CALCULATION OF HIGH ORDER OPERATOR TERMS IN VARIATIONAL MANY-BODY THEORIES

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Abstract.. - A recursion relation method capable of treating high order operator terms, in variational many-body theories with operator correlations, is suggested. As an illustration of the method two simple cases are solved exactly. First is the case of Fermi hypernetted σ(or τ) chains; second is the case of direct double σ(or τ) chains. The method can be extended to treat other interesing cases as well, since is attacks counting problems common to many calculations.

1. - Introduction.-

In variational many-body theories of Nuclear matter (NM), with operator correlations, such as those of ref. 1 (from here on called PW), and of ref. 2, the trial wavefunction is of the form:

$$| \Psi > = |S \prod_{i>j} F_{ij}| | \phi > \qquad (1.1)$$

where $|\phi>$ is the non-interacting ground state wavefunction, F_{ij} is the correlation two-body operator and S it the appropriate symmetrizer since the operators F_{ij}, F_{jk} do not in general commute. In PW theory the correlation operator is taken to be:

$$F_{ij} = \sum_{P=1}^{8} f^P(r_{ij}) 0^P_{ij} \qquad (1.2)$$

where $f(r_{ij})$ are functions of the internucleon distance and 0^P_{ij} are the operators:

$$0^P_{ij} =1,8 =1, \sigma_{ij}, \tau_{ij}, \sigma_{ij}\tau_{ij}, t_{ij}, t_{ij}\tau_{ij}, b_{ij}$$
$$b_{ij}\tau_{ij} \qquad (1.3)$$

$$\sigma_{ij}=\vec{\sigma}_i\cdot\vec{\sigma}_j, \quad \tau_{ij}=\vec{\tau}_i\cdot\vec{\tau}_j, \quad t_{ij}=\frac{3\vec{\sigma}_i\cdot\vec{r}_{ij} \ \vec{\sigma}_j\cdot\vec{r}_{ij}}{r_{ij}^2}-\vec{\sigma}_i\cdot\vec{\sigma}_j$$

$$b_{ij} = \frac{1}{2} (\vec{\sigma}_i + \vec{\sigma}_j)\cdot \vec{L}_{ij}$$

$\vec{\sigma}$ & $\vec{\tau}$ are the Pauli spin-isospin matrices, t_{ij} is the tensor operator and b_{ij} is the spin-orbit operator.
Then one calculates and minimizes:

$$E = \frac{< \Psi |H| \Psi >}{< \Psi | \Psi >}$$

to get an upper bound for the ground state energy of NM. The method employs a diagrammatic cluster expansion, described in PW, which has been proven to be very convenient for calculations of this kind. Since the exact calculation is a impossible task, several approximations are used. For instance only central chains are hypernetted, while operator chains are not. Furthermore, the operator chains are calculated in the 'single operator' scheme (SOC), while multiple operator chains are neglected. Wiringa[3] tested the validity of those approximations, by evaluating the supposedly leading terms of higher order corrections. The net contribution to the energy from those terms was found to be quite small indeed, inspite the fact that separately some of them were appreciable, due to cancelation of different corrections. Wiringa calculated these terms at densities around the equilibrium density of NM. However at higher densities these terms become more important. For asymmetric NM or for Neutron-matter calculations, much higher densities are relevant and so one may need a more accurate calculation.
Fantoni et al[4] developed an approximate treatment of hyperneted operator chains (HOC) which neglects various different operator orders. Their results for the Reid V-6 model are quite different (as quoted in PW) from the results of other calculations, such as Owen's[5], PW, BBG[6], which are in resonable agreement. This suggests that one has to take seriously in account the various orders in the operator products.

The present work intents to illustrate the general idea of a method which may lead to an accurate calculation of higher order operator terms of the cluster expansion. We picked two examples to illustrate the technique. First is the hypernation of the simplest σ(or τ) chain (which can be extended to more complicated σ(or τ) chains). This is described in section 3. Second is the calculation of double σ(or τ) chains (without any exchange links). This is described in section 4. The necessary mathematical notation is presented in section 2.

The weight is put on the development of the method and our choice of what to calculate at a first stage was made on these grounds. So no claim is made about the importance of the contribution to the energy of the above particular terms.

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2. - Notation and formalism.-

Since we deal with spin operators

$$\vec{\sigma}_1, \vec{\sigma}_2, \ldots, \vec{\sigma}_n$$

that correspond to particles $1, 2, \ldots, n$, it is proper to introduce a convenient notation. Let $\vec{\sigma}_1$ be denoted simply by $\vec{1}$, $\vec{\sigma}_2$ by $\vec{2}$ and so on. Then one can write the scalar product of two spin operators as:

$$\sigma_{13} \equiv \vec{\sigma}_1 \cdot \vec{\sigma}_3 = \vec{1} \cdot \vec{3} = 1_i 3_i \qquad (2.1)$$

where the summation convention over repeated indices is implied. Also the Pauli Identity is written as:

$$1_i 1_j = \delta_{ij} + i\varepsilon_{ijk} 1_k \qquad (2.2)$$

From here on we will denote the product

$$1_j 1_j 1_k \ldots 1_s$$

by

$$1_{ijk\ldots s}$$

The C-part of the ith -component of the operator $\vec{1}$, i.e. 1_i is defined as:

$$C(1_i) \equiv \langle 1_i \rangle \equiv \frac{\langle \uparrow | 1_i | \uparrow \rangle + \langle \downarrow | 1_i | \downarrow \rangle}{\langle \uparrow | \uparrow \rangle + \langle \downarrow | \downarrow \rangle} \qquad (2.3)$$

obviously: $\langle 1_i \rangle = 0$

and $\langle 1_{ij} \rangle = \langle \delta_{ij} + i\varepsilon_{ijk} 1_k \rangle = \delta_{ij} + i\varepsilon_{ijk} \langle 1_k \rangle = \delta_{ij}$

$$\qquad (2.4)$$

As example note that:

$$\langle \sigma_{12} \sigma_{12} \rangle = \langle 1_i 2_i 1_j 2_j \rangle = \langle 1_{ij} 2_{ij} \rangle = \langle 1_{ij} \rangle \langle 2_{ij} \rangle$$

$$= \delta_{ij} \delta_{ij} = 3$$

$$\langle \sigma_{13} \sigma_{32} \sigma_{12} \rangle = \langle 1_i 3_i 3_j 2_j 1_k 2_k \rangle = \langle 1_{ik} \rangle \langle 2_{jk} \rangle \langle 3_{ij} \rangle =$$

$$= \delta_{ik} \delta_{jk} \delta_{ij} = 3$$

In the above example the C-part operation was extended for two and three particles correspondingly. The subscripted C-part:

$$\langle \sigma_{13} \sigma_{23} \rangle_{12}$$

stands for: $\langle 1_i 3_i 2_j 3_j \rangle_{12} \equiv 1_i 2_j \langle 3_i 3_j \rangle$ (2.5)

i.e. C-part operation over the states of par ticles indicated by the subscripts is inhi bited. So one obtains:

$$\langle \sigma_{13} \sigma_{23} \rangle_{12} = 1_i 2_j \delta_{ij} = 1_i 2_i = \sigma_{12} \qquad (2.6)$$

Generalizing, the C-part of an operator product is:

$$C(\prod_{ij} \sigma_{ij}) \equiv \langle (\prod_{ij} \sigma_{ij}) \rangle \qquad (2.7)$$

where the brackets denote expectation over all particles appearing in the operator pro- duct. Note that since:

$$\langle 1_{ij\ldots k} \rangle = \frac{1}{2} \sum_m \langle m | 1_i 1_j \ldots 1_k | m \rangle =$$

$$= \frac{1}{2} \sum_{m,m'} \langle m | 1_i | m' \rangle \langle m' | 1_{j\ldots k} | m \rangle =$$

$$= \frac{1}{2} \sum_{m,m'} \langle m' | 1_{j\ldots k} | m \rangle \langle m | 1_i | m' \rangle =$$

$$= \frac{1}{2} \sum_{m} \langle m | 1_{j\ldots k_i} | m \rangle = \langle 1_{j\ldots ki} \rangle$$

$$\qquad (2.8)$$

One realizes that under the C-part operation cyclic permutations are allowed.
In what follows some useful quantities are defined.

$$D_{iji'j'} \equiv \langle 1_i 1_j 1_{i'} 1_{j'} \rangle = \langle 1_{iji'j'} \rangle \qquad (2.9)$$

$$\tilde{D}_{iji'j'} \equiv D_{ijj'i'} = \langle 1_{ijj'i'} \rangle \qquad (2.10)$$

$$I_{iji'j'} \equiv \delta_{ii'} \delta_{jj'} \qquad (2.11)$$

Explicitly one obtains:

$$D_{iji'j'} = \delta_{ij} \delta_{i'j'} - \delta_{ii'} \delta_{jj'} + \delta_{ij'} \delta_{i'j} \qquad (2.12)$$

Some properties of the above quantities are given below:

$$D_{iji'j'} D_{jkj'k'} = 2 D_{iki'k'} + \delta_{ii'} \delta_{kk'} \qquad (2.13)$$

or in shorthand: $D^2 = 2D + I$

$$D_{iji'j'} I_{jkj'k'} = -\delta_{ii'} \delta_{kk'} \qquad (2.14)$$

or in shorthand: $DI = -I$

Similarly one can show that:

$$\tilde{D} D = D\tilde{D} = -I$$

$$\tilde{D}^2 = 2 \tilde{D} + I \qquad (2.15)$$

$$\tilde{D}I = 3I$$

$$II = 3I$$

By repeated application of the above "multi- plication" properties one obtains:

$$D^n = 2^{n-1} D + \frac{1}{3}(2^{n-1} + (-1)^n) I$$

$$\tilde{D}^n = 2^{n-1} \tilde{D} + (3^{n-1} - 2^{n-1}) I \qquad (2.16)$$

and $D^k \tilde{D}^s = (-1)^k 3^{s-1} I$

Also note that:

$$1_{ii'} 2_{jj'} I_{iji'j'} = 9$$

$$1_{ii'} 2_{jj'} D_{iji'j'} = -3 \qquad (2.17)$$

$$1_{ii'} 2_{jj'} \tilde{D}_{iji'j'} = 9 - 4\sigma_{12}$$

3. - Fermi hyperneted σ-chains.

3.a Preliminary analysis

In this and in the following sections we adopt the diagrammatic technique and terminology of PW. Some of the diagrams that we are interested in, are displayed in fig. 1.
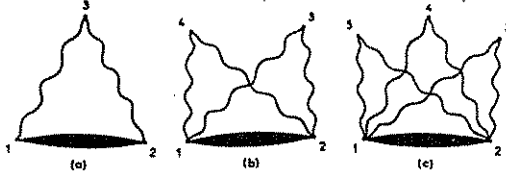
Figure 1

Diagrammatic representation on terms in the cluster expansion - Diagram 1(a) is contained in the SOC calculation of PW - Diagrams (1(b) and 1(c) are examples of terms associated with the hypernetted σ (or τ) chains.

Note that each wiggly line corresponds to:

$$F^{\sigma}_{ij} \; \sigma_{ij} \quad \text{with} \quad F^{\sigma}_{ij} = 2f^{C}_{ij} \; f^{\sigma}_{ij}$$

and the thick line, between the interacting particles 1 and 2, corresponds to: $f^{C}_{12} \; H_{12} \; f^{C}_{12}$.

It is instructive to examine in detail a simple diagram. Look for example at diagram 1(b). The relevant operators are: $\sigma_{12}, \; \sigma_{14}, \; \sigma_{23}, \; \sigma_{24}$, and they can come from either side of the Hamiltonian in the expression: $<\Psi|H|\Psi>$. The possible operator configurations are listed in table 1.

	Configuration	Number of terms	weight
i)	$H_{12} \; S(\sigma_{13}\sigma_{14}\sigma_{23}\sigma_{24})$	4!	1/4!
ii)	$\sigma_{13}H_{12} \; S(\sigma_{23}\sigma_{14}\sigma_{24})$	3!	1/3!
	$\sigma_{14}H_{12} \; S(\sigma_{13}\sigma_{24}\sigma_{23})$	3!	1/3!
	$\sigma_{23}H_{12} \; S(\sigma_{13}\sigma_{24}\sigma_{14})$	3!	1/3!
	$\sigma_{24}H_{12} \; S(\sigma_{13}\sigma_{23}\sigma_{14})$	3!	1/3!
iii)	$S(\sigma_{13}\sigma_{23}) \; H_{12} \; S(\sigma_{14}\sigma_{24})$	2x2	1/4
	$S(\sigma_{13}\sigma_{14}) \; H_{12} \; S(\sigma_{23}\sigma_{24})$	2x2	1/4
	$S(\sigma_{13}\sigma_{24}) \; H_{12} \; S(\sigma_{23}\sigma_{14})$	2x2	1/4
	$S(\sigma_{14}\sigma_{23}) \; H_{12} \; S(\sigma_{24}\sigma_{13})$	2x2	1/4
	$S(\sigma_{14}\sigma_{24}) \; H_{12} \; S(\sigma_{13}\sigma_{23})$	2x2	1/4
	$S(\sigma_{23}\sigma_{24}) \; H_{12} \; S(\sigma_{13}\sigma_{14})$	2x2	1/4
iv)	$S(\sigma_{23}\sigma_{14}\sigma_{24}) \; H_{12} \; \sigma_{13}$	3!	1/3!
	$S(\sigma_{13}\sigma_{24}\sigma_{23}) \; H_{12} \; \sigma_{14}$	3!	1/3!
	$S(\sigma_{13}\sigma_{24}\sigma_{14}) \; H_{12} \; \sigma_{23}$	3!	1/3!
	$S(\sigma_{13}\sigma_{23}\sigma_{14}) \; H_{12} \; \sigma_{24}$	3!	1/3!
v)	$S(\sigma_{13}\sigma_{14}\sigma_{23}\sigma_{24}) \; H_{12}$	4!	1/4!

Table 1

The various different cases can be grouped as follows:

   i) All four operators are on the right side of H
  ii) Three operators are on the right side of H   one on the left
 iii) Two operators are on the right side of H   and two on the left
  iv) One operator is on the right side of H   and three on the left
   v) All four operators are on the left side of H

In table I, H_{12} stands symbolicaly instead of $f^{C}_{12} \; H_{12} \; f^{C}_{12}$. Also the spatial product:

$$f^{C}_{13} \; f^{C}_{23} \; f^{C}_{24} \; f^{C}_{24} \; f^{\sigma}_{13} \; f^{\sigma}_{23} \; f^{\sigma}_{14} \; f^{\sigma}_{24} = \frac{1}{16} F^{\sigma}_{13} F^{\sigma}_{23} F^{\sigma}_{14} F^{\sigma}_{24}$$

has been omitted.

Since we are interested in calculating the C-parts of the operator configurations of table I, we are allowed to perform cyclic permulations of the operators. For instance, the C-part of:

$$S(\sigma_{13}\sigma_{23}) \; H_{12} \; S(\sigma_{14}\sigma_{24})$$

equals to the C-part of:

$$H_{12} \; S(\sigma_{14}\sigma_{24}) \; S(\sigma_{13}\sigma_{23})$$

If one does that to all configurations shown in table I, one realizes that all groups have on the right side of the Hamiltonian the same 24 terms, each one being a product of the operators $\sigma_{13}, \; \sigma_{14}, \; \sigma_{23}, \; \sigma_{24}$ in all 24 possible orders. Each term has a weight W, with:

$$W = \frac{1}{4!} + \frac{1}{3!} + \frac{1}{4} + \frac{1}{3!} + \frac{1}{4!} = \frac{16}{24}$$

i.e. there is no prefered operator order since all orders have the same weight. Each order is multiplied by the weight W, the $f^{C}_{12}H_{12}f^{C}_{12}$ factor as well as by $\frac{1}{16} F^{\sigma}_{13} F^{\sigma}_{23} F^{\sigma}_{14} F^{\sigma}_{24}$.

This results to:

$$\frac{16}{24} \times (\frac{1}{16} F^{\sigma}_{13} F^{\sigma}_{23} F^{\sigma}_{14} F^{\sigma}_{24}) \times (f^{C}_{12} \; H_{12} \; f^{C}_{12}) \times$$
$$\times \text{(All orders)}$$
$$= (F^{\sigma}_{13} F^{\sigma}_{23} F^{\sigma}_{14} F^{\sigma}_{24}) \; (f^{C}_{12} \; H_{12} \; f^{C}_{12}) \; S(\sigma_{13} \; \sigma_{23} \; \sigma_{14} \; \sigma_{24})$$

The quantity of interest is:

$$C(H_{12} \; S(\sigma_{13} \; \sigma_{23} \; \sigma_{14} \; \sigma_{24})) = C(H_{12} \; 0_{12}) \quad (3.1)$$

with

$$0_{12} \equiv <S(\sigma_{13} \ \sigma_{23} \ \sigma_{14} \ \sigma_{24})>_{12} \quad (3.2)$$

One can easily generalize this result for any diagram of the structure shown in fig. 2. Hence one has always to calculate the key-quantity:

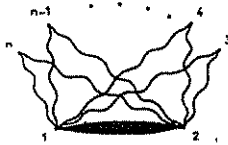$$0_{12} \equiv S(\sigma_{13} \ \sigma_{14}\cdots \ \sigma_{23} \ \sigma_{24}\cdots)_{12} \quad (3.3)$$

Figure 2

Diagrammatic representation of a general term considered in the hyperneted $\sigma(\tau)$ chain calculation.

The general diagram of fig. 2, consists of two factors. One is the correlation spatial part involving the products of F^σ's integrated over $\vec{r}_3$, $\vec{r}_4$,..., which is trivial to calculate, (see PW); the other involves the C-part of $(f^C_{12} H_{12} f^C_{12})0_{12}$ the calculation of which is the main task of the following paragraph.

3.b Calculation of 0_{12}

Starting from the definition for 0_{12} (equation (3.3)), and noting that:

$$<|\sigma_{1i}, \ \sigma_{2i}|>_{12} = 0 \quad i \neq 1,2 \quad (3.4)$$

one realizes that 0_{12} remains unaffected upon commutation of the σ_{1i} and σ_{2i} operators. That means that one can symmetrize as follows:

$$0_{12} = <S(\sigma_{13}\sigma_{14}\cdots) \ S(\sigma_{23}\sigma_{24}\cdots)>_{12} \quad (3.5)$$

Using the notation of section 2 one can write:

$$\sigma_{13}\sigma_{14}\cdots\sigma_{23}\sigma_{24}\cdots = 1_{s_1 s_2}\cdots 2_{r_1 r_2}\cdots 3_{s_1 r_1}$$

$$4_{s_2 r_2}\cdots$$

and since: $<3_{s_1 r_1}> = \delta_{s_1 r_1}$, $4_{s_2 r_2} = \delta_{s_2 r_2}$ etc.

one obtains:

$$0_{12} = S(1_{s_1 s_2}\cdots) \ S(2_{s_1 s_2}\cdots) \quad (3.6)$$

Let n be the number of indices $s_1, s_2\cdots, s_n$ in each of the symmetrized products of eq. (3.6). Clearly 0_{12} depends on n. It will

be shown that:

$$0^{(n)}_{12} = \begin{cases} n+1 & \text{,if } n \text{ is even} \\ \frac{1}{3}(n+2)\sigma_{12} & \text{,if } n \text{ is odd} \end{cases} \quad (3.7)$$

where the superscript n is added to explicitly display the dependence of 0_{12} on the number of indices. Consider first the case where n is even. Then:

$$S(1_{s_1 s_2}\cdots) = S(1_{s_1 s_2} 1_{s_3 s_4}\cdots) = S((\delta_{s_1 s_2} +$$

$$+i\epsilon_{s_1 s_2 k} 1_k)(\delta_{s_3 s_4} + i\epsilon_{s_1 s_2 m} 1_m)\cdots) =$$

$$= S(\delta_{s_1 s_2} \delta_{s_3 s_4}\cdots) \quad (3.8)$$

This is so because the $\epsilon_{s_1 s_2 k}$, $\epsilon_{s_3 s_4 m}$,..., terms drop out since they are antisymmetric in the (s_1, s_2), (s_3, s_4),... indices. The number of terms in $S(\delta_{s_1 s_2} \delta_{s_3 s_4}\cdots)$ is $(n-1)!!$

Consider the quantity $S^{(n)}_{123\dots n}$ defined by:

$$S(\delta_{12} \ \delta_{34}\cdots \ \delta_{n-1,n}) \ \frac{S^{(n)}_{12\dots n}}{(n-1)!!} \quad (3.9)$$

Where δ_{12}, δ_{34},... stand for $\delta_{s_1 s_2}$, $\delta_{s_3 s_4}$ =

$$0^{(n)}_{12} = \frac{S^{(n)}_{12\dots n} \ S^{(n)}_{12\dots n}}{|(n-1)!!|^2} \quad (3.10)$$

The quantity $S_{123\dots n, n+1, n+2}$ can be constructed as:

$$S^{(n+2)}_{12\dots n, n+1, n+2} = S^{(n)}_{12\dots n}\delta_{n+1, n+2} +$$

$$+ S^{(n)}_{n+1, 2,\dots, n}\delta_{1, n+2} +\cdots+$$

$$+ S^{(n)}_{12,\dots n-1, n+1} \delta_{n, n+2} \quad (3.11)$$

$$|S^{(n+2)}|^2 \ S^{(n+2)}_{12\dots n+2} \ S^{(n+2)}_{12\dots n+2} =$$

$$= 3(n+1)|S^{(n)}|^2 + n(n+1)|S^{(n)}|^2$$

$$= (n+1)(n+3)|S^{(n)}|^2 \quad (3.12)$$

(contraction over all repeated indices is implied)

In the first term of eq. (3.12) the factor of 3 comes from contracting two identical Kronecker deltas. There are $(n+1)$ such term in $|S^{(n+2)}|^2$ and thus the factor $n+1$. The second term contains all the "cross" terms of

the form:

$$S^{(n)}_{12\ldots k,n+1,k+2,\ldots n}\delta_{k,n+2}$$

$$S^{(n)}_{12\ldots \ell,n+1,\ell+2,\ldots n}\delta_{\ell,n+2} = |S^{(n)}|^2$$

There are $n(n+1)$ terms of this kind and hence the factor of $n(n+1)$.

$$0^{(n+2)}_{12} = \frac{|S(n+2)|^2}{|(n+1)!!|^2} = (n+3)(n+1)\frac{|S^{(n)}|^2}{|(n-1)!!|^2} =$$

i.e.: $\quad 0^{(n+2)}_{12} = \frac{n+3}{n+1}\, 0^{(n)}_{12}$ \hfill (3.13)

Since $\quad 0^{(2)}_{12} = \dfrac{|S^{(2)}|^2}{(1!!)^2} = \delta_{12}\delta_{12} = 3,$

the above recursion relation, (3.13), for $0^{(n)}_{12}$, is easily solved to give: $0^{(n)}_{12} = n+1$ (for even n). Now for odd number of indices, (n+1), one should calculate

$$0^{(n+1)}_{12} = \frac{S^{(n+1)}_{12\ldots,n,n+1}\, \tilde{S}^{(n+1)}_{12\ldots n,n+1}}{|(n+1)!!|^2}$$ \hfill (3.14)

with $S^{(n+1)}_{12\ldots n,n+1} = S^{(n)}_{12\ldots n}1_{n+1} + S^{(n)}_{n+1,2,\ldots,n}1_1 +$

$+ \ldots + S^{(n)}_{12\ldots n-1,n+1}1_n$ \hfill (3.15)

and $\tilde{S}^{(n+1)}_{12\ldots n,n+1} = S^{(n)}_{12\ldots n}2_{n+1} + S^{(n)}_{n+1,2,\ldots n}2_1 +$

$+ \ldots + S^{(n)}_{12\ldots n-1,n+1}2_n$ \hfill (3.16)

$$S^{(n+1)}_{12\ldots n+1}S^{(n+1)}_{12\ldots n+1} = (n+1)\sigma_{12}|S^{(n)}|^2 +$$

$$+ \frac{1}{3}n(n+1)\sigma_{12}|S^{(n)}|^2$$ \hfill (3.17)

The first piece comes from contracting terms in which the operators 1 and 2 carry the same index. For instance:

$$S^{(n)}_{12\ldots n}1_{n+1}S^{(n)}_{12\ldots n}2_{n+1} = |S^{(n)}|^2\sigma_{12}$$

There are (n+1) such terms and hence the factor (n+1). The second piece comes from "cross" terms.

For istance: $S^{(n)}_{12\ldots n}1_{n+1}\ S^{(n)}_{n+1,2,\ldots,n}2_1$

Since $S^{(n)}_{12\ldots n}\ S^{(n)}_{n+1,2,\ldots,n}$ is symmetric with respect to the indices 1 and (n+1) it must be proportional to $\delta_{1,n+1}$. I.e. one has:

$$S^{(n)}_{12\ldots n}\ S^{(n)}_{n+1,2,\ldots n} = \beta\delta_{1,n+1}$$

Then: $S^{(n)}_{12\ldots n}\ S^{(n)}_{12\ldots n} = \beta\delta_{1,1} = 3\beta$

or $\beta = \frac{1}{3}S^{n^2}$ and

$$S^{(n)}_{12\ldots n}\ S^{(n)}_{n+1,2\ldots n}\ 1_{n+1}2_1 =$$

$$= \frac{1}{3}|S^{(n)}|^2\delta_{1,n+1}\ 1_{n+1}2_1 = \frac{\sigma_{12}}{3}|S^{(n)}|^2$$

There are $n(n+1)$ such terms and hence the factor $n(n+1)$. From eq. (3.14) and (3.17) one obtains:

$$0^{(n+1)}_{12} = \frac{1}{n+1}\left(\frac{n+3}{3}\right)\ 0^{(n)}_{12}\ \sigma_{12}\quad \text{or}$$

$$0^{(n+1)}_{12} = \frac{1}{3}(n+3)\sigma_{12}\quad \text{or if m=n+1 (m is odd)}$$

$$0^{(m)}_{12} = \frac{1}{3}(m+2)\ \sigma_{12}$$

If by X_{12} we denote the spatial part of the diagram of figure 3, the quantity of interest is given by:

$$h^\sigma_{12} = \sum_{n=2,4\ldots}\frac{X^n_{12}}{n!}(n+1) + \sum_{n=3,5,\ldots}\frac{X^n_{12}}{n!}\frac{(n+2)}{3}\sigma_{12}$$ \hfill (3.18)
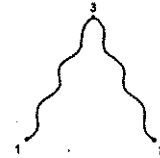
Figure 3

The basic $\sigma(\tau)$ chain-diagram that is hyperneted in the present work.

Which is trivial to calculate. One otains:

$$h^\sigma_{12} = \cosh(X_{12}) + X_{12}\sinh(X_{12}) - 1 + \frac{1}{3}\sigma_{12}|2\sinh(X_{12}) +$$

$$+ X_{12}\cosh(X_{12}) - 3X_{12}|$$

4. - Direct, double σ-chains.-

4.a Preliminary analysis

The general diagram whose C-part we wish to calculate is shown in figure 4. The quantity of interest is:
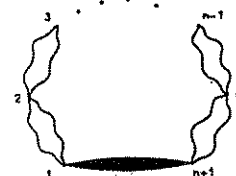
Figure 4

A general double $\sigma(\tau)$ diagram whose c-part is considered in the present work.

$$C\{S(\sigma_{12}\sigma_{23}\cdots\sigma_{n,n+1})H_{1,n+1}S(\sigma_{12}\sigma_{23}\cdots\sigma_{n,n+1})\} =$$

$$= C\{H_{1,n+1}0_{1,n+1}\} \qquad (4.1)$$

with

$$0_{1,n+1} \equiv <S(\sigma_{12}\sigma_{23}\cdots\sigma_{n,n+1})$$

$$S(\sigma_{12}\sigma_{23}\cdots\sigma_{n,n+1})>_{1,n+1} \qquad (4.2)$$

This quantity contains (n!)x(n!) terms. Using the notation of section 2 we write:

$$\sigma_{12}\sigma_{23}\cdots\sigma_{n,n+1} = (1_{i_1}2_{i_1})(2_{i_2}3_{i_2})\cdots$$

$$(n_{i_n}(n+1)_{i_n}) \qquad (4.3)$$

We choose the indices $i_1, i_2 \ldots i_n$ for the symmetrized product on the left in (4.2) and the primed indices $i_1', i_2', \ldots i_n'$ for the symmetrized product on the right correspondingly. Then any term in (4.2) will consist of a factor $1_{i_1 i_1'}(n+1)_{i_n i_n'}$ and a product of the form:

$$< 2_{i_1 i_2 i_1' i_2'} > < 3_{i_2 i_3 i_2' i_3'} > \cdots$$

or with some other ordering of the indices depending on the particular term in question. So in general, the structure of any single term in (4.2) will be:

$$1_{i_1 i_1'}(n+1)_{i_n i_n'}|D^{n-1-s}\tilde{D}^s|_{i_1 i_n i_1' i_n'} \qquad (4.4)$$

where the quantities D and $\tilde{D}$ are those defined in section 2.
Then one can write:

$$0_{1,n+1} = 1_{i_1 i_1'}(n+1)_{i_n i_n'}\sum_{s=0}^{n-1}\frac{M_{n,s}}{(n!)^2}$$

$$|D^{n-1-s}\tilde{D}^s|_{i_1 i_n i_1' i_n'} \qquad (4.5)$$

where $M_{n,s}$ the number or terms in (4.2) whose contribution is that given by (4.4). Using the properties listed in section 2 for the quantities I, $\tilde{D}$ and D one obtains:

$$0_{1,n+1} = \sum_{s=0}^{n-1}\frac{M_{n,s}}{(n!)^2}(-1)^{n-1-s}3^{s+1} -$$

$$- 2^n\frac{M_{n,n-1}}{(n!)^2}\sigma_{1,n+1} \qquad (4.6)$$

One now needs to find a way of calculating the $M_{n,s}$ coefficients, which is the subject of the next paragraph.

4.b The calculation of $M_{n,s}$

The quantity $0_{1,n+1}$,defined by (4.2), involves two symmetrized operator products. Each of these products contains n! terms, so that $0_{1,n+1}$ contains a total of $(n!)^2$ terms. Each of these terms consists of two parts, one comes from the left and the other comes from the right symmetrizer. If two operators that share a common particle index (for instance $\sigma_{i-1,i}$ and $\sigma_{i,i+1}$) are arranged with the same, relative to each other, order in both the left and the right part of same term, a D-factor will be associated with that index, otherwice a $\tilde{D}$-factor will result. The relative orders of operators that do not share a comon index are irrelevant. Let P(n) be a set with elements the $(n!)^2$ operator products associated with $0_{1,n+1}$. Any element of P(n) whose left part has s different relevant orders from its right part, and hence it will contribute according to (4.4), is said to be of order s. Let P(n,s) be a subset of P(n) that consists of all elements of P(n) of order s. The number of elements of P(n,s) is the quantity $M_{n,s}$ we wish to calculate.

Let $\lambda_{i,j}^{n,s}$ be the number of elements of P(n,s) that have the $\sigma_{n,n+1}$ operator placed at the ith position in their left part and at the jth position in their right part. Clearly then:

$$M_{n,s} = \sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_{i,j}^{n,s} \qquad (4.7)$$

Then $\lambda_{i,j}^{n+1,s}$, i.e. the number of elements of P(n+1,s) that have the operator $\sigma_{n+1,n+2}$ at the ith and j^{th} position in their left and right parts respectively is given by:

$$\lambda_{i,j}^{n+1,s} = \sum_{\ell=1}^{i-1}\sum_{r=1}^{j-1}\lambda_{\ell,r}^{n,s} + \sum_{\ell=i}^{n}\sum_{r=j}^{n}\lambda_{\ell,r}^{n,s} +$$

$$+ \sum_{\ell=1}^{i-1}\sum_{r=j}^{n}\lambda_{\ell,r}^{n,s-1} + \sum_{\ell=i}^{n}\sum_{r=1}^{j-1}\lambda_{\ell,r}^{n,s-1} \qquad (4.8)$$

The first (second) term in (4.8), takes in account all elements of P(n,s) that have the $\sigma_{n,n+1}$ operator in the left part before (after) the ith position and in the right part before (after) the jth position, thus when inserting at the ith and j^{th} positions, in the left and right parts respectively, the $\sigma_{n+1,n+2}$ operator we obtain elements of the set P(n+1,s), since the relevant relative orders of $\sigma_{n,n+1}$ and $\sigma_{n+1,n+2}$ are the same in both parts of every element. The third (fourth) term, takes in account all terms of P(n,s-1) that have the $\sigma_{n,n+1}$ operator in the left part before (after) the ith position and in the right part after (before) the jth position, thus when inserting at the ith and j^{th} positions, in the left and right parts respectively, the $\sigma_{n+1,n+2}$ operator, we obtain elements of the P(n+1,s) set since the relevant relative orders of $\sigma_{n+1,n+2}$ are different in the two parts of every element.

There is no other scheme by which one can ge‌nerate elements of P(n+1,s), and so (4.8) is complete. Using the recursion relation (4.8) along with (4.7) one can easily compute $M_{n,s}$. Initial values for n=1 and n=2 are easily calculated. We find:

$$\lambda^{1,0}_{1,1} = 1, \quad \lambda^{2,0}_{1,1} = \lambda^{2,0}_{2,2} = \lambda^{2,1}_{1,2} = \lambda^{2,1}_{2,1} = 1$$

$$\lambda^{2,0}_{1,2} = \lambda^{2,0}_{2,1} = \lambda^{2,1}_{1,1} = \lambda^{2,1}_{2,2} = 0$$

In table II we give the first few $M_{n,s}$ numbers calculated using the method described above.

s \ n	2	3	4	5	6	7	8
0	2	10	88	1216	24176	654424	23136128
1	2	16	200	3536	85872	2743728	111842432
2		10	200	4896	149152	5714472	270769536
3			88	3536	149152	7176352	407103104
4				1216	85872	5714472	407103104
5					24176	2743728	270769536
6						654424	111842432
7							23136128

Table II

Tabulation of the $M_{n,s}$ coefficients for n=2,3,...,8 and for the corresponding rele‌vant s-values.

5. - Discussion.-

The hypernation of σ (or τ) chains presented in section 3, can be rather easily extended to treat $\sigma\tau$ chains as well. Inclusion of exchanges, or of more complicated chains, as well as provision for ring diagrams can be carried out following the same general line with a few modifications in the details of the calculation. Hypernation of chains including tensor operators is certainly more involved.

It is straight forward to extend the method presented in section 4 to treat double $\sigma\tau$-chains or σ-σ , τ-$\sigma\tau$ or σ-τ double operator chians. Inclusion of exhanges is possible but not as easy. For double tensor chains the counting part is the same as for double -chains but the spatial part needs special merit. We want to remark that since it is not always easy to derive a recursion relation that will solve the enumeration problem, one can explicitly generate the various permutations imposed by the symmetrizers and count the required orders one by one using a fast digital computer. A method for generating all permutations of n-different objects is given by Johnson[7] and Trotter[8].

Although these methods as they are described above, are suitable for symmetric Nuclear Matter calculations, they can be extended to facilitate spin and/or isospin polarized matter calculations; also they can play the role of a guide in approximating other more complicated terms of the cluster expansion.

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