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"THE RELATIONSHIP BETWEEN THE JOHNSON-BARANGER TIME DEPENDENT FOLDED DIAGRAM EXPANSION AND THE TIME INDEPENDENT METHODS OF PERTURBATION THEORY"

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THE RELATIONSHIP BETWEEN THE JOHNSON-BARANGER TIME DEPENDENT FOLDED DIAGRAM EXPANSION AND THE TIME INDEPENDENT METHODS OF PERTURBATION THEORY

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A B S T R A C T

We investigate the relationship between the Johnson-Baranger time-dependent folded diagram (JBFD) expansion and the time independent methods of perturbation theory.

In the non degenerate case we show that the JBFD expansion and the Rayleigh-Schroedinger perturbation expansion for the ground state energy are identical.

In the degenerate case we show that when the last time of the box is chosen as its time base the JBFD expansion of the effective interaction is equal to the perturbation expansion of the effective interaction of the non hermitian eigenvalue problem of Bloch and Brandow-Des Cloizeaux; for the two simplest symmetrical choices of the box time base the JBFD expansion of the effective interaction differs from the perturbation expansion of the effective interaction of the hermitian eigenvalue problem of Des Cloizeaux.

I. INTRODUCTION

In degenerate and quasi-degenerate perturbation theory the idea of an effective hamiltonian is of great utility in the studies of the properties of nuclei (see reference [5] for a review).

The are many different approaches for deriving the effective interaction and the equivalence of these various approaches is not at all obvious.

In the degenerate case, Bloch [2], Des Cloizeaux [3] and Brandow [4] derived the effective hamiltonian for ordinary (non-many body) quantum systems.

We give below a bief outline of the work of references [2,3,4]. Consider the hamiltonian

$$H = H_o + V \tag{1.1}$$

where H_o is the unperturbed hamiltonian and V is the perturbation. We suppose the eigenvalue problem for H_o solved, therefore we know its eigenfunctions and eigenvalues. We decompose the full Hilbert space into a model space Ω_o and its complement which is a space orthogonal to Ω_o. The projection operators in the model space and in the orthogonal space are P_o and Q_o respectively. P_o and Q_o satisfy the usual relations

$$P_o+Q_o = 1 \qquad P_oQ_o = Q_oP_o = 0 \qquad P_o^2 = P_o \qquad Q_o^2 = Q_o$$

The eigenfunctions of H_o which belong to the model space are called active states and the ones which belong to the orthogonal space, passive states.

As an example of this decomposition suppose that one of the eigenvalues of H_o, ε_o, is D fold degenerate. The D degenerate eigenfunctions span the model space Ω_o, and the projection operator P_o is equal to

$$P_o = \sum_{a_o \in \Omega_o} |a_o><a_o| \tag{1.2}$$

All the other eigenfunctions belong to the orthogonal space. When we introduce the interaction in general the degeneracy is lifted and we obtain D eigenfunctions of H.

$$H\,|\psi_a\rangle = E_a\,|\psi_a\rangle \tag{1.3}$$

These D eigenfunctions of H span a sub-space Ω of the full Hilbert space of dimension D and the projection operator on Ω is

$$P = \sum_{a \in \Omega} |\psi_a\rangle \langle\psi_a|$$

In references [2,3,4] the eigenvalue problem (1.3) which is defined in the full Hilbert space, is replaced by an eigenvalue problem defined in the model space Ω_o.

$$\begin{aligned}(P_o H_o P_o + \bar{H}_1)|\phi_{a_o}\rangle &= E_a\,|\phi_{a_o}\rangle \\ &= \bar{H}\,|\phi_{a_o}\rangle\end{aligned} \tag{1.4}$$

where $\bar{H}$ is the model hamiltonian and $\bar{H}_1$ is the energy independent effective interaction. This replacement is done only for the D eigenfunctions in Ω. In the Bloch equation [2], the eigenvalue problem (1.4) is written as:

$$(\varepsilon_o P_o + W^B - E_a)|\phi_{a_o}\rangle = 0 \tag{1.5}$$

where $|\phi_{a_o}\rangle$ is the projection of $|\psi_a\rangle$ on Ω_o

$$|\phi_{a_o}\rangle = P_o|\psi_a\rangle \tag{1.6}$$

W^B is the non-hermitian effective interaction which is equal to

$$W^B = P_o V U \tag{1.7}$$

and U is given by

$$\begin{aligned}U &= P_o + Q_o / a\ (VU - UVU) \\ UQ_o &= 0 \\ a &= \varepsilon_o - H_o\end{aligned} \tag{1.8}$$

The equation of Brandow [4] and Des-Cloizeaux [3] is

$$(\varepsilon_o P_o + W^{B-DC} - E_a)|\phi_{a_o}> = 0 \qquad (1.9)$$

where W^{B-DC} is given by

$$W^{B-DC} = \sum_{n=0}^{\infty} \frac{1}{n!} P_o \left(\frac{d^n}{d\varepsilon_o^n} K(\varepsilon_o)\right) (W^{B-DC})^n \qquad (1.10)$$

and $K(\varepsilon_o)$ is the reaction matrix [5]

$$K(\varepsilon_o) = VP_o + VQ_o/a\, K(\varepsilon_o) \qquad (1.11)$$

The perturbation expansion of (1.10) is given in reference [3]

$$W^{B-DC} = \sum_{n=0}^{\infty} W_n \qquad (1.12)$$

W_n is equal to

$$W_n = \sum_{\mu_1, \mu_2 \ldots \mu_n} \{\mu_1, \mu_2 \ldots \mu_n\} \qquad (1.13)$$

where $\{\mu_1, \mu_2, \ldots \mu_n\}$ is [3]

$$\{\mu_1, \mu_2, \ldots \mu_n\} = \frac{1}{\mu_1! \mu_2! \ldots \mu_n!} \frac{P_o d^{\mu_1}}{d\varepsilon_o^{\mu_1}} K(\varepsilon_o) \frac{P_o d^{\mu_2}}{d\varepsilon_o^{\mu_2}} K(\varepsilon_o) \ldots$$

$$\ldots \frac{P_o d^{\mu_n}}{d\varepsilon_o^{\mu_n}} K(\varepsilon_o) P_o \qquad (1.14)$$

$\frac{d^{\mu} K(\varepsilon_o)}{d\varepsilon_o^{\mu}}$ means the μ^{th} derivative of the reaction matrix.

The μ's are positive integers satisfying the relations

$$\mu_1 + \mu_2 + \ldots + \mu_n = n-1$$
$$\mu_1 + \mu_2 + \ldots + \mu_p > p-1 \qquad 1 \leq p < n \qquad (1.15)$$

The perturbation expansion (1.12) gives rise to the folded diagram expansion of Brandow.

In references [3,6] it is shown that $W^{B-DC} = W^B$.

The proof given in reference [6] is based on eqs. (1.7) and (1.8).

In order to transform the non hermitian eigenvalue problem (1.5) in a hermitian one Des-Cloizeaux rewrites eq. (1.5) in the following form [2,3] :

$$(B\varepsilon_o + A - E_a) \mid \bar{\phi}_{a_o} > = 0 \tag{1.16}$$

A and B are hermitian operators and

$$W^B = AB^{-1} \tag{1.17}$$

The states $\{|\bar{\phi}_{a_o}>\}$ are the states biorthogonal to the states $\{|\phi_{a_o}>\}$. The operator B is a positive definite operator [2,3,4] which transforms the states $\{|\bar{\phi}_{a_o}>\}$ into the states $\{|\phi_{a_o}>\}$

$$B\,|\bar{\phi}_{a_o}> = |\phi_{a_o}> \tag{1.18}$$

Considered as an operator acting in Ω_o it has an inverse [2,3,4].

$$|\bar{\phi}_{a_o}> = B^{-1}|\phi_{a_o}> \tag{1.19}$$

Defining the square root operator $B^{1/2}$ which is hermitian and positive definite the equation (1.15) can be written as

$$(B^{-1/2}\ AB^{-1/2} - (E_a - \varepsilon_o))\ |\hat{\phi}_{a_o}> = 0 \tag{1.20}$$

where $|\hat{\phi}_{a_o}> = B^{1/2}\,|\phi_{a_o}>$ are the so called half-way bases states [3,4].

$$W^{DC} = B^{-1/2}\ A\ B^{-1/2}$$

$$= B^{-1/2}\ W^B\ B^{1/2} \tag{1.21}$$

is the hermitian effective interaction of Des Cloizeaux [3].

In the approach of Johnson and Baranger [1] the effective interaction is derived by a time-dependent method and up to now there is no investigation about the relationship of the Johnson-Baranger folded diagram expansion (JBFD) [1] and the approaches of references [2,3,4]. In this paper we make an analysis of the relationship between the work of reference [1] and references [2,3,4] . In the case of non-degenerate perturbation theory we compare the JBFD expansion to the Rayleigh-Schroedinger expansion [5].

In the case of degenerate perturbation theory we compare the perturbation expansion of the non-hermitian effective interation of Bloch, eq (1.5), to the JBFD expansion of the effective interaction when the last time of the box is chosen as its time base. In the hermitian case we compare the perturbation expansion of the effective interaction of Des Cloizeaux, eq. (1.20), to the JBFD expansion of the effective interaction for the two simplest symmetrical choices of the box time base: an average of the first and last time of each box and a linear combination of the first and last time of each box.

II. OUTLINE OF THE JOHNSON-BARANGER FOLDED DIAGRAM EXPANSION

The basic point in the Johnson-Baranger derivation of the folded diagram expansion of the effective interaction is the exact replacement of the matrix elements of the time-evolution operator $T(+\infty,-\infty)$ between states in the model space by a model time evolution operator $\bar{T}(+\infty,-\infty)$. The intermediate states of the model time evolution operator are active states only. The active states are connected by the effective interaction $\bar{H}_1$. It is shown in reference [1] that the eigenvalues of the model hamiltonian $\bar{H}$, $\bar{H} = P_o H_o + \bar{H}_1$, are equal to the true eigenvalues, E_a. We give below an outline of the Johnson-Baranger derivation. Consider the matrix elements of $T(t,t')$ between states in the model space as shown in fig. 1. The perturbation expansion of $T(t,t')$ is calculated according to the usual Feynman rules. In the evolution of the system the intermediate states can be active or passive states. However the matrix element shown in fig. 1 can be written in such a way that the intermediate states are active states only as shown in fig. 2. The active states are connected by a "box", whose Fourier transform is the reaction

matrix, eq. (1.11). The reaction matrix is not instantaneous it has an extent in time. The next step is to replace everywhere the box by an instantaneous interaction as shown in fig. 3. The time at which the instantaneous interaction will act, the "box" time base, is completely arbitrary. However the instantaneous interaction is hermitian only if the choice of time base preserves the symmetry between past and future.

In the above replacement we have to make sure that the model description is equivalent to the true description. This is easily seen not to be the case since in the model description the "boxes" can overlap and this does not occur in the true description.

As an example consider the model diagram shown in fig.4. This diagram does not occur in the true description so it must be removed. To do so we define an instantaneous interaction, the double box diagram as shown in fig. 5. Now it is easily seen that in general in the model description we can have n overlapping "boxes" whose removal gives rise to the n^{th} "box" folded diagram. These diagrams are calculated according to the usual Feynman rules. Therefore the perturbation expansion of the effective interaction is

$$\bar{H}_1 = \sum_{n=1}^{\infty} \bar{H}_{1_n} \tag{2.1}$$

where $\bar{H}_{1_n}$ is the n^{th} box folded diagram.

In the case of degenerate perturbation theory the term having n overlapping boxes has a very simple structure.

$$\bar{H}_{1_n} = (-1)^{n+1} (-i)^{2n-1} \int_o^{\infty} dT_1 dT_3 \ldots dT_{2n-1} \; P_o K(T_1) P_o K(T_3) P_o \ldots$$
$$P_o K(T_{2n-1}) P_o \; e^{i\varepsilon_o (T_1+T_3+\ldots+T_{2n-1})} \int_{\Gamma} dT_2 dT_4 dT_{2n-2} \tag{2.2}$$

The difference among the various prescriptions for the box time base is only in the region of integration Γ. In what follows we will calculate the perturbation expansion of the effective interaction for specific choices of the box time base.

1) <u>Perturbation expansion of the effective interaction in the non-hermitian case</u>

In this case the time base of the various boxes is the last time of the diagrams.

The value of $\bar{H}_1$ up to the triple box diagram is given by

$$\bar{H}_1 = \{0\} + \{10\} + \{110\} + \{200\} + \ldots. \qquad (2.3)$$

The region of integration is given below (in all cases $T_1, T_3, \ldots, T_{2n-1} > 0$).

1.1) $T_1 > 0$ for the single-box diagram

1.2) $-T_1 < T_2 < 0$ for the double-box diagram

1.3) a) $-T_1 < T_2 < 0$ b) $-T_1 < T_2 < 0$

$-T_3 < T_4 < 0$ $\quad -(T_1+T_2+T_3) < T_4 < -T_3$

for the triple-box diagram.

The calculation of the higher order folded diagrams is straightforward but lengthy. However the following rule emerges from an order by order calculation which has been checked up to n=5.

Consider n overlapping boxes:

1) Draw all the overlapping boxes;
2) Consider all the permutations of the relative order of the boxes time base (the last time of the box) keepping the time base of the first box (from left to right) as the latest time.
   Therefore if we have n boxes, there are (n-1)! possibilities.
3) Draw horizontal lines from right to left leaving the boxes time base and finishing when a box is reached. Let μ_i be the number of lines reaching the i^{th} box. Consider together all the permutations leading to the same set of numbers $\mu_1, \mu_2, \ldots, \mu_n$. The sum of the contributions of all these diagrams calculated according to the usual Feynman rules, is $\{\mu_1, \mu_2, \ldots, \mu_n\}$.

We have not analysed Kuo et al. [7] folded diagram expansion, however it seems that the rule given in ref. [7] is identical to the rule given above.

Therefore $\bar{H}_{1_n}$ is equal to

$$\bar{H}_{1_n} = \sum_{\mu_1, \mu_2, \ldots, \mu_n} \{\mu_1, \mu_2, \ldots, \mu_n\} \qquad (2.4)$$

Considering the rule given above, it is easily seen that the μ's satisfy any one of the relations.

$$\mu_1 + \mu_2 + \ldots + \mu_n = n-1$$
$$\mu_1 + \mu_2 + \ldots + \mu_p > p-1 \qquad 1 \leq p < n \tag{2.5}$$

$$\mu_1 + \mu_2 + \ldots + \mu_n = n-1$$
$$\mu_p \leq n - p \qquad 1 < p \leq n \tag{2.6}$$

2) <u>Perturbation expansion of the effective interaction in the hermitian case: the time base is the average of the first and last time of each box.</u>

The value of $\bar{H}_1$ up to the triple box diagram is given by

$$\bar{H}_1 = \{0\}+1/2\{10\}+1/2\{01\}+1/8\{200\}+1/8\{002\}+3/4\{020\}+3/8\{011\}+$$
$$+3/8\{110\}+1/4\{101\} + \ldots \tag{2.7}$$

The region of integration is equal to:

2.1) $T_1 > 0$ for the single-box diagram

2.2) $-(T_1+T_3)/2 < T_2 < 0$ for the double-box diagram

2.3) a) $-(T_1+T_3)/2 < T_2 < 0$

$-(T_3+T_5)/2 < T_4 < 0$

b) $-(T_3+T_5)/2 < T_4 < 0$

$-(T_1/2+3T_3/4+T_5/4+T_4/2) < T_2 < -(T_3+T_1)/2$

c) $-(T_1+T_3)/2 < T_2 < 0$

$-(T_1/4+T_2/2+3T_3/4+T_5/2) < T_4 < -(T_3+T_5)/2$

for the triple-box diagram.

3) <u>Perturbation expansion of the effective interaction in the hermitian case: the time base as a linear combination of the first and last time of the box.</u>

The value of $\bar{H}_1$ up to the triple box diagram is given

$$\bar{H}_1 = \{0\}+1/2\{10\}+1/2\{01\}+1/4\{200\}+1/4\{002\}+1/2\{020\}+3/8\{011\} +$$
$$+3/8\{110\}+1/4\{101\} + ... \qquad (2.8)$$

The region of integration is equal to:

3.1) $T_1 > 0$ for the single-box diagram

3.2) a) $-T_1 < T_2 < 0$

b) $-(T_1+T_3) < T_2 < 0$

c) $-T_3 < T_2 < 0$

for the double-box diagram.

In this case there is a factor of 1/2 multiplying each contribution.

3.3) a) $-T_1 < T_2 < 0$
$-T_3 < T_4 < 0$

b) $-T_3 < T_2 < 0$
$-T_5 < T_4 < 0$

c) $-T_1 < T_2 < 0$
$-(T_3+T_5) < T_4 < 0$

d) $-(T_1+T_3) < T_2 < 0$
$-T_5 < T_4 < 0$

e) $-(T_1+T_3+T_5) < T_2 < 0$
$-(T_1+T_3+T_5+T_2) < T_4 < 0$

f) $-(T_3+T_5) < T_2 < 0$
$-(T_2+T_3+T_5) < T_4 < 0$

g) $-(T_1+T_3) < T_2 < 0$
$-(T_1+T_2+T_3) < T_4 < 0$

h) $-T_3 < T_2 < 0$
$-(T_2+T_3) < T_4 < 0$

There is a factor of 1/16 multiplying the first four contributions and one of 1/8 multiplying the last four.

It is worth mentioning that we have many more possibilities for choice two than for choice three . As an example, for the triple-box diagram, we have three possibilities in case two and twenty four in case three. So, between the two hermitian prescriptions, the easiest to calculate is case two.

In what follows we will compare the perturbation expansion (2.4), (2.7) and (2.8) to the perturbation expansion of the effection interaction of Bloch, eq. (1.12) and Des Cloizeaux, eq. (1.21).

III. NON DEGENERATE PERTURBATION THEORY

In the case of non-degenerate perturbation theory the model space has only one dimension, so the projection operator P_o is equal to

$$P_o = |0><0|$$

The eigenvalue is given by

$$E_o = \varepsilon_o + <0|\bar{H}_1|0> \tag{3.1}$$

In the non-hermitian case $\bar{H}_1$ is equal to eq. 4.1.

In the case of one dimension eq. (4.1) reduces to

$$<0|\bar{H}_1|0> = \sum_{n=o}^{\infty} \frac{1}{n!} \left(\frac{d^n}{d\varepsilon_o^n} <0|K(\varepsilon_o)|0>\right) \left(<0|\bar{H}_1|0>\right)^n \tag{3.2}$$

Using (3.1) and (3.2) the energy E_o is given by

$$\begin{aligned} \Delta E &= E_o - \varepsilon_o \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d^n}{d\varepsilon_o^n} <0|K(\varepsilon_o)|0>\right)(\Delta E)^n \end{aligned} \tag{3.3}$$

Using a formula of Lagrange [3,5], (3.3) reduces to

$$\Delta E = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{d^{n-1}}{d\varepsilon_o^{n-1}} \left(<0|K(\varepsilon_o)|0>\right)^n \tag{3.4}$$

which is equal to the Rayleigh-Schroedinger perturbation theory [5].

In the hermitian case $\bar{H}_1$ is given up to the triple-box diagram by the equations (2.7) and (2.8). In both cases, the expectation value of $\bar{H}_1$ is equal to eq. (3.2) to the order considered. So, to this order they are equal to the Rayleigh-Schroedinger perturbation theory. It is certainly plausible that the equality remains at higher orders.

IV. DEGENERATE PERTURBATION THEORY-NON-HERMITIAN CASE

The effective interaction when the last time of the diagram is chosen as its time base is given to all orders of perturbation theory by eqs. (2.1), (2.4) and (2.5). This is equal to the perturbation expansion of W^{B-DC} given by eqs. (1.12), (1.13) and (1.15). Therefore:

$$\bar{H}_{1_n} = \sum_{n=0}^{\infty} \frac{1}{n!} P_o \left(\frac{d^n K(\varepsilon_o)}{d\varepsilon_o^n}\right) (\bar{H}_1)^n \qquad (4.1)$$

So when we chose the last time of the diagram as its time base, the JBFD expansion of the effective interaction is identical order by order to the Brandow- Des Cloizeaux effective interaction and to the Bloch effective interaction since the last two are equal [3,6].

Therefore, the Johnson-Baranger folded diagram expansion is identical to the Brandow folded diagram expansion of the effective interaction.

V. DEGENERATE PERTURBATION THEORY-HERMITIAN CASE

The perturbation expansion of the Des Cloizeaux hermitian effective interaction is [3]

$$W^{DC} = \{0\}+1/2\{10\}+1/2\{01\}+3/8\{110\}+3/8\{011\}+1/4\{101\}+1/2\{200\}+ \\ +1/2\{002\}+ \ldots \qquad (5.1)$$

If we compare (5.1) to eqs. (2.7) and (2.8) we see that

they are all different. This tell us that W^{DC} is not equal to the JBFD expansion of the effective interaction for the two symmetrical choices of the box time base considered in this paper. The three effective interactions, (2.7), (2.8) and (5.1) are related by an unitary transformation in the model space Ω_o.

We did not attempt to find what symmetrical choice of the box time base gives rise to the Des Cloizeaux effective interaction.

It is interesting to notice that to compare the different hermitian prescriptions we should consider at least the triple-box diagram since the way to make the double box diagram hermitian is unique.

VI. CONCLUSIONS

In this paper we have shown that in the case of ordinary (non-many body) quantum systems the perturbation expansion of the Bloch effective interaction is equal order by order to the JBFD expansion of the effective interaction when the last time of the box is chosen as its time base. In the hermitian case, the perturbation expansion of the Des Cloizeaux effective interaction differs from the JBFD expansion for the two symmetrical choices of the box time base considered in this paper.

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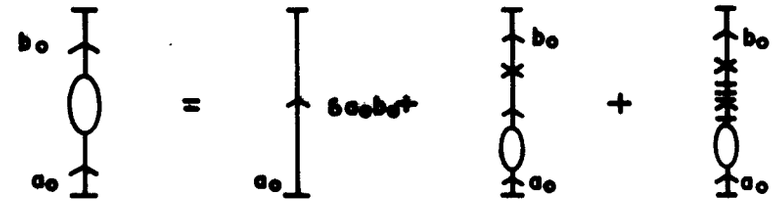

Fig. 1 – The states $\{|a_o\rangle\}$ belong to the model space. The hatched and non-hatched lines represent the propagation of a passive and an active state respectively The cross is the interaction H_1.

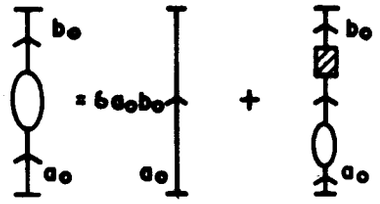

Fig. 2

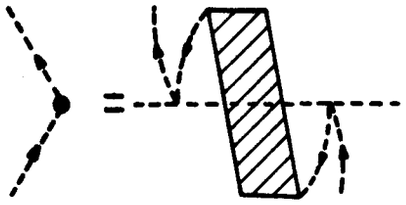

Fig. 3 – A dashed line means that it does not belong to the diagram whereas a full line does. The ends of the "boxes" are integrated to $\pm \infty$.

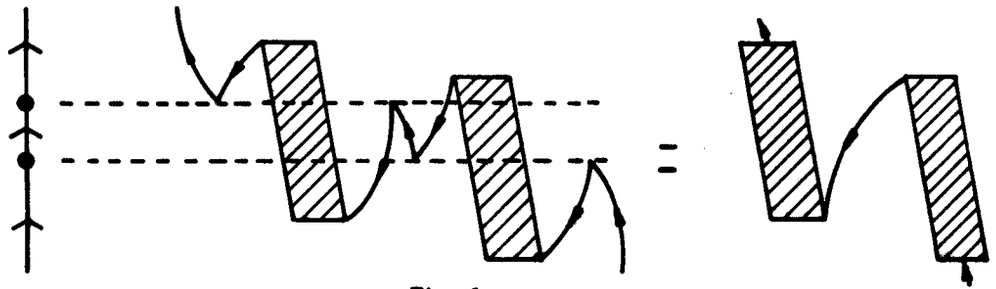

Fig. 4

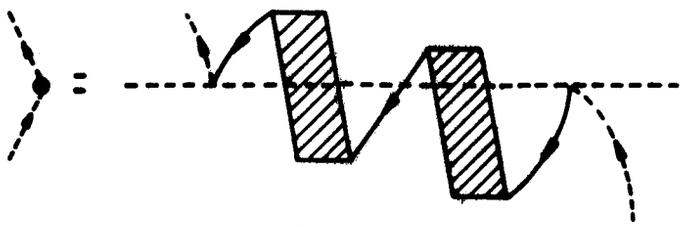

Fig. 5

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