

A PASCAL-TYPE TRIANGLE FOR THE NUMBER OF TOPOLOGICALLY DISTINCT MANY-ELECTRON FEYNMAN GRAPHS

F. BATTAGLIA* and T.F. GEORGE

*Departments of Chemistry and Physics and Astronomy, 239 Fronczak Hall,
State University of New York at Buffalo, Buffalo, New York 14260, USA*

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Abstract

By expressing the Green function for a many-body system in terms of a perturbative expansion written as a sum over all connected and topologically distinct Feynman graphs, it is shown that the number of such diagrams can be iteratively obtained from a Pascal-type triangle. The key to the problem is to notice that it is possible to define on the set of graphs an equivalence relation, and that, from a well-known theorem of set theory, an equivalence relation on a set partitions it into disjoint classes.

Second quantization is the quantum theory technique that correctly describes a system of many particles whose total number is not conserved. Even if the number of particles in a many-body system is a constant of the motion, the technique turns out to be very useful because their statistics are taken into account without the need for symmetrizing or antisymmetrizing products of single-particle wave functions. Only a few cases can be solved exactly with a second-quantized Hamiltonian [1]. In general, one must resort to approximate methods in which part of the Hamiltonian is considered exactly soluble and the remainder is treated as a perturbation. In many-particle physics, the perturbative expansion becomes quite cumbersome, but can be written in an elegant and concise form using the language of Feynman diagrams [2]. The main utility of such diagrams lies in the fact that one can represent graphically various terms in a particular series expansion, give a physical interpretation to them, and easily perform sums of an infinite class of perturbation terms. In fact, in many-body theory the interaction between particles is not necessarily weak, so that a perturbation theory in which one considers only the first term, or even the first few terms, will not give satisfactory results.

*Permanent address: Dipartimento di Chimica, Università delle Basilicata, 85100 Potenza, Italy.

In the treatment of many-particle systems, a fundamental role is played by the Green function, defined as [3]

$$iG_{\alpha\beta}(z, y) = \langle \Psi | T[\psi_{\alpha}(z)\psi_{\beta}^{\dagger}(y)] | \Psi \rangle, \quad (1)$$

where $|\Psi\rangle$ is the exact Heisenberg normalized ground state. This function contains observable properties of great interest, for from it one can compute expectation values of any single-particle operator in the ground state of the system and the ground-state energy of the total Hamiltonian H . The construction of the Green function for a non-trivial physical system is, however, a formidable task, and the usual approach is to use perturbation techniques.

The perturbative approach splits the Hamiltonian into two parts,

$$H = H_0(t) + H_I(t), \quad (2)$$

where the problem for H_0 is assumed to be already solved. Perturbative techniques are most conveniently applied in the interaction picture (herein denoted by a tilde) in which the displacement operator satisfies the integral equation

$$\tilde{U}(t, t_0) = T \exp \left[-i \int_t^{t_0} dt' \tilde{H}_I(t') \right], \quad (3)$$

where T is the time-ordering operator.

For a two-body interaction $V(\mathbf{x}_1, \mathbf{x}_2)$, such as the mutual Coulombic repulsion among the electrons in a molecule, eq. (1) becomes

$$iG_{\alpha\beta}(z, y) = [\langle 0 | S | 0 \rangle]^{-1} \left\{ iG_{\alpha\beta}^0(z, y) + \frac{(-i)^2}{2!} \sum_{\substack{\lambda\lambda' \\ \mu\mu'}} d^4x_1 d^4x_2 V_{\lambda\lambda'\mu\mu'}(x_1, x_2) \right. \\ \left. \times \langle 0 | T[\tilde{\psi}_{\lambda}^{\dagger}(x_1)\tilde{\psi}_{\mu}^{\dagger}(x_2)\tilde{\psi}_{\mu'}(x_2)\tilde{\psi}_{\lambda'}(x_1)\tilde{\psi}_{\alpha}(z)\tilde{\psi}_{\beta}^{\dagger}(y)] | 0 \rangle + \dots \right\}, \quad (4)$$

where we have defined

$$S \equiv \tilde{U}(+\infty, -\infty) \quad (5)$$

and

$$V(x_1, x_2) = \delta(t_1 - t_2)V(\mathbf{x}_1, \mathbf{x}_2). \quad (6)$$

We then see that, in order to compute the n th-order contribution to $G_{\alpha\beta}(z, y)$, we must find the expectation value in the unperturbed ground state $|0\rangle$ of the time-ordered product of $4n + 2$ ladder operators of the form

$$\langle 0 | T [\underbrace{\tilde{\psi}^\dagger \dots \tilde{\psi}}_{4n} \tilde{\psi}_\alpha(z) \tilde{\psi}_\beta^\dagger(y)] | 0 \rangle . \tag{7}$$

To compute those kinds of terms, we make use of Wick’s theorem [4], according to which, if we define the contraction between two operators A and B as

$$AB = T(AB) - N(AB),$$

then

$$T(ABC\dots XYZ) = N(ABC\dots XYZ) + N \left[\sum \text{all possible pairs of contractions} \right], \tag{8}$$

where N is the normal ordering operator which arranges the product AB so that the creation operator is on the left and the destruction operator on the right. Clearly, given that in eq. (4) we compute *vacuum* expectation values, terms of the type (7) become

$$\langle 0 | T [\tilde{\psi}^\dagger \dots \tilde{\psi} \tilde{\psi}_\alpha(z) \tilde{\psi}_\beta^\dagger(y)] | 0 \rangle = \sum \text{all fully contracted terms} . \tag{9}$$

Each contraction gives a Green function, so for the n th order there are $2n + 1$ Green functions and n interactions integrated over all internal coordinates. Therefore, there are $(2n + 1)!$ terms in the sum.

It is possible to give a pictorial representation for these terms by generating what are better known as Feynman diagrams. Such diagrams are constructed by means of the following correspondence: (i) a dot for each coordinate which is integrated over; (ii) a wavy line between two dots for each corresponding interaction; (iii) an oriented segment for each free Green function. It is possible to show that, in the numerator of eq. (4), the vacuum polarization graphs can be factorized out and cancel exactly, at any order, with the denominator $\langle 0 | S | 0 \rangle$, so that only the connected diagrams contribute to the Green function [5]. Among the connected diagrams, the topologically equivalent ones give the same numerical value, so that in order to write the Green function to any given order, one must follow a set of rules. The first of these rules is: write all topologically distinct connected Feynman diagrams. Other rules give a prescription of how to associate with each geometrical element of a diagram a unique analytic expression. Equation (4) then becomes

$$iG_{\alpha\beta}(z, y) = \sum_{n=0}^{\infty} (-2i)^n \int_{-\infty}^{\infty} dt_n \langle 0 | T [\tilde{V}(t_1) \dots \tilde{V}(t_n) \tilde{\psi}_\alpha(z) \tilde{\psi}_\beta^\dagger(y)] | 0 \rangle', \tag{10}$$

where the prime stands for "connected and topologically distinct".

We are now in a position to present a rule for the total number of topologically distinct diagrams that can be drawn for a system of many identical fermions interacting via a two-body potential [6]. Let $\bar{N}(n)$, $\bar{C}(n)$ and $\bar{D}(n)$ be, respectively, the sets of n th-order diagrams, connected diagrams, and disconnected diagrams, and let $N(n)$, $C(n)$ and $D(n)$ be the number of diagrams in those sets:

$$\bar{N}(n) = \bar{C}(n) \cup \bar{D}(n), \tag{11}$$

$$N(n) = C(n) + D(n). \tag{12}$$

In order to find $C(n)$, we recognize that it is possible to define in $\bar{N}(n)$ a partition into disjoint classes. Such a partition is performed by means of the following relation R_p defined in $\bar{N}(n)$: two n th-order diagrams belonging to $\bar{N}(n)$ belong to the relation R_p if and only if p is the total number of interactions appearing in the connected part of the diagram which contains $\psi_\alpha(z)$ and $\psi_\beta^\dagger(y)$. It is straightforward to realize that R_p is an equivalence relation (i.e. it is reflexive, symmetric, and transitive) and therefore defines in $\bar{N}(n)$ a partition into disjoint classes. Obviously, $0 \leq p \leq n$, so that in $\bar{N}(n)$ there are $n + 1$ classes. Indicating by $d_p(n)$ the number of n th-order terms belonging to the class p , we can write

$$d_n(n) = C(n) = N(n) - \sum_{p=0}^{n-1} d_p(n). \tag{13}$$

Denoting a free Green function by a set of parentheses $(,)$, each of which contains a pair of 4-space coordinates, we can write a generic term of order n belonging to the class p as

$$\underbrace{(x,) (,) \dots (,) (, y) (,) \dots (,)}_{2p + 1} \underbrace{}_{2(n - p)}$$

and

$$\begin{aligned} d_p(n) &= (\text{number of terms of order } p \text{ belonging to class } p) \\ &\times (\text{number of permutations of } 2(n - p) \text{ internal coordinates}) \\ &\times (\text{number of ways of connecting } n \text{ interactions in groups of } p) \\ &= C(p) [2(n - p)]! \binom{n}{p} \\ &= \left[(2p + 1)! - \sum_{k=0}^{p-1} d_k(p) \right] [2(n - p)]! \binom{n}{p}, \end{aligned} \tag{14}$$

$$C(n) = (2n + 1)! - \sum_{p=0}^{n-1} \left\{ [2(n-p)]! \binom{n}{p} \left[2p + 1! - \sum_{k=0}^{p-1} d_k(p) \right] \right\}. \tag{15}$$

We note that eq. (14) gives the number of disconnected diagrams of order n and class p in terms of the number of disconnected diagrams of lower order, provided $p < n$. For $p = n$, the equation simply says that $d_n(n) = C(n)$ is given by subtracting the total number of disconnected diagrams from the total number of diagrams. For this reason, we give both eqs. (14) and (15), where the latter gives $C(n)$ in terms of $d_k(p)$ with $p < n$. In order to obtain topologically distinct diagrams, we note that: (i) the number of permutations of n interactions is $n!$, and (ii) the number of ways the coordinates in each interaction can be interchanged is given by $\sum_{k=0}^n \binom{n}{k} = 2^n$. The number of topologically distinct Feynman graphs for a many-fermion system interacting via a two-body potential is thus

$$F(n) = C(n)/n! 2^n, \tag{16}$$

which is tabulated in table 1 for values of n up to 7.

Table 1
Number of topologically distinct Feynman graphs up to 7th order

n	0	1	2	3	4	5	6	7
$F(n)$	1	2	10	74	706	8 162	110 410	1 708 394

It is interesting to observe that in order to obtain the number $C(n)$ of connected diagrams at a given order n according to eq. (13), one could construct a Pascal-type triangle. More than being a mere curiosity, this is very helpful in the numerical evaluation of $C(n)$, which can be somewhat troublesome due to the abundance of factorials appearing in eqs. (14) and (15). $C(n)$ can instead be directly read along the diagonal of the triangle, which is constructed, row by row, by making a direct product of three numerical triangles and by following rules that are obviously obtained from a glance at table 2, where the triangle is shown up to $n = 4$.

From table 1, we see that the number of topologically distinct diagrams grows rapidly, and it has been shown [7] that $F(n)$ grows asymptotically as $(2n + 1)!!$. One could therefore question the practicality of taking the approach of computing the perturbation expansion terms up to a given order n , even for a small value of n . The answer to this question depends on the specific problem one is dealing with.

Table 2

Pascal-type triangle for the number of connected Feynman graphs. $C(p)$ is obtained by subtracting from $(2p+1)!$ the sum of the first p terms of the $n=p$ row

n	p	0	1	2	3	4
0		1				
1		$2! \binom{1}{0}$	$C(1)$			
2		$4! \binom{2}{0}$	$C(1)2! \binom{2}{1}$	$C(2)$		
3		$6! \binom{3}{0}$	$C(1)4! \binom{3}{1}$	$C(2)2! \binom{3}{2}$	$C(3)$	
4		$8! \binom{4}{0}$	$C(1)6! \binom{4}{1}$	$C(2)4! \binom{4}{2}$	$C(3)2! \binom{4}{3}$	$C(4)$
.	
.	
.	

It could happen that, under certain physical conditions to be specified case by case, the perturbation series converges quickly, so that one might still want to compute all the terms in the perturbation expansion until convergence is achieved. In such a situation, even though those terms might seem to be large in number, the problem is usually still within the capabilities of the computing facilities currently available. For example, we have successfully applied such an approach to model a charge-transfer process in ion-surface scattering [8,9]. Here, the utility of a general formula for the number of topologically distinct diagrams involved in the description of the process was shown, and the conditions under which the perturbation expansion converges quickly were given.

However, it might also happen that one has to face the difficulties of an extremely poor convergence of the perturbation series. In such a case, the diagrammatic approach is, in general, totally different: one looks for suitable classifications of the various terms and retains only the most important classes. Even in this situation, one must usually deal with a new diagrammatic expansion in which each diagram might represent an infinite number of diagrams in the original expression [eq. (10)], where the problem of counting diagrams might still arise. Hence, the approach suggested by us would again be helpful.

In conclusion, our aim in this paper has been to point out to the chemistry community a general approach that might be taken whenever one is interested in counting diagrams, regardless of whether they arise from the perturbation expansion of the Schrödinger equation or from the virial expression for real gases, or from any

other problem treated by iterative techniques. The common rule is to first find the appropriate equivalence relationship on the set of diagrams at hand. We have shown that our method, applied to a many-electron system, yields the same results as given by other methods, such as functional derivative ones [7]. Finally, the possibility of building up a Pascal-type triangle allows an easy listing of the number of diagrams in each of the classes generated by the equivalence relationship, and an easy way of numerically generating $F(n)$.

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