Perturbation Theory for Spin Systems

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1. Introduction

The methods of quantum field theory applied to the many body problems have had an extensive success in the last years[1,2]. The application of these methods to spin systems raises difficult problems, which, since the pioneering work of F. J. Dyson[3], have been the subject of many publications. Among other methods[4,5,6], one should cite particularly the double time temperature dependent Green's function method[7,8,9], which has been successfully applied to the ferromagnetic problem[10,11].

To study the properties of spin impurities in metals, it has appeared useful to develop a perturbation theoretic method analogous to the Feynman graph technique[1,12]. The main difficulty rises from the fact that Wick's theorem[13] is not valid for spin operators, because the commutator of two S operators is not a C number, but an operator. It is possible though to formulate a theorem very similar to Wick's theorem and to develop the corresponding diagram technique.

The purpose of this paper is to prove the modified Wick's theorem, to introduce the corresponding diagrams and to illustrate the technique by a simple example. Applications of the method presented here to physically interesting cases will be the subject of separate publication[14].

2. Generalized Wick's Theorem for Spin Operators

In time dependent perturbation theory, one is lead to evaluate quantities of the type[1]:

$$\langle 0|\mathrm{T}\{A(t_1)B(t_2)\cdots P(t_m)\}|0\rangle \ ,$$

where T is the time ordering operator, $A(t_1)\cdots P(t_m)$ are operators written in a suitable interaction picture

$$A(t)=e^{i\mathscr{H}_0 t}Ae^{-i\mathscr{H}_0 t} \ ,$$

and $|0\rangle$ is the ground state of $\mathscr{H}_0$.

Wick's theorem then allows to transform the time ordered product into a sum of normal products, the expectation value of which is particularly simple to calculate.

Let us consider now a system of interacting spins $S^1, S^2, \cdots S^N$; the simplest way to define the free Hamiltonian $\mathscr{H}_0$ is to introduce a static homogenous magnetic field in z direction. Then

$$\mathscr{H}=\mathscr{H}_0+\mathscr{H}'$$
$$\mathscr{H}_0=-\mu g H_z \sum S_z{}^n$$
$$\mathscr{H}'=F(S^1, S^2\cdots S^N) \;.$$

$\mathscr{H}'$ is the spin-spin interaction and is supposed to be a polynomial expression in the $S_x{}^i$, $S_y{}^r$, $S_z{}^t$ operators. From now on all operators are supposed to be written in interaction picture.

One defines then as the normal product of a set of S operators the set for which the S_+ operators stand on the left, the S_- operators in the middle and the S_z operators on the right (the place assigned to the S_z operators is of course arbitrary but must be fixed in order to have definite rules). The contraction of two S operators, i.e. the difference between the time ordered product and the normal product, is given by

$$\begin{aligned}\underbrace{S_+^n(t)S_-^{n'}}(t')&=\mathrm{T}\{S_+^n(t)S_-^{n'}(t')\}-\mathrm{N}\{S_+^n(t)S_-^{n'}(t')\}\\&=-2S_z^n e^{i\mu g H_z(t'-t)}\vartheta(t'-t)\delta_{nn'}\\ \underbrace{S_+^n(t)S_z^{n'}}(t')&=S_+^n(t)\vartheta(t'-t)\delta_{nn'}\\ \underbrace{S_-^n(t)S_z^{n'}}(t')&=-S_-^n(t)\vartheta(t'-t)\delta_{nn'}\;.\end{aligned}\tag{1}$$

Note that S_z is independent of time as an operator but that the time variable is necessary to indicate the ordering of the operators in the set.

If one tries to transform explicitly a given set of S operators into a normal set by using the commutation rules (1), one sees that one given operator can be the subject of many contractions. In order to formulate the theorem, one must introduce S operators depending on many "*time variables*", namely $S_-(t;t_1\cdots t_m)$ and $S_z(t';t'')$. In this, t is the only true time variable; the dummy time variables $t_1\cdots t_m$ and t', t'' are merely indices; they "*remember*" preceding contractions.

The generalization of equations (1)

$$\begin{aligned}&\underbrace{S_+^n(t)S_-^{n'}}(t';t_1\cdots t_m)=-2S_z^n(t;t')\vartheta(t'-t)\vartheta(t_1-t)\cdots\vartheta(t_m-t)e^{i\mu g H_z(t'-t)}\delta_{nn'}\\&\underbrace{S_-^n(t;t_1\cdots t_m)S_z^{n'}}(t';t'')=-S_-^n(t;t_1\cdots t_m t')\vartheta(t''-t)\delta_{nn'}\\&\underbrace{S_+^n(t)S_z^{n'}}(t';t'')=S_+^n(t)\vartheta(t'-t)\delta_{nn'}\end{aligned}\tag{2}$$

together with the definitions

$$S_z(t;t)\equiv S_z(t)$$
$$S_-(t)\ \equiv S_-(t;\ )\qquad (\text{i.e. } m=0)$$

explain by themselves how the dummy time variables are constructed. $S_-(t;t_1\cdots t_m)$ is defined as symmetric in the dummy time variables, whereas $S_z(t';t'')$ is not symmetric.

THEOREM: *The time ordered product of a set of S operators is equal to the sum of the normal products of all sets of operators one can construct by contracting parts of the initial set in all possible ways, including the set without* *contraction. These normal products are multiplied by the scalar factors—defined by* (2)*—which occur in the contractions leading to them.*

In general, there are many different scalar factors to the same operator set, but each different scalar factor must occur only once, even if there are topologically different contractions leading to it. In this we suppose all time variables to be different.

Before proving the theorem, it may be useful to illustrate it by a simple example, e. g. the set $S_z^n(t)S_+^{n'}(t')S_-^{n''}(t'')$.

The construction of the different terms is done in the two columns below:

Possible set (in normal form)	Contractions leading to them
$S_+^{n'}(t')S_-^{n''}(t'')S_z^n(t)$	
$S_+^{n'}(t')S_-^{n''}(t'')$	$S_+^{n'}(t')S_z^n(t)$
$S_+^{n'}(t')S_-^{n''}(t'';t)$	$S_-^{n''}(t'')S_z^n(t)$
$S_z^n(t)S_z^{n''}(t';t'')$	$S_+^{n'}(t')S_-^{n''}(t'')$
$S_z(t';t'')$	$S_+^{n'}(t')S_z^n(t)S_-^{n''}(t'')$ $S_+^{n'}(t')S_z^n(t)S_-^{n''}(t'')$

We get therefore

$$\begin{aligned}
\mathrm{T}\{S_+^{n'}(t')S_z^n(t)S_-^{n''}(t'')\} &= S_+^{n'}(t')S_-^{n''}(t'')S_z^n(t) \\
&+S_+^{n'}(t')S_-^{n''}(t'')\{\vartheta(t-t')\delta_{nn'}-\vartheta(t-t'')\delta_{nn''}\} \\
&+S_z^nS_z^{n'}\{-2e^{i\mu gH_z(t''-t')}\vartheta(t''-t')\delta_{n''n'}\} \\
&+S_z^n\{-2e^{i\mu gH_z(t''-t')}\vartheta(t''-t')\delta_{n''n'}\}\{\vartheta(t-t')\delta_{nn'}-\vartheta(t-t'')\vartheta(t-t')\delta_{nn'}\}.
\end{aligned}$$

Note that the dummy time variables have been dropped in the final expression. One can explicitly check that this formula gives the right value for all possible orderings of the times t, t', t''.

To illustrate the second part of the theorem, let us consider the set

$$S_+^n(t)S_z^{n'}(t')S_z^{n''}(t'') .$$

The contractions

$$S_+^n(t)S_z^{n'}(t')S_z^{n''}(t'') \quad \text{and} \quad S_+^n(t)S_z^{n'}(t')S_z^{n''}(t'')$$

lead to the same scalar factor and must therefore not give rise to two different terms.

3. Proof of the Theorem for the Simplest Sets

The proof of the theorem follows the line of a classical proof of the Wick's theorem[15].

Let us consider a normal product of p operators

$$S_+(t_1)\cdots S_+(t_m)S_-(t_{m+1};t_{m+1}^1\cdots t_{m+1}^{i_{m+1}})\cdots S_-(t_{m+j};t_{m+j}^1\cdots t_{m+j}^{i_{m+j}})$$
$$S_z(t_{m+j+1};t_{m+j+1}^1)\cdots S_z(t_p;t_p^1)$$

and let us multiply it from the right by an operator $S(t_{p+1})$ with

$$t_{p+1}<t_r, t_m^k \quad \text{for all } r,\ m,\ k\,. \tag{3}$$

The indices m in S^m have been dropped for simplicity.

LEMMA: *The product*

$$S^+(t_1)\cdots S_z(t_p;t_p^1)S(t_{p+1}) \tag{4}$$

is equal to the sum of the normal products of all sets of operators one can construct by contracting $S(t_{p+1})$ with the other operators in all possible ways, except one which will be specified later, including the set without contraction. The normal products are multiplied by the scalar factors defined by (2) which occur in the contractions leading to them. Each different scalar factor to a specific set must occur only once.

Note that not all contractions have to be considered but only those generated by $S(t_{p+1})$. The exception will be specified during the proof.

Proof. There are three cases to consider:

(a) $S(t_{p+1})=S_z(t_{p+1})$

In this case the product (4) is already under normal form and the lemma is obviously right, since all contractions of $S_z(t_{p+1})$ with S_- or S_+ operators contain ϑ-functions which are identically zero because of (3).

(b) $S(t_{p+1})=S_-(t_{p+1})$

The proof proceeds as follows:

I: analysis of the non-zero terms predicted by the lemma,

II: explicit transformation of the product (4) in a sum of normal products and comparison of the result with the terms predicted by the lemma.

I. Following contraction systems are to be considered:

i) contraction of $S_-(t_{p+1})$ with an $S_+(t_r)$ is identically zero because of condition (3);

ii) contraction of $S_-(t_{p+1})$ with an $S_z(t_{m+j+s};t^1_{m+j+1})$ produces an $S_-(t_{p+1};t_{m+j+s})$ which can be contracted with an S_+ or an S_z operator;

iii) contraction of $S_-(t_{p+1};t_{m+j+s})$ with an $S_+(t_r)$ is identically zero, because of (3);

iv) contraction of $S_-(t_{p+1};t_{m+j+s})$ with an $S_z(t_{m+j+f};t^1_{m+j+f})$ produces an $S_-(t_{p+1};t_{m+j+s}t_{m+j+f})$.

Proceeding the same analysis until all S_z operators have been contracted, one sees that the only non-zero contractions are repeated contractions of the $S_-(t_{p+1})$ operator with S_z operators. All different systems of repeated contractions will be generated by choosing all possible different subsets of the S_z set and contracting them with $S_-(t_{m+1})$. Since by definition S_- is symmetric in the dummy time variables, one can see from rules (2) that the order in which the contractions are performed in a given subset has no influence on the final result and therefore each different subset must give rise to only one term.

One can express the result by writing

$$\begin{aligned} &S_+(t_1)\cdots S_z(t_p;t_p^1)S_-(t_{p+1}) \\ &\quad =S_+(t_1)\cdots S_-(t_{m+j};t_{m+j}^1\cdots t_{m+j}^{i m+j})L_-\{S_-(t_{p+1};t_{m+j+s}\cdots t_{m+j+q}); \\ &\quad S_z(t_{m+j+r};t_{m+j+r}^1)\cdots S_z(_{m+j+f};t_{m+j+f}^1)\} \end{aligned}$$

where $L_-\{A(t);S_z(t_{m+j+r};t_{m+j+r}^1)\cdots\}$ is a symbol representing the sum of all different possible subsets of the S_z operators multiplied by the scalar factors coming from the repeated contractions of $S_-(t_{p+1})$ with the complementary subset, and multiplied from the left by the operator $A(t)$; the reason why $A(t)$ is written instead of S_- will be clear shortly.

II. Since in the case considered the operators S_+ and S_- play no role in the explicit transformation of (4) into a normal product, one needs only consider the product

$$S_z(t_{m+j+1};t_{m+j+1}^1)\cdots S_z(t_p;t_q^1)S_-(t_{p+1}) .$$

If only one operator S_z is present, one has

$$\begin{aligned} S_z(t_p;t_p^1)S_-(t_{p+1}) &= S_-(t_{p+1})S_z(t_p;t_p^1)+S_-(t_{p+1};t_p)\{-\vartheta(t_p-t_{p+1})\} \\ &= L_-\{S_-(t_{p+1};t_p);S_z(t_p;t_p^1)\} , \end{aligned}$$

which is in agreement with the lemma. Strictly speaking, one should not include ϑ-functions nor dummy time variables in the expression constructed in this way, since one merely uses ordinary commutation rules. They are written down to show in a clearer way the identity of the results with those predicted by the lemma.

One supposes now the lemma to be correct for k S_z-operators present and proves it for $k+1$. Then

$$\begin{aligned} &S_z(t_{p-k};t_{p-k}^1)\cdots S_z(t_p;t_p^1)S_-(t_{p+1}) \\ &=S_z(t_{p-k};t_{p-k}^1)L_-\{S_-(t_{p+1};t_{p-k+q});S_z(t_{p-k+r};t_{p-k+r}^1)\cdots S_z(t_{p-k+f};t_{p-k+f}^1)\} \\ &\qquad\qquad s,\ q,\ r,\ f\geqslant 1 \qquad (5) \\ &=L_-\{S_z(t_{p-k};t_{p-k}^1)S_-(t_{p+1};t_{p-k+s}\cdots t_{p-k+q});S_z(t_{p-k+r};t_{p-k+r}^1)\cdots\} \\ &=L_-\{S_-(t_{p+1};t_{p-k+s}\cdots t_{p-k+q})S_z(_{p-k};t_{p-k}^1);S_z(t_{p-k+r};t_{p-k+r}^1)\cdots\} \\ &\quad +L_-[S_-(t_{p+1};t_{p-k+s}\cdots t_{p-k+q}t_{p-k})\{-\vartheta(t_{p-k}^1-t_{p+1})\};S_z(t_{p-k+r};t_{p-k+r}^1)\cdots] . \qquad (6) \end{aligned}$$

Considering a set of two objects, say a and b, one can explicitly construct all subsets, namely

$$\phi \quad a \quad b \quad a\,b \qquad (7)$$

where ϕ is the empty subset. If one adds a third object, c, then the subsets of the set $a\ b\ c$ are

$$\begin{matrix} \phi & a & b & a\,b \\ c & a\,c & b\,c & a\,b\,c\,. \end{matrix}$$

One sees that to construct these subsets, one must add to the preceding subsets, given by (7), those obtained by joining c to them. This can be proved to be true when one goes from k to $k+1$ objects.

It follows that

$$(6)=L_-\{S_-(t_{p+1};t_{p-k+s}\cdots t_{p-k+q});S_z(t_{p-k+r};t^1_{p-k+r})\cdots\}\,. \qquad s,\ q,\ r\geqslant 0$$

This proves the lemma in this case.

(**c**) $S(t_{p+1})=S_+(t_{p+1})$

The analysis proceeds as under (**b**):

I. Let us examine first the different systems of contractions which give non-zero contribution:

i) repeated contractions of $S_+(t_{p+1})$ with S_z operators. This kind of contraction system is completely similar to the one analysed above for the case $S_-(t_{p+1})$. These contractions merely reproduce the operator $S_+(t_{p+1})$.

ii) contraction of $S_+(t_{p+1})$ with $S_-(t_{m+k};t^1_{m+k}\cdots t^{i_{m+k}}_{m+k})$. This produces an operator $S_z(t_{p+1};t_{m+k})$ which can be contracted with an S_+ or an S_- operator.

iii) the contraction of $S_z(t_{p+1};t_{m+k})$ with an $S_+(t_r)$ is identically zero because of condition (3);

iv) contraction of $S_z(t_{p+1};t_{m+k})$ with an $S_-(t_{m+s};t^1_{m+s}\cdots t^{i_{m+s}}_{m+s})$ gives an operator $S_-(t_{m+s};t^1_{m+s}\cdots t^{i_{m+s}}_{m+s}t_{p+1})$;

v) contraction of this $S_-(t_{m+s};t^1_{m+s}\cdots t_{p+1})$ operator with an S_+ operator is identically zero because of (3).

vi) further contractions of $S_-(t_{m+s};t^1_{m+s}\cdots t_{p+1})$ with S_z operators must be explicitly excluded at this point. The reason why these contractions have to be ruled out in the lemma will be clear below.

The non-zero contraction systems predicted by the lemma are therefore the following:

[1] multiple contraction of $S_+(t_{p+1})$ with S_z operators,

[2] contraction of the resulting $S_+(t_{p+1})$ with an S_- operator,

[3] contraction of the resulting S_z operator with an S_- operator.

These contractions are not all different from zero; if one orders the S_- operators so that

$$t_{m+j}<t_{m+j-1}<\cdots<t_{m+1}\ , \tag{8}$$

then non-zero contractions are obtained by contracting $S_z(t_{p+1};t_{m+k})$ with S_- operators which follow $S_-(t_{m+k};t^1_{m+k}\cdots)$ in the set.

One can express the contractions described under [2] and [3] by

$$\begin{aligned}&S_-(t_{m+1};t^1_{m+1}\cdots)\cdots S_-(t_{m+j};t^1_{m+j}\cdots)S_+(t_{p+1})\\ &=S_+(t_{p+1})S_-(t_{m+1};t^1_{m+1}\cdots)\cdots S_-(t_{m+j};t^1_{m+j}\cdots)\\ &\quad+\sum_k p(k)\{\prod_{i;\hat{k}}S_-(t_{m+i};t^1_{m+1}\cdots)\}S_z(t_{p+1};t_{m+k})\\ &\quad+\sum_{k<s}g(k,s)\{\prod_{i;\hat{k};\hat{s}}S_-(t_{m+i};t^1_{m+i}\cdots)\}S_-(t_{m+s};t^1_{m+s}\cdots t_{p+1})\ ,\end{aligned} \tag{9}$$

where $\prod_{i;\hat{k}\hat{s}}$ means that in the product the terms k and s have to be omitted, and p and g are defined by

$$p(k)=-2e^{i\mu_gH_z(t_{m+k}-t_{p+1})}\vartheta(t_{m+k}-t_{p+1})\vartheta(t^1_{m+k}-t_{p+1})\cdots\vartheta(t^{i_{n+k}}_{m+k}-t_{p+1})$$

$$g(k,s)=-\vartheta(t_{m+k}-t_{m+s})p(k)\ .$$

One can express the contraction described under [1] by

$$S_z(t_{m+j+1};t^1_{m+j+1})\cdots S_z(t_p;t^1_p)S_+(t_{p+1})$$
$$=S_+(t_{p+1})L_+\{S_z(t_{m+j+1};t^1_{m+j+1})\cdots S_z(t_p;t^1_p)\}$$

where L_+ represents the sum of all different possible subsets of the S_z operators multiplied by the scalar factors coming from the repeated contractions of $S_+(t_{m+1})$ with the complementary subset.

Then

$$(4)=S_+(t_1)\cdots S_+(t_m)S_+(t_{p+1})S_-(t_{m+1};t^1_{m+1}\cdots)\cdots S_-(t_{m+j};t^1_{m+j}\cdots)L_+\{S_z(t_{m+j+1};t^1_{m+j+1})\cdots\}$$
$$+S_+(t_1)\cdots S_+(t_m)\sum_k p(k)\{\prod_{i\hat{k}} S_-(t_{m+i};t^1_{m+i}\cdots)\}S_z(t_{p+1};t_{m+k})L_+\{S_z(t_{m+j+1};t^1_{m+j+1})\cdots\}$$
$$+S_+(t_1)\cdots S_+(t_m)\sum_{k<s}g(k,s)\{\prod_{i;\hat{k}\hat{s}}S_-(t_{m+i};t^1_{m+i}\cdots)\}S_-(t_{m+s};t^1_{m+s}\cdots t_{p+1})L_+\{S_z(t_{m+j+1};t^1_{m+j+1})\cdots\}. \tag{10}$$

II. As in case (**b**), the lemma is proved to be correct by explicit transformation of the product (4) into a sum of normal products. In a first step, one can write, as proved under (**b**)

$$S_+(t_1)\cdots S_z(t_p;t^1_p)S_+(t_{p+1})$$
$$=S_+(t_1)\cdots S_-(t_{m+j};t^1_{m+j}\cdots t^{i_{m+j}}_{m+j})S_+(t_{p+1})L_+\{S_z(t_{m+j+1};t^1_{m+j+1})\cdots\}\ .$$

Since the S_+ and S_z operators play no role in the following, one needs only consider the product

$$S_-(t_{m+1};t^1_{m+1}\cdots t^{i_{m+1}}_{m+1})\cdots S_-(t_{m+j};t^1_{m+j}\cdots t^{i_{m+j}}_{m+j})S_+(t_{p+1})\ . \tag{11}$$

The lemma is obviously right for $j=1$. Let us consider the case $j=2$. In this case,

$$(11)=S_+(t_{p+1})S_-(t_{m+1};t^1_{m+1}\cdots)S_-(t_{m+2};t^1_{m+2}\cdots)$$
$$+S_-(t_{m+2};t^1_{m+2}\cdots)S_z(t_{p+1};t_{m+1})p(1)$$
$$+S_-(t_{m+1};t^1_{m+1}\cdots)S_z(t_{p+1};t_{m+2})p(2)$$
$$+S_-(t_{m+2};t^1_{m+2}\cdots t_{p+1})g(1,2)\ . \tag{12}$$

The result one can obtain by explicit construction is not unique. To obtain the result predicted by the lemma one needs first commute the S_- operators so that condition (8) is satisfied.

To prove the lemma, one proceeds again by induction: supposing the lemma to be true for $j=r-1$, one proves it for $j=r$. Then

$$S_-(t_{m+1};t^1_{m+1}\cdots)\cdots S_-(t_{m+r};t^1_{m+r}\cdots)S_+(t_{p+1})$$
$$=S_-(t_{m+1};t^1_{m+1}\cdots)\sum_{k\geqq 2}p(k)\{\prod_{\substack{i;\hat{k}\\ i\geqq 2}}S_-(t_{m+i};t^1_{m+i}\cdots)\}S_z(t_{p+1};t_{m+k})$$
$$+S_-(t_{m+1};t^1_{m+1}\cdots)\sum_{\substack{k<s\\ k\geqq 2}}g(k,s)\{\prod_{\substack{i;\hat{k}\hat{s}\\ i\geqq 2}}S_-(t_{m+i};t^1_{m+i}\cdots)\}S_-(t_{m+s}\cdots t_{p+1})$$
$$+S_-(t_{m+1};t^1_{m+1}\cdots)S_+(t_{p+1})S_-(t_{m+2};t^1_{m+2}\cdots)\cdots S_-(t_{m+r};t^1_{m+r}\cdots)\ . \tag{13}$$

The first two terms are already under normal form. The last term is equal to

$$
\begin{aligned}
&S_+(t_{p+1})S_-(t_{m+1};t^1_{m+1}\cdots)\cdots S_-(t_{m+r};t^1_{m+r}\cdots)+\\
&\quad +p(1)S_z(t_{p+1};t_{m+1})S_-(t_{m+2};t^1_{m+2}\cdots)\cdots S_-(t_{m+r};t^1_{m+r}\cdots)\ .
\end{aligned}
\tag{14}
$$

To put the second term of (14) in normal form, one must push S_z on the right step by step. Each step will produce two terms; a term without contraction whereby S_z is a step further on the right and a term containing the contraction with one of the S_-. Written shortly the procedure is the following:

$$
\begin{aligned}
&S_z(1)S_-(2)S_-(3)\cdots\\
&=S_-(2)S_z(1)S_-(3)\cdots+\underbrace{S_-(2)S_z}(1)S_-(3)\cdots\\
&=S_-(2)S_-(3)S_z(1)\cdots+S_-(2)\underbrace{S_-(3)S_z}(1)\cdots+\underbrace{S_-(2)S_z}(1)S_-(3)\cdots
\end{aligned}
$$

and so on. At the end,

$$
\begin{aligned}
(14)=&S_+(t_{p+1})S_-(t_{m+1};t^1_{m+1}\cdots)\cdots S_-(t_{m+r};t^1_{m+r}\cdots)\\
&+p(1)S_-(t_{m+2};t^1_{m+2}\cdots)\cdots S_-(t_{m+r}\cdots;t^1_{m+r}\cdots)S_z(t_{p+1};t_{m+1})\\
&+\sum_{s\geqq 2}g(1,s)\{\prod_{\substack{i,\ \hat{s}\\ i\geqq 2}}S_-(t_{m+i};t^1_{m+i}\cdots)\}S_-(t_{m+s};t^1_{m+s}\cdots t_{p+1})\ .
\end{aligned}
\tag{15}
$$

Adding (15) to the first two terms of (13) then gives

$$
\begin{aligned}
&S_+(t_{p+1})S_-(t_{m+1};t^1_{m+1}\cdots)\cdots S_-(t_{m+r};t^1_{m+r}\cdots)\\
&\quad+\sum_{k\geqq 1}p(k)\{\prod_{i;\ \hat{k}}S_-(t_{m+i};t^1_{m+i}\cdots)\}S_z(t_{p+1};t_{m+k})\\
&\quad+\sum_{\substack{k<s\\ k\geqq 1}}g(k,s)\{\prod_{i;\ \hat{k}\,\hat{s}}S_-(t_{m+i};t^1_{m+i}\cdots)\}S_-(t_{m+s};t^1_{m+s}\cdots t_{p+1})\ .
\end{aligned}
$$

Multiplying this equation from the left by the $S_+(t_1)\cdots$ operators and from the right by $L_+\{S_z(t_{n+j+1};t^1_{n+j+1})\cdots\}$ clearly gives the same result as predicted by (10) and achieves the proof of the lemma.

4. Proof of the Theorem—General Case

Since the thorem is valid for the simplest sets, namely the single operators $S_+(t)$, $S_-(t)$ and $S_z(t)$, one can suppose it right for k operators present and prove it for $k+1$ operators.

One must prove that the expression

$$
\mathrm{T}\{S(t_1)\cdots S(t_{k+1})\}
$$

will be given by the sum of the normal products which can be generated by all possible contractions.

For any ordering of the times $t_1\cdots t_{k+1}$ there will be an earliest time which is denoted by t_{k+1}. Then

$$
\mathrm{T}\{S(t_1)\cdots S(t_{k+1})\}=\mathrm{T}\{S(t_1)\cdots S(t_k)\}S(t_{k+1})\ .
$$

Since the theorem is supposed to hold for k operators, this expression is equal to a sum of normal products multiplied from the right by $S(t_{k+1})$ and each of these normal products satisfies the conditions of the lemma (conditions (3)). One can therefore transform each term into a sum of normal products, and the whole sum will be under normal form. To prove the theorem, one must prove:

(**a**) that all possible systems of contractions predicted by the theorem are effectively constructed;

(**b**) that no term occurs twice.

(**a**) Clearly any contraction system of the $k+1$ operators can be constructed by contracting first the k operators between them and then contracting the $(k+1)^{th}$ operator with some of the contracted operators. All possible contractions of the k operators are present because the theorem is supposed to be valid for k operators, and, but for the exception the role of which will be made clear below, all contraction systems dependent on $S(t_{k+1})$ are present in the sum, and therefore any system of contraction can be explicitly constructed.
(**b**) One has to prove now that the same term never occurs twice in the expansion constructed above. Since the theorem is supposed to be true for k operators present, all terms of the expansion of $\mathrm{T}\{S(t_1)\cdots S(t_k)\}$ are different. On the other hand, the terms generated by the lemma from one specific normal product of the k operators are all different. The only case therefore where double terms could be produced would be the case whereby one of the terms generated by $S(t_{k+1})$ from one specific normal product is equal to a term generated from another specific normal product; in another words, one of the contractions generated by $S(t_{k+1})$ must be equivalent to a contraction between the k first operators. Let us consider again the three cases:

[1] $S(t_{k+1})=S_z(t_{k+1})$
Only one term is non zero, so the case is trivial.

[2] $S(t_{k+1})=S_-(t_{k+1})$
Non zero systems of contractions are repeated contractions with S_z operators. They involve therefore the variable t_{k+1} at each step in an essential way and cannot be equivalent to a contraction between the k other operators.

[3] $S(t_{k+1})=S_+(t_{k+1})$
Referring to the cases analysed under (c) during the proof of the lemma, cases i) to v) are excluded for the same reason as under [2].

The contractions described under vi) do not involve the variable t_{k+1} in an essential way. They can be generated by first contracting a $S_-(t_{m+s};t^1_{m+s}\cdots)$ with S_z operators independent of $S_+(t_{k+1})$ and then contracting with $S_z(t_{k+1};t_{n+r})$, namely

$$S_-(t_{m+r};t^1_{m+r}\cdots)\cdots S_-(t_{m+s};t^1_{m+s}\cdots)\cdots S_z(t_{p-q};t^1_{p-q})\cdots S_+(t_{k+1})$$

$$=S_-(t_{m+r};t^1_{m+r}\cdots)\cdots S_-(t_{m+s};t^1_{m+s}\cdots)\cdots S_z(t_{p-q};t^1_{p-q})\cdots S_+(t_{k+1})\ .$$

This explains why these contractions have to be explicitly excluded in the lemma and shows that all systems of contractions predicted by the theorem are effectively present in the expansion. This completes the proof of the theorem.

In spite of the heavy complications which occur in the proof, the theorem is a natural generalization of Wick's theorem and this allows for a graphical representation of the different contractions completely similar to the Feynman diagram technique. This is done in the next section.

5. Diagram Technique and Calculation Rules

Apart from the expansion theorem, no special difficulty arises in the perturbation theory. Two points however must be kept in mind:

(**a**) Permutations of the time variables in

$$\mathrm{T}\{\mathscr{H}'(t_1)\cdots\mathscr{H}'(t_p)\}$$

generate terms of the expansion theorem which can be automatically taken into account by multiplying by a factor $p!/r$ where r is the number of time permutations which do not generate new terms in the expansion[16]; in usual theory r is generally ignored because it is always equal to one for diagrams connected to external lines. In this theory, r is often different from one, because, as seen above, it happens that topologically different contractions lead to only one term in the expansion. This occurs when S_+ or S_- operators are repeatedly contracted with S_z operators.

(**b**) Because of rules (2) the value corresponding to a given contraction is not independent of the other contractions occuring in the same diagram.

To introduce diagrams in a clear way, the best perhaps is to choose a simple Hamiltonian, say

$$\begin{aligned}\mathscr{H}'=-J\sum_{j\neq r}S^jS^r&=-J\sum_{j\neq r}S^j_zS^r_z-J\sum_{j\neq r}S^j_+S^r_-\\&=\qquad A\qquad+\qquad B\end{aligned}\tag{16}$$

and to give the rules for the calculation of the Green's function defined by

$$D_{nn'}(t-t')=-i\langle|\{\mathrm{T}\,S^n_-(t)S^{n'}_+(t')\}|\rangle\ ,$$

where $|\rangle$ is the ground state of $\mathscr{H}_0+\mathscr{H}'$.

A. Graphology.

(i) to each S operator associate a point in the plane;

(ii) to each $\underbrace{S_+S_-}$ contraction associate the line given in Fig. 1a;

(iii) to each $\underbrace{S_+S_z}$ contraction associate the line given in Fig. 1b;

(iv) to each $\underbrace{S_-S_z}$ contraction associate the line given in Fig. 1c;

(v) draw a wavy line between operators connected by $\mathscr{H}'$.

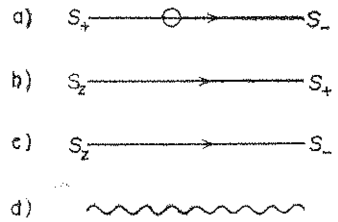

Fig. 1. Symbols used in the diagrams to represent spin contractions:

(a) $\underline{S_+S_-}$ contraction (c) $\underline{S_-S_z}$ contraction

(b) $\underline{S_+S_z}$ contraction (d) $\mathscr{H}'$ interaction line

No confusion can arise between $\underline{S_+S_z}$ and $\underline{S_-S_z}$ lines, because they are connected in different ways in the diagrams.

B. Calculation rules.

To calculate the p^{th} order contribution to $D_{nn'}(t-t)$:

(i) draw all possible non-equivalent connected diagrams containing p interation vertices which start with $S_+^{n'}(t')$ and end with $S_-^{n}(t)$. To have a non-zero expectation value, all S_+ and S_- operators have to be contracted; this is not true for the S_z operators.

(ii) to each $\underline{S_+^n(t')S_-^{n'}}(t;t_1\cdots t_m)$ contraction associate a factor

$$-2\delta_{nn'}e^{i\mu_gH_z(t-t')}\vartheta(t-t')\vartheta(t_1-t')\cdots\vartheta(t_m-t')\ .$$

(iii) to each $\underline{S_z^n(t'';t)S_+^{n'}}(t')$ contraction, associate a factor

$$\vartheta(t''-t')\delta_{nn'}\ .$$

(iv) to each $\underline{S_-^{n'}(t';t_1\cdots t_m)S_z^n}(t'';t)$ contraction, associate a factor

$$-\vartheta(t-t')\delta_{nn'}\ .$$

(v) to each interaction line associate a factor iJ.

(vi) divide by a factor r, which is defined by the number of repeated contractions of S_+ and S_- operators with S_z operators.

(vii) sum over the $2p$ internal indices and integrate over the p internal time variables.

(viii) include the right power of $\langle 0|S_z|0\rangle$, keeping in mind that S_z is "destroyed" when contracted.

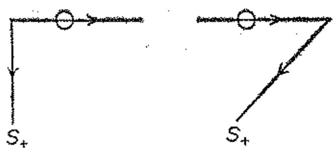

Fig. 2. The two diagrams drawn in the figure have identical meanings.

Following points may be useful:

(a) "Non-equivalent diagrams" means "non equivalent under time permutation". This qualification depends on the interaction Hamiltonian, and diagrams which are non-equivalent for a given Hamiltonian can well be equivalent for another.

(**b**) Since an S_+S_- contraction produces an S_z operator, each S_+S_- line (figure 1 a) can be contracted with an S_+ or an S_- operator (figure 2).

(**c**) Each S_+S_- line can have many incoming $S_zS_\pm$ lines but only one outgoing line.

(**d**) There must be no closed loop of S_z lines (Fig. 3).

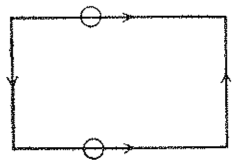

Fig. 3. Example of a diagram with closed loop of S_zS_+ lines. This kind of diagram is meaningless.

6. Simple Application

As a simple application of the rules stated above, let us prove to first order (the result is known to be correct in all orders) that this type of interaction gives nor shift nor broadening to the resonance line induced by a homogenous alternating magnetic field perpendicular to the z-axis. This resonance line is essentially given by $\mathrm{Im}\sum_{nn'} D_{nn'}(\omega)$[14].

To zero-th order:

$$D^0_{nn'}(\omega)=\frac{2S\delta_{nn'}}{\omega-\omega_0+i\delta}$$

where ω_0 is the Larmor frequency and S is equal to $-\langle 0|S_z|0\rangle$.

To first order:

The possible connected diagrams are drawn in Fig. 4 and Fig. 5. Quite happily, most of the diagrams give zero contribution because the terms S^jS^j do not occur in the Hamiltonian.

Only diagrams a, b, c, d of Fig. 4 and diagram a of Fig. 5 give non-zero contributions:

From Fig. 4:

$$\begin{aligned}\mathrm{a+c}&=2jJ\sum_{n_1n_1'}\int dt_1\vartheta(t_1-t')(-2)e^{-i\omega_0(t-t')}\vartheta(t-t')\delta_{n'n_1}\delta_{n'n}\langle S_z\rangle^2\\&=-4iJN\delta_{nn'}\vartheta(t-t')e^{-i\omega_0(t-t')}\langle S_z\rangle^2\int dt_1\vartheta(t_1-t')\end{aligned} \tag{17}$$

where $\langle S_z\rangle\equiv\langle 0|S_z|0\rangle$.

Similarly:

$$\mathrm{b+d}=-4iJN\delta_{nn'}\vartheta(t-t')e^{-i\omega_0(t-t')}\langle S_z\rangle^2\int dt_1\{-\vartheta(t_1-t)\}\ . \tag{18}$$

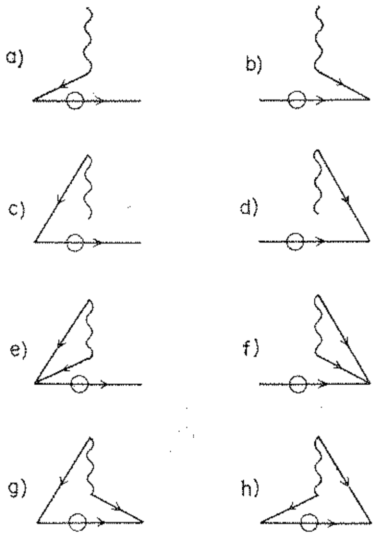

Fig. 4. Diagrams constructed from part A of the Hamiltonian $\mathscr{H}'$ (Eq. (16)).

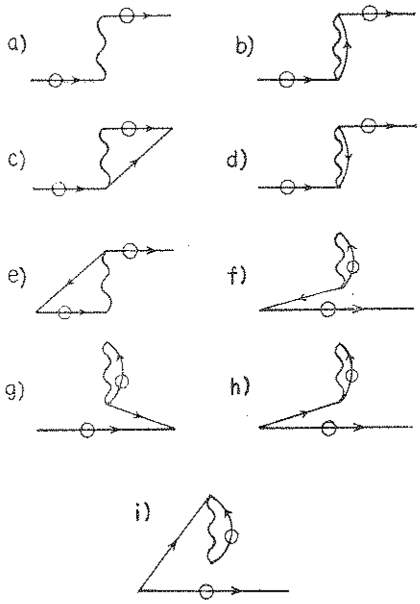

Fig. 5. Diagrams constructed from part B of the Hamiltonian $\mathscr{H}'$ (Eq. (16)).

The sum of (17) and (18) gives

$$(17)+(18)=-4iJN\delta_{nn'}\vartheta(t-t')e^{-i\omega_0(t-t')}\langle S_z\rangle^2(t-t') \ .$$

From Fig. 5:

$$\begin{aligned} \mathrm{a}&=iJ\sum_{n_1n_1'}\delta_{n_1n}\delta_{n_1'n'}\int dt_1 4e^{-i\omega_0(t_1-t')-i\omega_0(t-t_1)}\vartheta(t_1-t')\vartheta(t-t_1) \\ &=4iJ\vartheta(t-t')e^{-i\omega_0(t-t')}(t-t')\langle S_z\rangle^2 \ . \end{aligned} \tag{19}$$

It follows that

$$\sum_{nn'}\{(17)+(18)+(19)\}=0 \ .$$

The technique presented in this paper has been used in the problem of the resonance of spin impurities in metals[14]. Other problems, as well as the extension of this method to finite temperature, are under study.

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