Quantum algorithms (VQE) and nuclear physics with applications, parts I and II

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Overview

In these two lectures we will derive the essential elements for using the VQE algorithm applied to a selected nuclear physics model, in our case the so-called pairing Hamiltonian. In order to do so, we will need to present the so-called Jordan-Wigner transformation first. We will apply this to the pairing Hamiltonian discussed previously. This Hamiltonian is writen in second quantization and we will use the Pauli matrices discussed earlier in order to rewrite the second-quantization creation and annihilation operators in terms of Pauli matrices.

The unitary coupled cluster approach is discussed below here.

Thereafter, in the second lecture, we discuss how to implement the VQE algorithm. The results obtained with the VQE algorithm will be compared to those obtained by using FCI and the unitary coupled cluster method (as well as the standard coupled cluster method with doubles excitations only).

The Jordan-Wigner transformation

The Jordan-Wigner transformation is a transformation that maps the Pauli gates discussed earlier onto fermionic creation and annihilation operators. The creation and annihilation operators from second quantization can then be represented on quantum computers, and we will be able to rewrite our Hamiltonians in a second quantization representation in terms of quantum gates.

Explicit expressions

Suppose that we represent a qubit in state $|0\rangle$ as a state occupied with a single fermion and $|1\rangle$ as a state with no fermion. We then see that the operators

$$\sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$\sigma_- = \frac{1}{2}(\sigma_x - i\sigma_y) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \tag{1}$$

have the following effect on the qubit basis states

$$\sigma_+|1\rangle = |0\rangle \qquad \sigma_-|0\rangle = |1\rangle,$$

and

$$\sigma_+|0\rangle = 0 \qquad \sigma_-|1\rangle = 0.$$

Replacing creation and annihilation operators with Pauli matrices

The term σ_+ acts as a creation operator and σ_- acts as an annihilation operator. However, since fermionic states are anti-symmetric, $a_a^\dagger a_b^\dagger|c\rangle = -a_b^\dagger a_a^\dagger|c\rangle$, we need our quantum gate representation of the creation/annihilation operators to preserve this property. This can be achieved by multiplying the σ_z matrix on all the occupied states except for the one we operate on. The complete creation and annihilation operators can then be represented as

$$a_n^\dagger \equiv \left(\prod_{k=1}^{n-1} \sigma_z^k\right)\sigma_+^n \qquad a_n \equiv \left(\prod_{k=1}^{n-1} \sigma_z^k\right)\sigma_-^n \tag{2}$$

where the superscript tells us which qubit the operator acts on.

Representations of spin states

For convenience, we let odd qubits to be in a spin up state, while even qubits are in spin down state. The following state

$$\textit{Qubit state:}|0 \quad 0 \quad 1 \quad 1\rangle$$
$$\textit{Spin state:} + \quad - \quad + \quad -$$
$$\textit{Spacial state:} 1 \quad 1 \quad 2 \quad 2 \, ,$$

the first spacial state is occupied with a fermion pair with opposite spin, while the second state is not occupied with any fermions. The equivalent of the reference state for our qubit-state is then

$$|\Psi_0\rangle = |0\rangle^{\otimes^n}|1\rangle^{\otimes^k}, \tag{3}$$

where n is the number of particles and $n + k$ is the number of spin-orbitals.

Jordan-Wigner transformation of Pairing Hamiltonian

We can write the pairing Hamiltonian in second quantized representation in terms of the Pauli matrices. A detailed derivation is provided below. Here we simply state the result: For the one body part of the Hamiltonian we have the terms

$$\hat{H}_{0p} = \frac{1}{2}\delta(p - 1 - I[p\%2 = 0])(I^p + \sigma_z^p), \tag{4}$$

where we sum over each qubit p and $\%$ is the modulo operator. We have that $I[f(x) = y] = 1$ if $f(x) = y$ and zero otherwise.

Interaction part

For the interaction term we have two possibilities. First for $p = q$ we have:

$$\begin{aligned}
\hat{V}_p = -\frac{1}{8}g\Big[&I^{\otimes 2p-2} \otimes I \otimes I \otimes I^{\otimes n-2p} \\
+&I^{\otimes 2p-2} \otimes I \otimes \sigma_z \otimes I^{\otimes n-2p} \\
+&I^{\otimes 2p-2} \otimes \sigma_z \otimes I \otimes I^{\otimes n-2p} \\
+&I^{\otimes 2p-2} \otimes \sigma_z \otimes \sigma_z \otimes I^{\otimes n-2p}\Big].
\end{aligned} \tag{5}$$

And the remaining contribution to the two-body interaction

For $q - p \geq 1$ we get:

$$\begin{aligned}
\hat{V}_{pq} = -\frac{1}{16}g[&I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q} \\
-&I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q} \\
+&I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q} \\
+&I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q} \\
+&I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q} \\
+&I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q} \\
-&I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q} \\
+&I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q}].
\end{aligned} \tag{6}$$

We have included a factor of two so the sum over p and q here can be restricted to $q > p$. The complete Jordan-Wigner transformed pairing Hamiltonian can then be written as

$$\hat{H} = \sum_p \hat{H}_{0p} + \sum_p \hat{V}_p + \sum_{q>p} \hat{V}_{pq}, \tag{7}$$

where $\hat{H}_{0p}$, $\hat{V}_p$ and $\hat{V}_{pq}$ is given by the one-body part and two-body part, respectively.

3

Details behind the derivation of the Jordan-Wigner transformed Pairing Hamiltonian

Here we show how we can rewrite our pairing Hamiltonian in terms of the Pauli matrices. First, we observe that

$$a_i^\dagger a_i = \left(\prod_{k=1}^{i-1} \sigma_z^k\right) \sigma_+^i \left(\prod_{k=1}^{i-1} \sigma_z^k\right) \sigma_-^i$$

$$= \sigma_+^i \sigma_-^i = \frac{1}{2}(I^i + \sigma_z^i),$$

and see that the one-body part of the Hamiltonian can be written as

$$\hat{H}_0 = \frac{1}{2}\xi \sum_p ([(p-1) - (p-1)\%2]/2)(I^p + \sigma_z^p).$$

where p now runs over each qubit and $\%$ is the modulo operator. For the interaction term, we get

$$\hat{V} =$$
$$-\frac{1}{2}g \sum_{pq} \left(\prod_{k=1}^{2p-2} \sigma_z^k\right) \sigma_+^{2p-1} \left(\prod_{k=1}^{2p-1} \sigma_z^k\right) \sigma_+^{2p} \left(\prod_{k=1}^{2q-1} \sigma_z^k\right) \sigma_-^{2q} \left(\prod_{k=1}^{2q-2} \sigma_z^k\right) \sigma_-^{2q-1}.$$

$$(8)$$

Rewriting the Pairing Hamiltonian

We have that

$$\left(\prod_{k=1}^{2p-2} \sigma_z^k\right) \sigma_+^{2p-1} \left(\prod_{k=1}^{2p-1} \sigma_z^k\right) \sigma_+^{2p} =$$
$$\sigma_z^{\otimes 2p-2} \otimes \sigma_+ \otimes I^{\otimes n-2p-1} \times \sigma_z^{\otimes 2p-1} \otimes \sigma_+ \otimes I^{\otimes n-2p} =$$
$$I^{\otimes 2p-2} \otimes \sigma_+ \sigma_z \otimes \sigma_+ \otimes I^{\otimes n-2p},$$

which can be rewritten as

$$\hat{V} =$$
$$-\frac{1}{2}g \sum_{pq} \left[I^{\otimes 2p-2} \otimes \sigma_+ \otimes \sigma_+ \otimes I^{\otimes n-2p}\right] \left[I^{\otimes 2q-2} \otimes \sigma_- \otimes \sigma_- \otimes I^{\otimes n-2q}\right].$$

Two possibilities

We have two possibilities here. First for $p = q$:

$$-\frac{1}{2}g\left[I^{\otimes 2p-2} \otimes \sigma_+\sigma_- \otimes \sigma_+\sigma_- \otimes I^{\otimes n-2p}\right], \qquad (9)$$

and for $q - p \geq 1$ we have

$$-\frac{1}{2}g\left[I^{\otimes 2p-2} \otimes \sigma_+ \otimes \sigma_+ \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_- \otimes \sigma_- \otimes I^{\otimes n-2q}\right]. \qquad (10)$$

For $p - q \geq 1$ we simply exchange p with q and σ_+ with σ_-.

More details

To continue, we insert the expressions for $\sigma_\pm$ into these equations. For $p = q$ we then have:

$$
\begin{aligned}
V_{p=q} &= -\frac{1}{8}g\left[I^{\otimes 2p-2} \otimes (I + \sigma_z) \otimes (I + \sigma_z) \otimes I^{\otimes n-2p}\right] \\
&= -\frac{1}{8}g\left[I^{\otimes 2p-2} \otimes I \otimes I \otimes I^{\otimes n-2p} \right.\\
&\quad + I^{\otimes 2p-2} \otimes I \otimes \sigma_z \otimes I^{\otimes n-2p} \\
&\quad + I^{\otimes 2p-2} \otimes \sigma_z \otimes I \otimes I^{\otimes n-2p} \\
&\quad \left. + I^{\otimes 2p-2} \otimes \sigma_z \otimes \sigma_z \otimes I^{\otimes n-2p}\right],
\end{aligned}
$$

and for $q - p \geq 1$ we get

$$-\frac{1}{32}g\left[I^{\otimes 2p-2} \otimes (\sigma_x + i\sigma_y) \otimes (\sigma_x + i\sigma_y) \otimes I^{\otimes 2(q-p-1)} \otimes (\sigma_x - i\sigma_y) \otimes (\sigma_x - i\sigma_y) \otimes I^{\otimes n-2q}\right].$$

Rewriting as four-qubit operations

This can be rewritten as sixteen four-qubit operations

$$-\frac{1}{32}g[I^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$\mp iI^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q_p}$$

$$\mp iI^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$- I^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q_p}$$

$$\pm iI^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$+ I^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q_p}$$

$$+ I^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$\mp iI^{\otimes 2p_q-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q_p}$$

$$\pm iI^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$+ I^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q_p}$$

$$+ I^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$\mp iI^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q_p}$$

$$- I^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$\pm iI^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q_p}$$

$$\pm iI^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q_p}$$

$$+ I^{\otimes 2p_q-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q_p-p_q-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q_p}],$$

where the subscript is used if $p > q$.

Final expression

Computing the sum over p and q, the terms with $\pm$ and $\mp$ sign in front will cancel. Also, we can include a factor 2 and limit the sum to $p < q$. Our final expression is then

$$V_{p \neq q} = -\frac{1}{16}g[I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q}$$

$$- I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q}$$

$$+ I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q}$$

$$+ I^{\otimes 2p-2} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q}$$

$$+ I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_y \otimes I^{\otimes n-2q}$$

$$+ I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_x \otimes I^{\otimes n-2q}$$

$$- I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_x \otimes \sigma_x \otimes I^{\otimes n-2q}$$

$$+ I^{\otimes 2p-2} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes 2(q-p-1)} \otimes \sigma_y \otimes \sigma_y \otimes I^{\otimes n-2q}].$$

Variational Quantum Eigensolvers

As discussed in the lecture on the VQE algorithm, the variational principle states that the expectation value of the Hamiltonian has to be larger than or equal to the ground state energy of the system. Mathematically this can be expressed as

$$\langle \psi | H | \psi \rangle \geq E_0. \tag{11}$$

We can understand this principle intuitively by considering that no single measurement of the energy can be lower than the ground state energy. Hence, the expectation value of the energy can neither. Variational methods make use of this principle by calculating the expectation value in the baove equation for what we call a trial wavefunction $|\psi_T(\boldsymbol{\theta})\rangle$ given by

$$\langle \psi_T(\boldsymbol{\theta}) | H | \psi_T(\boldsymbol{\theta}) \rangle = E(\boldsymbol{\theta}).$$

Variational parameters

The variational parameters $\boldsymbol{\theta} = [\theta_1, \theta_2, \cdots, \theta_p]$ are then varied to minimize $E(\boldsymbol{\theta})$, which hopefully makes a good approximation for E_0. For variational quantum eigensolvers (VQE), the trial wave function is given by a parametrized n-qubit state

$$U(\boldsymbol{\theta})|\psi_0\rangle = |\psi_T(\boldsymbol{\theta})\rangle,$$

where $U(\boldsymbol{\theta})$ is some parametrized multi-qubit gate and $|\psi_0\rangle$ is the initial state of the qubits. As long as the Hamiltonian can be rewritten as a sum of quantum gates O_i

$$H = \sum_{i=1}^{m} h_i O_i,$$

we can find its expectation value by considering the expectation of each term

$$\langle\psi_T(\boldsymbol{\theta})|H|\psi_T(\boldsymbol{\theta})\rangle = \sum_{i=1}^{m} h_i\langle\psi_T(\boldsymbol{\theta})|O_i|\psi_T(\boldsymbol{\theta})\rangle. \tag{12}$$

The implementation details will be discussed in the next lecture.

Unitary Coupled Cluster ansatz

The coupled cluster ansatz is given by

$$|\psi_{CC}\rangle = e^{\hat{T}}|c\rangle,$$

with the cluster operator $\hat{T}$ and $|c\rangle$ being our reference state. This type of ansatz is not implementable on a quantum computer since $e^{\hat{T}}$ is not a unitary operator. Unitary coupled cluster instead suggest that we write our ansatz as

$$|\psi_{UCC}\rangle = e^{\hat{T}-\hat{T}^{\dagger}}|\psi_0\rangle, \tag{13}$$

where $\hat{T}$ is the usual coupled cluster operator and the state $|\psi_0\rangle$ is the reference state. One can show that $e^{\hat{T}-\hat{T}^{\dagger}}$ is unitary citeUCCDArticle.

New cluster operator

The unitary coupled cluster doubles (UCCD) method introduces the cluster operator

$$\hat{T}_{UCCD} = \hat{T} - \hat{T}^{\dagger} =$$
$$\sum_{ijab} t_{ij}^{ab}(a_a^{\dagger}a_b^{\dagger}a_j a_i - a_i^{\dagger}a_j^{\dagger}a_b a_a), \tag{14}$$

where we vary the trial wavefunction over the real cluster amplitudes t_{ij}^{ab}. Note that this ansatz depends on the number of particles in our system as we sum over i and j. Hence, we can specify the specific configuration we wish to solve for, unlike the previously discussed ansatzes. Rewriting eq. (14) in terms of Pauli gates by utilizing the Jordan-Wigner transformation results in

$$t_{ij}^{ab}(a_a^{\dagger}a_b^{\dagger}a_j a_i - a_i^{\dagger}a_j^{\dagger}a_b a_a) = \frac{it_{ij}^{ab}}{8}\bigotimes_{k=i+1}^{j-1}\sigma_z^k\bigotimes_{l=a+1}^{b-1}\sigma_z^l$$
$$(\sigma_x^i\sigma_x^j\sigma_y^a\sigma_x^b + \sigma_y^i\sigma_x^j\sigma_y^a\sigma_y^b$$
$$+\sigma_x^i\sigma_y^j\sigma_y^a\sigma_y^b + \sigma_x^i\sigma_x^j\sigma_x^a\sigma_y^b$$
$$-\sigma_y^i\sigma_x^j\sigma_x^a\sigma_x^b - \sigma_x^i\sigma_y^j\sigma_x^a\sigma_x^b$$
$$-\sigma_y^i\sigma_y^j\sigma_y^a\sigma_x^b - \sigma_y^i\sigma_y^j\sigma_x^a\sigma_y^b), \tag{15}$$

where we can assume that $i < j < a < b$. The subscript denotes which qubit we act upon with the Pauli gates.

Preparing for quantum computing, Suzuki-Trotter approximation

The preparation of this trial wavefunction is by first utilizing the Suzuki-Trotter approximation on the operator. Denoting

$$\hat{Z}_{ij}^{ab} = i\frac{t_{ij}^{ab}}{8p}(\bigotimes_{k=i+1}^{j-1}\sigma_z^k)(\bigotimes_{l=a+1}^{b-1}\sigma_l^z),$$

the Suzuki-Trotter approximation gives

$$|\psi(\boldsymbol{t})\rangle \approx \left(\prod_{ijab} e^{\hat{Z}_{ij}^{ab}\sigma_x^i\sigma_x^j\sigma_y^a\sigma_x^b}e^{\hat{Z}_{ij}^{ab}\sigma_y^i\sigma_x^j\sigma_y^a\sigma_y^b}e^{\hat{Z}_{ij}^{ab}\sigma_x^i\sigma_y^j\sigma_y^a\sigma_y^b}e^{\hat{Z}_{ij}^{ab}\sigma_x^i\sigma_x^j\sigma_x^a\sigma_y^b}\right.$$

$$\left. e^{-\hat{Z}_{ij}^{ab}\sigma_y^i\sigma_x^j\sigma_x^a\sigma_x^b}e^{-\hat{Z}_{ij}^{ab}\sigma_x^i\sigma_y^j\sigma_x^a\sigma_x^b}e^{-\hat{Z}_{ij}^{ab}\sigma_y^i\sigma_y^j\sigma_y^a\sigma_x^b}e^{-\hat{Z}_{ij}^{ab}\sigma_y^i\sigma_y^j\sigma_x^a\sigma_y^b}\right)^p|c\rangle, \quad (16)$$

where p decides the step size in the Suzuki-Trotter approximation and will be restricted to $p = 1$ in our discussions.

More details

Since we are dealing with the pairing Hamiltonian as an example system in this school, we can reduce the number of terms in our ansatz by not allowing to break particle pairs. The Taylor expansion of the UCCD operator gives us

$$e^{\sum_{ijab}t_{ij}^{ab}(a_a^\dagger a_b^\dagger a_j a_i - a_i^\dagger a_j^\dagger a_b a_a)} = I + \sum_{ijab}t_{ij}^{ab}(a_a^\dagger a_b^\dagger a_j a_i - a_i^\dagger a_j^\dagger a_b a_a)$$

$$+ [\sum_{ijab}t_{ij}^{ab}(a_a^\dagger a_b^\dagger a_j a_i - a_i^\dagger a_j^\dagger a_b a_a)]^2/2!$$

$$+ \cdots. \quad (17)$$

We can immediately see that the first sum over i, j, a, b will break pairs if we do not introduce a restriction on the sum. This can be explained by the fact that any non zero t_{ij}^{ab} will include the following term

$$t_{ij}^{ab}(a_a^\dagger a_b^\dagger a_j a_i - a_i^\dagger a_j^\dagger a_b a_a)|c\rangle,$$

which will break pairs if $j \neq i + 1$ and $b \neq a + 1$. Hence we make the restriction $j = i + 1$ and $b = a + 1$.