} \exp\left[\frac{i}{2}\theta_{ij} \bigotimes_{a=j+1}^{i-1} Z_a (Y_j X_i - X_j Y_i)\right] && (14)\\
&= \prod_{i>j} \exp\left[\frac{i}{2}\theta_{ij} \bigotimes_{a=j+1}^{i-1} Z_a (Y_j X_i)\right] \exp\left[-\frac{i}{2}\theta_{ij} \bigotimes_{a=j+1}^{i-1} Z_a (X_j Y_i)\right] && (15)
\end{aligned}
$$

2.2.5 Heuristic Ansatz

3 non-MO