Many-body methods for nuclear physics, from structure to reactions

Group-8


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Training in Advanced Low Energy Nuclear Theory
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I. PART 1A

Show that the unperturbed Hamiltonian H_0 and V commute with both the spin projection S_z and the total spin S^2, and Hamiltonian commutes with the product of the pair creation and annihilation operators. That is

$$\left[\hat{H}_0 \quad \hat{S}_z\right] = 0 \qquad \left[\hat{H}_0 \quad \hat{S}^2\right] = 0$$
$$\left[\hat{V}_0 \quad \hat{S}_z\right] = 0 \qquad \left[\hat{V}_0 \quad \hat{S}^2\right] = 0$$
$$\left[\hat{H} \quad \sum_p \hat{P}_p^+ \hat{P}_p^-\right] = 0$$

(1)

$$\begin{aligned}
\left[\hat{H}_0 \qquad \hat{S}_z\right] &= \left[\sum_{p\sigma}(p-1)a^+_{p\sigma}a_{p\sigma} \qquad \frac{1}{2}\sum_{p\sigma}\sigma a^+_{p\sigma}a_{p\sigma}\right] \\
=&\frac{1}{2}\sum_{p\sigma}(p-1)\sigma a^+_{p\sigma}a_{p\sigma}a^+_{p\sigma}a_{p\sigma} - \frac{1}{2}\sum_{p\sigma}(p-1)\sigma a^+_{p\sigma}a_{p\sigma}a^+_{p\sigma}a_{p\sigma} \\
=&0
\end{aligned}$$

(2)

$$\begin{aligned}
\left[\hat{H}_0 \qquad \hat{S}_+\right] &= \left[\sum_{p\sigma}(p-1)a^+_{p\sigma}a_{p\sigma} \qquad \sum_p a^+_{p+}a_{p-}\right] \\
=&\left[\sum_p(p-1)(a^+_{p+}a_{p+} + a^+_{p-}a_{p-}) \qquad \sum_p a^+_{p+}a_{p-}\right] \\
=&\sum_p(p-1)(a^+_{p+}a_{p+}a^+_{p+}a_{p-} + a^+_{p-}a_{p-}a^+_{p+}a_{p-} - a^+_{p+}a_{p-}a^+_{p+}a_{p+} - a^+_{p+}a_{p-}a^+_{p-}a_{p-}) \\
=&\sum_p(p-1)(a^+_{p+}(1-a^+_{p+}a_{p+})a_{p-} - a^+_{p-}a^+_{p+}a_{p-}a_{p-} + a^+_{p+}a^+_{p+}a_{p-}a_{p+} - a^+_{p+}(1-a^+_{p-}a_{p-})a_{p-}) \\
=&\sum_p(p-1)(a^+_{p+}a_{p-} - a^+_{p+}a_{p-}) \\
=&0
\end{aligned}$$

In a similar way, we can prove that

$$\left[\hat{H}_0 \qquad \hat{S}_-\right] = 0$$

So

$$\begin{aligned}
&\left[\hat{H}_0 \quad \hat{S}^2\right] = \left[\hat{H}_0 \quad \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+)\right] \\
=&\left[\hat{H}_0 \quad \hat{S}_z^2\right] + \frac{1}{2}\left[\hat{H}_0 \quad \hat{S}_+\hat{S}_-\right] + \frac{1}{2}\left[\hat{H}_0 \quad \hat{S}_-\hat{S}_+\right] \\
=&\hat{S}_z\left[\hat{H}_0 \quad \hat{S}_z\right] + \left[\hat{H}_0 \quad \hat{S}_z\right]\hat{S}_z + \frac{1}{2}\left(\hat{S}_+\left[\hat{H}_0 \quad \hat{S}_-\right] + \left[\hat{H}_0 \quad \hat{S}_+\right]\hat{S}_- + \hat{S}_-\left[\hat{H}_0 \quad \hat{S}_+\right] + \left[\hat{H}_0 \quad \hat{S}_-\right]\hat{S}_+\right) \\
=&0
\end{aligned}$$

(3)

$$\begin{aligned}
&\left[\sum_p \hat{P}_p^+ \quad \hat{S}_z\right] = \left[\sum_p \hat{P}_p^+ \quad \frac{1}{2}\sum_{p\sigma}\sigma a_{p\sigma}^+ a_{p\sigma}\right] \\
&= \left[\sum_p a_{p+}^+ a_{p-}^+ \quad \frac{1}{2}\sum_p \left(a_{p+}^+ a_{p+} - a_{p-}^+ a_{p-}\right)\right] \\
&= \frac{1}{2}\sum_p \left[\left(a_{p+}^+ a_{p-}^+ a_{p+}^+ a_{p+} - a_{p+}^+ a_{p-}^+ a_{p-}^+ a_{p-}\right) - \left(a_{p+}^+ a_{p+} a_{p+}^+ a_{p-}^+ - a_{p-}^+ a_{p-} a_{p+}^+ a_{p-}^+\right)\right] \\
&= \frac{1}{2}\sum_p - \left(a_{p+}^+(1 - a_{p+}^+ a_{p+}) a_{p-}^+ - (1 - a_{p-} a_{p-}^+) a_{p+}^+ a_{p-}^+\right) \\
&= \frac{1}{2}\sum_p - \left(a_{p+}^+ a_{p-}^+ - a_{p+}^+ a_{p-}^+ - a_{p-} a_{p+}^+ a_{p-}^+ a_{p-}^+\right) \\
&= 0
\end{aligned}$$

$$\begin{aligned}
&\left[\sum_q \hat{P}_q^- \quad \hat{S}_z\right] = \left[\sum_q a_{q-} a_{q+} \quad \frac{1}{2}\sum_p \left(a_{p+}^+ a_{p+} - a_{p-}^+ a_{p-}\right)\right] \\
&= \frac{1}{2}\sum_{pq}\left[a_{q-} a_{q+} a_{p+}^+ a_{p+} - a_{q-} a_{q+} a_{p-}^+ a_{p-} - a_{p+}^+ a_{p+} a_{q-} a_{q+} + a_{p-}^+ a_{p-} a_{q-} a_{q+}\right] \\
&= \frac{1}{2}\sum_{pq}\left[a_{q-} a_{q+} a_{p+}^+ a_{p+} - a_{q-} a_{q+} a_{p-}^+ a_{p-} - a_{q-} a_{q+} a_{p+}^+ a_{p+} + a_{q-} a_{q+} a_{p-}^+ a_{p-}\right] \\
&= 0
\end{aligned}$$

$$\begin{aligned}
&\left[\hat{V} \quad \hat{S}_z\right] = -g\left[\sum_{pq} \hat{P}_p^+ \hat{P}_q^- \quad \hat{S}_z\right] \\
&= -g\left(\sum_p \hat{P}_p^+ \left[\sum_q \hat{P}_q^- \quad \hat{S}_z\right] + \left[\sum_p \hat{P}_p^+ \quad \hat{S}_z\right]\sum_q \hat{P}_q^-\right) \\
&= 0
\end{aligned}$$

(4)

$$
\begin{aligned}
&\left[\sum_p \hat{P}_p^+ \quad \hat{S}_+\right] = \left[\sum_p a_{p+}^+ a_{p-}^+ \qquad \sum_p a_{p+}^+ a_{p-}\right] \\
&= \sum_p \left(a_{p+}^+ a_{p-}^+ a_{p+}^+ a_{p-} - a_{p+}^+ a_{p-} a_{p+}^+ a_{p-}^+\right) \\
&= \sum_p \left(-a_{p+}^+ a_{p+}^+ a_{p-}^+ a_{p-} + a_{p+}^+ a_{p+}^+ a_{p-} a_{p-}^+\right) \\
&= 0
\end{aligned}
$$

In a similar way, we can prove that

$$\left[\sum_p \hat{P}_p^+ \quad \hat{S}_-\right] = 0$$

$$
\begin{aligned}
&\left[\sum_q \hat{P}_q^+ \quad \hat{S}_+\right] = \left[\sum_q a_{q+}^+ a_{q-}^+ \qquad \sum_p a_{p+}^+ a_{p-}\right] \\
&= \sum_p \left(a_{q+}^+ a_{q-}^+ a_{p+}^+ a_{p-} - a_{p+}^+ a_{p-} a_{q+}^+ a_{q-}^+\right) \\
&= 0
\end{aligned}
$$

and

$$\left[\sum_q \hat{P}_q^+ \quad \hat{S}_-\right] = 0$$

So

$$
\begin{aligned}
&\left[\hat{V} \quad \hat{S}^2\right] = -g\left[\sum_{pq} \hat{P}_p^+ \hat{P}_q^- \qquad \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+)\right] \\
&=0
\end{aligned}
$$

(5)

$$
\begin{aligned}
&\left[\hat{H}_0 \quad \sum_p \hat{P}_P^+\right] = \left[\sum_p (p-1)(a_{p+}^+ a_{p+} + a_{p-}^+ a_{p-}) \quad \sum_p a_{p+}^+ a_{p-}^+\right] \\
&=\sum_p (p-1)\left(a_{p+}^+ a_{p+} a_{p+}^+ a_{p-}^+ + a_{p-}^+ a_{p-} a_{p+}^+ a_{p-}^+ - a_{p+}^+ a_{p-}^+ a_{p+}^+ a_{p+} - a_{p+}^+ a_{p-}^+ a_{p-}^+ a_{p-}\right) \\
&=\sum_p (p-1)\left(a_{p+}^+ a_{p-}^+ + a_{p+}^+ a_{p-}^+ - a_{p-} a_{p+}^+ a_{p-}^+ a_{p-}^+ - a_{p+}^+ a_{p-}^+ a_{p+}^+ a_{p+} - a_{p+}^+ a_{p-}^+ a_{p-}^+ a_{p-}\right) \\
&=\sum_p 2(p-1) a_{p+}^+ a_{p-}^+
\end{aligned}
$$

$$
\begin{aligned}
&\left[\hat{H}_0 \quad \sum_p \hat{P}_P^-\right] = \left[\sum_p (p-1)(a_{p+}^+ a_{p+} + a_{p-}^+ a_{p-}) \quad \sum_p a_{p-} a_{p+}\right] \\
=&\sum_p (p-1)\left(a_{p+}^+ a_{p+} a_{p-} a_{p+} + a_{p-}^+ a_{p-} a_{p-} a_{p+} - a_{p-} a_{p+} a_{p+}^+ a_{p+} - a_{p-} a_{p+} a_{p-}^+ a_{p-}\right) \\
=&-\sum_p 2(p-1) a_{p+} a_{p-}
\end{aligned}
$$

$$
\begin{aligned}
&\left[\hat{V} \quad \sum_p \hat{P}_P^+\right] = -g\left[\sum_{pq} \hat{P}_p^+ \hat{P}_q^- \quad \sum_p \hat{P}_P^+\right] \\
=&-g\left(\sum_p \hat{P}_p^+ \left[\sum_q \hat{P}_q^- \quad \sum_p \hat{P}_P^+\right] + \left[\sum_p \hat{P}_p^+ \quad \sum_p \hat{P}_P^+\right] \sum_q \hat{P}_q^-\right) \\
=&-g\sum_p \left(a_{p+}^+ a_{p-}^+ \left(a_{p-} a_{p+} a_{p+}^+ a_{p-}^+ - a_{p+}^+ a_{p-}^+ a_{p-} a_{p+}\right)\right)
\end{aligned}
$$

$$
\begin{aligned}
&\left[\hat{V} \quad \sum_p \hat{P}_P^-\right] = -g\left[\sum_{pq} \hat{P}_p^+ \hat{P}_q^- \quad \sum_p \hat{P}_P^-\right] \\
=&-g\left(\sum_p \hat{P}_p^+ \left[\sum_q \hat{P}_q^- \quad \sum_p \hat{P}_P^-\right] + \left[\sum_p \hat{P}_p^+ \quad \sum_p \hat{P}_P^-\right] \sum_q \hat{P}_q^-\right) \\
=&-g\sum_p \left(\left(a_{p+}^+ a_{p-}^+ a_{p-} a_{p+} - a_{p-} a_{p+} a_{p+}^+ a_{p-}^+\right) a_{p-} a_{p+}\right)
\end{aligned}
$$

$$
\begin{aligned}
&\left[\hat{H} \quad \sum_p \hat{P}_P^+ \hat{P}_P^-\right] = \left[\hat{H}_0 + \hat{V} \quad\quad \sum_p \hat{P}_P^+ \hat{P}_P^-\right] \\
=&\left[\hat{H}_0 \quad \sum_p \hat{P}_P^+ \hat{P}_P^-\right] + \left[\hat{V} \quad\quad \sum_p \hat{P}_P^+ \hat{P}_P^-\right] \\
=&\sum_p \hat{P}_P^+ \left[\hat{H}_0 \quad \sum_p \hat{P}_P^-\right] + \left[\hat{H}_0 \quad \sum_p \hat{P}_P^+\right] \sum_p \hat{P}_P^- + \sum_p \hat{P}_P^+ \left[\hat{V} \quad\quad \sum_p \hat{P}_P^-\right] + \left[\hat{V} \quad\quad \sum_p \hat{P}_P^+\right] \sum_p \hat{P}_P^- \\
=&\sum_p 2(p-1) a_{p+}^+ a_{p-}^+ a_{p+} a_{p-} - \sum_p 2(p-1) a_{p+}^+ a_{p-}^+ a_{p+} a_{p-} + 0 \\
=&0
\end{aligned}
$$

II. PART 1B

Simpler case: 2 particals 4 sp. Find the eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for selected values of $g \in [-1, 1]$ and comment your results. First, some rules:

$$
\begin{aligned}
&H = H_0 + V = \sum_p (p-1)(a_{p+}^+ a_{p+} + a_{p-}^+ a_{p-}) - g \sum_{pq} \hat{P}_p^+ \hat{P}_q^- \\
&a_p^+|0\rangle = |p\rangle \qquad \langle 0|a_p = \langle p| \\
&\hat{P}_p^+ = a_{p+}^+ a_{p-}^+ \qquad \hat{P}_p^- = a_{p-} a_{p+}
\end{aligned}
$$

Assume $\varepsilon = 1$

Two particles only occupied the lowest orbit, so p=1,q=1

$$
\begin{aligned}
H_{11} &= \langle 0|a_{1+}a_{1-} H a_{1-}^+ a_{1+}^+|0\rangle \\
&= \langle 0|a_{1+}a_{1-}(-g\sum_{pq} \hat{P}_p^+ \hat{P}_q^-) a_{1-}^+ a_{1+}^+|0\rangle \\
&= \langle 1+1-| - g\hat{P}_1^+ \hat{P}_1^- |1+1-\rangle \\
&= \langle 1+1-| - g a_{1+}^+ a_{1-}^+ a_{1-} a_{1+} |1+1-\rangle \\
&= -g
\end{aligned}
$$

One state is that two particles occupied the lowest orbit, another state is that two particles occupied the second orbit.

$$
\begin{aligned}
H_{12} &= \langle 0|a_{1+}a_{1-} H a_{2-}^+ a_{2+}^+|0\rangle \\
&= \langle 0|a_{1+}a_{1-}(a_{2+}^+ a_{2+} + a_{2-}^+ a_{2-}) a_{2-}^+ a_{2+}^+|0\rangle + \langle 0|a_{1+}a_{1-}(-g\sum_{pq} \hat{P}_p^+ \hat{P}_q^-) a_{2-}^+ a_{2+}^+|0\rangle \\
&= \langle 1+1-|2+2-\rangle - g\langle 1+1-|P_1^+P_1^- + P_1^+P_2^- + P_2^+P_1^- + P_2^+P_2^-|2+2-\rangle \\
&= -g\langle 1+1-|P_1^+P_2^-|2+2-\rangle \\
&= -g\langle 1+1-|a_{1+}^+ a_{1-}^+ a_{2-} a_{2+}|2+2-\rangle \\
&= -g\langle 1+1-|1+1-\rangle \\
&= -g
\end{aligned}
$$

One state is that two particles occupied the second orbit, another state is that two particles occupied the lowest orbit.

$$
\begin{aligned}
H_{21} &= \langle 0|a_{2+}a_{2-}Ha_{1-}^{+}a_{1+}^{+}|0\rangle \\
&= \langle 0|a_{2+}a_{2-}(-g\sum_{pq}\hat{P}_p^{+}\hat{P}_q^{-})a_{1-}^{+}a_{1+}^{+}|0\rangle \\
&= -g\langle 2+2-|P_1^{+}P_1^{-} + P_1^{+}P_2^{-} + P_2^{+}P_1^{-} + P_2^{+}P_2^{-}|1+1-\rangle \\
&= -g\langle 2+2-|P_2^{+}P_1^{-}|1+1-\rangle \\
&= -g\langle 2+2-|a_{2+}^{+}a_{2-}^{+}a_{1-}a_{1+}|1+1-\rangle \\
&= -g\langle 2+2-|2+2-\rangle \\
&= -g
\end{aligned}
$$

Both states are occupied the second orbit

$$
\begin{aligned}
H_{22} &= \langle 0|a_{2+}a_{2-}Ha_{2-}^{+}a_{2+}^{+}|0\rangle \\
&= \langle 0|a_{2+}a_{2-}(a_{2+}^{+}a_{2+} + a_{2-}^{+}a_{2-})a_{2-}^{+}a_{2+}^{+}|0\rangle + \langle 0|a_{2+}a_{2-}(-g\sum_{pq}\hat{P}_p^{+}\hat{P}_q^{-})a_{2-}^{+}a_{2+}^{+}|0\rangle \\
&= 2\langle 2+2-|2+2-\rangle - g\langle 2+2-|P_1^{+}P_1^{-} + P_1^{+}P_2^{-} + P_2^{+}P_1^{-} + P_2^{+}P_2^{-}|2+2-\rangle \\
&= 2 - g\langle 2+2-|P_2^{+}P_2^{-}|2+2-\rangle \\
&= 2 - g\langle 2+2-|a_{2+}^{+}a_{2-}^{+}a_{2-}a_{2+}|2+2-\rangle \\
&= 2 - g\langle 2+2-|2+2-\rangle \\
&= 2 - g
\end{aligned}
$$

So, the matrix element is

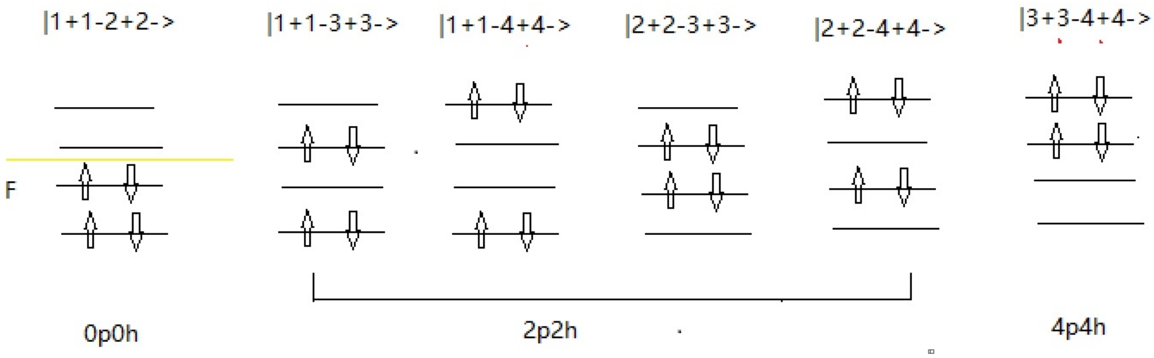
$$
H = \begin{bmatrix} -g & -g \\ -g & 2-g \end{bmatrix}
$$

, by diagonalizing the Hamiltonian matrix, we can get the eigenvalues

III. PART 1C

Setting up the Hamiltonian matrix : 4 particles 8 orbits, we also assume $\varepsilon = 1$. There are six particle occupied situation.

$$
H = \begin{bmatrix}
\langle 1+1-2+2-|H|1+1-2+2-\rangle & \langle 1+1-2+2-|H|1+1-3+3-\rangle & \dots & \langle 1+1-2+2-|H|3+3-4+4-\rangle \\
\langle 1+1-3+3-|H|1+1-2+2-\rangle & \langle 1+1-3+3-|H|1+1-3+3-\rangle & \dots & \langle 1+1-3+3-|H|3+3-4+4-\rangle \\
\dots & \dots & .. & \dots \\
\dots & \dots & .. & \dots \\
\langle 3+3-4+4-|H|1+1-2+2-\rangle & \langle 3+3-4+4-|H|1+1-3+3-\rangle & .. & \langle 3+3-4+4-|H|3+3-4+4-\rangle
\end{bmatrix}
$$



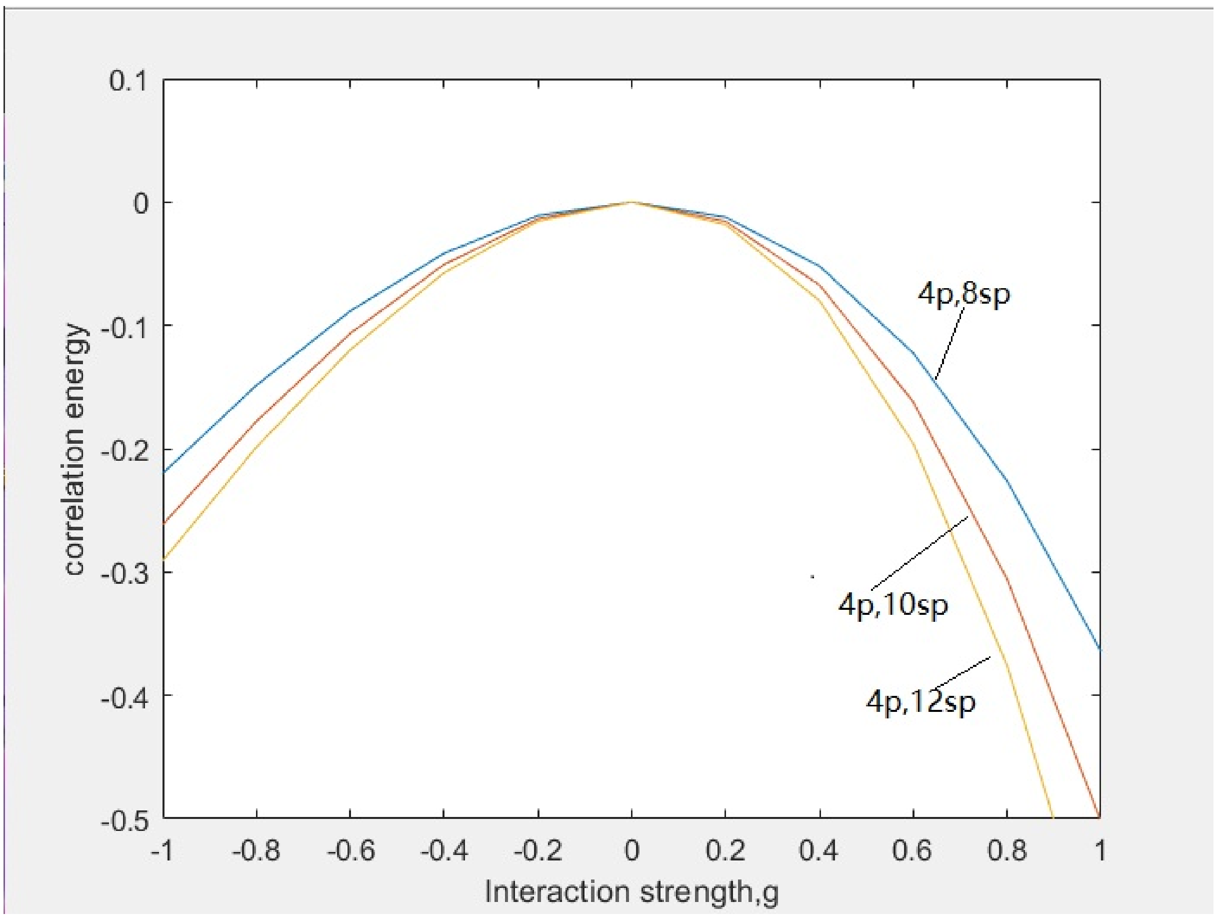
$$H_{11} = \langle 0|a_{1+}a_{1-}a_{2+}a_{2-}Ha^+_{2-}a^+_{2+}a^+_{1-}a^+_{1+}|0\rangle$$
$$= \langle 0|a_{1+}a_{1-}a_{2+}a_{2-}(a^+_{2+}a_{2+} + a^+_{2-}a_{2-})a^+_{2-}a^+_{2+}a^+_{1-}a^+_{1+}|0\rangle$$
$$+\langle 0|a_{1+}a_{1-}a_{2+}a_{2-}(-g\sum_{pq}\hat{P}^+_p\hat{P}^-_q)a^+_{2-}a^+_{2+}a^+_{1-}a^+_{1+}|0\rangle$$
$$= 2 - g\langle 1+1-2+2-|P^+_1P^-_1 + P^+_1P^-_2 + P^+_1P^-_3 + P^+_2P^-_1 + P^+_2P^-_2$$
$$+P^+_2P^-_3 + P^+_3P^-_1 + P^+_3P^-_2 + P^+_3P^-_3|1+1-2+2-\rangle$$
$$= 2 - g\langle 1+1-2+2-|P^+_1P^-_1 + P^+_2P^-_2|1+1-2+2-\rangle$$
$$= 2 - 2g$$

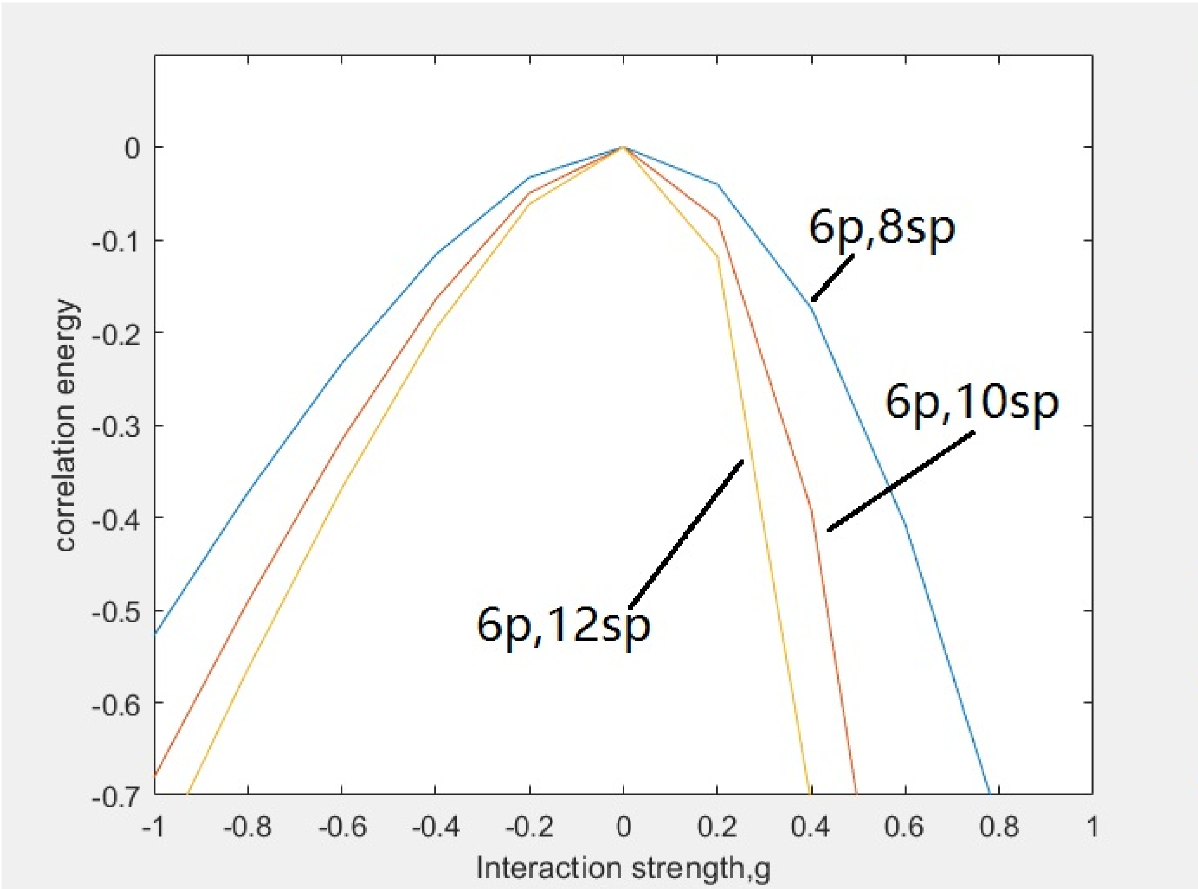
$$H_{12} = \langle 0|a_{1+}a_{1-}a_{2+}a_{2-}Ha^+_{3-}a^+_{3+}a^+_{1-}a^+_{1+}|0\rangle$$
$$= \langle 0|a_{1-}a_{1+}a_{2-}a_{2+}(-g\sum_{pq}\hat{P}^+_p\hat{P}^-_q)a^+_{3-}a^+_{3+}a^+_{1-}a^+_{1+}|0\rangle$$
$$= -g\langle 1+1-2+2-|P^+_1P^-_1 + P^+_1P^-_2 + P^+_1P^-_3 + P^+_2P^-_1 + P^+_2P^-_2$$
$$+P^+_2P^-_3 + P^+_3P^-_1 + P^+_3P^-_2 + P^+_3P^-_3|1+1-3+3-\rangle$$
$$= -g\langle 1+1-2+2-|P^+_2P^-_3|1+1-3+3-\rangle$$
$$= -g$$

In the similar way, we can get other matrix elements. finally, we can get the matrix.

$$H = \begin{bmatrix} 2-2g & -g & -g & -g & -g & 0 \\ -g & 4-g & -g & -g & 0 & -g \\ -g & -g & 6-g & 0 & -g & -g \\ -g & -g & 0 & 6-g & -g & -g \\ -g & 0 & -g & -g & 8-g & -g \\ 0 & -g & -g & -g & -g & 10-g \end{bmatrix}$$

,




6p,8sp
6p,10sp
6p,12sp
correlation energy
Interaction strength,g
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1