Linked Cluster Expansions in the Statistical Theory of Ferromagnetism*

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(Received 27 November 1961)

A general perturbation theory of the statistics of spin interactions is developed in the form of a linked cluster expansion with particular emphasis on the Ising model. The theory applies to the evaluation of the expectation value of arbitrary spin functions as well as of the free energy. The thermodynamical consistency of the perturbation expansion is shown to arise from (1) variational principles satisfied by the free energy after a "renormalization procedure" has been carried out and (2) a generalized "Ward Identity" between renormalized quantities. These results are used to discuss inconsistencies in recent high-density theories of ferromagnetism and an improved theory obtained by the summation of all the convolution diagrams (nodal expansion) is briefly presented. The applicability of the method to general quantum mechanical many-body problems, including the theory of the Heisenberg model of ferromagnetism, is shown.

I. INTRODUCTION

RECENTLY, a perturbation approach to the study of spin interaction has been developed by Brout[1] based on a semi-invariant expansion of the partition function. The graphical representation of this expansion has been further analyzed by Horwitz and Callen.[2] In a subsequent study of the free energy of a many-fermion system by Brout and the author,[3] it appeared that the semi-invariant expansion of the partition function was conveniently supplemented by a method relying primarily on the use of quantum mechanical propagators. This established a link with the more usual many-body techniques analogous of those used in quantum field theory.

In this paper we develop a complete perturbation theory from a propagator-type point of view with the Ising model Hamiltonian serving as a reference. This is done for the following purposes:

(a) A greater simplicity and generality is achieved as compared to the original expansion for the Ising model. Many results of Sec. II, III, and IV are generalization of those obtained by Horwitz and Callen.[2]

(b) The thermodynamical consistency of the perturbation expansion can be discussed.

(c) The method can be immediately generalized to other problems as, for instance, thes tudy of the Heisen berg quantum mechanical model of ferromagnetism or the many-body fermion or boson system.

In Sec. II, a linked cluster expansion for any average of functions of spin operators is established for the Ising model of arbitrary spin in presence of an external magnetic field. The result is analogous to the Horwitz-Callen[2] rearrangement of Brout's[1] original theory.

In Sec. III, all the reducible linked graphs are eliminated essentially by a "renormalization procedure" similar to that of Horwitz and Callen.[2] In particular, simple expressions for the magnetization and the energy in terms of renormalized quantities are given.

The free energy is then expressed in terms of the renormalized quantities in Sec. IV. It is shown, in general, that the free energy satisfies an infinity of variational principles and that these principles insure that the magnetization can be obtained correctly from the free energy. This can also be easily satisfied without summing the complete set of graphs provided this is done in a consistent way defined in the paper.

The thermodynamical requirement that the susceptibility be equal to the fluctuation of the magnetization is studied in detail in Sec. V. This important consistency condition is shown to be a consequence of a generalized "Ward identity"[4] between renormalized quantities. The violation of this theorem in high-density limit theories of ferromagnetism[2,5] is related in Sec. VI, to inconsistencies of those theories. This is the motivation of presenting the sum of all the convolution diagrams (nodal expansions) as an improved high-density expansion.

Finally in Sec. VII, the general structure of the perturbation approach is shown to be valid in quantum statistics and, in particular, for the Heisenberg model.

II. LINKED CLUSTER EXPANSION FOR p-SPIN OPERATORS

We are interested in the calculation of the expectation value $\langle O_p \rangle$ of a p-spin operator O_p. O_p is a product of $p\mu_i$ where μ_i may take the values 1, $1-1/s$, $1-2/s$, $\cdots$, -1 and $i=1, 2, \cdots, n$; the value s of the spin is here taken arbitrary instead of the conventional value $\frac{1}{2}$ for the Ising model in order to stress the generality of the expansion. Typical O_p are μ_i and $\mu_i\mu_j$: The former gives the magnetization and the latter enters the calculation for the energy and the susceptibility. The Hamiltonian is

$$H=-\tfrac{1}{2}\sum_{ij} v_{ij}\mu_i\mu_j-\mathfrak{IC}\sum_i \mu_i, \qquad (2.1)$$

* This work has been supported in part by the Office of Naval Research.

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[1] R. Brout, Phys. Rev. **115**, 824 (1959).

[2] G. Horwitz and H. Callen (to be published).

[3] R. Brout and F. Englert, Phys. Rev. **120**, 1519 (1960).

[4] J. C. Ward, Phys. Rev. **78**, 182 (1950).

[5] R. Brout, Phys. Rev. **118**, 1009 (1960); **122**, 469 (1961).

where v_{ij} is the exchange integral taken between two spins and $\mathfrak{H}$ is an external magnetic field (measured in suitable units); then

$$\langle O_p\rangle = \mathrm{tr}\exp(-\beta H)O_p/\mathrm{tr}\exp(-\beta H) = \mathrm{tr}\rho O_p, \quad (2.2)$$

where ρ is the density matrix of the canonical ensemble.

We take now as the unperturbed Hamiltonian H_0 the term $-\mathfrak{H}\sum_i \mu_i$ in (2.1) where $\mathfrak{H}$ is to be put eventually to zero at the end of the calculation if no external field is present; then from (2.2)

$$\langle O_p\rangle = \frac{\mathrm{tr}\exp(-\beta H_0)\exp[\beta(\tfrac{1}{2}\sum_{ij} v_{ij}\mu_i\mu_j)]O_p}{\mathrm{tr}\exp(-\beta H_0)\exp[\beta(\tfrac{1}{2}\sum_{ij} v_{ij}\mu_i\mu_j)]} \quad (2.3)$$

or

$$\langle O_p\rangle = \frac{\langle\exp[\beta(\tfrac{1}{2}\sum_{ij} v_{ij}\mu_i\mu_j)]O_p\rangle_0}{\langle\exp[\beta(\tfrac{1}{2}\sum_{ij} v_{ij}\mu_i\mu_j)]\rangle_0}, \quad (2.4)$$

where we have defined the unperturbed average

$$\langle O_p\rangle_0 = \frac{\mathrm{tr}\exp(-\beta H_0)O_p}{\mathrm{tr}\exp(-\beta H_0)} = \mathrm{tr}\rho_0 O_p. \quad (2.5)$$

The reason for the above-mentioned choice of H_0 is, of course, that the density matrix ρ_0 is factorizable into a product $\rho_0 = \prod_{i=1}^{N}\rho_0{}^i$ of density matrices $\rho_0{}^i$ relative to a single spin i.

We begin the perturbation development from Eq. (2.4) by expanding both numerator and denominator as power series in β. Thus

$$\langle O_p\rangle = \sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\langle H_{\mathrm{int}}{}^n O_p\rangle_0 \Big/ \sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\langle H_{\mathrm{int}}{}^n\rangle_0, \quad (2.6)$$

with

$$H_{\mathrm{int}} = -\tfrac{1}{2}\sum_{ij} v_{ij}\mu_i\mu_j. \quad (2.7)$$

This leaves us with the evaluation of averages of product of the form

$$\langle\mu_i\mu_k\mu_k\mu_k\mu_l\cdots\mu_p\rangle_0 = \langle\mu_i\rangle_0\langle\mu_k\mu_k\mu_k\rangle_0\langle\mu_l\rangle_0\cdots\langle\mu_p\rangle_0, \quad i\neq k\neq l\neq\cdots p, \quad (2.8)$$

where the equalities result from the factorizability of ρ_0. Clearly, were it not for the occurrence in the expansions of the numerator or indices already contained in O_p the average $\langle O_p\rangle_0$ would by (2.8), factorize out of the numerator and the factor multiplying $\langle O_p\rangle_0$ would cancel against the denominator leaving $\langle O_p\rangle = \langle O_p\rangle_0$. More generally, the possibility of finding factors in the expansion of the numerator canceling against the denominator is prohibited by the fact that $\langle\mu_k{}^n\rangle \neq \langle\mu_k\rangle^n$. A similar situation arises in the theory of quantum mechanical propagators and there a cancellation theorem (the linked cluster expansion) can still be obtained by the use of Wick's theorem; here we use a more general procedure analogous to the one used in a previous study of the free energy of a many-body fermion system.[3]

We represent $\langle\mu_k{}^n\rangle$ as a sum of products of semi-invariants in the well known Ursell-Mayer fashion[6]

$$\langle\mu_k{}^n\rangle_0 = \sum_{\{p_i\}}\prod_i M_{p_i}{}^0(k), \quad (2.9)$$

where the sum is of all splits of the n factors into groups of p_i factors; for instance:

$$\begin{aligned}\langle\mu\rangle_0 &= M_1{}^0,\\ \langle\mu\mu\rangle_0 &= M_1{}^0M_1{}^0 + M_2{}^0,\\ \langle\mu\mu\mu\rangle_0 &= M_1{}^0M_1{}^0M_1{}^0 + 3M_1{}^0M_2{}^0 + M_3{}^0.\end{aligned} \quad (2.10)$$

We have not written the index k since the averages as well as the semi-invariants are independent of the particular spin considered. Equation (2.9) [or (2.10)] may be inverted in a well known way[6] to give M_p in terms of the moment $\langle\mu^n\rangle$; the first few M_p are given, for example, below:

$$\begin{aligned}M_1{}^0 &= \langle\mu\rangle_0,\\ M_2{}^0 &= \langle\mu^2\rangle_0 - \langle\mu\rangle_0{}^2,\\ M_3{}^0 &= \langle\mu^3\rangle_0 - 3\langle\mu^2\rangle_0\langle\mu\rangle_0 + 2\langle\mu\rangle_0{}^3.\end{aligned} \quad (2.11)$$

For spin $\frac{1}{2}$ these may be expressed in terms of the reduced unperturbed magnetization R_0:

$$\begin{aligned}M_1{}^0 &= R_0,\\ M_2{}^0 &= 1 - R_0{}^2,\\ M_3{}^0 &= -2R_0(1-R_0{}^2).\end{aligned} \quad (2.12)$$

In general, the evaluation of $M_p{}^0$ is greatly simplified if one uses the following formula

$$M_p{}^0 = d^p\ln Z_0{}^i(x)/dx^p, \quad (2.13)$$

where $x=\beta\mathfrak{H}$ and $Z_0{}^i(x)$ is the "unperturbed partition function" (evaluated for $H_{\mathrm{int}}=0$) for one spin i, that is,

$$Z_0{}^i(x) = \mathrm{tr}\exp(\mu_i x) = \frac{\sinh[x(2s+1)/2s]}{\sinh(x/2s)}. \quad (2.14)$$

[We have, of course, $\ln Z_0(x) = \sum_i \ln Z_0{}^i(x)$ for the total unperturbed partition function.] Indeed, from (2.14) we have

$$\langle\mu_i{}^n\rangle_0 = \frac{1}{Z_0{}^i(x)}\frac{d^n Z_0{}^i(x)}{dx^n}, \quad (2.15)$$

from which (2.13) follows immediately by straightforward differentiation, as shown in detail in reference (3).

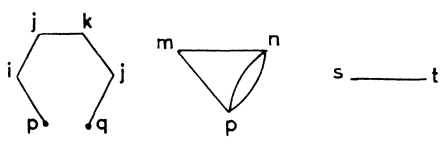

FIG. 1. Graphical representation of $(1/10!)(\frac{1}{2})^{10}\beta v_{pi}v_{ij}v_{kj}{}^2 \times v_{jq}v_{pm}v_{mn}v_{np}{}^2v_{st}(M_1{}^0)^4(M_2{}^0)^5(M_3{}^0)^2$.

[6] B. Kahn, thesis, Amsterdam 1938 (N. V. Noord-Hollandsche Uitgevers-maatschappij), Chap. III.

We now represent each term of the power series expansion of the numerator of (2.4) in terms of graphs after expanding the averages in terms of semi-invariant following (2.8) and (2.9). To each factor $\frac{1}{2}\beta v_{ij}$ we associate a bond i—j and to each semi-invariant $M_p{}^0(i)$ we associate a vertex labeled (i) with p lines coming to it. Such factors in the nth order of the power series expansion arise from

$$\frac{1}{n!}(\tfrac{1}{2})^n(\beta v_{ij})(\beta v_{kl})\cdots(\beta v_{mn})\langle\mu_i\mu_j\mu_k\mu_l\cdots\mu_m\mu_n O_p\rangle_0, \quad (2.16)$$

where some indices may be equal. We have shown in Fig. 1 a graphical representation of such a term where O_p is taken to be $\mu_p\mu_q$. The total contribution of a given graph to the numerator can then be obtained by (1) multiplying all the $\frac{1}{2}\beta v_{ij}$ related to the lines by all the $M_p{}^0$ related to the vertices, (2) dividing by $n!$, (3) summing over all spin indices without any restriction, and (4) multiplying the graph by the number of terms G in the expansion that give rise to the same graph. In Appendix A, we show that this number is $G=2^n n!/g$ when g is the number of symmetry operations transforming the graph into itself (the order of the symmetry group of the graph).

We define now a *linked graph* as a graph that does not contain any disconnected part; for instance the graph of Fig. 1 is unlinked and the graph of Fig. 2(a) is linked (a graph is linked even if it is connected only through the spins contained in O_p as in Fig. 2(b). From the above-mentioned rules it is clear that the $1/n!$ coming from the expansion of $\exp[\beta\sum_{i,j}\frac{1}{2}v_{ij}\mu_i\mu_j]$ cancels with the $n!$ arising from the G factor of the graph. So an unlinked graph is equal to the product of all the parts unlinked to the first (the one containing O_p) and the first one. But the contribution in an unlinked graph of *all* the parts unlinked to the first is exactly the contribution of the denominator. Thus only the linked graphs that contain O_p contributes to $\langle O_p\rangle$.

We now summarize the linked cluster theorem which we write in the symbolic form

$$\langle O_p\rangle=\sum_{n=0}^{\infty}\langle(\beta H_{\text{int}})^n; O_p\rangle_{0,L} \quad (2.17)$$

by giving a set of rules exemplified at Fig. 3.

(a) Draw all the possible *linked* graphs ending at p fixed points (the p spins contained in O_p).

(b) To each line i—j attribute a factor βv_{ij}.

(c) To each vertex attribute a semi-invariant $M_n{}^0$, n being the number of lines arriving at the vertex. (Each fixed point is to be counted as a line.)

(d) To each graph attribute a factor $1/g$.

(e) Sum without restriction over all spin indices (except, of course, over the p fixed ones).

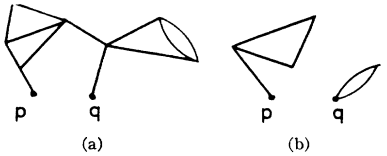

FIG. 2. Linked graphs contributing to $\langle\mu_p\mu_q\rangle$.

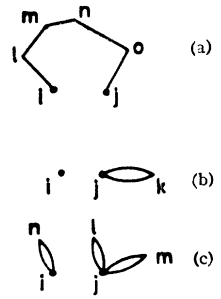

FIG. 3. Contributions to $\langle\mu_i\mu_j\rangle$. (a) $\beta^5\sum_{l,m,n,o}(v_{il}v_{lm}v_{mn}v_{no}v_{oj})\times(M_2{}^0)^6$, $[g=1]$; (b) $\beta^2\frac{1}{2}\sum_k(v_{jk})^2M_1{}^0M_2{}^0M_3{}^0$, $[g=2]$; (c) $\beta^6\frac{1}{16}\times\sum_{n,l,m}(v_{jl})^2(v_{jm})^2(v_{in})^2(M_2{}^0)^3M_3{}^0M_5{}^0$, $[g=16]$.

These results are analogous to the graphical expansion of the free energy obtained by Horwitz and Callen[2] by a rearrangement of Brout's[1] initial expansions.

One may notice that the above expansion is given in terms of the $M_p{}^0$ which are given functions of the external field $\mathcal{H}$ [for spin $\frac{1}{2}$, for instance, $M_p{}^0=M_p{}^0(R_0)$ and $R_0=\tanh\beta\mathcal{H}$]. The linked cluster expansion is thus in a certain sense analogous to an expansion in a grand ensemble where $\mathcal{H}$ plays the role of a chemical potential and where the magnetization $\langle\mu\rangle$ is not held fixed during the perturbation.

III. RENORMALIZATION—ENERGY AND MAGNETIZATION

We shall call a graph reducible at a vertex i if it can be split into different pieces by cutting the graph at i by a line that does not cut any bond. The parts left after the graph has been completely reduced will be called the irreducible parts of the graphs (Fig. 4) and a

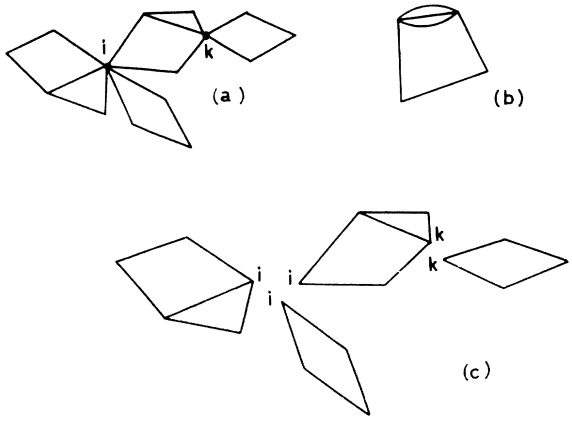

FIG. 4. Reducible and irreducible graphs. (a) Reducible graph; (b) irreducible graph; (c) irreducible parts.

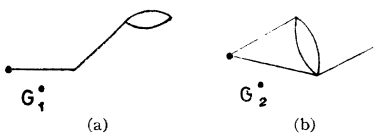

FIG. 5. Self-energy diagrams.

graph that cannot be reduced will be called irreducible. The vertex i will be called a point of reducibility.

It is clear that we could obtain an expansion involving only irreducible graphs if we were able to sum all the irreducible parts articulated to a given vertex. We shall show that such a procedure amounts to a simple redefinition M_n of the semi-invariants M_n^0 attached to an n-order vertex and we shall call M_n the renormalized semi-invariant of order n.[7]

We define the nth order self-energy G_n^0 as the sum of all linked diagrams fixed at an nth order vertex, which is not a point of reductibility, evaluated following the previous rules, except for the fixed vertex which receives a factor of 1 (Fig. 5). The contribution to M_n of the parts terminating with k lines is by (2.13)

$$G_k{}^0 M_{n+k}{}^0=[G^0(\partial^k/\partial x^k)]\partial^n/\partial x^n \ln Z_0{}^i(x).$$

For instance, the contribution of $G_3{}^0$ to M_2 is given by (Fig. 6)

$$M_5{}^0 G_3{}^0=[G_3{}^0(\partial^3/\partial x^3)]\partial^2/\partial x^2 \ln Z_0{}^i(x).$$

In general, the total contribution of m_k irreducible parts of the $G_k{}^0$ type will be

$$\frac{1}{m_k!}[G_k{}^0(\partial^k/\partial x^k)]\partial^n/\partial x^n \ln Z_0{}^i(x),$$

where $m_k!$ arises from the symmetry factor of the graph. It is understood that $\partial/\partial x$ operates only on $\ln Z_0{}^i(x)$. Summing all the reducible parts attached to an nth order vertex we have

$$\sum_{m_k,m_l\cdots=0}^{\infty} \frac{1}{m_k!}\frac{1}{m_l!}\cdots\left[G_k{}^0\frac{\partial^k}{\partial x^k}\right]^{m_k} \times\left[G_l{}^0\frac{\partial^l}{\partial x^l}\right]^{m_l}\cdots\frac{\partial^n}{\partial x^n}\ln Z_0{}^i(x) \quad (3.1)$$

or

$$M_n=\exp\left[\sum_k G_k{}^0\frac{\partial^k}{\partial x^k}\right]M_n{}^0(x). \quad (3.2)$$

We may now reduce all the self-energy parts and express (3.2) in terms of the renormalized self-energy parts G_k so obtained; thus the equations

$$M_n=\exp[\textstyle\sum_k G_k(\partial^k/\partial x^k)]M_n{}^0(x), \quad (3.3)$$

[7] M_n is analogous to a renormalized *propagator* in field theory because our graphs are essentially analogous to the *dual* of the graphs used in field theory. That is our interaction *lines* corresponds to *points* where propagators touch; these propagators are drawn as lines because of the necessity of keeping track of time ordering in quantum field theory. In our classical theory, however, these lines collapse into a point which is our $M_n{}^0$ or M_n.

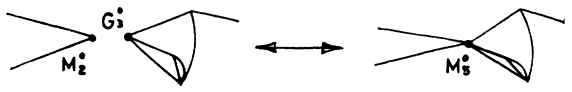

FIG. 6. Contribution to M_2. A self-energy part $G_3{}^0$ attached to a vertex $M_2{}^0$ gives a $M_5{}^0$ contribution to M_2.

together with the graph giving the irreducible G_k in terms of the M_n define the renormalized semi-invariant. We have thus obtained an irreducible cluster expansion for all the $\langle O_p\rangle$ if we replace everywhere in our previous rule $M_n{}^0$ by M_n and draw only the graphs *irreducibly linked* to the fixed p vertices. We write this symbolically as

$$\langle O_p\rangle=\sum_{n=0}^{\infty}\langle(\beta H_{\rm int})^n; O_p\rangle_{\rm I.L.}. \quad (3.4)$$

Many results can be expressed simply in terms of the G_k and M_k; for instance, the *magnetization* is directly given by M_1 as obtained from (3.3).

We now express the *energy* in terms of the G_n. The energy is given by the 2-spin operator average $\langle\mu_i\mu_j\rangle$ multiplied by $\frac{1}{2}v_{ij}$ and summed over i and j. Equivalently, we may also consider only all *closed* topologically different diagrams and sum all the different graphs obtained by fixing in these diagrams each line successively in both directions and by multiplying the result by $\frac{1}{2}$. Instead of fixing a line we may calculate the total contribution of the closed topologically different diagrams by fixing a vertex, thus expressing the result in terms of the G_n. As there are n lines arriving to a nth order vertex, the following formula for the energy appears plausible

$$\left(-\frac{E}{N}\right)=\frac{1}{2\beta}\sum_{n=1}^{\infty} nM_nG_n. \quad (3.5)$$

Actually (3.5) is correct even when the symmetry of the graphs are taken into account. This is shown in Appendix B together with other topological properties of the graphs that will be used later.

We illustrate formulas (3.3) and (3.5) by a simple example. Let us neglect all the G_i but G_1; the justification of such an approximation will be discussed in Sec. VI. We thus have

$$\begin{aligned} &G_1=(1/N)\textstyle\sum_{ij}\beta v_{ij}M_1=\beta v(0)M_1,\\ &G_n=0, \quad n>1 \end{aligned} \quad (3.6)$$

with $v(0)=(1/N)\sum_{ij}v_{ij}$. We then obtain the magnetization curve

$$\begin{aligned} &M_1=\exp[G_1(\partial/\partial x)]M_1{}^0(x),\\ &M_1=M_1{}^0(x+\beta v(0)M_1), \end{aligned} \quad (3.7)$$

which is the well-known result of the molecular field theory[8] with the Curie temperature given by Curie-

[8] C. Kittel, *Introduction to Solid-State Physics* (John Wiley & Sons, Inc., New York, 1956), 2nd ed., Chap. 15.

Weiss value $\beta v(0)=1$. Similarly, the same approximation in (3.5) gives the molecular field energy

$$(-E/N)=\tfrac{1}{2}v(0)M_1^2. \tag{3.8}$$

IV. FREE ENERGY AND VARIATIONAL PRINCIPLES

The free energy $F=E-TS$ may be obtained from the energy by integrating over β. It is, however, more instructive to deduce an explicit cluster expansion for the free energy because this will show the origin, in terms of graphs, of the variational principles that the free energy satisfies.

We define

$$Z(\xi)=\mathrm{tr}\exp[-\beta(H_0+H_{\mathrm{int}}(\xi))], \tag{4.1}$$

with

$$H_{\mathrm{int}}(\xi)=\xi H_{\mathrm{int}}=-\tfrac{1}{2}\textstyle\sum_{ij}\xi v_{ij}\mu_i\mu_j; \tag{4.2}$$

so

$$-\beta[\partial F(\xi)/\partial\xi]=\partial\ln Z(\xi)/\partial\xi=-\beta\langle(1/\xi)H_{\mathrm{int}}(\xi)\rangle_\xi, \tag{4.3}$$

where the average is taken at the value ξ of the coupling constant. Then

$$\ln Z=N\ln\frac{\sinh[\beta\mathfrak{H}(2s+1)/2s]}{\sinh(\beta\mathfrak{H}/2s)}-\beta\int_0^1\left\langle\frac{1}{\xi}H_{\mathrm{int}}(\xi)\right\rangle_\xi d\xi. \tag{4.4}$$

Applying (2.17) to (4.4) with

$$O_p=H_{\mathrm{int}}(\xi)=-\tfrac{1}{2}\textstyle\sum_{ij}\xi v_{ij}\mu_i\mu_j,$$

one finds

$$\ln Z=N\ln\frac{\sinh[\beta\mathfrak{H}(2s+1)/2s]}{\sinh(\beta\mathfrak{H}/2s)}+\sum_{n=0}^{\infty}\beta\frac{1}{2(n+1)}\langle(-\beta H_{\mathrm{int}})^n;\textstyle\sum_{ij}v_{ij}\mu_i\mu_j\rangle_{0,L}. \tag{4.5}$$

However, $1/2(n+1)$ is precisely the ratio of the sum of symmetry factors of all the graphs obtained by fixing, in a closed graph, a line in all possible ways, to the symmetry factor of a free graph (see Appendix B). We may then consider $1/2(n+1)$ as a symmetry factor for a free graph. The evaluation of $F(1)-F(0)$ is then identical to the evaluation of any O_p except that the graphs are closed and considered as free. We thus write symbolically

$$\ln Z=\ln Z_0(\beta\mathfrak{H})+\sum_{n=1}^{\infty}\langle(-\beta H_{\mathrm{int}})^n\rangle_{0,L}. \tag{4.6}$$

The expansion (4.6) is given in terms of $M_n{}^0$, that is, in terms of the unrenormalized semi-invariants. In order to have an expansion in terms of the M_n we must reduce the graphs. This operation is here, however, not straightforward because the free energy graphs are free and the reduction procedure was carried out for fixed graphs. Thus, the result (4.6) applied to irreducible graphs with renormalized vertices would amount to an overcounting. Instead of "counting" the overcounting we shall prove that the following expansion is correct:

$$(1/N)\ln Z=M_0-\sum_{n=1}^{\infty}M_nG_n+(1/N)\sum_{n=1}^{\infty}\langle(-\beta H_{\mathrm{int}})^n\rangle_{\mathrm{I.L.}}, \tag{4.7}$$

where M_0 is obtained from (3.2) where $M_0{}^0(x)$ is defined as $\ln Z_0(x)$. Thus the overcounting introduces two effects: (a) a renormalization of $M_0{}^0(x)$; (b) a counter term $-\sum_{n=1}^{\infty}M_nG_n$ which may be interpreted as the sum of all the graphs with one point fixed. In terms of the G_n (4.7) may be written explicitly by using (3.5)

$$\left(\frac{1}{N}\right)\ln Z=M_0-\sum_{n=1}^{\infty}M_nG_n+\sum_{n=1}^{\infty}\tfrac{1}{2}\int_0^1\frac{d\xi}{\xi}nM_nG_n(\xi), \tag{4.8}$$

where the $G_n(\xi)$ are functions of the coupling constant ξ only through the explicit dependence of G_n on the v_{ij}-bonds.

We first prove that the right-hand side of (4.8), where the G_n are considered as functions of independent variables α_n, is stationary with respect to variations of the α_n for $\alpha_n=M_n$ where M_n is given by (3.3). Thus, we consider the function

$$\phi(\alpha_n)=M_0[G_k(\alpha_n)]-\sum_{n=1}^{\infty}\alpha_nG_n(\alpha_k)+\sum_{n=1}^{\infty}\frac{1}{2}\int_0^1\frac{d\xi}{\xi}n\alpha_nG_n(\xi,\alpha_k). \tag{4.9}$$

In general, we have from (3.3) for any variation that does not affect x,

$$\delta M_n=\exp\left[\sum_{k=1}^{\infty}G_k\frac{\partial^k}{\partial x^k}\right]\left(\sum_{j=1}^{\infty}\frac{\partial^j}{\partial x^j}\delta G_j\right)M_n{}^0(x),$$

or

$$\delta M_n=\sum_{j=1}^{\infty}M_{n+j}\delta G_j. \tag{4.10}$$

In particular,

$$\delta M_0=\sum_{j=1}^{\infty}M_j\delta G_j. \tag{4.11}$$

Thus,

$$\delta\phi(\alpha_n)=\sum_{n=1}^{\infty}[M_n(\alpha_k)-\alpha_n]\delta G_n(\alpha_k)-\sum_{n=1}^{\infty}G_n(\alpha_k)\delta\alpha_n+\delta\sum_{n=1}^{\infty}\frac{1}{2}\int\frac{d\xi}{\xi}n\alpha_nG_n(\xi,\alpha_k). \tag{4.12}$$

To evaluate the variation of the last term we notice

that this term is the sum of all irreducible closed graphs evaluated using the symmetry factor of the free graph. The variation is equivalent to fixing *all* the vertices successively and replacing the α_n relative to it by a $\delta\alpha_n$. We still evaluate the graph with the symmetry factor of the free graph. This is, however, equivalent to counting only the topologically different graphs with one fixed vertex together with the correct symmetry factor of such a graph. Thus we see that the variation of the last term is simply $\sum_{n=1}^{\infty} G_n(\alpha_k)\delta\alpha_n$. We have thus obtained

$$\delta\phi(\alpha_n)=\sum_{n=1}^{\infty}[M_n(\alpha_k)-\alpha_n]\delta G_n(\alpha_k), \tag{4.13}$$

and if all the $\alpha_k=M_k$, then

$$\delta\phi(\alpha_n)\,|_{\alpha_n=M_n}=0. \tag{4.14}$$

So $\phi(\alpha_n)$ is stationary with respect to any variation of the α_n around the value M_n.

Next we evaluate $d\phi[M_n(\xi)]/d\xi$, where α_n is replaced by the correct M_n for a given coupling constant ξ. In calculating the derivative we only have to consider the explicit dependence of $G_n(\xi)$ in the last integral because of (4.14); thus,

$$\frac{d\phi[M_n(\xi)]}{d\xi}=\frac{1}{2\xi}\sum_{n=1}^{\infty} nM_n(\xi)G_n(\xi)$$

$$=(1/N)\langle(-\beta/\xi)H_{\text{int}}(\xi)\rangle_\xi; \tag{4.15}$$

so

$$Nd\phi[M_n(\xi)]/d\xi=d\ \ln Z(\xi)/d\xi. \tag{4.16}$$

Moreover for $\xi=0$, $N\phi$ is equal to $\ln Z_0$ so we have proved that $N\phi=\ln Z$ and the validity of the relation (4.7) for the free energy is established. The free energy is then stationary with respect to any variation of the renormalized semi-invariant around their correct value; these variational principles are equivalent to the equations (3.3) defining these M_n.

The importance of these variational principles is that they insure automatically the thermodynamical relation

$$(1/N)\partial\ \ln Z/\partial x=M_1. \tag{4.17}$$

In order to establish this we first calculate the derivative of M_n with respct to x; this differs from the result obtained in (4.10) because we now have to vary x in (3.3). This simply adds a derivative of $M_n{}^0(x)$ with respect to x to the previous result and thus,

$$\frac{dM_n}{dx}=\sum_{j=1}^{\infty} M_{n+j}\frac{dG_j}{dx}+M_{n+1}, \tag{4.18}$$

and, in particular,

$$\frac{dM_0}{dx}=\sum_{j=1}^{\infty} M_j\frac{dG_j}{dx}+M_1. \tag{4.19}$$

With the help of (4.19) we obtain by differentiation of (4.7)

$$\frac{d\ \ln Z}{Ndx}=M_1-\Big[\sum_{j=1}^{\infty} G_j(dM_j/dx)$$

$$-\sum_{j=1}^{\infty}\frac{d}{dx}\tfrac{1}{2}\int_0^1\frac{d\xi}{\xi}nM_nG_n(\xi)\Big].$$

The same reasoning that led to the variational principles now leads to the vanishing of the quantity between the brackets so that (4.1) is proved.

We now state the theorem: In any order of perturbation theory (of the evaluation of the G_n), the free energy obtained by (4.7) satisfies the variational principles and thus the relation (4.17) if one uses a "complete set" of self-energies G_n; that is all the G_n deduced from any member of the set by fixing any vertex in a defining graph.

This theorem is an immediate consequence of the proof of the variational principle given above. It provides a criterion of consistency for the use of the set of graphs to be included in a given approximation to the free energy, namely, one must use only a "complete set" of G_n. We shall see, however, in the next section that such a criterion is not sufficient to define a completely thermodynamically consistent approximation to the free energy.

V. SUSCEPTIBILITY AND THE GENERALIZED "WARD IDENTITY"

Differentiating (4.17) with respect to x we obtain the well-known thermodynamical relation

$$(1/N)d^2\ \ln Z/dx^2=dM_1/dx=\chi, \tag{5.1}$$

where χ is the isothermal susceptibility. On the other hand we obtain by differentiating (4.1) twice with respect to x:

$$N\chi=\langle(\textstyle\sum_i\mu_i)^2\rangle-\langle\sum_i\mu_i\rangle^2. \tag{5.2}$$

This is the usual type of relation relating response functions to fluctuations; its physical significance is very important because (5.2) guarantees that the susceptibility is always positive and that infinities in the susceptibility and in the distribution function occur simultaneously. We shall investigate the translation of (5.2) into perturbation theory.

We write (4.18) in the following form:

$$\frac{dM_n}{dx}=\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} M_{n+j}\left(\frac{\partial G_j}{\partial M_k}\right)_{\text{gr}}\frac{dM_k}{dx}+M_{n+1}, \tag{5.3}$$

where $(\partial G_j/\partial M_k)_{\text{gr}}$ means the derivative of G_j considered as a function of the independent variables M_k through the graphical definition of G_j. That is, more precisely,

$$(\partial G_j/\partial M_k)_{\text{gr}}=(\partial G_j/\partial\alpha_k)_{\alpha_k=M_k}. \tag{5.4}$$

We may also write

$$M_{n+j}=(\partial M_n/\partial G_j)_{\text{funct}}=(\partial M_j/\partial G_n)_{\text{funct}}, \quad (5.5)$$

where here the M_n are considered as a function of the G_j through the functional dependence (3.3). We now define the matrices $\mathbf{R}$ and $\mathbf{S}$ such that

$$(\mathbf{R})_{nm}=(\mathbf{R})_{mn}=M_{n+m}=(\partial M_n/\partial G_m)_{\text{funct}}, \quad (5.6)$$

$$(\mathbf{S})_{nm}=(\partial G_n/\partial M_m)_{\text{gr}}, \quad (5.7)$$

and the vectors $\mathbf{M}$ and $\mathbf{M}^+$ defined by

$$\begin{aligned}(\mathbf{M})_n&=M_n,\\ (\mathbf{M}^+)_n&=M_{n+1}.\end{aligned} \quad (5.8)$$

Equation (5.3) can then be solved as a matrix equation

$$d\mathbf{M}/dx=[1-\mathbf{RS}]^{-1}\mathbf{M}^+. \quad (5.9)$$

The first component of (5.9) is the susceptibility; it is easily seen that dM_1/dx becomes infinite if

$$\det[1-\mathbf{RS}]=0. \quad (5.10)$$

Thus (5.10) may be considered as an equation defining the possible phase transitions of the system. We finally note that from (5.3)

$$\begin{aligned}\frac{dM_1}{dx}&=\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\left(\frac{\partial G_n}{\partial M_k}\right)_{\text{gr}}M_{n+1}\frac{dM_k}{dx}+M_2\\ &=\mathbf{M}^+\mathbf{S}\frac{d\mathbf{M}}{dx}+M_2,\end{aligned} \quad (5.11)$$

or, with the help of (5.9),

$$\chi=dM_1/dx=\mathbf{M}^+\mathbf{S}[1-\mathbf{RS}]^{-1}\mathbf{M}^++M_2. \quad (5.12)$$

We now evaluate the right-hand side of (5.2) directly from the propagator formalism. This involves the calculation of $O_2=\langle\mu_i\mu_j\rangle$. We have (Fig. 7)

$$\langle\mu_i\mu_j\rangle=\sum_n\sum_m M_{n+1}G_{ij}{}^{nm}M_{m+1}+M_1{}^2+\delta_{ij}M_2, \quad (5.13)$$

where $G_{ij}{}^{nm}$ is the contribution to $\langle\mu_i\mu_j\rangle$ from graphs linked to i with n lines and to j with m lines, the semi-invariant relative to the extremities i and j being replaced by 1. Introduction of the matrix $\mathbf{G}_{ij}$ such that

$$(\mathbf{G}_{ij})_{nm}=G_{ij}{}^{nm} \quad (5.14)$$

leads to

$$\langle\mu_i\mu_j\rangle=\mathbf{M}^+\mathbf{G}_{ij}\mathbf{M}^++(M_1)^2+\delta_{ij}M_2 \quad (5.15)$$

and

$$(1/N)[\langle(\textstyle\sum_i\mu_i)^2\rangle-\langle\sum_i\mu_i\rangle^2]=\mathbf{M}^+\mathbf{G}(0)\mathbf{M}^++M_2, \quad (5.16)$$

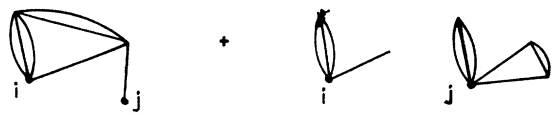

FIG. 7. Contributions to $\langle\mu_i\mu_j\rangle$ for $i\neq j$.

where we have introduced the Fourier transform of $\mathbf{G}_{ij}$:

$$\mathbf{G}(\mathbf{q})=\frac{1}{N}\sum_{ij}\mathbf{G}_{ij}e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}. \quad (5.17)$$

We now express $\mathbf{G}_{ij}$ in terms of *renormalized bond matrix* $\mathbf{C}_{ij}$ such that $(\mathbf{C}_{ij})_{mn}=C_{ij}{}^{mn}$ represents the sum of all the graphs connecting i and j, respectively, with m lines arriving at i and n lines arriving at j and containing no articulation point. An articulation point is a point where the graph can be cut into two pieces, one linked to i, the other to j, by a single line not cutting any line of the diagram (Fig. 8). We readily express $\mathbf{G}_{ij}$ in terms of $\mathbf{C}_{ij}$:

$$G_{ij}{}^{mn}=C_{ij}{}^{mn}+\sum_k\sum_{\gamma,\alpha}C_{ik}{}^{m\gamma}M_{\gamma+\alpha}C_{kj}{}^{\alpha n}+\cdots,$$

or

$$\mathbf{G}_{ij}=\mathbf{C}_{ij}+\sum_k\mathbf{C}_{ik}\mathbf{R}\mathbf{C}_{kj}+\cdots. \quad (5.18)$$

In terms of the Fourier transform $\mathbf{C}(\mathbf{q})$ of $\mathbf{C}_{ij}$,

$$\mathbf{C}(\mathbf{q})=(1/N)\textstyle\sum_{ij}\mathbf{C}_{ij}e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}, \quad (5.19)$$

we have

$$\mathbf{G}(\mathbf{q})=\mathbf{C}(\mathbf{q})+\mathbf{C}(\mathbf{q})\mathbf{R}\mathbf{C}(\mathbf{q})+\cdots$$

or

$$\mathbf{G}(\mathbf{q})=\mathbf{C}(\mathbf{q})[1-\mathbf{R}\mathbf{C}(\mathbf{q})]^{-1}. \quad (5.20)$$

This equation appears as a matrix generalization of a similar relation obtained by Meeron in the study of the nodal expansion of a gas.[9] We shall come back to the nodal expansion later.

Using (5.20), we may write (5.16) as

$$\begin{aligned}&\frac{1}{N}[\langle(\textstyle\sum_i\mu_i)^2\rangle-\langle\sum_i\mu_i\rangle^2]\\ &\qquad=\mathbf{M}^+\mathbf{C}(0)[1-\mathbf{R}\mathbf{C}(0)]^{-1}\mathbf{M}^++M_2.\end{aligned} \quad (5.21)$$

Comparing (5.12) and (5.21), we see that (5.2) will be verified if

$$\mathbf{S}=\mathbf{C}(0), \quad (5.22)$$

or, equivalently,

$$\left(\frac{\partial G_n}{\partial M_m}\right)_{\text{gr}}=\left(\frac{\partial G_m}{\partial M_n}\right)_{\text{gr}}=[\mathbf{C}(0)]_{mn}=(1/N)\sum_{ij}C_{ij}{}^{mn}. \quad (5.23)$$

The identity (5.23) follows from the definition of G_n: Taking the derivative with respect to M_n is equivalent to taking the sum of all graphs connecting two points, one with n lines arriving at it, the other with m lines,

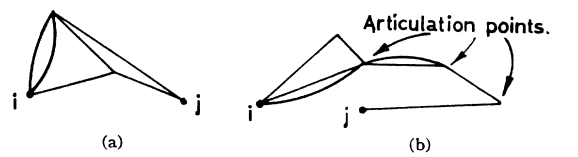

FIG. 8. Renormalized bonds. (a) Contribution to the renormalized bond $C_{ij}{}^{32}$; (b) Contribution to $G_{ij}{}^{31}$ containing three articulation points.

[9] E. Meeron, Phys. Fluids **1**, 189 (1958).

and then summing freely on the indices relative to the two points. This is precisely $\sum_{ij} C_{ij}$. We notice that if by fixing ρ different M_m in a graph contributing to G_n we obtain the same contribution to $[C(0)]_{mn}$, the result is automatically divided by ρ because of the symmetry factor of the graph.

The relation (5.22) which insures the thermodynamical consistency condition (5.2) is very similar to the "Ward Identity" in Quantum Electrodynamics.[4] It relates the renormalization of the semi-invariant M_n to the bond-renormalization: These renormalizations must be carried out simultaneously in order to satisfy the theorem. The fact that this is realized if one sums the whole perturbation series but generally it is not satisfied for a partial summation of graphs is related to inconsistencies that have appeared in recent theories of ferromagnetism. This problem will be examined now.

VI. HIGH DENSITY LIMIT EXPANSIONS AND THE NODAL EXPANSION

If we define z qualitatively as the number of spins in the "range" of the exchange potential v_{ij}, one may argue on physical grounds that if $z \to \infty$ the Weiss molecular field theory of ferromagnetism becomes valid.[5] This then implies that in the neighborhood of the Curie point we have, for a high-density system of spin (high Z),

$$(1/N)\sum_{ij} \beta v_{ij} \simeq (1/N)\beta j z \simeq 1, \qquad (6.1)$$

where j is an average exchange potential. From (6.1) we see that we may classify, in the region of the Curie point, unrenormalized graphs by means of powers of $1/z$. Each bond carries a factor of $1/z$ and each summation but one carries a factor of z. To check the consistency of this method we first have to sum all the graphs or order 1 and show that we obtain the molecular field results. The only graphs of order 1 are open chains (Fig. 9) and, in terms of renormalized graphs, this means that all G_i but G_1 are to be put equal to zero. We know from Sec. III that this leads precisely to the Weiss theory so that the validity of the $1/z$ classification is established.

One may then try to evaluate the first correction to the Weiss molecular field, that is the $1/z$ terms. This has been done by Brout[5] and by Horwitz and Callen[2] in two different, but nearly equivalent, ways. We shall discuss here once more the argument.

At first it appears that only the rings (and chains) contribute a factor $1/z$ (to the free energy, for instance). [Fig. 10(a)]. However, for large rings (with more than z vertices) any correction of the type 10(b) which would be of order $1/z^2$ might appear with the second ring attached to any $n \geq z$ vertices, thus restroring a contribution of order $1/z$. Thus, an accurate evaluation of the free energy to order $1/z$ must include vertex renormalization not only by means of chains but also by means of rings. This, however, does not necessarily include all the graphs of order $1/z$ for if the ring becomes increasingly large, any vertex renormalization or any renormalization may finally contribute to the order considered.

FIG. 9. Graphs of order 1.

As one may expect that in the ordered phase, large rings may be very important, a correct evaluation of all the $1/z$ graphs becomes impossible and the $1/z$ expansion itself probably loses its meaning. The best one may hope for is an approximate high density theory if one sums all the rings and chains, together with the appropriate vertex renormalization by means of rings and chains. This is the Horwitz-Callen theory and may be obtained from our general formalism by neglecting all the G_i but G_1 and G_2 (Fig. 11).

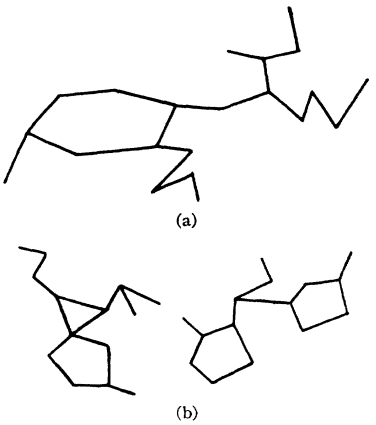

FIG. 10. (a) $1/z$ contribution; (b) $1/z^2$ contributions.

We now discuss the consistency of such an approximation. First, as was already established by these authors, it is clear that the variational principle is obeyed as a consequence of the fact any graph obtained by fixing a vertex in one of the graphs of Fig. 11 is still a contribution to G_1 or G_2. Thus, the thermodynamical relation $d \ln Z/dx = M_1$ is verified. On the other side the "Ward Identity" is not verified because no bond renormalization has been done. Thus we have no guarantee that the Curie point obtained by the divergence in long-range order (or in the specific heat) coincides with the infinity of the susceptibility. In fact, the inconsistency of the model is even worse because it had appeared[10] that the infinity of the susceptibility occurs for finite magnetic field above the Curie point obtained by the singularity in the specific heat. This is not only thermodynamically inconsistent but the second result violates a general theorem due to Lee and Yang.[11]

[10] This was first observed by M. Coopersmith. A detailed analysis of the nature of the inconsistency will be given elsewhere by G. Horwitz to whom we are very much indebted for many contributions to the analysis of this section.

[11] T. D. Lee and C. N. Yang, Phys. Rev. 87, 410 (1956).

In order to correct this inconsistency we then have to renormalize the bonds by means of rings with renormalized bonds. This leads to the sum of all the graphs with no crossing lines; it is the generalization of the "convolution approximation" or "nodal expansion" recently studied in the theory of imperfect gases.[9]

The convolution approximation will obviously satisfy the variational principle because the consistency requirement is verified. The Ward identity will, however, *not* be exactly satisfied because the renormalization of a bond by a graph of the convolution expansion may lead to a graph not contained in the original approximation. The convolution approximation is thus not a completely thermodynamically consistent approximation and this will also be true for the imperfect gas. However, it will in fact be impossible to have a consistent bond and vertex renormalization without summing *all* the graphs. This shows the difficulty of handling a perturbation theory in the neighborhood of a phase transition. Indeed, anywhere else, such discrepancies would be small effects, for if we stick to our initial $1/z$ classification we find that any nonconvolution correction is at least of order $1/z^3$. But as this expansion is meaningless for large rings, this cannot be trusted in a phase transition region and trouble may occur in the analytic behavior of the

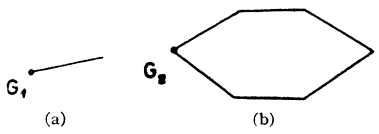

FIG. 11. Self-energy graphs in the Horwitz-Callen theory.

divergent function. Thus, in short, the convolution approximation appears, qualitatively, as the simplest theory of a high-density expansion: it satisfies the variational principle and contains all the first required bond renormalized corrections to the Horwitz-Callen theory. This is why, despite the lack of complete consistency of the convolution approximation, we shall give here the formal summation of all the convolution graphs.

Finally, we shall close this discussion by mentioning that Brout's theory of the high density suffers exactly from the same inconsistencies as the Horwitz-Callen theory and for the same reasons. In fact, the two theories are nearly equivalent, the difference being a rather unimportant difference in the vertex renormalization.

We evaluate the correlation function $\langle\mu_i\mu_j\rangle$ for $i\neq j$; and from this the energy, hence all the thermodynamical quantities may be determined. From (5.15) we have

$$\langle\mu_i\mu_j\rangle=\mathbf{M}^+\mathbf{G}_{ij}\mathbf{M}^+ + M_1^2, \quad i\neq j. \tag{6.2}$$

The problem is thus to evaluate the correlation matrix $\mathbf{G}_{ij}$.

We separate the contributions to $\mathbf{G}_{ij}$ into two parts:

(a) The graphs with no articulation points. This is given by the bond-renormalization matrix $\mathbf{C}_{ij}$.

(b) The graphs with articulation points. These contribute a matrix $\mathbf{T}_{ij}$ to $\mathbf{G}_{ij}$. Thus

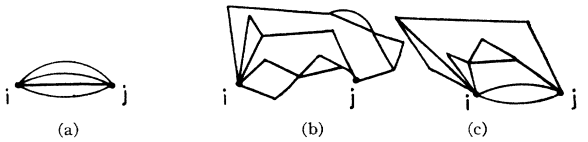

FIG. 12. Contribution to C_{ij} in the convolution approximation. (a) ladders of v_{ij} bonds contributing to C_{ij}; (b) ladders of $\mathbf{T}_{ij}$ bonds contributing to C_{ij}; (c) mixed ladders of v_{ij} bonds and $\mathbf{T}_{ij}$ bonds.

$$\mathbf{G}_{ij}=\mathbf{C}_{ij}+\mathbf{T}_{ij}. \tag{6.3}$$

From (6.3) and (5.20) we obtain the general relation between $\mathbf{C}_{ij}$ and $\mathbf{T}_{ij}$ in terms of their Fourier transform $\mathbf{C}(\mathbf{q})$ and $\mathbf{T}(\mathbf{q})$:

$$\mathbf{RT}(\mathbf{q})=[\mathbf{RC}(\mathbf{q})]^2\frac{1}{1-\mathbf{RC}(\mathbf{q})}. \tag{6.4}$$

Equation (6.4) is general. We now determine $\mathbf{C}_{ij}$ in terms of $\mathbf{T}_{ij}$ in the convolution approximation. If only graphs without crossing lines are to be counted, then only the following contribution to $\mathbf{C}_{ij}$ arise

(a) any number of v_{ij} bonds between i and j; that is, all "ladders" of v_{ij} [Fig. 12(a)];
(b) any ladders of graphs with articulation points with the exception of a single T_{ij}-type of graph [Fig. 12(b)];
(c) any mixture of (a) and (b) graphs [Fig. 12(c)].
In order to sum these graphs we multiply each line arriving at i by p and each line arriving at j by p', p and p' being arbitrary variables. Then we evaluate

$$\sum_{\alpha=1}^{\infty}\sum_{\beta=1}^{\infty} p^\alpha C_{ij}{}^{\alpha\beta}p'^\beta. \tag{6.5}$$

The contribution to (6.5) of the graphs with $n_{\alpha\beta}$ $T_{ij}{}^{\alpha\beta}$ bonds and the graphs with m v_{ij} bonds is then

$$\frac{1}{m!}[pv_{ij}p']^m\frac{1}{n_{\alpha\beta}!}[p^\alpha T_{ij}{}^{\alpha\beta}p'^\beta]^{n_{\alpha\beta}}.$$

The sum of all the ladders of v_{ij} and $\mathbf{T}_{ij}$ bonds then contributes

$$\sum_{m=0}^{\infty}\sum_{n_{\alpha\beta}=0}^{\infty}\frac{1}{m!}[pv_{ij}p']^m\prod_{\alpha=1,\beta=1}^{\infty}\frac{1}{n_{\alpha\beta}!}[p^\alpha T_{ij}{}^{\alpha\beta}p'^\beta]^{n_{\alpha\beta}}-1$$
$$=\exp[pv_{ij}p'+\textstyle\sum_{\alpha,\beta}p^\alpha T_{ij}{}^{\alpha\beta}p'^\beta]-1.$$

Then

$$\textstyle\sum_{\alpha\beta}p^\alpha G_{ij}{}^{\alpha\beta}p'^\beta=\exp[pv_{ij}p'+\sum_{\alpha,\beta}p^\alpha T_{ij}{}^{\alpha\beta}p'^\beta]$$
$$-1-\textstyle\sum_{\alpha,\beta}p^\alpha T_{ij}{}^{\alpha\beta}p'^\beta \tag{6.6}$$

for arbitrary p and p'.

The relation (6.6) may be written in a more concise form if we introduce an angle representation $\mathbf{A}(\phi,\phi')$ of

a matrix $\mathbf{A}$ by the reciprocal relations

$$\mathbf{A}(\phi,\phi')=\sum_{n=-\infty}^{+\infty}\sum_{m=-\infty}^{+\infty}[\mathbf{A}]^{nm}e^{-in\phi}e^{+im\phi'},$$
$$[\mathbf{A}]^{nm}=\left(\frac{1}{2\pi}\right)^2\int_0^{2\pi}d\phi\int_0^{2\pi}d\phi'\,e^{+in\phi}e^{-im\phi'}\mathbf{A}(\phi,\phi'), \tag{6.7}$$

where $[\mathbf{A}]^{nm}=0$ for n or $m\leq 0$. Writing $p=e^{-i\phi}$ and $p'=e^{+i\phi'}$, we obtain

$$\mathbf{G}_{ij}(\phi,\phi')=\exp[\beta\mathbf{v}_{ij}+\mathbf{T}_{ij}(\phi,\phi')]-1-\mathbf{T}_{ij}(\phi,\phi'), \tag{6.8}$$

where the matrix $\mathbf{v}_{ij}$ has only its 1-1 element nonvanishing and equal to v_{ij}. Equations (6.4) and (6.8) define a nonlinear convolution integral equation both in configuration and angle space for $\mathbf{C}_{ij}$ or $\mathbf{T}_{ij}$. If the $\mathbf{R}$ matrix is calculated by approximating all the semi-invariants by a single constant, Eqs. (6.4) and (6.8) reduce to scalar equations for a single nonvanishing component (ϕ_0,ϕ_0) in angle space and are then equivalent formally to Meeron's equation for imperfect gases.[9] These equations lead then to the remarkable result proved by Green[12] that $\mathbf{G}(\mathbf{q})(\phi_0,\phi_0)$ diverges for $q\to 0$ like $1/q$, thus giving an order correlation varying like $1/r^2$. This result is reminiscent of the value $1/r^{7/4}$ obtained by Domb and Sykes.[13] Of course, the averaging of the semi-invariants is not *a priori* a valid approximation but it is interesting to note that due to the nonlinear character of the relations (6.4) and (6.8) a behavior like a $1/q$ divergence (which might be related to a logarithmic divergence for the specific heat) may arise while this would never be the case in an approximation of the perturbation series such as that of Callen and Horwitz or Brout's spherical model. This, in our opinion, would justify a more extensive study of the nodal expansion of the Ising model but this is outside the scope of this paper.

VII. GENERALIZATION OF THE LINKED-CLUSTER EXPANSION—QUANTUM STATISTICS

Our analysis of perturbation expansions is based on the "propagator" formalism developed in Sec. II. It is clear that this analysis is not restricted to the Ising Model Hamiltonian. First the possible values that can be taken by μ_i are irrelevant. More important is the fact that the introduction of quantum mechanics does not alter fundamentally the formalism. Namely, if the μ_i are replaced by noncommuting operators (for instance, the components s_i^x, s_i^y, s_i^z of the spin i in the Heisenberg model of Ferromagnetism) one has to consider the operators in the "interaction representation"

$$\bar{\mu}_i(\beta')=\exp(\beta' H_0)\mu_i\exp(-\beta' H_0), \tag{7.1}$$

and, in the "Heisenberg representation,"

$$\mu_i(\beta')=\exp(\beta' H)\mu_i\exp(-\beta' H), \tag{7.2}$$

where β' is a real parameter. We have still used μ_i instead of s_i^x, s_i^y, s_i^z to simplify the notation and keep the generality of the reasoning.

One may then ask to evaluate the quantum mechanical propagator,

$$\langle O_p(\beta_1\beta_2\cdots\beta_p)\rangle=\langle T\mu_i(\beta_1)\cdots\mu_p(\beta_p)\rangle, \tag{7.3}$$

where T is the usual "time-ordering" operator placing $\mu_k(\beta_k)$ on the left or on the right of $\mu_l(\beta_l)$, respectively, if $\beta_k>\beta_l$ or $\beta_k<\beta_l$. The analysis may now be carried through entirely following the pattern of Sec. II, using time-ordered product of operator. For instance, (2.6) becomes

$$\langle O_p(\beta_1\cdots\beta_p)\rangle=\sum_{n=0}^{\infty}\frac{1}{n!}\left\langle\int_0^\beta\cdots\int_0^\beta\cdots d\beta_n T\bar{H}_{\rm int}(\beta_1)\cdots\bar{H}_{\rm int}(\beta_n)O_p\right\rangle_0\Bigg/$$
$$\sum_{n=0}^{\infty}\frac{1}{n!}\left\langle\int_0^\beta\cdots\int_0^\beta\cdots d\beta_n T\bar{H}_{\rm int}(\beta_1)\cdots\bar{H}_{\rm int}(\beta_n)\right\rangle_0. \tag{7.4}$$

If one then defines time-ordered semi-invariant by using the time-ordered generalization of (2.9), one obtains the linked-cluster expansion (2.11) in its time-ordered generalization. General expansions for thermodynamical quantities follow in a straightforward manner as well as variational principles[14] and "Ward identities".

A detailed example of the quantum mechanical linked cluster expansion as applied to the Heisenberg model of ferromagnetism is differed to a separate publication. If one applies this method to a system of fermions by using the creation and annihilation of a particle a_k, $a_k^\dagger$ one obtains again the expansion used by Brout and the author[3] and its generalization to bosons as well.

ACKNOWLEDGMENTS

We wish to thank R. Brout, G. Horwitz and R. Stinchcombe for many discussions covering all parts of this work.

APPENDIX A

G Factor of Graph

Consider a term arising from the nth order term in the expansion of the numerator of (2.4). We write this term symbolically in the following way

$$\langle\bar{a}\cdot\bar{b}\cdot\cdot;\bar{c}\cdot\cdot\bar{d}\cdot;e\cdot f\cdot\cdot;g\cdot h\cdot\cdot;O_p\cdot\cdot\rangle_0. \tag{A1}$$

[12] M. Green, J. Chem. Phys. **33**, 1403 (1960).

[13] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A235**, 247 (1956).

[14] See for instance J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

FIG. 13. Graph corresponding to the term represented by (A1).

Here, each semicolon separates two interactions $v_{ij}\mu_i\mu_j$. The μ_i factors are represented by letters a, b, c, d, e, f. and an mth order semi-invariant by a contraction sign of bars and superscript dots, etc. O_p is any p-body operator and in example (A1) has only one spin index contracted with interaction factors. The graph corresponding to (A1) is the fourth-order graph represented in Fig. 13.

All the terms of the expansion are obtained if one draws all possible sets of contraction signs in any order. Many of these however give rise to an identical graph representation.
These are

(1) All the terms differing from a given one by a permutation of the n interactions. This contributes a factor $n!$ to G;
(2) All the terms differing by an interchange of the two contractions ending in the same interaction. For instance, the two terms

$$\langle \bar{a}\cdot\bar{b}^{\cdot\cdot};\ \bar{c}^{\cdot\cdot}\bar{d}^{\cdot};\ e^{\cdot}f^{\cdot\cdot};\ g^{\cdot}h^{\cdot\cdot};\ O_p^{\cdot\cdot}\rangle_0,$$
$$\langle \bar{a}\cdot\bar{b}^{\cdot\cdot};\ \bar{c}^{\cdot\cdot}\bar{d}^{\cdot};\ e^{\cdot\cdot}f^{\cdot};\ g^{\cdot}h^{\cdot\cdot};\ O_p^{\cdot\cdot}\rangle_0,$$

are represented by the same diagram drawn in Fig. 13. In general, this contributes a factor 2^n to G.
(3) In counting all the diagrams with a factor $2^n n!$ we have overcounted all the terms which are transformed into themselves under the operations performed in (1) and (2). For instance, a permutation of a, b and c, d or of e, f and g, h in the term (A1) does not lead to a new term of the expansion. Thus, we must divide the combinatorial factor $2^4\cdot 4!$ by 4. In general, we clearly have to divide the factor $2^n n!$ by the number g of symmetry operations that transform the graph into itself. So

$$G=2^n n!/g. \tag{A2}$$

APPENDIX B

We shall prove (3.5) and some topological properties of the diagrams.

We recall from Sec. III that the energy may be evaluated by considering all closed topologically different

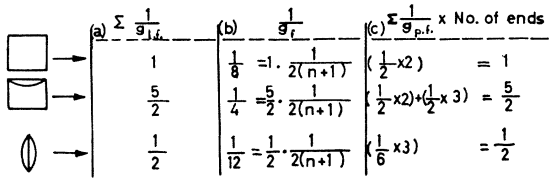

FIG. 14. Symmetry factor of graphs.

diagrams and summing all the different graphs (with their corresponding factors) obtained by fixing in these diagrams successively each line. The result is to be multiplied by $\frac{1}{2}$.

(a) We characterize the sum $\sum 1/g$ obtained in that way by the index l.f. (line fixed). If we compare this factor with the g factor of the same topological graph considered as free ($g_{f.}$), we have

$$\sum 1/g_{l.f.}=2(n+1)/g_{f.}, \tag{B1}$$

where $(n+1)$ is the number of lines of the closed graph. (Fig. 14). Indeed, (3.5) is obvious if all the graphs obtained by the fixing of a line are different, if some graphs are identical, this is still true because the factor reducing the left hand side of (3.5) is then accounted for by the enlarged symmetry factor $g_{f.}$. Relation (B1) was used in Sec. IV in order to study the free energy.

(b) Consider now the sum of $1/g$ obtained by fixing a vertex instead of line and multiplying each graph by the number of lines terminating at the fixed vertex. The same reasoning that led to (B1) leads to

$$\sum(1/g_{p.f.})\times\text{number of ends}$$
$$=\text{total number of ends}\times(1/g_{f.})=2(n+1)/g_{f.}, \tag{B2}$$

where the index p.f. means "point fixed" (Fig. 14). The last equality in (B2) results from the fact that the total number of each is equal to twice the number of lines. Comparing (B1) to (B2), we have

$$\sum 1/g_{l.f.}=\sum(1/g_{p.f.})\times\text{number of ends.} \tag{B3}$$

From (B3) it follows immediately that we may express the energy in the form

$$\left(-\frac{E}{N}\right)=\frac{1}{2\beta}\sum_{n=1}^{\infty} nM_nG_n,$$

which is Eq. (3.5).