An Algorithm for Generating Goldstone and Bloch-Brandow Diagrams*

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An algorithm for the automatic generation of Goldstone and Bloch–Brandow diagrams, needed for diagrammatic perturbation expansions, is described (the Bloch–Brandow diagrams are required for degenerate perturbations). Diagrams are produced in sets, each set consisting of members related by exchanges about interaction lines. Only distinct connected diagrams are generated. Applications are described.

I. Introduction

The Brueckner–Goldstone [1] many-body perturbation theory, with perturbation corrections expressed in terms of Feynman-like diagrams [2], has found widespread application in many fields. It was first applied to atomic systems by Kelly [3] a decade ago, and has since been successfully used to calculate a variety of atomic and molecular properties. An extension of the method to systems having a degenerate or nearly degenerate unperturbed state was put forward by Bloch and Horowitz [4], and recast in a connected-diagram, energy-independent form by Brandow [5]. Similar methods have since been described [6], and the Brandow technique has recently been applied to molecular excited states [7].

The first step in implementing these methods is listing all topologically distinct connected diagrams. Their number rises rapidly with the order of the perturbation, and the process soon becomes tedious and error-prone. This happens, in our experience, when the number of diagrams of a given order considerably exceeds 10, usually in the fourth order for nondegenerate states (Goldstone diagrams) and already in the third order for degenerate states (Bloch–Brandow diagrams). It is desirable, therefore, to have an algorithm for the automatic generation of all needed diagrams, especially if investigation of an open-shell system is attempted. Such an algorithm is described in the present paper.

Paldus and Wong [8] have described a method for the automatic generation

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of all distinct linked Hugenholtz-type [9] vacuum and Green function diagrams. We prefer to generate the widely used Goldstone diagrams [2] and their generalization to degenerate systems, the Bloch–Brandow diagrams [4, 5]. A Hugenholtz diagram of order n is equivalent to up to 2^n Goldstone diagrams, obtainable from each other by exchanges about one or more interaction lines. We first generate these sets of diagrams, or "exchange sets" (Section II), and then list all distinct members. Only two-particle interactions are considered; a single-particle interaction may be incorporated, if needed, by replacing a "bubble" (a hole line that starts and ends on the same interaction line) by an appropriate one-electron operator. The Paldus and Wong [8] approach produces a smaller set of "essentially distinct" Hugenholtz diagrams, from which all Goldstone diagrams may be found; it also leads to a more efficient evaluation of the diagrams, based on the so-called "double projection" scheme [10]. An important advantage of our procedure, on the other hand, is the added capability of generating Bloch–Brandow diagrams with any desired number of incoming and outgoing lines, needed for handling open-shell systems. Any limitations on the allowed number of hole lines, particle lines and bubbles, dictated by the particular problem at hand, are easily applied.

The accepted definition of distinct diagram is adopted with one alteration. Two diagrams are considered distinct if not obtainable from each other by an allowed deformation, which is defined as (i) any deformation not changing the time-ordering of the interaction lines, or (ii) a reflection in a horizontal plane while keeping the direction of the fermion lines ("time reversal" or "Hermitian conjugation").

For convenience, the algorithm for generating the Goldstone diagrams is described first (Section II). The extension to Bloch–Brandow diagrams is shown in Section III, and applications are discussed in Section IV.

II. Goldstone Diagrams

A. Exchange Sets

The eight Goldstone diagrams in Fig. 1 are obtainable from one another by performing exchanges about one or more interaction lines. A set of all such diagrams will be named an exchange set. It corresponds to a single Hugenholtz diagram [8, 9]. The first part of the algorithm, described in this subsection, generates all these sets of distinct, connected diagrams.

An exchange set of Goldstone diagrams (or a single Hugenholtz diagram) is completely defined by specifying the number of hole and particle lines, and the ordinal number of interaction lines on which each fermion line starts and ends
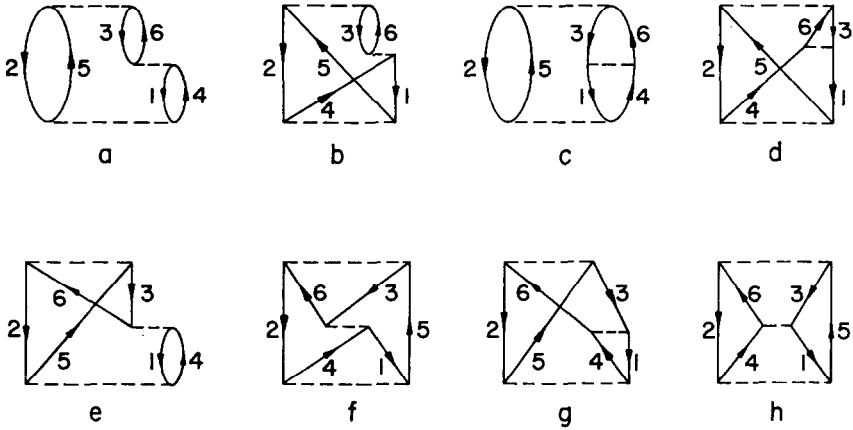
FIG. 1.   The "exchange set" of the third-order ring diagram. (b) and (e) are Hermitian conjugates of each other, as are (d) and (g). (h) is an "$\alpha\beta$-contributing" diagram.

(interaction lines are numbered from the bottom up). A vector K is defined so that the fermion line i starts on interaction line $K(2i-1)$ and ends on interaction $K(2i)$. Hole lines precede particle lines in the vector, and standard order, to be maintained within each group (hole or particle lines) is defined by

$$K(2i-1) \leqslant K(2i);\tag{1}$$

for $i < j$, $K(2i-1) \leqslant K(2j-1)$, and if

$$K(2i-1) = K(2j-1), \quad \text{then } K(2i) \leqslant K(2j).\tag{2}$$

Note that (1) means that a fermion line is considered to begin at the lower of the two interactions to which it is connected, regardless of its actual direction, and (2) determines the numbering of the fermion lines. The exchange set of Fig. 1 carries the K vector 121323121323.

A standard order of K vectors (or exchange sets) having the same number of hole and particle lines is also defined. The vector K_1 precedes K_2 if there is an i_m so that

$$K_1(i) = K_2(i), \quad \text{for all} \quad i < i_m,$$
$$K_1(i_m) < K_2(i_m).\tag{3}$$

Thus, Fig. 2(a), associated with the vector 121333121223, follows the diagram of Fig. 1 (here $i_m = 5$).

It is easy to list all vectors satisfying Eqs. (1) and (2), but many of them do not correspond to actual Goldstone diagrams, and some of the diagrams obtained

are redundant. The remaining part of this subsection describes a procedure for weeding out these spurious vectors. An important time-saving device in the algorithm is that vector elements are checked consecutively, and if a violation of some sort is discovered upon reaching the element $K(i)$, other vectors with the same i first elements need not be considered.
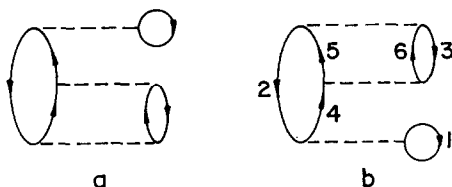

FIG. 2. Two diagrams related by Hermitian conjugation. (b) precedes (a) in standard order, and is the only one retained.

The validity test for a given vector consists of the following steps:

1. A particle line cannot start and end on the same interaction (there are no particle bubbles).

2. A hole line comes into interaction line $K(2i - 1)$ and goes out of interaction $K(2i)$, while the reverse holds for a particle line. Each interaction line must then have two incoming and two outgoing fermion lines.

3. The Hermitian conjugate (or time-reverse) of a diagram is obtained by turning it upside down but keeping line directions (see Fig. 2). A diagram preceded in standard order by its Hermitian conjugate is discarded. This check is used also to set a flag for Hermitian diagrams.

4. The number of hole lines and the number of particle lines found between two consecutive interactions must be equal.

5. The vectors surviving steps 1–4 correspond to sets of distinct diagrams; some of these may however be disconnected (i.e., consist of two or more parts connected by neither fermion nor interaction lines). The loop structure of one Goldstone diagram belonging to the set has to be elucidated to determine connectedness; it will also be needed later (Section IIC). A loop consists of all fermion lines that may be traversed without going along an interaction line. Thus, Fig. 2(b) consists of three loops, viz. (1), (2, 4, 5), (3, 6).

The following procedure is used for loop construction: (i) Start with a hole line that goes from interaction i to interaction j. If $i = j$, the loop is closed. If not, then (ii) look for a line that closes the loop, i.e., a particle line going between the same interactions. If such a line is found, the next hole line is taken in step (i).

If not, then (iii) look for a line that starts or ends on interaction i or j. The existence of such a line is guaranteed by step 4 above. If, say, a particle line is found going from interaction i to i', it is added to the loop and we go back to (ii) with i' substituted for i (and with a hole line looked for if $i' > j$). The procedure ends when all lines have been assigned to loops. As an example, consider the set represented by Fig. 2(b) and associated with the K-vector 111323122323. Line 1 forms a loop by itself. Line 2 is then taken; since no particle line with K elements 13 can be found, line 4 with K elements 12 is added to the loop, and a search for a particle line with K elements 23 produces line 5. Finally, the loop started with line 3 is completed by line 6. It should be noted that a particular member of an exchange set is singled out at this stage. The procedure followed tends to produce the diagram with the largest number of loops, to be referred to as the direct Goldstone diagram.

The connectedness of the diagram is now easily tested. Two loops are connected if they include lines starting or ending on a common interaction. A string of connected loops may be constructed by checking this property, and if the string comprises all loops the diagram is connected.

B. Generating all Goldstone Diagrams

The procedure described above produces a list of all distinct, connected exchange sets or Hugenholtz diagrams. In this subsection, a method for expanding this list to obtain all distinct, connected Goldstone diagrams is given.

Not all 2^n Goldstone diagrams included in an exchange set of order n need be distinct. Thus, Fig. 3 shows eight diagrams obtainable from one another by exchanges; however, 3(a), (d), (f) and (g) are identical, and so are 3(b), (c), (e)
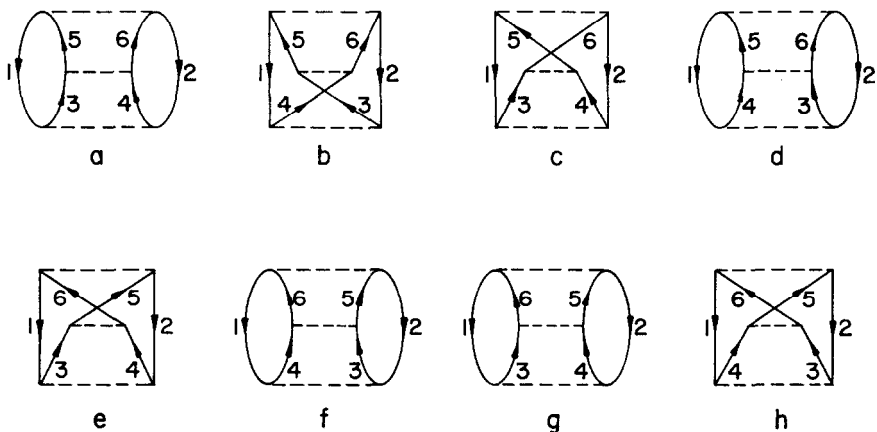

FIG. 3. The "exchange-set" of the third-order p–p ladder. (a), (d), (f), and (g) are identical, as are the other four.

and (h), so that only two distinct diagrams remain. Another case is that of the third-order ring diagram (Fig. 1), where 1(b) and (e) are related by Hermitian conjugation, as are 1(d) and (g). The following convention for numbering the individual members of an exchange set is adopted, greatly facilitating the elimination of redundant diagrams: Each member is given the ordinal number $\sum_i 2^{i-1}$, where the summation goes over interaction lines about which exchanges with respect to the direct diagrams have to be taken to get this member. Thus, the diagrams in Fig. 1 and 3 carry the numbers 0 to 7 in consecutive order.

The procedure for eliminating the redundant set members consists of two steps:

1. If the set is Hermitian (with a flag set in Section IIA, step 3) the Hermitian conjugate of each member belongs also to the set. For each interaction i about which an exchange has taken place to produce a particular member from the direct diagram, the conjugate will have an exchange about interaction $n + 1 - i$, n being the order. The ordinal number of the conjugate is thus found, and a member preceded by its conjugate is discarded. As an example, Fig. 3(g) has exchanges about interactions 2 and 3, and its ordinal number is 6. Its exchange will have exchanges about interactions 1 and 2 and the ordinal number 3 (Fig. 3(d)). Therefore, 3(g) is discarded.

2. Two fermion lines starting on the same interaction, ending on the same interaction, and going in the same direction are called equivalent lines (e.g., lines 1 and 2, 3 and 4, 5 and 6 in Fig. 3). Performing exchanges about two interaction lines connected by a pair of equivalent lines leaves the diagram invariant (see, e.g., Fig. 3(a) and 3(d)). All members of the exchange set fall into classes, each of which consists of diagrams connected by such spurious exchanges, and only one diagram of each class is retained (e.g., only diagrams (a) and (b) of Fig. 3). The partitioning of diagrams into classes is easy, noting that carrying out an exchange about interaction i will change the ith bit of the ordinal number of the diagram from 0 to 1, or vice versa.

C. $\alpha\beta$-contributing Diagrams

Considerable computational savings may be realized during the actual calculation of the perturbation corrections if several members of an exchange set are summed simultaneously. This may be done by interpreting some or all interaction lines of the direct diagram as direct–minus-exchange integrals. If diagrams are summed over spinorbitals (this is particularly convenient for open-shell systems), a diagram will vanish unless all lines in a loop are associated with the same spin. Starting with the direct diagram of Fig. 1(a), ignoring spinorbital combinations for which it vanishes, and taking the direct-minus-exchange integral for all interactions (the exchange integral vanishes, of course, if two ends of the interaction have different spins), diagrams 1(a)–1(h) are computed together. The

only contribution not included is Fig. 1(h) when lines 1, 3, and 5 are associated with spin α and lines 2, 4, and 6 with β (or vice versa). Such a member of an exchange set, which does not necessarily vanish even though its parent direct diagram does, will be labeled "$\alpha\beta$-contributing". It must be identified for the computational savings discussed above to be realized. For this purpose, the loop structure of all set members is analized. If all the lines in a loop of diagram A belong to the same loop of diagram B, and this holds for all loops of A, then B is said to be "included" in A. A diagram (besides the direct one) not included in any of the other members is $\alpha\beta$-contributing. It is easily seen that diagrams 1(b)–1(g) are included in 1(a), but 1(h) is not.

III. Bloch–Brandow Diagrams

The algorithm described above for the generation of Goldstone diagrams is applied with certain modifications to Bloch—Brandow diagrams [4, 5, 7], needed to obtain perturbation corrections if the unperturbed state of interest is degenerate or nearly degenerate. The use of these diagrams has been described in detail [5] and will not be discussed here. The feature distinguishing them from Goldstone diagrams is the existence of an equal number of incoming and outgoing lines, called valence lines. The number of incoming (or outgoing) lines may go up to the number of fermions outside closed shells in the state investigated.

It is convenient to regard a pair of valence lines, one incoming and one outgoing, as a single line during the first stages of the generation procedure. A similar practice has been suggested by Brandow [5] to determine the overall sign of the diagram and its denominators. Two examples are shown in Fig. 4. With this convention, steps 1–3 of Section IIA are followed, the only modification being that three line types (valence, core and particle) are now recognized. The next step is:

4.   Valence lines are assigned as core-like or particle-like so that the number of core and core-like lines between two consecutive interactions is made equal to the number of particle and particle-like lines. Thus, line 1 in Fig. 4(a) is core-like, while line 1 in 4(c) is particle-like. If this balance cannot be obtained, the vector K does not correspond to a legitimate diagram and is discarded. Any valence line remaining unassigned after balance is achieved must start and end on the same interaction (see line 2 in Fig. 4(a) and 4(c)) or the vector is discarded. Such a line is arbitrarily assigned as particle-like for purposes of step 6 below.

5.   Connectedness is tested as in step 5 of Section IIA. A diagram with several pairs of valence lines may be connected when each pair is regarded as a single line (Fig. 5(a)) but disconnected when pairs are separated (Fig. 5(b)). Pair separation takes place, therefore, before this test is applied.
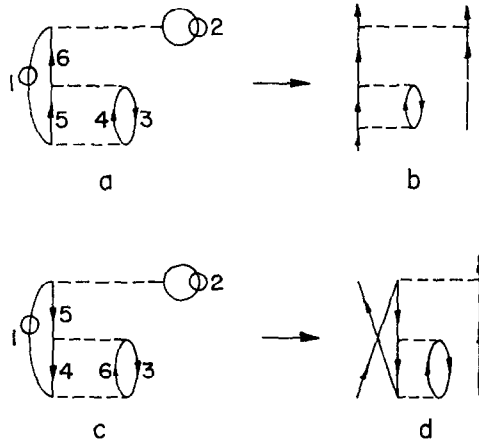
FIG. 4. Bloch–Brandow diagrams. Pairs of valence lines are considered single lines (denoted by small open circles) in (a) and (c), and separated in (b) and (d). Line 1 is core-like in (a), particle-like in (c).

6. An additional complication peculiar to diagrams with several valence-line pairs is that two different diagrams (5(c), (d)) might yield the same diagram upon pair separation (Fig. 5(e)). This redundancy is avoided by requiring each pair of valence-like pairs i and j, with $i < j$, to satisfy the following condition: If i and j are both particle-like or both core-like, then $K(2i - 1) \leqslant K(2j - 1)$, and
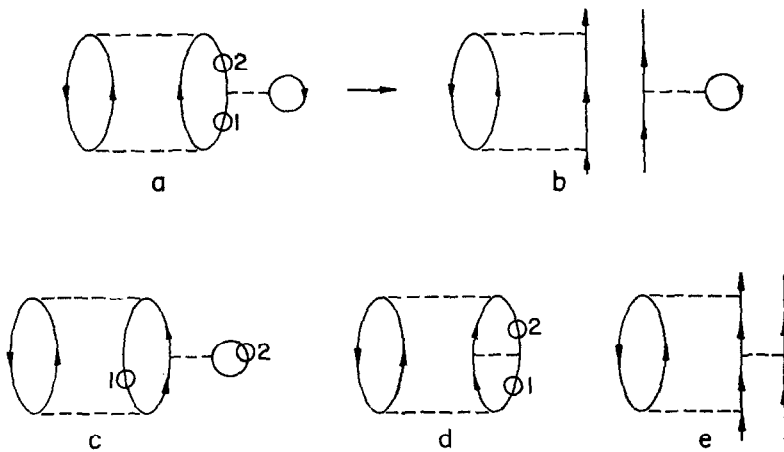

FIG. 5. Complications occurring in Bloch–Brandow diagrams with several valence line pairs. 1. The connected diagram (a) turns disconnected (b) upon pair separation. 2. Two distinct diagrams (c) and (d), yield the same diagram (e).

$K(2i) \leqslant K(2j)$; if one is core-like and the other particle-like, then $K(2i - 1) \leqslant K(2j)$, and $K(2i) \leqslant K(2j - 1)$. The K elements for the valence lines of Fig. 5(c) and 5(d) are 1322 and 1223, respectively, and only 5(d) satisfies this condition.

Up to this stage, exchange sets have been generated. The procedure for generating all Bloch–Brandow diagrams is similar to that described in Section IIB, and is applied after valence-line separation. The definition of equivalent lines is generalized to include two valence lines that start (or end) on the same interaction and go in the same direction, such as the two outgoing lines in Fig. 4(b) or the two incoming lines in 4(d). An exchange about an interaction attached to two equivalent valence lines (the uppermost interaction in Fig. 4(b) or 4(d)) therefore, is spurious, which is taken into account in step 2 of Section IIB. The testing for $\alpha\beta$-contributing diagrams is done as in Section IIC.

Finally, it should be mentioned that so-called "folded" diagrams are required in the Brandow formalism [5]. Their generation from the regular diagram is straight-forward [5, 7] and will not be discussed here.

IV. APPLICATIONS

A computer program implementing the algorithm described above has been written. It is capable of generating diagrams up to 5th order (inclusive), with a desired number of core, particle, and valence lines and bubbles. The number of

TABLE I

Numbers of distinct connected diagrams

Order	Exchange sets	All diagrams	$\alpha\beta$-contributing	Run time (CDC6600 sec)
Goldstone diagrams without bubbles				
1–3	4	12	1	0.25
4	31	222	20	4
5	422	6668	611	180
Goldstone diagrams with bubbles				
1–3	14	60	1	0.7
4	132	1348	45	20
Bloch–Brandow, 1–2 valence line pairs, no bubbles				
1–3	41	148	22	2
4	442	4016	581	73
Bloch–Brandow, 3–4 valence line pairs, no bubbles				
1–3	27	63	20	2
4	446	2806	1004	146

diagrams and run times for several cases are shown in Table I. No major changes are required to generate diagrams of higher orders, but computer times become prohibitive. More important, the cost of actually calculating the diagrams is several orders of magnitude higher than that of generating them, so that the program is more than adequate for present needs.

The diagram generation program for the CDC6600 computer will be made available through the Quantum Chemistry Program Exchange, University of Indiana.

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