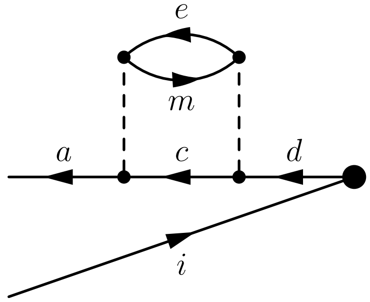
CEM 993 **Spring 2023**

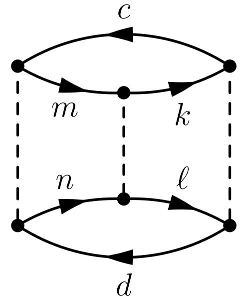
Assignment No. 4 (20 pts.) **Due Date: March 29, 2023**

1. (3 pts.) Assign weights (w_R), signs (s_R), scalar factors ($d^{(R)}_{\chi'_R,\chi''_R}$), and operator expressions ($\hat{O}^{(R)}_{\chi''_R}$) to the Goldstone diagrams shown below. Write the complete algebraic expressions for each of the diagrams. We use the notation, in which a, i represent fixed indices, while c, d, e, k, l, m, n are free (summation) labels. The rightmost vertex in diagram (a) should be interpreted as the single excitation operator $\hat{C}_1$.

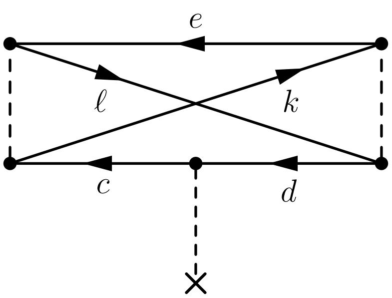
(a)



(b)



(c)



2. (4 pts.) Use the diagrammatic method based on drawing the resulting Goldstone diagrams to calculate

   (a) $\langle\Phi|V_N Z_N V_N|\Phi\rangle$,

   (b) $V_N|\Phi_i^a\rangle$.

   It is strongly recommended that you use the non-oriented and oriented Hugenholtz skeletons/diagrams in the initial steps. Remember, however, that the final product of your work should be all admissible non-equivalent resulting Goldstone diagrams and the corresponding algebraic expressions.

3. (4 pts.) Use the diagrammatic method to rederive Eq. (6) from Assignment No. 3.

4. (4 pts.) Use the diagrammatic arguments based on drawing the relevant non-oriented Hugenholtz skeletons to explain why matrix element $\langle \Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n} | \, [Z_N, T_1] \, | \Phi \rangle$, where Z_N and T_1 are the one-body operators defined by Eqs. (4) and (5) in Assignment No. 3, vanishes when $n \geq 2$ (see Problem 3 in Assignment No. 3). As usual, $[,]$ is the commutator, $|\Phi\rangle$ is the Fermi vacuum state, and $|\Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n}\rangle$ is the n-tuply excited determinant relative to $|\Phi\rangle$. Use a similar simplified diagrammatic analysis to determine the range of n values for which $\langle \Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n} | \, [V_N, T_1] \, | \Phi \rangle$ is nonzero, where V_N is a two-body operator in the normal-ordered form. In providing your answer, you can use a convention in which the $n = 0$ determinant is equivalent to $|\Phi\rangle$ (no excitations).

5. (3 pts.) Draw the Hugenholtz diagrams that would correspond to the Goldstone diagrams (a)–(c) in Problem 1. Write the complete algebraic expressions for each of the resulting Hugenholtz diagrams. In reading the Hugenholtz diagrams, use the same notation as in Problem 1. Remember that the rightmost vertex in diagram (a) should be interpreted as the single excitation operator $\hat{C}_1$.

6. (2 pts.) Redo Problem 2 using the diagrammatic method based on the Hugenholtz-Brandow diagrams.

SOLUTIONS

1. (a) $w_R = 1$, $s_R = (-1)^{1+1} = +1$ $(l_R = 1, h_R = 1)$

$$d^{(R)}_{\chi_R' \chi_R''} = \langle am|\hat{v}|ce\rangle\langle ce|\hat{v}|dm\rangle \times \langle d|\hat{c}_1|i\rangle$$

$$\hat{O}^{(R)}_{\chi_R''} = N[X_a^\dagger X_i]$$

Expression:

$$\left(\sum_{c,d,e,m} \langle am|\hat{v}|ce\rangle\langle ce|\hat{v}|dm\rangle\langle d|\hat{c}_1|i\rangle\right) \times N[X_a^\dagger X_i]$$

(b) $w_R = \frac{1}{2}$, $s_R = (-1)^{2+4} = +1$ $(l_R = 2, h_R = 4)$

$$d^{(R)}_{\chi_R' \chi_R''} = \langle mn|\hat{v}|cd\rangle\langle kl|\hat{v}|mn\rangle\langle cd|\hat{v}|kl\rangle$$

$$\hat{O}^{(R)}_{\chi_R''} = N[\emptyset] = 1$$

Expression:

$$\frac{1}{2}\sum_{\substack{k,l,m,n\\c,d}} \langle mn|\hat{v}|cd\rangle\langle kl|\hat{v}|mn\rangle\langle cd|\hat{v}|kl\rangle$$

$$= \frac{1}{2} \sum_{klmncd} \langle cd|\hat{v}|kl\rangle\langle kl|\hat{v}|mn\rangle \times \langle mn|\hat{v}|cd\rangle$$

(c) $H_R = 1, \quad S_R = (-1)^{1+2} = -1 \quad (l_R = 1, h_R = 2)$.

$$d^{(R)}_{\chi_R' \chi_R''} = \langle kl|\hat{v}|ce\rangle\langle c|\hat{z}|d\rangle\langle de|\hat{v}|lk\rangle$$

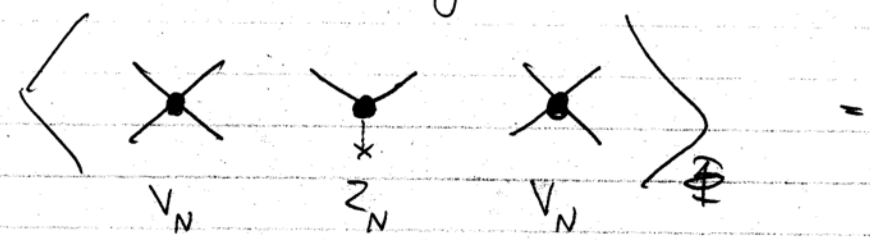
$$\hat{O}^{(R)}_{\chi_R''} = N[\emptyset] = 1$$

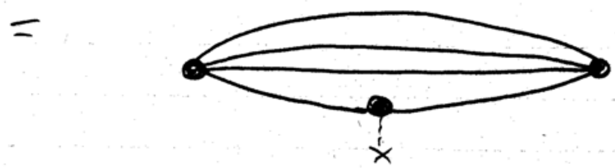
Expression:

$$- \sum_{klcde} \langle kl|\hat{v}|ce\rangle\langle c|\hat{z}|d\rangle\langle de|\hat{v}|lk\rangle$$

2. We can start constructing the final Goldstone diagrams directly from the Goldstone vertices or we can use the Hugenholtz skeletons and diagrams as intermediate steps. We will do the latter.

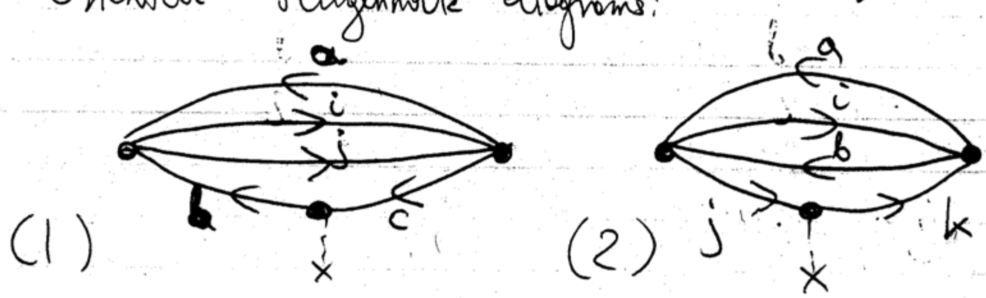
(a) Nonoriented Hugenholtz skeletons:





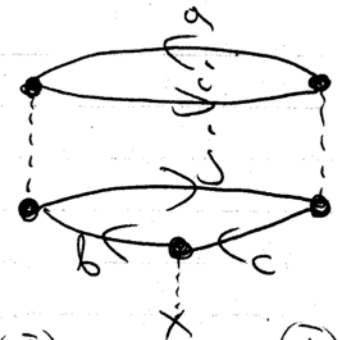
(a, b, c, i, j, k - free labels)

Oriented Hugenholtz diagrams:



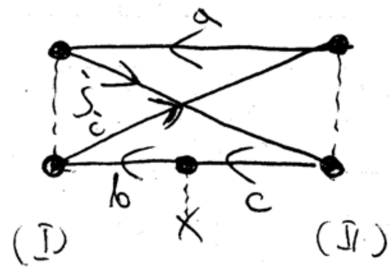
Goldstone diagrams (from (1)):

(1A)



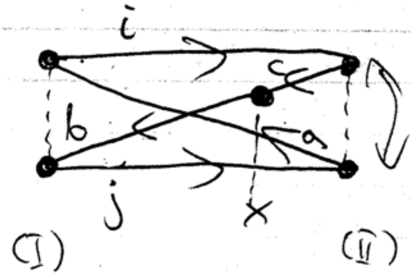
vertices (I) (II)

(1B)



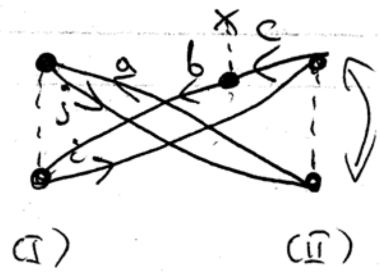
exchange of outgoing lines at (I)

(1C)



exchange of outgoing lines at (II)

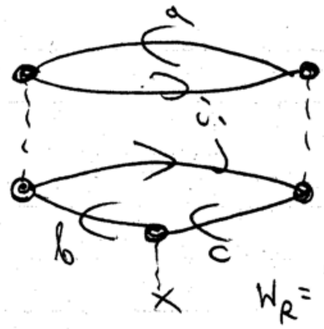
(1D)



exchanges at (I) & (II)

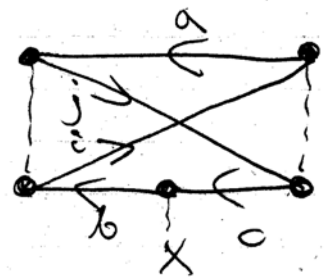
Since all labels are free, we can see that diagrams (1A) and (1D) are the same. Similarly, diagrams (1B) and (1C) are equivalent.
We are left with two diagrams resulting from the Hugenholtz diagram (1):

(1A)



$W_R = 1, S_R = 1$

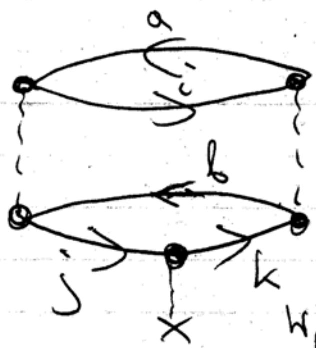
(1B)



$W_R = 1, S_R = -1.$

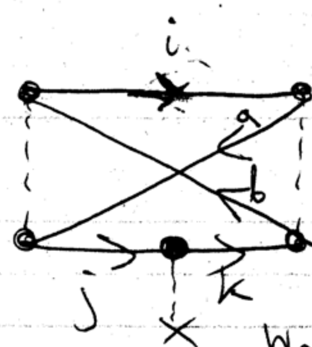
Similar arguments allow us to draw two nonequivalent diagrams resulting from the Hugenholtz diagram (2):

(2A)



$W_R = 1, S_R = -1$

(2B)



$W_R = 1, S_R = 1$

Diagrams (2A) and (2B) are the <u>p-h (particle-hole) variants</u> of diagrams (1A) and (1B), respectively.

By recoding weights, signs, and scalar factors, we obtain:

$$(1A) + (1B) + (2A) + (2B) =$$

$$= \sum_{abcij} \langle ac|\hat{v}|ij\rangle \langle b|\hat{z}|c\rangle \langle ij|\hat{v}|ab\rangle$$
$$- \sum_{abcij} \langle ac|\hat{v}|ij\rangle \langle b|\hat{z}|c\rangle \langle ij|\hat{v}|ba\rangle$$
$$- \sum_{abijk} \langle ab|\hat{v}|ik\rangle \langle k|\hat{z}|j\rangle \langle ij|\hat{v}|ab\rangle$$
$$+ \sum_{abijk} \langle ab|\hat{v}|ik\rangle \langle k|\hat{z}|j\rangle \langle ij|\hat{v}|ba\rangle$$

$$= \sum_{abcij} \langle ac|\hat{v}|ij\rangle \langle b|\hat{z}|c\rangle \langle ij|\hat{v}|ab\rangle_A$$
$$- \sum_{abijk} \langle ab|\hat{v}|ik\rangle \langle k|\hat{z}|j\rangle \langle ij|v|ab\rangle_A$$

$$= \sum_{abij} \langle ij|\hat{v}|ab\rangle_A \times$$

$$\times \left(\sum_{c} \langle b|\hat{z}|c\rangle \langle ac|\hat{v}|ij\rangle - \right.$$

$$\left. - \sum_{k} \langle k|\hat{z}|j\rangle \langle ab|\hat{v}|ik\rangle \right)$$

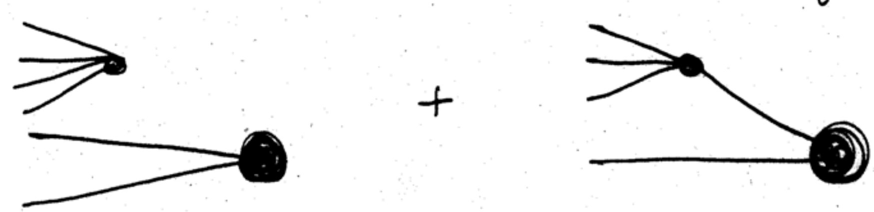
(b) $V_N |\Phi_i^a\rangle$:

Nonoriented Hugenholtz skeletons:

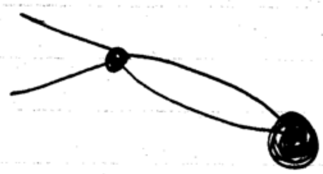
V_N $\quad X_a^\dagger X_i$

 $|\Phi\rangle$

all external lines must extend to the left

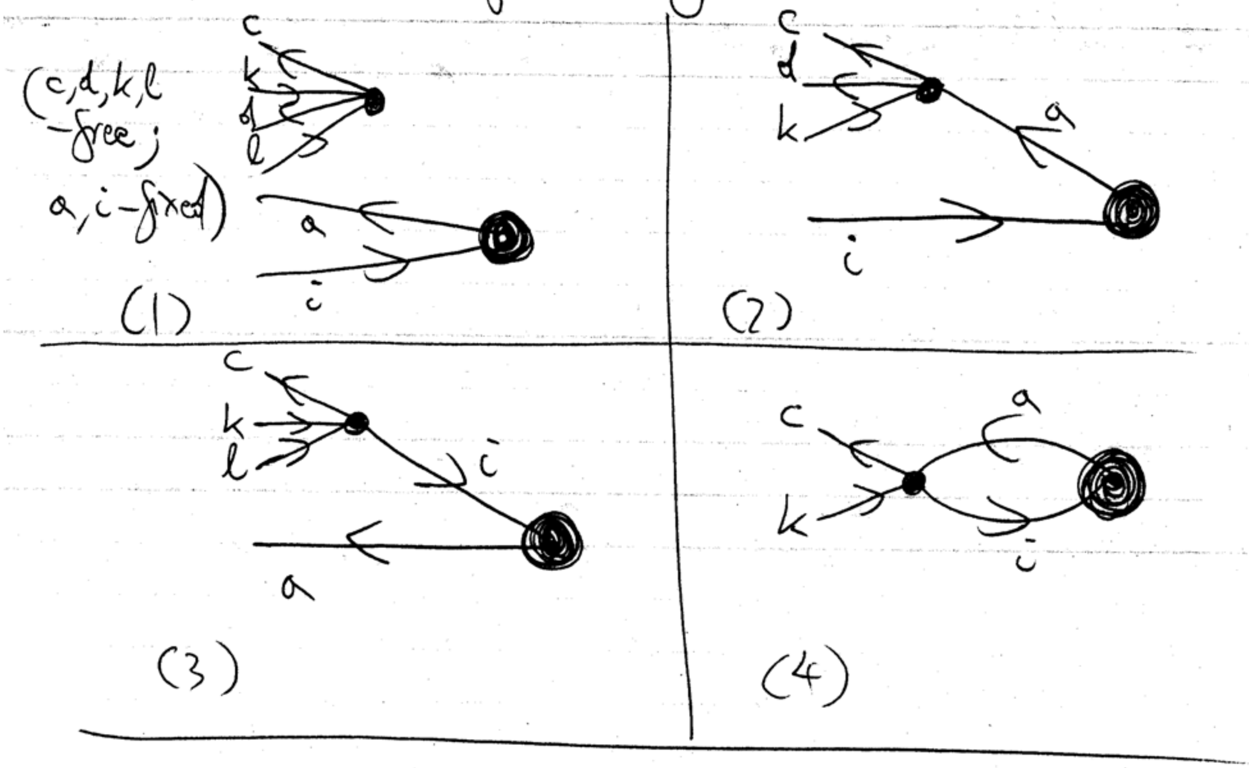
= 

no contractions $\qquad$ + $\qquad$ 1 contraction

+ 

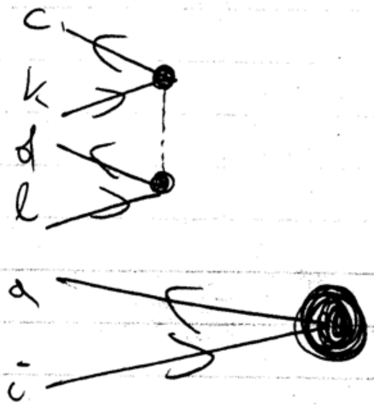
2 contractions

Hugenholtz diagrams (adding arrows...):



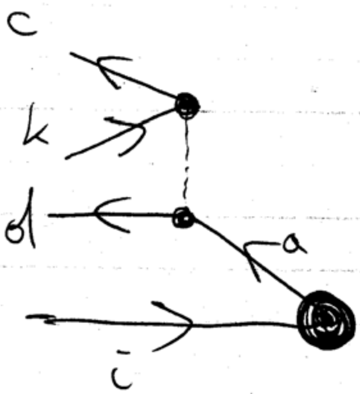
Goldstone diagrams (from (1) – (4)):

(c, d, k, l – <u>free</u>; a, i – <u>fixed</u>)

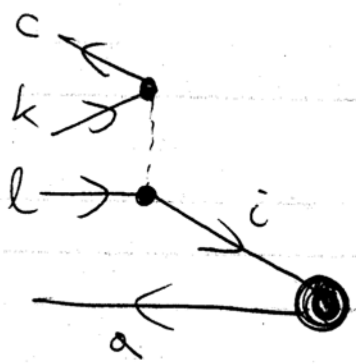


lines going out of V_N

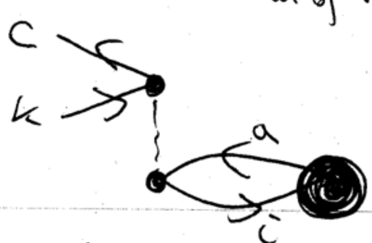
(1) (exchange of c and d produces the same diagram)



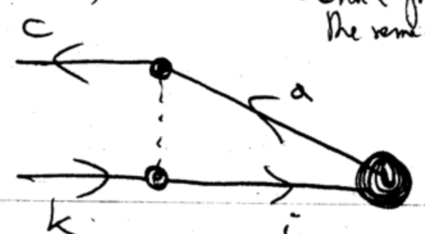
(2) (exchange of c and d going out of V_N produces the same d–m)



(3) (exchange of c and i produces the same d–m)



(4A)



(4B) (lines i and c going out of V. exchanged)

Diagram weights and signs:

(1) $w_R = \frac{1}{2}$, $s_R = 1$

(2) $w_R = 1$, $s_R = 1$

(3) $w_R = 1$, $s_R = -1$

(4A) $w_R = 1$, $s_R = 1$

(4B) $w_R = 1$, $s_R = -1$

The formula for $V_N|\Phi_i^a\rangle$ is:

$$V_N|\Phi_i^a\rangle = \frac{1}{2}\sum_{cdkl} \langle cd|\hat{v}|kl\rangle N[X_a^\dagger X_i X_c^\dagger X_k X_d^\dagger X_l]|\Phi\rangle$$

$$+ \sum_{cdk} \langle cd|\hat{v}|ka\rangle N[X_c^\dagger X_k X_d^\dagger X_i]|\Phi\rangle$$

$$- \sum_{ckl} \langle ci|\hat{v}|kl\rangle N[X_c^\dagger X_k X_a^\dagger X_l]|\Phi\rangle$$

$$+ \sum_{ck} \left(\langle ci|\hat{v}|ka\rangle - \langle ci|\hat{v}|ak\rangle\right) \times$$

$$\times N[X_c^\dagger X_k]|\Phi\rangle$$

$$= \frac{1}{2} \sum_{cdkl} \langle cd|\hat{v}|kl\rangle |\Phi^{acd}_{ikl}\rangle$$

$$+ \sum_{cdk} \langle cd|\hat{v}|ka\rangle |\Phi^{cd}_{ki}\rangle$$

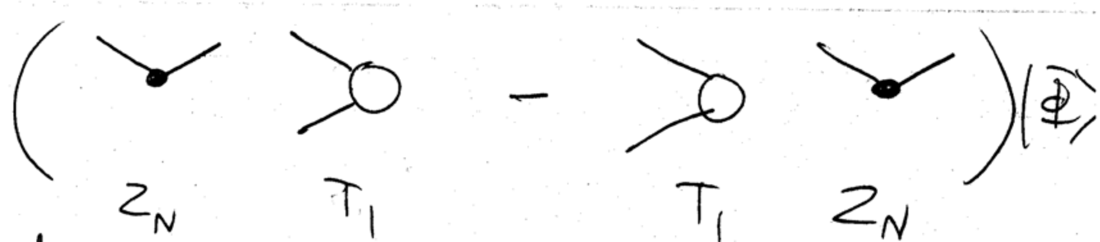
$$- \sum_{ckl} \langle ci|\hat{v}|kl\rangle |\Phi^{ca}_{kl}\rangle$$

$$+ \sum_{ck} \langle ci|\hat{v}|ka\rangle_A |\Phi^{c}_{k}\rangle \, .$$

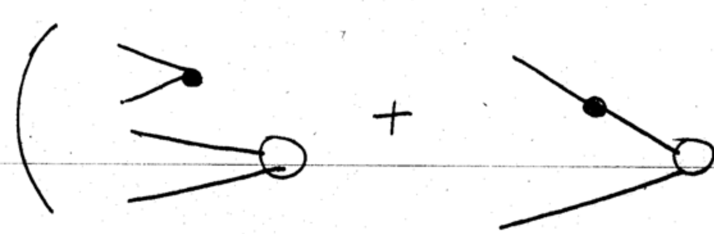
3. Hugenholtz skeletons (nonoriented):

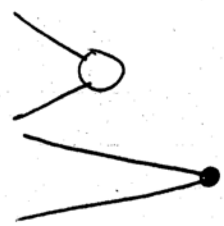
$$[Z_N, T_1]|\Phi\rangle = (Z_N T_1 - T_1 Z_N)|\Phi\rangle$$

=

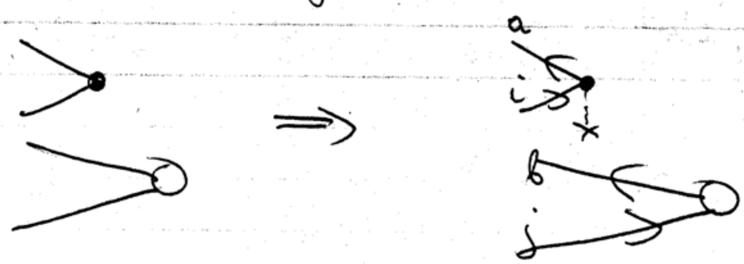


external
all lines must
extend to the left



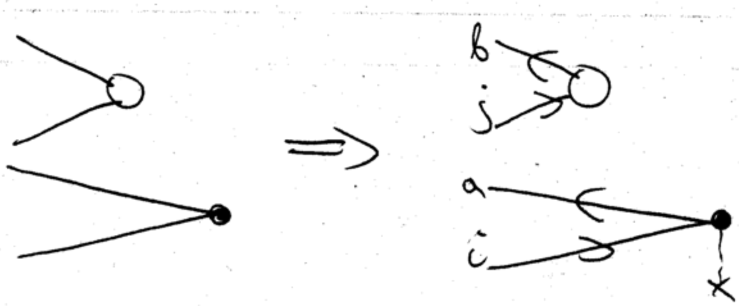
$+$  $-$  $\Big)|\Phi\rangle$

Please note that the first and the last terms (disconnected diagrams!) cancel out; indeed,



(a, b, i, j - free)

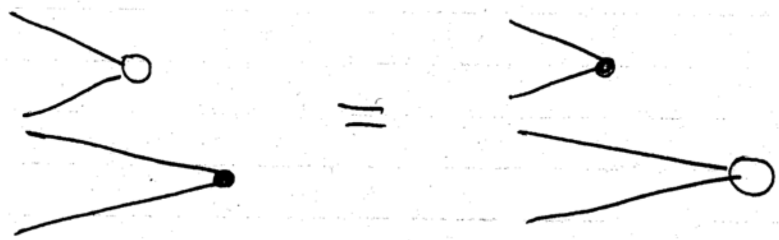
$$= \sum_{abij} \langle a|\hat{z}|i\rangle \langle b|\hat{t}_1|j\rangle N[X_a^\dagger X_i X_b^\dagger X_j]|\Phi\rangle$$



(a, b, i, j - free)

$$= \sum_{abij} \langle a|\hat{z}|i\rangle \langle b|\hat{t}_1|j\rangle N[X_a^\dagger X_i X_b^\dagger X_j]|\Phi\rangle$$

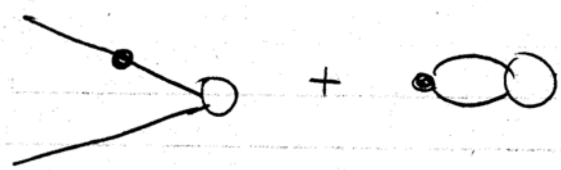
This shows that



In other words, $[Z_N, T_1]|\Phi\rangle$ contains the CONNECTED DIAGRAMS ONLY (<u>this is true for all commutator expressions</u>).

Thus, we are left with:

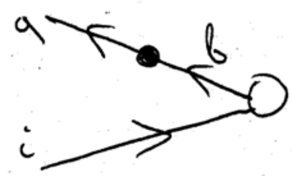
$[Z_N, T_1]|\Phi\rangle =$



$=$

$=$ (oriented Hugenholtz diagrams) $=$

$=$



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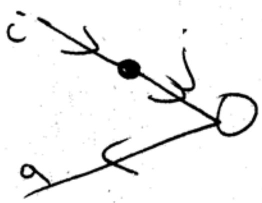

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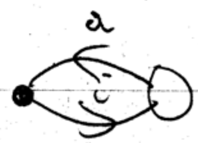
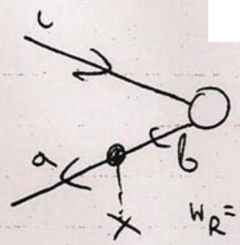
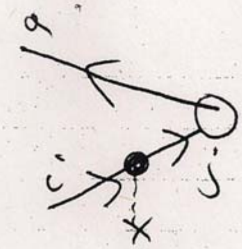


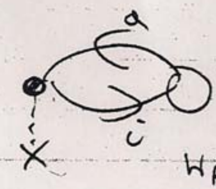
← a, b, i, j – free labels

$=$ 

$W_R = 1,\ S_R = 1$

$+$ 

$W_R = 1,\ S_R = -1$

$+$ 

$W_R = 1,\ S_R = 1$

$=$

$$= \sum_{abi} \langle a|\hat{z}|b\rangle \langle b|\hat{t}_1|i\rangle N[X_a^\dagger X_i]|\Phi\rangle$$

$$- \sum_{aij} \langle j|\hat{z}|i\rangle \langle a|\hat{t}_1|j\rangle N[X_a^\dagger X_i]|\Phi\rangle$$

$$+ \sum_{ai} \langle i|\hat{z}|a\rangle \langle a|\hat{t}_1|i\rangle\ |\Phi\rangle$$

$$= \sum_{ai} \left(\sum_b \langle a|\hat{z}|b\rangle \langle b|\hat{t}_1|i\rangle - \sum_j \langle a|\hat{t}_1|j\rangle \langle j|\hat{z}|i\rangle \right)$$

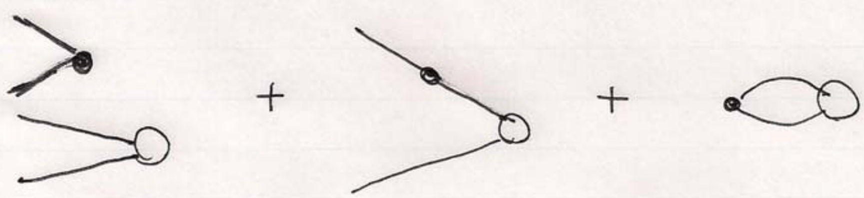
$$\times |\Phi_i^a\rangle + \sum_{a,i} \langle a|\hat{t}_1|i\rangle \langle i|\hat{z}|a\rangle |\Phi\rangle$$

4. The non-oriented Hugenholtz skeletons representing Z_N and T_1 are

 and , respectively.

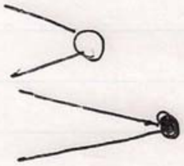
Note that both lines of T_1 extend to the left (T_1 is a particle-hole excitation operator).

Let us determine the skeletons representing $[Z_N, T_1]|\Phi\rangle = (Z_N T_1 - T_1 Z_N)|\Phi\rangle = Z_N T_1|\Phi\rangle$:

 (A)

We used the fact that all resulting diagrams must have external lines, if any, extending to the left ($Z_N T_1$ acts on $|\Phi\rangle$).

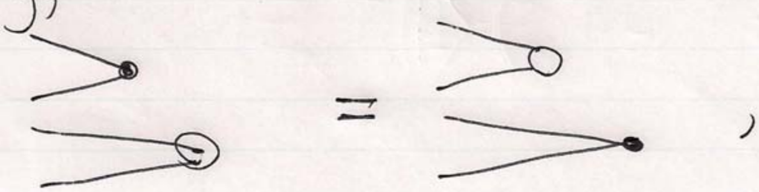
$T_1 Z_N |\Phi\rangle$:



(B)

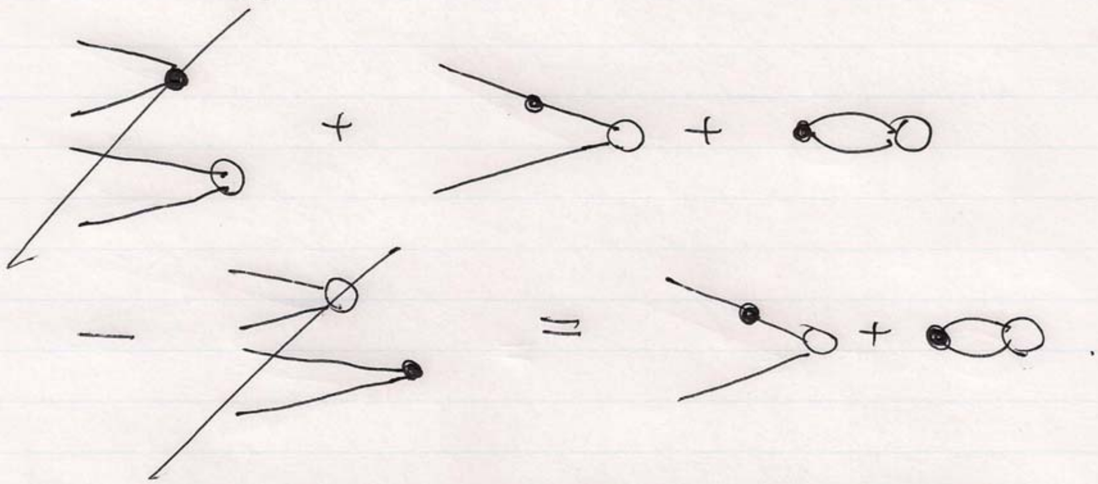
Here, we cannot connect lines of T_1, which extend to the left, with lines of Z_N.

Clearly,

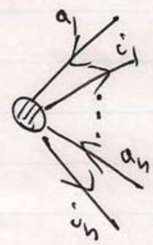


since in each case the operator part is of the $N[X_a^\dagger X_i X_b^\dagger X_j] = N[X_b^\dagger X_j X_a^\dagger X_i]$ type ($X_a^\dagger X_i$ and $X_b^\dagger X_j$ pairs can be interchanged inside $N[\ldots]$).

Thus, the non-oriented Hugenholtz skeletons representing $[Z_N, T_1]|\Phi\rangle$ are :



In order to form $\langle \Phi^{a_1 \ldots a_n}_{i_1 \ldots i_n} | [Z_N, T_1] | \Phi \rangle$, we must connect all of the external lines of

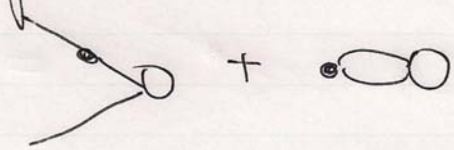


with the diagrams (lines of diagrams) representing $[Z_N, T_1]|\Phi\rangle$.
The latter contain at most two external lines, i.e., $\langle \Phi^{a_1 \ldots a_n}_{i_1 \ldots i_n} | [Z_N, T_1] | \Phi \rangle$ can

be non-zero only when $n=0$ (projection on $|\Phi\rangle$) or $n=1$ (projection on $|\Phi_{i_1}^{a_1}\rangle$).
When $n \geqslant 2$, we obtain

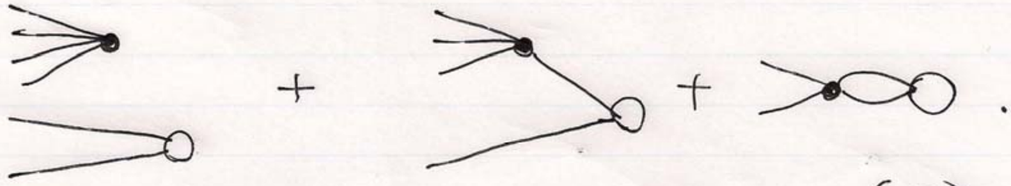
$$\langle \Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n} | [Z_N, T_1] | \Phi \rangle = 0 .$$

Note that we've also proved that

$$[Z_N, T_1]|\Phi\rangle =$$ 

$$= (Z_N T_1)_C |\Phi\rangle$$, where C designates connected product.

Let us now consider $\langle \Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n} | [V_N, T_1] | \Phi \rangle$.
Again, we begin with $[V_N, T_1]|\Phi\rangle =$
$= (V_N T_1 - T_1 V_N)|\Phi\rangle$. The non-oriented skeletons (Hugenholtz-style) of $(V_N T_1)|\Phi\rangle$ are:

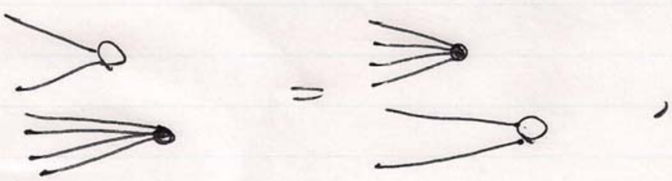


(C)

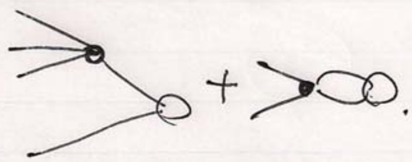
Those of $(T_1 V_N)|\Phi\rangle$ are (only one):

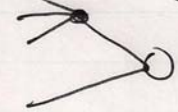
(D)

Again, all diagrams or skeletons have lines extending to the left, since we have $(V_N T_1)$ and $(T_1 V_N)$ acting on $|\Phi\rangle$ and, in the case of $(T_1 V_N)$, we cannot connect lines of T_1 and V_N. Also,



as in the case of Z_N and T_1, so that

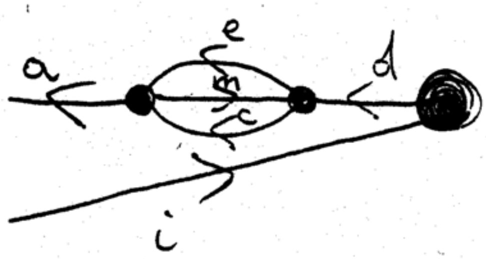
$$(V_N T_1 - T_1 V_N)\,|\Phi\rangle =$$ 

In order to form $\langle \Phi^{a_1 \cdots a_n}_{i_1 \cdots i_n} | [V_N, T_1]_C |\Phi\rangle$, we must connect the external lines of $[V_N, T_1]|\Phi\rangle$ with  (all lines of $\langle \Phi^{a_1 \cdots a_n}_{i_1 \cdots i_n}|$) which means that n can only be 1 (the  skeleton) or 2 (the  skeleton).

$$\langle \Phi^{a_1 \cdots a_n}_{i_1 \cdots i_n} | [V_N, T_1] |\Phi\rangle = 0 \text{ if } n = 0 \text{ and } n \geq 3.$$

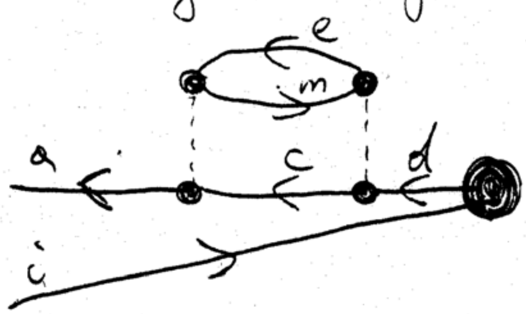
Again, we've demonstrated that $[V_N, T_1]|\Phi\rangle = (V_N T_1)_C |\Phi\rangle$.

5. (a)



a, i - fixed
c, d, e, m - free

Hugenholtz diagram



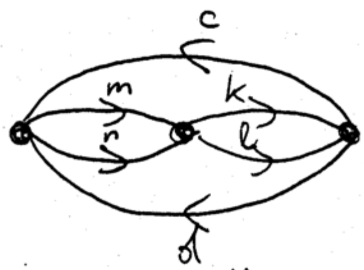
Brandow diagram

$w = \frac{1}{2}, \quad S = +1$

Expression:

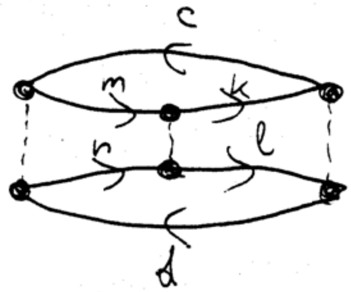
$$\frac{1}{2} \sum_{cdem} \langle am|\hat{v}|ce\rangle_A \langle ce|\hat{v}|dm\rangle_A \langle d|c_1|i\rangle \times X_a^\dagger X_i$$

(b).



all labels are free

Hugenholtz diagram



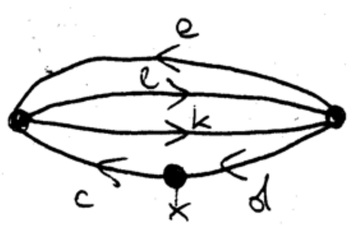
Brandow diagram

$w = \frac{1}{8}, \quad s = +1$

Expression:

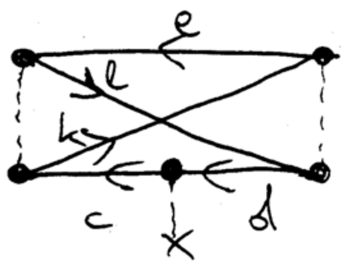
$$\frac{1}{8} \sum_{cdklmn} \langle cd|\hat{v}|kl\rangle_A \langle kl|\hat{v}|mn\rangle_A \langle mn|\hat{v}|cd\rangle_A$$

(c)



all labels are free

Hugenholtz diagram



Brandow diagram

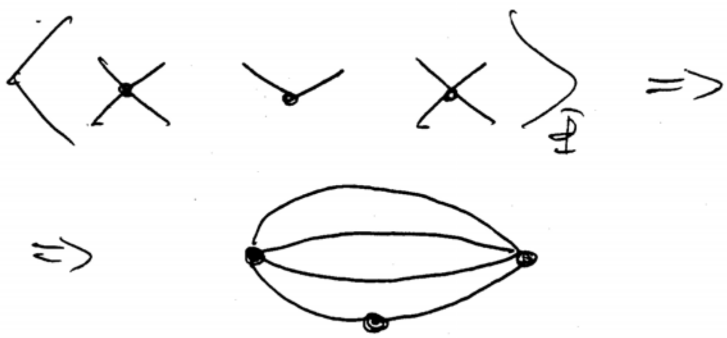
$$w = \frac{1}{2}, \quad S = -1$$

Expression:

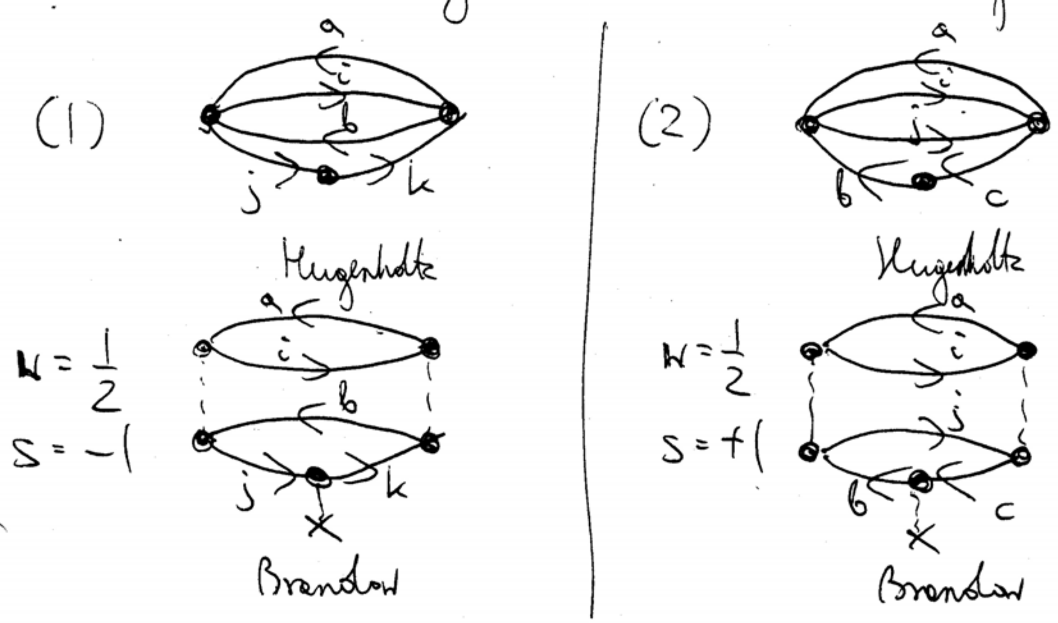
$$-\frac{1}{2} \sum_{cdekl} \langle kl|\hat{v}|ce\rangle_A \langle c|\hat{z}|d\rangle \langle de|\hat{v}|lk\rangle_A$$

6. (a) $\langle \Phi | V_N Z_N V_N | \Phi \rangle$.

Nonoriented Hugenholtz skeletons:



Oriented Hugenholtz and Brandow diagrams:



$$\langle \Phi | V_N Z_N V_N | \Phi \rangle = (2) + (1)$$

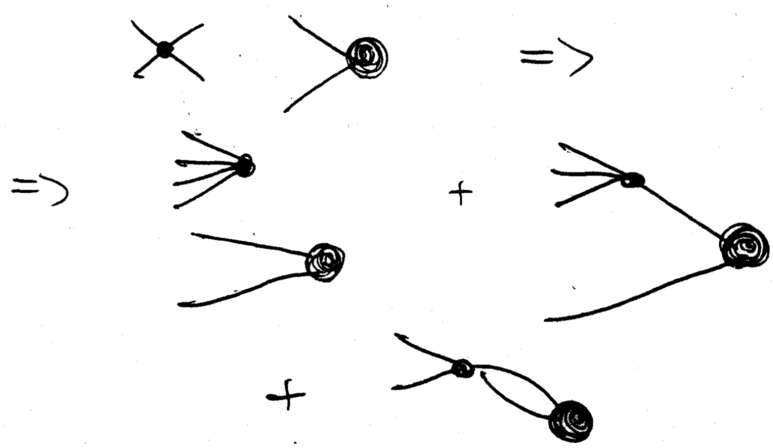
$$= \frac{1}{2} \sum_{abcij} \langle ij|\hat{v}|ab\rangle_A \langle b|\hat{z}|c\rangle \langle ac|\hat{v}|ij\rangle_A$$

$$- \frac{1}{2} \sum_{abijk} \langle ab|\hat{v}|ik\rangle_A \langle k|\hat{z}|j\rangle \langle ij|\hat{v}|ab\rangle_A$$

$$= \frac{1}{2} \sum_{abij} \langle ij|\hat{v}|ab\rangle_A \left(\sum_c \langle b|\hat{z}|c\rangle \langle ac|\hat{v}|ij\rangle_A - \sum_k \langle ab|\hat{v}|ik\rangle_A \langle k|\hat{z}|j\rangle \right)$$

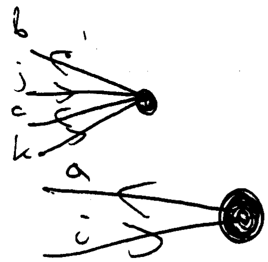
(b) $V_N |\Phi_i^a\rangle$:

Nonoriented Hugenholtz skeletons

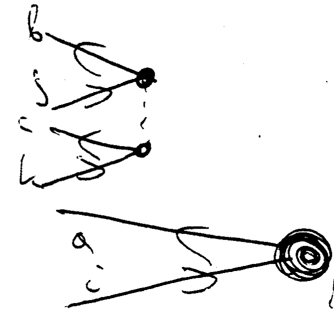


Oriented Hugenholtz and Brandow diagrams:

(1)



Hugenholtz



Brandow

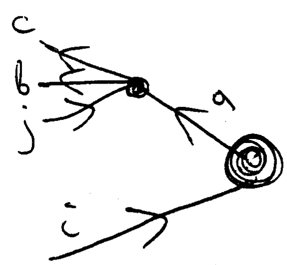
$bcjk$ - free

a, i - fixed

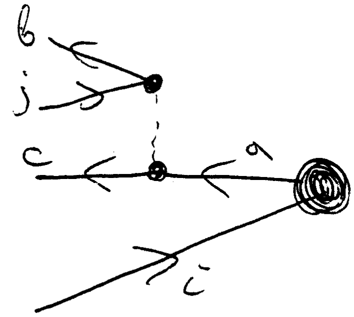
scalar = 1

$w = \frac{1}{4}$, $s = +1$

(2)



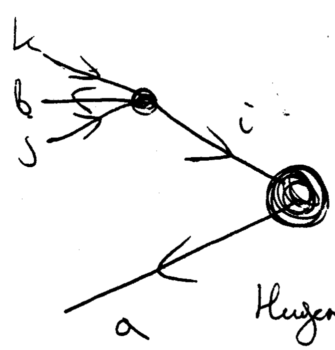
Hugenholtz



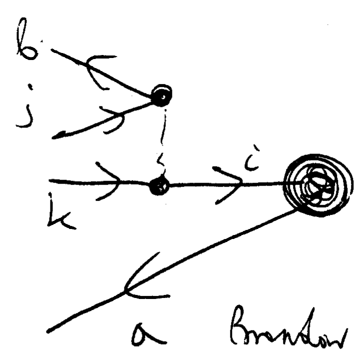
Brandow

$w = \frac{1}{2}$, $s = +1$

(3)



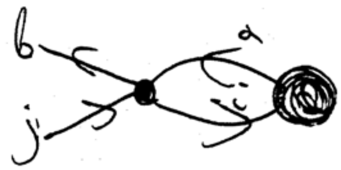
Hugenholtz



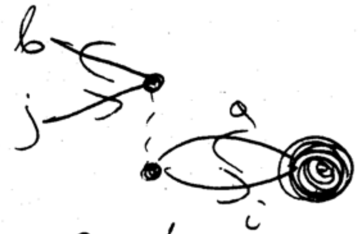
Brandow

$w = \frac{1}{2}$, $s = -1$

(4)



Hugenholtz



Brandow

$$w = 1, \quad s = +1$$

Expression:

$$V_N|\Phi_i^a\rangle = \left(\frac{1}{4} \sum_{bcjk} \langle bc|\hat{v}|jk\rangle_A\right)|\Phi_{ijk}^{abc}\rangle$$

$$+ \frac{1}{2} \sum_{bcj} \langle bc|\hat{v}|ja\rangle_A \, |\Phi_{ij}^{cb}\rangle$$

$$- \frac{1}{2} \sum_{jkb} \langle bi|\hat{v}|jk\rangle_A \, |\Phi_{jk}^{ba}\rangle$$

$$+ \sum_{bj} \langle ib|\hat{v}|aj\rangle_A \, |\Phi_{j}^{b}\rangle$$