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A Formula Related to Irreducible Diagram Expansions

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A formula is presented which can be regarded as the analytic basis for irreducible diagram expansions. It expresses the off-diagonal elements of the inverse of a matrix of operators by the off-diagonal elements and by diagonal elements of various inverses of the original operator. The formula can be obtained by purely analytic means without reference to statistical considerations. No infinite processes are involved if one deals with a finite matrix of operators.

KEY WORDS: Kraichnan's model equation; stochastic systems; irreducible diagrams.

In an internal report[1] written a few years ago, some equations occurring in a paper by Kraichnan[2] were rederived. Basic is one algebraic relation which possesses an essential property of irreducible diagrams. This note is written to emphasize its significance. Recently, the derivation of diagram expansions has been reexamined by Lee.[3] In his abstract, he expresses the hope that his paper will give some insight into the analytic structure of irreducible diagram

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expansions. In my opinion, this insight has already been provided by the relation mentioned above. The formula refers to operators arising from larger operators by partitioning. It is just one step away from irreducible diagram expansions as they usually appear; yet it has been derived without reference to the statistical nature of the problem and without the use of perturbations or series expansions. If the operator in question is partitioned into a finite number of suboperators, then the relation contains only a finite number of terms. The mathematical nature of such expansions can therefore be explored without reference to the physical context. This point which I regard as conceptually important cannot be recognized in Lee's treatment, for he uses mathematical and physical arguments in combination.

Diagrams are used to symbolize a sequence of operations by means of vertices to which a subscript is assigned and lines connecting the vertices. The subscripts serve to identify the operators involved. In irreducible diagrams, no repetition of subscripts is admitted. This is the property which is reproduced in the basic formula mentioned above. Whether this formula and its derivation reveal the analytic structure of diagram expansions is a moot question; it is, of course, conceivable that the derivation can be simplified, so that the logical lines are displayed more clearly. The injection of physical arguments may help the intuitive side, but if it is used as a substitute for a mathematical argument, then it is likely to break the line of thought. The present note defines the notation and shows the basic formula; moreover, it applies this formula to some simple examples where the operators are matrices, in order to illustrate the meaning of different terms. For the derivation and the physical application, reference is made to the original report.

Let B be an operator and ψ and f elements of some function space. Usually an element of this function space consists of M functions defined in the $\mathbf{x},t$ space, where $\mathbf{x}$ is the local vector and t the time. The number M is very large; in the applications, it is taken to be infinite; in this note, we take M to be finite. It is natural to consider the individual functions as components of the "vectors" ψ and f. One might also say that one has carried out a partitioning of the elements ψ and f of the function space. This partitioning induces a partitioning in the matrix B. In practice B appears directly in the partitioned form; that is, B appears as a matrix of operators. Then one has

$$B = \left(\begin{array}{cc|cc|cc} B_{1,1} & B_{1,2} & B_{1,3} & \cdots & B_{1,M-1} & B_{1,M} \\ B_{2,1} & B_{2,2} & B_{2,3} & \cdots & B_{2,M-1} & B_{2,M} \\ \hline \vdots & & & & & \\ B_{M,1} & B_{M,2} & B_{M,3} & \cdots & B_{M,M-1} & B_{M,M} \end{array}\right)$$

$$\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ --- \\ \psi_3 \\ \vdots \\ --- \\ \psi_{M-1} \\ \psi_M \end{bmatrix}, \qquad f = \begin{bmatrix} f_1 \\ f_2 \\ --- \\ f_3 \\ \vdots \\ --- \\ f_{M-1} \\ f_M \end{bmatrix}$$

One might also combine the components of ψ and f in pairs or triplets and partition the original matrix B accordingly. A partitioning in pairs is indicated by the dashed lines. One of the operators obtained by the partitioning then consists of four operators of the original form. One wants to solve the problem

$$B\psi = f$$

In Kraichnan's work, the diagonal operators are usually differential operators, for instance, they may be given by $\partial/\partial t + \nabla^2$, the off-diagonal operators may also be differential operators, but usually only with respect to the space coordinates. In simpler cases, the operation performed by the off-diagonal elements is multiplication of the function to which the operator is applied by a given function. Usually the statistical nature of the problem is introduced by the off-diagonal elements. However, statistically considerations play a role only after the matrix inversion has been carried out; they are of no concern in the present note. The operators (or matrices of operators) which arise by the partitioning are numbered in the same manner as one numbers matrix elements. Thus the four operators which are combined in the coarser partitioning by the dashed lines as shown above, taken together would be denoted by $B_{1,1}$, $B_{1,2}$, etc., and a corresponding notation would be applied to ψ and f. The diagonal elements of the partitioned matrix B are given by a square matrix of operators. From now on, we consider B as given and assume that a certain partitioning has been carried out which divides ψ and f into M and B into M^2 elements.

Let $B^{-1} = C$ and let C be partitioned in the same manner as B. The relation which we shall quote connects the off-diagonal elements of B with the off-diagonal elements of C. For this purpose, the diagonal elements of C and of a number of other auxiliary inverses of B are needed. The introduction of these auxiliary inverses is the device by which one can establish the crucial relation for cases where M is finite.

In defining these inverses, we replace systematically rows and the corresponding columns of B by zeros. This is accomplished in the following manner: Let E be the identity operator belonging to B and let E_α be the identity operator belonging to the αth diagonal operator of the partitioned operator B. Let D^{α} be an operator partitioned in the same manner as B and C; D^{α} is defined by

$$D^{\alpha}_{k_1 k_2} = 0, \quad k_1 \neq \alpha \quad \text{or} \quad k_2 \neq \alpha; \qquad \text{and} \qquad D^{\alpha}_{\alpha,\alpha} = E_{\alpha}$$

One has, of course, $D^{\alpha}D^{\alpha} = D^{\alpha}$; $D^{\alpha}D^{\beta} = 0$, $\alpha \neq \beta$; $D^{\alpha}(E - D^{\alpha}) = 0$. A matrix which arises from B by replacing rows and columns with subscripts $\alpha_1 \cdots \alpha_n$, $n < M$ by zero, is then given by

$$B^{\alpha_1,\alpha_2,\cdots,\alpha_n} = (E - D^{\alpha_1}) \cdots (E - D^{\alpha_n})\, B(E - D^{\alpha_n}) \cdots (E - D^{\alpha_1})$$

The sequence of the operators with which B is premultiplied and postmultiplied is unessential. We define an inverse $C^{\alpha_1\cdots\alpha_n}$ of $B^{\alpha_1\cdots\alpha_n}$ as a matrix of operators which has zeros in the rows and columns with subscripts $\alpha_1 \cdots \alpha_n$ and which satisfies

$$C^{\alpha_1\cdots\alpha_n} B^{\alpha_1\cdots\alpha_n} = (E - D^{\alpha_1}) \cdots (E - D^{\alpha_n})$$

To obtain $C^{\alpha_1\cdots\alpha_n}$, one would form the inverse of $B^{\alpha_1\cdots\alpha_n}$ after the rows and columns with subscripts $\alpha_1 \cdots \alpha_n$ have been removed and then place the resulting elements of C into the position in which the elements of B appeared originally. With this definition, one has the following relation:

$$\begin{aligned} C_{\alpha,\beta} = &- C^{\beta}_{\alpha\alpha} B_{\alpha\beta} C_{\beta\beta} + \sum_{k_1=1\cdots M}{}' C^{\beta k_1}_{\alpha\alpha} B_{\alpha k_1} C^{\beta}_{k_1 k_1} B_{k_1 \beta} C_{\beta\beta} \\ &- \sum_{k_1,k_2=1\cdots M}{}'' C^{\beta k_1 k_2}_{\alpha\alpha} B_{\alpha k_2} C^{\beta k_1}_{k_2 k_2} B_{k_2 k_1} C^{\beta}_{k_1 k_1} B_{k_1 \beta} C_{\beta\beta} + \cdots \end{aligned} \tag{1}$$

where the prime on the first sum indicates that all subscripts α, β, and k_1 are different and the double prime on the second sum indicates that all subscripts α, β, k_1, and k_2 are different. In this equation the subscripts follow the rule of matrix multiplication: the first subscript of the first operator agrees with the first subscript of C on the left, the last subscript of the last operator on the right agrees with the second subscript of C on the left. Superscripted diagonal operators C alternate with off-diagonal operator of B. The rule by which the superscripts of the operators C are chosen is best recognized if one reads the sums from the right to left: Each new C has one additional superscript which agrees with the second subscript of B at the right of the operator C. The rightmost operator C has no superscript. The formula terminates with the sum in which the number of superscripts of the first operator matrix C is $M - 1$. The structure of irreducible diagrams can be recognized in the fact that no subscripts are repeated. Equation (1) is, with some changes of notation, the formula on top of p. 13 of Ref. 1. It is obvious that this formula does not give the inverse of B, for it contains the diagonal terms of the inverse $C^{\alpha_1 \cdots \alpha_n}$.

We consider a few simple examples. The matrix

$$B = \left(\begin{array}{c|c} 1 & 2 \\ \hline 3 & 4 \end{array}\right)$$

has the inverse

$$C = \left(\begin{array}{c|c} -2 & 1 \\ \hline \frac{3}{2} & -\frac{1}{2} \end{array}\right)$$

Considering the partitioning as indicated by the dashed lines, one has

$$B_{1,2} = (1), \qquad B_{2,1} = (3), \qquad C_{1,1} = (-2), \qquad C_{2,2} = (-\tfrac{1}{2})$$

$$B^1 = \begin{pmatrix} 0 & 0 \\ 0 & 4 \end{pmatrix}, \quad C^1 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{4} \end{pmatrix}, \quad B^2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad C^2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

In (1) only the first term on the right will be present. One has $C_{1,2} = 1$, $C_{2,1} = \frac{3}{2}$, and, according to (1),

$$C_{1,2} = -C^2_{1,1} B_{1,2} C_{2,2} = (-1)(2)(-\tfrac{1}{2}) = (1)$$

$$C^1_{2,1} = -C^1_{2,2} B_{2,1} C_{1,1} = -\tfrac{1}{4} \cdot 3 \cdot -2 = \tfrac{3}{2}$$

In a slight generalization, we consider a larger matrix B, partitioned into four matrices. The diagonal matrices must be square:

$$B = \begin{pmatrix} B_{1,1} & B_{1,2} \\ B_{2,1} & B_{2,2} \end{pmatrix}$$

Then

$$B^1 = \begin{pmatrix} 0 & 0 \\ 0 & B_{2,2} \end{pmatrix}, \quad C^1 = \begin{pmatrix} 0 & 0 \\ 0 & B^{-1}_{2,2} \end{pmatrix}, \quad B^2 = \begin{pmatrix} B_{1,1} & 0 \\ 0 & 0 \end{pmatrix}, \quad C^2 = \begin{pmatrix} B^{-1}_{1,1} & 0 \\ 0 & 0 \end{pmatrix}$$

Then one obtains

$$C_{1,2} = -B^{-1}_{1,1} B_{1,2} C_{2,2}, \qquad C_{2,1} = -B^{-1}_{2,2} B_{2,1} C_{1,1}$$

As a check, we form $M = B \cdot C$; M ought to be the unit matrix

$$M = \begin{pmatrix} B_{1,1} & B_{1,2} \\ B_{2,1} & B_{2,2} \end{pmatrix} \begin{pmatrix} C_{1\,1} & -B^{-1}_{1,1} B_{1,2} C_{2,2} \\ -B^{-1}_{2,2} B_{2,1} C_{1,1} & C_{2,2} \end{pmatrix}$$

Then

$$M_{1,2} = -B_{1,1}B_{1,1}^{-1}B_{1,2}C_{2,2} + B_{1,2}C_{2,2} = 0, \qquad M_{2,1} = 0$$

The first diagonal terms gives

$$M_{1,1} = (B_{1,1} - B_{1,2}B_{2,2}^{-1}B_{2,1})\, C_{1,1}$$

$M_{1,1}$ is not automatically E_1, but it gives a relation from which C^1 can be computed,

$$C_{1,1} = (B_{1,1} - B_{1,2}B_{2,2}^{-1}B_{2,1})^{-1}$$

One might consider larger matrices and apply different partitionings to them. This would illustrate how the subscripts in the sums occurring in (1) must be chosen. For instance, for $M = 3$, only the first sum will appear and with α and β fixed, k_1 can assume only one value.

We add a few remarks about the further developments carried out in Ref. 1. The statistical element is brought in by the observation that, because of the nature of collective coordinates in Kraichnan's formulation, the individual components of the vector ψ are essentially equivalent, and that in the limit $M \to \infty$, it does not matter if a finite number of rows and columns in the partitioned matrix B are omitted. In the limit $M \to \infty$, the diagonal operators $C_{\alpha,\alpha}^{\alpha_1 \cdots \alpha_n}$ are the same and they are statistically sharp. It is therefore possible to replace them by one operator Γ. The formula which arises in this manner has been quoted by Lee. In the steps carried out so far, it is simpler to think in terms of an operator Γ rather than of a Green's function G which serves to represent the operator. The transition to the Green's function is carried out separately. The equations so obtained are taken as the starting point for the derivation of some formulas originally given by Kraichnan. This includes the application of an irreducible diagram expansion to Burger's equation. The special feature which occurs here lies in the nonlinear term of Burger's equation. The operator is split into a linear part and a remaining term which is treated as if it were an inhomogeneous term. One must, however, take into account that the randomness of the linear operator and of the driving term are related to each other. The splitting of the nonlinear operator is not free of arbitrariness, none of the existing possibilities is inherently preferable, and to each of the resulting equations, Kraichnan's justification for the truncation of the system can be applied. Unfortunately, the resulting equations, all presumably valid in the limit $M \to \infty$, are not the same, although all of them refer to the same model system. One is therefore confronted with a strange situation: While the method of introducing irreducible diagrams shown in Ref. 1 removes certain doubts which might exist if one applies a more intuitive approach, it also brings the technique into sharper focus and gives rise to new questions.

The fact that the matrix B can be partitioned in different ways might be used to introduce model equations which are closer to the physical reality. One might apply the randomizing factor ϕ of the type used by Kraichnan for each element of a coarser partitioning. Of course, the operator Γ would then be more complicated and the labor involved in obtaining actual solutions would be much larger.

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