Revista Brasileira de Física, Vol. 6, Nº 2, 1976

The Relationship between the Johnson-Baranger Time-Dependent Folded Diagram Expansion and the Time-Independent Methods of Perturbation Theory

EMERSON JOSÉ VELOSO DE PASSOS

Instituto de Física, Universidade de São Paulo, São Paulo SP*

Recebido em 15 de Março de 1976

We investigate the relationship between the Johnson-Baranger time-dependent folded diagram (JBFD) expansion, and the time independent methods of perturbation theory. In the nondegenerate case, we show that the JBFD expansion and the Rayleigh-Schrddinger perturbation expansion, for the ground state energy, are identical. On the other hand, we show, in the degenerate case, that, for the nonhermitian effective interaction considered in this paper, the JBFD expansion, of the effective interaction, is equal to the perturbative expansion of the effective interaction of the nonhermitian eigenvalue problem of Bloch and Brandow-Des Cloizeaux. For the two hermitian effective interactions, considered in this paper, the JBFD expansion of the effective interaction differs from the perturbation expansion of the effective interaction of the hermitian eigenvalue problem of Des Cloizeaux.

Neste trabalho, investigamos a conexão entre a expansão em "diagramas dobrados" de Johnson e Baranger (JBFD) e os métodos de teoria de perturbação independente do tempo. No caso não degenerado, mostramos que, a expansão de Rayleigh-Schrddinger e de JBFD são idênticas. No caso degenerado, mostramos que, para a interação efetiva não hermitiana, considerada neste trabalho, a expansão da interação efetiva em JBFD é idêntica à expansão da interação efetiva da equação de autovalores não hermitiana de Bloch e Brandow-Des Cloizeaux. Para as duas interações

* Postal address: C.P. 20516, 01000-São Paulo SP.

efetivas hermitianas, consideradas neste trabalho, a expansão da interação efetiva em JBFD difere da expansão da interação efetiva da equação de autovalores hermitiana de Des Cloizea[illegible]

1. INTRODUCTION

In degenerate and quasi-degenerate perturbation theory, the idea of an effective Hamiltonian is of great [illegible] ties of nuclei (see Ref. 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 brief outline of the work of Refs. 2, 3 and 4. Consider the Hamiltonian

$$H = H_0 + V, \qquad (1.1)$$

where H_0 is the unperturbed Hamiltonian, and V the perturbation. We suppose the eigenvalue problem for H_0 solved, therefore we know its eigenfunctions and eigenvalues. We decompose the full Hilbert space into a model space, Ω_0, and its complement which is a space orthogonal to Ω_0. The projection operators in the model space, and in the orthogonal space, are P_0 and Q_0, respectively. P_0 and Q_0 satisfy the usual relations

$$P_0 + Q_0 = 1, \quad P_0 Q_0 = Q_0 P_0 = 0, \quad P_0^2 = P_0, \quad Q_0^2 = Q_0$$

The eigenfunctions of H_0 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_0, we call it ε_0, is D-fold degenerate. The D degenerate eigenfunctions span the model space Ω_0, and the projection operator P_0 is equal to

$$P_0 = \sum_{a_0 \in \Omega_0} |a_0\rangle\langle a_0| \ . \tag{1.2}$$

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

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

These D eigenfunctions of H span a subspace, 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 Refs.2, 3 and 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_0:

$$(P_0 H_0 P_0 + \bar{H}_1)|\phi_{a_0}\rangle = E_a|\phi_{a_0}\rangle \tag{1.4}$$

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

$$(\varepsilon_0 P_0 + W^B - E_a)|\phi_{a_0}\rangle = 0, \tag{1.5}$$

where $|\phi_{a_0}\rangle$ is the projection of $|\psi\rangle$ on Ω_0 :

$$|\phi_{a_0}\rangle = P_0|\psi_a\rangle, \tag{1.6}$$

and W^B is the nonhermitian effective interaction, which is given by

$$W^{B} = P_0 VU \,, \tag{1.7}$$

and U is

$$U = P_0 + (Q_0/a)\ (VU - UVU),$$
$$UQ_0 = 0, \quad a = \varepsilon_0 - H_0 \,. \tag{1.8}$$

The equation of Brandow[4] and Des Cloizeaux[3] reads

$$(\varepsilon_0\ P_0 + W^{B-DC} - E_a)\,|\phi_{a_0}> = 0 \,, \tag{1.9}$$

where W^{B-DC} is given by

$$W^{B-DC} = \sum_{n=0} \frac{1}{n!}\ P_0\ \left(\frac{d^n}{d\varepsilon_0^n} K(\varepsilon_0)\right)\ \left(W^{B-DC}\right)^n \,, \tag{1.10}$$

$K(\varepsilon_0)$ being the reaction matrix[5]

$$K\ \varepsilon_0 = VP_0 + V(Q_0/a)K(\varepsilon_0) \ . \tag{1.11}$$

The perturbation expansion of (1.10) is given in Ref.3:

$$W^{B-DC} = \sum_{n=0}^{\infty} W_n \,, \tag{1.12}$$

where W_n is given *by*

$$W_n = \sum_{\mu_1,\ \mu_2 \ldots \mu_n} \{\mu_1, \mu_2, \ldots, \mu_n\}, \tag{1.13}$$

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

$$\{\mu_1, \mu_2, \ldots, \mu_n\} = \frac{1}{\mu_1 ! \mu_2 ! \ldots \mu_n !}\ P_0\ \frac{d^{\mu_1}}{d\varepsilon_0{}^{\mu_1}}\ K(\varepsilon_0)\ .\ \ P_0\ \frac{d^{\mu_2}}{d\varepsilon_0{}^{\mu_2}}\ \ K(\varepsilon_0) .\ \ldots$$
$$.\ P_0\ \frac{d^{\mu_n}}{d\varepsilon_0{}^{\mu_n}}\ \ K(\varepsilon_0)\ P_0 \ , \tag{1.14}$$

$\frac{d^{\mu}}{d\varepsilon_0} K(\varepsilon_0)$ denoting the μ^{th} derivative of the reaction matrix.

The μ's above are positive integers satisfying the relations

$$\mu_1 + \mu_2 + \ldots + \mu_n = n-1,$$

$$\mu_1 + \mu_2 + \ldots + \mu_p > p-1, \quad 1 \leq p < n. \tag{1.15}$$

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

In Refs. 3 and 6, it is shown that $W^{B-DC} = W^{B}$. Besides, the proof given in Ref.6 is based on Eqs. (1.7) and (1.8).

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

$$(B\varepsilon_0 + A - BE_\alpha) \mid \bar{\phi}_{\alpha_0} > = 0, \tag{1.16}$$

A and B being hermitian operators, and

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

The states $\{|\bar{\phi}_{\alpha_0}>\}$ are the stater biorthogonal to the states $\{|\phi_{\alpha_0}>\}$. The operator B is a positive definite operator[2,3,4] which transforrns the states $\{|\bar{\phi}_{\alpha_0}>\}$ into the states $\{|\phi_{\alpha_0}>\}$, namely,

$$B \, |\bar{\phi}_{\alpha_0}> = |\phi_{\alpha_0}> . \tag{1.18}$$

Considered as an operator acting in Ω_0, B has an inverse[2,3,4]:

$$|\bar{\phi}_{\alpha_0}> = B^{-1}|\phi_{\alpha_0}> . \tag{1.19}$$

üefining the square root operator, $B^{1/2}$, which is herrnitian and positive definite, Eq.(1.16) can be written as

$$(B^{-1/2}\ A\ B^{-1/2} - (E_{\alpha} - r,))|\hat{\phi}_{\alpha_0}> = 0, \tag{1.20}$$

where $|\hat{\phi}_{\alpha_0}> = B^{1/2}\ |\overline{\phi}_{\alpha_0}>$ are the so-called half-way bases states[3,4]. The operator

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

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

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 regarding the relationship between the Johnson-Baranger folded diagram expansion (JBFD), and the approaches of Refs.2, 3 and 4. In this paper, we analyze such a relationship.

In the case of nondegenerate perturbation theory, we compare the JBFD expansion with the Rayleigh-Schrödinger expansion[5].

For the degenerate perturbation theory, we compare the perturbation expansion of Bloch's nonhermitian effective interaction, Eq. (1.5), with 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 choiceç of the "box" time base : an average of the first and last times of each box, and a linear combination of the first and last times of each box.

2. 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

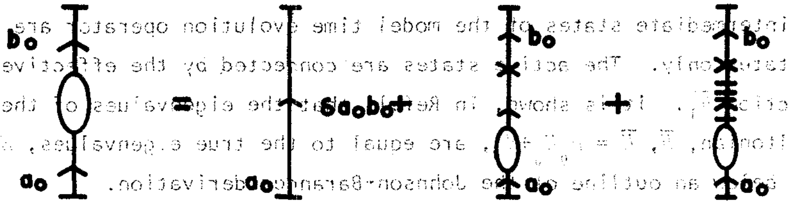

Fig.1 Matrix elements of the time evolution operator. The states $\{|a_0\rangle\}$ belong to the model space. The hatched and nonhatched lines represent the propagation of passive and nonpassive states, respectively.

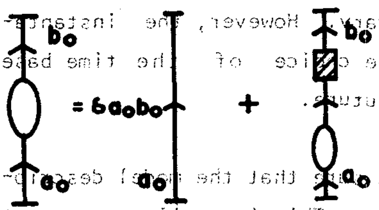

Fig.2 - Matrix elements of Fig.1 in terms of active states only.

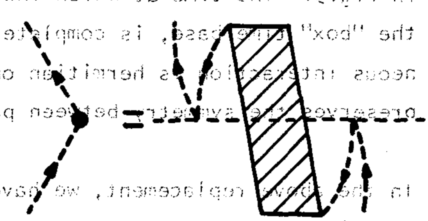

Fig.3 - A dashed line means that it does not belong to the diagram, whereas a full line does.

of the matrix elements of the time-evolution operator $T(+\infty,-\infty)$, between states in the model space, by a model time evolution operator $\overline{T}(+\infty,-\infty)$. The intermediate states of the model time evolution operator are active states only. The active states are connected by the effective interaction $\overline{H}_1$. It is shown, in Ref.I, that the eigenvalues of the model Hamiltonian, $\overline{H}$, $\overline{H} = P_0H_0+\overline{H}_1$, 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 elements 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 Fiy.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 the 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 has to be removed. To do so, we define an instantaneous interaction, the double box diagram shown in Fig.5. It is easily seen that, in general, we can have, in the model description, 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

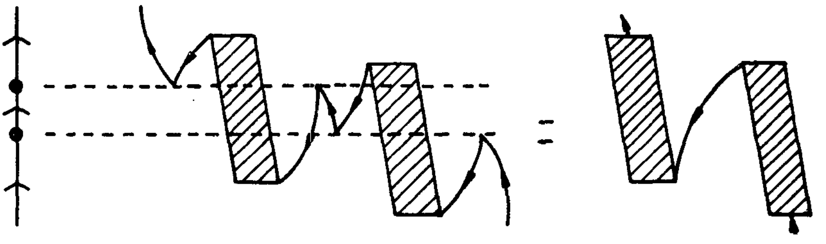

Fig.4 - A model diagram which does not occur in the full description.

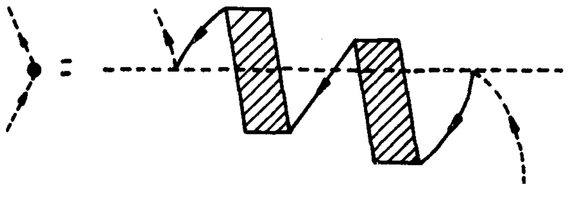

Fig. 5 - A double box diagram.

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

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

In the case of degenerate perturbation theory, the term having n overlapping "boxes" has a very simple expression for the specific choices of the "box" time base considered in this paper, which can easily be derived using the rules given in Ref.1. Doing so, $\overline{H}_{1_n}$ is seen to be equal to

$$\begin{aligned}\overline{H}_{1_n} = (-1)^{n+1}(-i)^{2n-1} \int_0^{\infty} dT_1 dT_3 \ldots dT_{2n-1}\ P_0 K(T_1) P_0 K(T_3) P_0 \ldots \\ \cdot P_0 K(T_{2n-1}) P_0 \ \exp\{i\varepsilon_0 (T_1 + T_3 + \ldots + T_{2n-1})\} \int_{\Gamma} dt_2 dt_4 \ldots dt_{2n-2}.\end{aligned} \tag{2.2}$$

The difference between 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.

(i) *Perturbation Expansion of the Effective Interaction in the Nonhermitian Case*

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

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

$$\overline{H}_1 = \{0\} + \{10\} + \{110\} + \{200\} + \ldots \tag{2.3}$$

The region of integration is given below, and again this is a straightforward application of the rules given in Ref.1 (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) $-T_1 < T_2 < 0$,

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

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 tp n=5.

Consider n overlapping boxes:

1) Draw all the overlapping boxes;

2) Consider all permutations of the relative order of the "boxes" time base (the last time of the "box") keeping the time base of the first "box" (froni 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 permutations leading to the same set of numbers $\mu_1, \mu_2, \ldots, \mu_n$. The sum of the contributions of all these diagrains, calculated according to the usual Feynman rules, is $\{\mu_1,\mu_2,\ldots,\mu_n\}$.

We have not analyzed the 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, $\bar{H}_{1_n}$ becomes

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

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

$$\mu_1+\mu_2+\ldots+\mu_n = n-1,$$
$$\mu_1+\mu_2+\ldots_p > p-1, \quad 1\leq p<n , \qquad (2.5)$$

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

(ii) Perturbation Expansion of the Effective Interaction in the Hermitian Case: the time base is the average of the first and Zast times of each box.

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 given by

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

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

2.3) a) $-(T_1+T_3)/2 < T_2 < 0$,
$-(T_3+T_5)/2 < T, < o$;

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.

(iii) Perturbation Expansion of the Effective Interaction in Hermitian Case: the time base as a linear combination of the first and Zast times of the "box".

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

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

The region of integration is as follows:

3.1) $T_1 > 0$, forthesingle-boxdiagram;

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 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 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 No.2 than for choice No.3. As an example, we note that we have, for the triple-box diagram, three possibilities in case No.2, and twenty four in case No.3. So, between the two hermitian prescriptions, the easiest to calculate is case No.2.

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

3. NONDEGENERATE PERTURBATION THEORY

In the case of nondegenerate perturbation theory, the model space has only one dimension, so the projection operator P_0 is, simply,

$$P_0 = |0\rangle\langle 0| .$$

The eigenvalue is given by

$$E_0 = \varepsilon_0 + \langle 0|\overline{H}_1|0\rangle . \tag{3.1}$$

In the nonhermitian case $\overline{H}_1$ is given by Eq. (4.1) of next Section.

For a single dimension, Eq. (4.1) reduces to

$$\langle 0|\overline{H}_1|0\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{d^n}{d\varepsilon_0^n} \langle 0|K(\varepsilon_0)|0\rangle\right) (\langle 0|\overline{H}_1|0\rangle)^n \tag{3.2}$$

Using (3.1) and (3.2), the energy E_0 is given by

$$\begin{aligned} \Delta E &= E_0 - \varepsilon_0 \\ &= \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{d^n}{d\varepsilon_0^n} \langle 0|K(\varepsilon_0)|0\rangle\right)(\Delta E)^n . \end{aligned} \tag{3.3}$$

Using a formula by Lagrange, given in Refs. 3 and 5, Eq. (3.3) reduces to

$$\Delta E = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{d^{n-1}}{d\varepsilon_0^{n-1}} (\langle 0|K(\varepsilon_0)|0\rangle)^n, \qquad (3.4)$$

which is equivalent to the Rayleigh-Schrödinger perturbation series[5].

In the hermitian case, $\bar{H}_1$ is given, up to the triple-box diagram, by Eqs. (2.7) and (2.8). In both cases, the expectation value of $\bar{H}_1$ is given by Eq. (3.2), to the order considered. So, to this order, they are equivalent to the Rayleigh-Schrödinger perturbation series. It is certainly plausible that the equality persists to higher orders.

4. DEGENERATE PERTURBATION THEORY: NONHERMITIAN 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 coincides with the perturbation expansion of W^{B-DC}, given by Eqs. (1.12), (1.13) and (1.15). Therefore,

$$\bar{H}_1 = \sum_{n=0}^{\infty} \frac{1}{n!} P_0 \left(\frac{d^n}{d\varepsilon_0^n} K(\varepsilon_0)\right) (\bar{H}_1)^n . \qquad (4.1)$$

So, when we choose 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 as well, since the last two do coincide[3,6].

The conclusion is, therefore, that the Johnson-Baranger folded diagram expansion is identical to the corresponding one by Brandow, for the effective interaction.

5. DEGENERATE PERTURBATION THEORY: HERMITIAN CASE

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

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

If we compare (5.1) to Eqs. (2.7) and (2.8), we see that they are all different. This tells us that W^{DC} does not coincide with 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, Eqs. (2.7), (2.8) and (5.1), are related by an unitary transformation in the model space R_o.

We did not attempt to find which symmetrical choice for the box time base gives rise to the Des Cloizeaux effective interaction. It is interesting to notice that when comparing the different hermitian prescriptions, we should consider at least the triple-box diagram, since the prescription, for making the double box diagram hermitian, is unique.

6. 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 coincides, 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 Des Cloizeaux's effective interaction differs from the JBFD expansion for the two symmetrical choices of the "box" time base made here.

The author wishes to thank Prof. M. Baranger for having suggested this research, and Drs. M.B. Johnson and C.P. Malta for a critical reading of the manuscript. Financial support from FAPESP and BNDE (Brazil) are gratefully acknowledged.

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