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Linked-Clusters Expansion in Quantum Statistics: Petit Canonical Ensemble*

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A linked-cluster expansion for the free energy in the petit canonical ensemble is presented and proved. It has the advantage of avoiding the introduction of the unknown chemical potential in the perturbation series. As a consequence of correlations among the population numbers $n(\mathbf{k})$, additional linkages representing these correlations appear. The result is used to find the ground-state energy of a many-body fermion system. This expression reduces to the Brueckner-Goldstone expansion only in the case of central forces in an isotropic system, a theorem due to Kohn, Luttinger, and Ward. It is also shown that in the random phase approximation, correlation bonds do not contribute. Finally the relation of our formalism to the Bloch-De Dominicis expansion for the grand partition function is discussed.

1. INTRODUCTION

THERE are now several studies concerning the cluster-perturbation development of quantum statistical mechanics in the grand canonical ensemble. The use of the grand ensemble is dictated by the mathematical convenience of avoiding the problem of the correlation between the population numbers $n(\mathbf{k})$ from one unperturbed state to another [i.e., $\langle n(\mathbf{k})n(\mathbf{k}')\rangle - \langle n(\mathbf{k})\rangle\langle n(\mathbf{k}')\rangle = 0$ for $\mathbf{k}\neq\mathbf{k}'$]. Here the average is taken with respect to an unperturbed grand canonical distribution. The unperturbed Hamiltonian has eigenstates which are products of one-particle eigenstates.

As is well known, there is a price to pay for this convenience. In this case, one introduces the unknown chemical potential μ which itself must be calculated in terms of the perturbing many-body forces. Thus the perturbation expansion of the grand partition function is a mixed expansion where each coefficient of a given power of the coupling constant ξ is in itself a function of ξ. Sometimes, this development is very useful; for example, in understanding the theory of quasi-particles it seems to be essential since it is μ itself which is the reference energy for quasi-particles and holes. In other cases, however, the appearance of μ is a calculational disadvantage and must be replaced by its power series in ξ. The resulting unscrambling problem is not easy. It is the purpose of this paper to present the perturbation cluster expansion in terms of the petit canonical ensemble directly and so avoid the problem of the chemical potential. Thus for direct calculation of thermodynamic functions, the present method will prove to be more useful.

It is shown in this paper, that as a consequence of correlations brought about by the condition $\Sigma n(\mathbf{k})=N$ in the petit ensemble, new kinds of cluster graphs appear in the normal development which contain "correlation" bonds. These arise because the so-called unlinked clusters do not quite factorize.

In Sec. 2, we present in detail the few lowest orders of perturbation theory together with obvious generalizations which then lead to a general statement of the cluster theorem, and the proof follows immediately. As an application in Sec. 3 we prove that the expansion of Brueckner and Goldstone[1] is valid for the ground-state energy of a Fermi gas in the case of central forces in an isotropic and homogeneous system (a theorem due to Kohn, Luttinger, and Ward[2,3]), but in general is not true. As another application we show in Sec. 4 that in the random phase approximation no correlation bonds occur and consequently in this approximation one may use the unperturbed chemical potential in each term

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[1] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).
[2] W. Kohn and J. M. Luttinger, Phys. Rev. **118**, 41 (1960).
[3] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

of the perturbation series, a result announced in a previous paper.[4]

It is of interest to establish the connection between the methods adopted in this paper and those of Bloch and De Dominicis.[5] This is presented in Appendix D.

Throughout this paper we use Fermi statistics only.

2. LINKED CLUSTER EXPANSION

A. Introductory Discussion

The starting point of our analysis is to write the difference between perturbed and unperturbed free energies as[4]

$$\Delta F=F(1)-F(0)=\int_0^1\langle V\rangle_\xi d\xi, \tag{2.1}$$

where ξ is the coupling constant given by $H=H_0+\xi V$. The angular bracket symbol in (2.1) is defined for an arbitrary operator O by

$$\langle O\rangle_\xi=\frac{\mathrm{tr}e^{-\beta(H_0+\xi V)}O}{\mathrm{tr}e^{-\beta(H_0+\xi V)}}. \tag{2.2}$$

For perturbation theory, it is useful to go into interaction representation and in the usual fashion we find

$$\xi\langle V\rangle_\xi=\frac{\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\xi^{n+1}\int_0^\beta\cdots\int_0^\beta d\beta_1\cdots d\beta_n\langle TV(\beta_n)\cdots V(\beta_1)V(0)\rangle_0}{\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\xi^{n}\int_0^\beta\cdots\int_0^\beta d\beta_1\cdots d\beta_n\langle TV(\beta_n)\cdots V(\beta_1)\rangle_0}, \tag{2.3}$$

where

$$V(\beta)=e^{\beta H_0}Ve^{-\beta H_0}.$$

For orientation, we examine the first few terms in perturbation theory. To do this the denominator in (2.3) must be brought into the numerator to get an explicit function of ξ. We write

$$\xi\langle V\rangle_\xi=-\frac{1}{\beta}\sum_{n=1}^{\infty}\frac{(-\xi)^n}{(n-1)!}M_n, \tag{2.4}$$

$$-\frac{1}{\beta}M_1=\langle V(0)\rangle_0,$$

$$-\frac{1}{\beta}M_2=\int_0^\beta d\beta_1 T[\langle V(\beta_1)V(0)\rangle_0-\langle V(\beta_1)\rangle_0\langle V(0)\rangle_0], \tag{2.5}$$

$$\begin{aligned}-\frac{1}{\beta}M_3=\int_0^\beta\int_0^\beta d\beta_1 d\beta_2 T[&\langle V(\beta_1)V(\beta_2)V(0)\rangle_0\\&-\langle V(\beta_2)\rangle_0\langle V(\beta_1)V(0)\rangle_0\\&-\langle V(\beta_1)\rangle_0\langle V(\beta_2)V(0)\rangle_0\\&-\langle V(0)\rangle_0\langle V(\beta_1)V(\beta_2)\rangle_0\\&+2\langle V(0)\rangle_0\langle V(\beta_1)\rangle_0\langle V(\beta_2)\rangle_0].\end{aligned} \tag{2.6}$$

M_n is the nth semi-invariant formed from the variables $V(\beta_{n-1})$, $\cdots$, $V(\beta_1)$, $V(0)$. This is seen from the fact that

$$(\partial/\partial\xi)\ln\{\mathrm{tr}\exp[-\beta(H_0+\xi V)]\}=(\partial/\partial\xi)\sum_{n=0}^{\infty}\frac{(-\xi)^nM_n}{n!}, \tag{2.7}$$

followed by one integration in β space. This last step is permissible because of homogeneity in β space. We remark in passing that (2.7) shows the connection between techniques which rely on denominator cancellation (after differentiation) and techniques which rely on the statistical properties of semi-invariants for independent variables[6] (before differentiation). In this paper both techniques are used since it was found to be pedagogically convenient to work with the M_n's in low order, but mathematically more convenient and transparent to work with denominator cancellation in the general proof. Of course, proofs are easily interchangeable from one method to the other.

For H_0 we take the set of single-particle states and the explicit form of V is a two-body local potential. Thus, in second quantization we have

$$H_0=\sum\epsilon_{\mathbf{k}}a^\dagger(\mathbf{k})a(\mathbf{k}), \tag{2.8}$$

$$V=1\sum[v(\mathbf{q})/\Omega]a^\dagger(\mathbf{k}_1+\mathbf{q})a^\dagger(\mathbf{k}_2-\mathbf{q})a(\mathbf{k}_2)a(\mathbf{k}_1), \tag{2.9}$$

$$[a^\dagger(\mathbf{k}),a(\mathbf{k}')]+\delta_{\mathbf{k}\mathbf{k}'} \tag{2.10}$$

or in interaction representation

$$V(\beta)=1\sum[v(\mathbf{q})/\Omega]a^\dagger(\mathbf{k}_1+\mathbf{q};\beta)a^\dagger(\mathbf{k}_2-\mathbf{q};\beta)\times a(\mathbf{k}_2;\beta)a(\mathbf{k}_1;\beta), \tag{2.11}$$

$$a^\dagger(\mathbf{k};\beta)=a^\dagger(\mathbf{k})\exp[\beta\epsilon_{\mathbf{k}}],\qquad a(\mathbf{k};\beta)=a(\mathbf{k})\exp[-\beta\epsilon_{\mathbf{k}}]. \tag{2.12}$$

We shall take the direct diagonal interaction $v(0)=0$. This amounts to absorbing a constant into all one-particle energies.

We now consider the first order term (2.4). This is the exchange diagram of Fig. 1(a). For the moment, we follow the obvious generalization of Goldstone's graph notation to finite temperature in the same manner

[4] F. Englert and R. Brout (to be published).

[5] C. Bloch and C. De Dominicis, Nuclear Phys. **7**, 459 (1958).

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

as Bloch and De Dominicis. A more precise graphical description will be presented below. Figure 1(a) is a member of the sum M_1 given by

$$\langle V\rangle_0=-\sum_{\mathbf{k}_1\mathbf{k}_2} v(\mathbf{k}_1-\mathbf{k}_2)\langle n_1n_2\rangle, \tag{2.13}$$

where we abbreviate $n_i=n(\mathbf{k}_i)$. For simplicity we ignore spin indices. Thus, for spin $\frac{1}{2}$ all exchange terms written in this paper are present for parallel spins only.

In Appendix B, we show the following:

$$\langle n_1n_2\rangle_0=\langle n_1\rangle_0\langle n_2\rangle_0+O(1/N);\quad \mathbf{k}_1\neq\mathbf{k}_2. \tag{2.14}$$

For the case $\mathbf{k}_1=\mathbf{k}_2$, then $\langle n_1^2\rangle_0-\langle n_1\rangle_0^2=O(1)$, however, this is of no interest since the term $\mathbf{k}_1=\mathbf{k}_2$ contributes only $O(1)$ to (2.13). Since it is desired to find $\lim_{N\to\infty}(F/N)$, such contributions may be neglected.

In going from (2.13) to (2.14), we are reducing an "operator" graph to a "c-number" graph. Since this reduction is the essential content of our analysis we shall now dwell at some length on this point.

Operator Graphs

It is required to characterize expectation values of products

$$\langle V(\beta_{n-1})\cdots V(\beta_1)V(0)\rangle_0.$$

This is easily done by noting that if a particle goes up it must come down, i.e., if a particle in a state is annihilated, at some later stage in the product a particle must be created in this same state and vice versa. If this occurs for a given state, then the term considered is the average of a product of number operators multiplied by a c-number function of $\beta_1,\ \cdots\beta_{n-1}$. We write it in the form

$$\varphi\{\beta_1,\cdots\beta_n;\, v(\mathbf{q}_1)\cdots v(\mathbf{q}_n)\}\langle g\rangle_0\quad g=n_1'n_2'\cdots n_n',$$

where

$$n_i'=n_i(=a_i^\dagger a_i)\quad\text{or}\quad n_i'=n_1-1(=-a_ia_i^\dagger),$$

according to whether the annihilation operator appears earlier or later than the creation operator. Such a term may be represented by a graph similar to a Goldstone

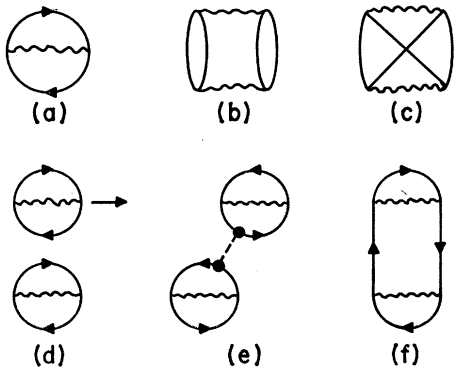

FIG. 1. Graphs arising in first and second order.

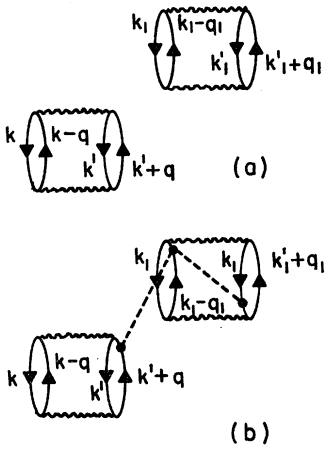

FIG. 2. A sample reduction from an "operator graph" to a "c-number graph."

graph except that the fermion line gives rise to an *operator* n_i'. For example, the g part of the graph Fig. 2(a) is

$$g=n'(\mathbf{k})n'(\mathbf{k}-\mathbf{q})n'(\mathbf{k}')n'(\mathbf{k}'+\mathbf{q})\times n'(\mathbf{k}_1)n'(\mathbf{k}_1-\mathbf{q}_1)n'(\mathbf{k}_1')n'(\mathbf{k}_1+\mathbf{q}_1).$$

If there are n ($n>1$) pairs of creation-destruction operators occurring for a given state, the term considered may be represented by the sum of the graphs obtained by pairing in all possible ways the creation and annihilation operators into number operators. This theorem, which enables us to treat on the same footing graphs with or without repeated indices when one performs sums is simply a reinterpretation of a theorem of Bloch and De Dominicis and is demonstrated in Appendix A. Such a statement implies ignoring exclusion principle in intermediate states, a point to be discussed in further detail on a specific example.

c-Number graphs

We now express the contribution of "operator" graphs in terms of "c-number" graphs. This is done by expanding the factor $\langle g\rangle_0$ in terms of the semi-invariants generated by the number operators.

The semi-invariants $M^{(\nu)}(\mathbf{k}_1\cdots\mathbf{k}_\nu)$ may be defined in analogy to the Ursell functions in statistical mechanics.

$$\begin{aligned}&\langle n'(\mathbf{k}_1)\rangle_0=M^{(1)}(\mathbf{k}_1),\\&\langle n'(\mathbf{k}_1)n'(\mathbf{k}_2)\rangle_0=M^{(2)}(\mathbf{k}_1,\mathbf{k}_2)+M^{(1)}(\mathbf{k}_1)M^{(1)}(\mathbf{k}_2),\\&\langle n'(\mathbf{k}_1)n'(\mathbf{k}_2)n'(\mathbf{k}_3)\rangle_0\\&\quad=M^{(3)}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)+M^{2}(\mathbf{k}_1,\mathbf{k}_2)M^{(1)}(\mathbf{k}_3)\\&\qquad+M^{(2)}(\mathbf{k}_1,\mathbf{k}_3)M^{(1)}(\mathbf{k}_2)+M^{(2)}(\mathbf{k}_2,\mathbf{k}_3)M^{(1)}(\mathbf{k}_1)\\&\qquad\quad+M^{(1)}(\mathbf{k}_1)M^{(1)}(\mathbf{k}_2)M^{(1)}(\mathbf{k}_3);\end{aligned} \tag{2.15}$$

the generalization in higher order is the usual Ursell prescription.[7]

We represent a semi-invariant of order ν by con-

[7] B. Kahn, thesis, Amsterdam, 1938 (N. V. Noord-Hollandsche Uitgeversmaatschappij), Chap. III.

necting the ν lines of momenta $k_1 \cdots k_\nu$ which represent the operators $n(k_1)\cdots n(k_\nu)$ by a dashed line.

In Appendix B, we prove two statements. The first is that Z_0 is the generating function of the M^ν:

$$M^{(\nu)}(\mathbf{k}_1,\cdots,\mathbf{k}_\nu) = \partial^\nu \ln Z_0/\partial(-\beta\epsilon(k_1))\cdots\partial(-\beta\epsilon(\mathbf{k}_\nu)), \quad (2.16)$$

where $Z_0=\mathrm{tr}e^{-\beta H_0}$. The second statement is with regard to the order of magnitude of $M^{(\nu)}$; if p is the number of distinct $\mathbf{k}_i$ in $M^{(\nu)}(\mathbf{k}_1,\mathbf{k}_2\cdots\mathbf{k}_\nu)$, one has

$$M^{(\nu)}(\mathbf{k}_1\cdots\mathbf{k}_\nu)=O(1/N^{p-1}). \quad (2.17)$$

Each operator graph gives rise to a large number of graphs generally with dashed lines. These graphs may be considered as representing c numbers and the g factors are products of occupation number averages and semi-invariants of order greater than one. For example the graph Fig. 2(a) gives rise to the graph of Fig. 2(b) among others, the g factor of which is

$$g=\langle n'(\mathbf{k})\rangle_0\langle n'(\mathbf{k}-\mathbf{q})\rangle_0\langle n'(\mathbf{k}')\rangle_0\langle n'(\mathbf{k}_1)\rangle_0 \times\langle n'(\mathbf{k}_1'+\mathbf{q}_1)\rangle_0 M^{(3)}(\mathbf{k}'+\mathbf{q},\,\mathbf{k}-\mathbf{q}_1,\,\mathbf{k}_1').$$

Substantial simplification occurs if one notices that the semi-invariants of order greater than 1 are the same when expressed either in terms of n or n'. This is established in Appendix C.

With this notation, we now turn to the first few terms in perturbation theory beginning with M_2. There are two kinds of "operator graphs" which arise in this order, the linked graphs of Fig. 1(b) and 1(c) and the unlinked graphs of Fig. 1(d). Note that Fig. 1(b) and 1(c) are not contained in $\langle V(\beta)\rangle_0\langle V(0)\rangle_0$. This is general. In nth order a totally linked graph is contained only in $\langle V(\beta_{n-1})\cdots V(\beta_1)V(0)\rangle_0$ and in no other products in M_n. Also note that Fig. 1(b) has a positive sign and Fig. 1(c) a negative sign because of one extra commutation. This is an example of Wick's theorem that the sign of a graph is $(-1)^l$ where l is the number of closed loops. Explicitly

$$\text{Fig. 1(b)} \to [v(\mathbf{q})]^2/\Omega^2\int_0^\beta d\beta'\{\exp[-\beta'(\epsilon(\mathbf{k}_1+\mathbf{q}) +\epsilon(\mathbf{k}_2-\mathbf{q})-\epsilon(\mathbf{k}_1)-\epsilon(\mathbf{k}_2))] \times\langle n'(\mathbf{k}_1+\mathbf{q})n'(\mathbf{k}_2-\mathbf{q})n'(\mathbf{k}_1)n'(\mathbf{k}_2)\rangle\} \quad (2.18)$$

$$\text{Fig. 1(c)} \to -[v(\mathbf{q})/\Omega][v(\mathbf{k}_1+\mathbf{k}_2-\mathbf{q})/\Omega] \times\int_0^\beta d\beta'\{\exp[-\beta'(\epsilon(\mathbf{k}_1+\mathbf{q}) +\epsilon(\mathbf{k}_2-\mathbf{q})-\epsilon(\mathbf{k}_1)-\epsilon(\mathbf{k}_2))] \times\langle n'(\mathbf{k}_1+\mathbf{q})n'(\mathbf{k}_2-\mathbf{q})n'(\mathbf{k}_1)n'(\mathbf{k}_2)\rangle\}. \quad (2.18a)$$

The reduction of (2.18) and (2.18a) to "c-number" graphs is immediate since both graphs give $O(N)$ to the energy and hence all semi-invariants of order ν ($\nu>1$) contained in $\langle n'(\mathbf{k}_1+\mathbf{q})n'(\mathbf{k}_2-\mathbf{q})n'(\mathbf{k}_1)n'(\mathbf{k}_2)\rangle$ may be set equal to zero in the infinite limit (Appendix B). We now turn to Fig. 1(d). This graph is contained in both $\langle V(\beta)V(0)\rangle_0$ and $\langle V(\beta)\rangle_0\langle V(0)\rangle_0$. Explicitly it arises in the term in M_2 which is

$$\text{Fig. 1(d)} \to [v(\mathbf{k}_1-\mathbf{k}_2)/\Omega][v(\mathbf{k}_3-\mathbf{k}_4)/\Omega] \times[\langle n(\mathbf{k}_1)n(\mathbf{k}_2)n(\mathbf{k}_3)n(\mathbf{k}_4)\rangle_0 -\langle n(\mathbf{k}_1)n(\mathbf{k}_2)\rangle_0\langle n(\mathbf{k}_3)n(\mathbf{k}_4)\rangle_0]. \quad (2.19)$$

This term contains four summations and two factors of $O(1/\Omega)$ and hence appears of $O(N^2)$. The square bracket however is $O(1/N)$ through the use of (2.15) and (2.17). In fact, reduction to "c-number" graphs gives this result automatically.

$$\begin{aligned}&\langle n(\mathbf{k}_1)n(\mathbf{k}_2)n(\mathbf{k}_3)n(\mathbf{k}_4)\rangle_0-\langle n(\mathbf{k}_1)n(\mathbf{k}_2)\rangle_0\langle n(\mathbf{k}_3)n(\mathbf{k}_4)\rangle_0\\ &\quad=M^{(2)}(\mathbf{k}_1,\mathbf{k}_3)M^{(1)}(\mathbf{k}_2)M^{(1)}(\mathbf{k}_4)\\ &\qquad+M^{(2)}(\mathbf{k}_1,\mathbf{k}_4)M^{(1)}(\mathbf{k}_2)M^{(1)}(\mathbf{k}_3)\\ &\qquad+M^{(2)}(\mathbf{k}_2,\mathbf{k}_3)M^{(1)}(\mathbf{k}_1)M^{(1)}(\mathbf{k}_4)\\ &\qquad+M^{(2)}(\mathbf{k}_2,\mathbf{k}_4)M^{(1)}(\mathbf{k}_1)M^{(1)}(\mathbf{k}_3)+O(1/N^2). \quad (2.20)\end{aligned}$$

Thus complete reductions to "c-number" graphs gives the linked term Fig. 1(e). Notice that there are no graphs with a dashed line connection within an already linked part [i.e., the term $M(\mathbf{k}_1,\mathbf{k}_2)$ in (2.19) is cancelled out]. In case the unlinked parts have indices in common, we note that

$$\begin{aligned}&\langle n(\mathbf{k}_1)n(\mathbf{k}_2)n(\mathbf{k}_1)n(\mathbf{k}_4)\rangle_0-\langle n(\mathbf{k}_1)n(\mathbf{k}_2)\rangle_0\langle n(\mathbf{k}_1)n(\mathbf{k}_4)\rangle_0\\ &\quad=M^{(2)}(\mathbf{k}_1,\mathbf{k}_1)M^{(1)}(\mathbf{k}_2)M^{(1)}(\mathbf{k}_4)+O(1/N). \quad (2.21)\end{aligned}$$

Comparing (2.21) and (2.20) we see that if two indices in the diagram are in common (contracted indices), the order of magnitude of the semi-invariant is increased by one factor of N. However, the number of terms with contracted indices is $1/N$ of those with noncontracted indices. The result is that one may use Eq. (2.20) even when two of the arguments in a $M^{(\nu)}$ are identical. This prescription in fact gives exactly the coefficient of $O(1/N)$ in the square bracket in (2.19). Thus Fig. 1(e) is also correct if the connected lines have identical indices.

Notice that in Eq. (2.17) there do not appear the "anomalous graphs" of Kohn and Luttinger,[2] a sample of which is drawn in Fig. 1(f) for reference. It will be shown in our general discussion that anomalous graphs do not appear. Rather, in the notation of the present paper they arise as dashed lines between fermion lines of the same momenta.

In other words the anomalous graph is a different graphical notation of one kind of our dashed line graphs. In the free energy, it is evidently more convenient to introduce the present notation and so include in one diagram both identical and different indices. In the grand partition function, however, the graphs with different indices vanish by virtue of the independence of the n_k so the anomalous graphs may be more convenient.

As the third order graphs contain no new principle, we draw a few dashed line graphs which arise directly in Fig. 3. We remark in passing that there are two kinds of dashed line graphs which occur when there are three unlinked parts, represented in Fig. 3(a) and 3(b). Fig. 3(b) contains M_{123} and Fig. 3(a) $M_{12}M_{35}$. Note both are the same order of magnitude in N, i.e., both contribute $O(N)$ to $F(1)$.

In fourth order, in addition to the types of terms already mentioned, there appears the first violation of the Pauli exclusion principle. As there appears to be inadequate discussion in the literature of this point, we go into some detail. The first point is that one is at freedom to include among intermediate states, wave functions which either obey or do not obey the exclusion principle. The reason for this freedom is the following. The perturbation Hamiltonian is a totally symmetric operator with respect to the permutation group. Thus, if one begins with an antisymmetrized product the only nonvanishing matrix elements are those which connect wave functions of the same symmetry type. Therefore, if the unperturbed wave function is an antisymmetrized product, the perturbation itself will pick out the antisymmetrized parts of the intermediate-state wave functions. As this argument is abstract, we shall illustrate both points of view in the fourth order calculation. The argument given is to be considered a pedagogical amplification of the excellent analysis contained in Goldstone's paper.

We first consider the case where the exclusion principle is built into the intermediate states from the outset. Now consider the operator graphs that arise in $\langle V^4\rangle_0$ and $\langle V^2\rangle_0\langle V^2\rangle_0$ corresponding to the two unlinked parts in Fig. 4(a).[8] Since the exclusion principle is obeyed in intermediate states, no indices may be in common in the unlinked parts in the expression for $\langle V^4\rangle_0$. This is, of course, not the case in $\langle V^2\rangle_0\langle V^2\rangle_0$. Therefore, there is incomplete cancellation in the contribution to M_4 from $\langle V^4\rangle_0-\langle V^2\rangle_0\langle V^2\rangle_0$ from diagrams of the type 4(a) with an index in common. The result may be rediagrammed in Goldstone's manner as Fig. 4(b), where the sign of the graph is correctly given by Wick's algebra.

The alternative approach is to ignore the exclusion principle in intermediate states. In this case both

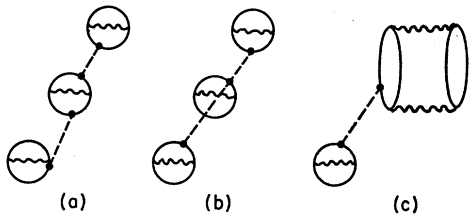

FIG. 3. Prototypes of the unlinked graphs arising in third order.

[8] Here we have considered as different those graphs which differ by a different ordering of the interaction (wavy) lines. This facilitates the discussion and, as will be shown in the formal proof, allows a complete elimination of anomalous graphs.

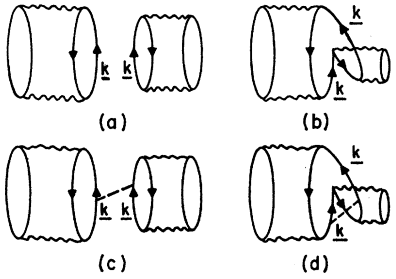

FIG. 4. Graphs which give rise to Pauli exclusion principle violating terms in the free energy.

diagrams 4(a) and 4(b) appear in $\langle V^4\rangle_0$ but with opposite signs and only 4(a) in $\langle V^2\rangle_0\langle V^2\rangle_0$ which again leaves only 4(b) with the factor $[-\langle n(\mathbf{k})\rangle_0^2]$.

The above notation turns out to be inconvenient in the general formulation of the problem. In fact, the Bloch-De Dominicis theorem on identical indices gives a total of three connected graphs in the formal reduction from "operator graphs" to "c-number" graphs. Firstly, Fig. 4(b) arises with the factor $[-\langle n(\mathbf{k})\rangle_0^2]$. Moreover, a graph which violates the Pauli exclusion principle has repeated indices within the graph; this means that a term $[-M^{(2)}(\mathbf{k},\mathbf{k})]$ arises which is an internal dashed line within the graph itself. This is Fig. 4(d). Finally, Fig. 4(c) which contains $[+M^{(2)}(\mathbf{k},\mathbf{k})]$ also appears. Figure 4(c) and 4(d) cancel one another leaving Fig. 4(b) alone.

The above cancellation is again inconvenient in the proof of reduction to the Brueckner-Goldstone expansion. For this reason, we shall present the final theorem in a manner which eliminates Fig. 4(d). This is to interpret Fig. 4(b) as an operator graph, with the factor $[-\langle n^2(\mathbf{k})\rangle_0]=[-\langle n(\mathbf{k})\rangle]$. Then Fig. 4(d) does not arise but Fig. 4(c) remains. Figure 4(b)+Fig. 4(c) gives the factor $[-\langle n(\mathbf{k})\rangle_0^2]$.

B. Theorem

With this qualitative sketch we are now in a position to state the general cluster expansion. This is given by a set of rules which corresponds to the formula (2.23) below.

1. In nth order draw all graphs, in a specified time-ordered sequence linked and unlinked, containing n interaction lines. Each interaction line carries a factor $-v(\mathbf{q})$. The linked parts contain all violations of the Pauli exclusion principle, but *no* anomalous graphs. The unlinked parts are singly connected by dashed lines. The definition of singly connected is a connection in which two otherwise unlinked parts are connected by one and only one dashed line.

2. To each hole or particle line not connected by a dashed line associate a factor of $\langle n(\mathbf{k})\rangle_0$ or $\langle 1-n(\mathbf{k})\rangle_0$, respectively. Here we drop our $n'(\mathbf{k})$ notation in favor of the conventional notation with the sign of Rule 4.[9]

[9] In this way, a Fourier analysis of the graphs becomes impossible due to the fact that the range of integration of intermediate β_i's are not independent. This may be an inconvenience especially when all dashed lines may be avoided, as is in the grand partition function.

To a dashed line connecting $\mathbf{k}_1\cdots\mathbf{k}_\nu$ associate the semi-invariant $M^{(\nu)}(\mathbf{k}_1,\cdots\mathbf{k}_\nu)$ including terms where $\mathbf{k}_1\cdots\mathbf{k}_\nu$ are the same states. [This rule is to be applied with the convention that Pauli exclusion graphs contain only *one* hole or particle for each repeated index in accordance with the above discussion. This is established below.]

3. A hole line running from β_i to β_j $(\beta_i>\beta_j)$ is associated with the propagator $\exp(\beta_i-\beta_j)\epsilon(\mathbf{k})$. A particle line running from β_i to β_j $(\beta_i<\beta_j)$ is associated with $\exp(\beta_i-\beta_j)\epsilon(\mathbf{k})$.

4. The sign of a graph is $(-1)^{l+k}$ where l is the number of closed fermion loops and k is the number of hole lines which are not connected by dashed lines. Here each hole line in a Pauli exclusion graph is counted separately. Divide the result by n and integrate over $\beta_1\cdots\beta_{n-1}$.

C. Proof

We now present a formal proof of these points. The program is the following. In the first paragraph below we establish that no disconnected graphs occur. In the second paragraph we isolate contributions of $O(N)$ and show that these are the singly connected graphs only. Rule 2 is an automatic consequence of this analysis. Rules 3 and 4 are automatic consequences of the Wick theorem as applied to the many-body problem by Goldstone and Bloch and De Dominicis and hence are not further discussed here. The division by n in Rule 4 is a consequence of integration with respect to the coupling constant as seen from Eq. (2.23). Finally, in the last paragraph we take up the question of the anomalous and Pauli exclusion violation graphs in our general formalism.

Reduction to Connected Graphs

Disconnected "operator" graphs do not give rise to factorized integrals in (2.1), but disconnected "c-number" graphs do (in this context a dashed line is considered a connection). Evidently, all the graphs which are not connected to the first one in the numerator of (2.1) comprise a sum of graphs multiplying each connected graph. This sum is obviously the value of the denominator and hence the usual cancellation argument of the disconnected graphs obtains. The expansion of the free energy may then be written, after integration over the coupling constant,

$$F(1)=F(0)+\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\frac{1}{n}\int_0^\beta\cdots\int_0^\beta d\beta_n\cdots d\beta_1 \times\langle TV(\beta_n)\cdots V(\beta_1)V(0)\rangle_{0,c}, \quad (2.22)$$

where the c index means restriction to connected graphs in the sense given above.

Elimination of Unnecessary Graphs

A large number of graphs which occur in (2.22) may be dropped because they give vanishingly small contributions in the limit of an infinitely large system. This comes from the two following facts

1. Each connected graph without dashed lines if of $O(N)$.

2. Each dashed line connecting fermion lines gives rise to a factor of order $O((1/N)^{\nu-1-s})$, where s is the number of identical indices (i.e., $\nu-s$ is the number of distinct indices.)

The first statement is a consequence of the conservation of momentum. The second is shown in Appendix B.

As we do not need graphs of order less than N, the following graphs may be disregarded without further discussion.

(1) All graphs containing dashed lines inside an otherwise connected graph (this means a graph which would be connected if all dashed lines were removed) except those connecting lines with identical indices ("anomalous" or "Pauli exclusion violating" graphs).

(2) All graphs in which otherwise disconnected graphs are connected by more than one dashed line. This is obviously true when the dashed lines connect states with different indices. It is also true when they connect states with same indices because these give rise to an extra power of $(1/N)$ for each restriction to identical indices. This gives rise to the same order of $(1/N)$ as those connecting fermion lines with different indices.

Thus, except for "anomalous" or "Pauli exclusion violating" graphs the only graphs which occur are

1. Connected graphs without dotted lines; these we call linked [e.g., Fig. 5(a)].

2. Linked graphs singly connected by dashed lines [Fig. 5(b)].

It is easily verified that all these graphs are of order N, so that the denominator in (2.22) automatically cancels all terms which are of higher order in N.

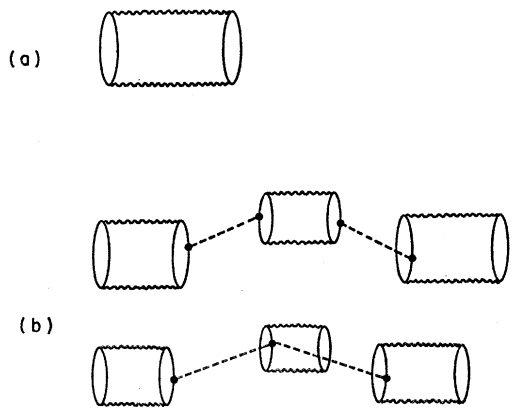

FIG. 5. Linked graphs and singly connected graphs.

Elimination of Anomalous Graphs and Discussion of Pauli Exclusion Violating Graphs

It is possible to eliminate linked graphs which contain dotted lines, within as well as anomalous graphs. This is more easily achieved if we consider separately the contributions of graphs with different time ordering or equivalently if we write (2.22) in the form

$$F(1)=F(0)+\sum_{n=0}^{\infty}\frac{(-1)^n}{n}\int_0^{\beta}\cdots\int_0^{\beta_2}d\beta_n\cdots d\beta_1 \times\langle V(\beta_n)\cdots V(\beta_1)V(0)\rangle_{0,c}.$$

The graphs for (2.23) are the same as those for (2.22) except that graphs with different time ordering are to be considered different. Now a graph with a dashed line inside occurs because a given $n'(\mathbf{k})$ occurs several times; however considered as an operator-graph $[n'(\mathbf{k})]^m=n'(\mathbf{k})$; $(-1)^{m+1}n'(\mathbf{k})$ or 0 according to whether all fermion lines with momentum k are going backwards in time (hole line), forward (particle line) or if some are going forward and some backward. We thus consider a graph with several hole lines (or particle lines) with the same momentum as containing only one hole (or one particle line). In this way all "anomalous" graphs vanish and "Pauli exclusion violating" graphs are simplified in such a way that no dashed lines occur inside a linked graph.[9]

3. THE BRUECKNER-GOLDSTONE EXPANSION

The previous expansion gives a perturbation series for the ground-state energy of a many-body fermion system when one takes the limit $\beta\rightarrow\infty$. This expansion contains in addition to the Brueckner-Goldstone expansion all the graphs connected by dashed lines in this limit; the latter contribution is generally finite (and has been evaluated to second order by Kohn and Luttinger[2]). This can be seen as follows: the contribution of a graph with m unlinked parts connected with m dashed lines (singly-connected graph) may be first integrated over all momenta except those involved in the dashed line connections and integrated over intermediate β, the result is of the form

$$\beta^m\sum_{\mathbf{k}_1\cdots\mathbf{k}_m}f_1(\mathbf{k}_1)f_2(\mathbf{k}_2)\cdots f_m(\mathbf{k}_m)M(\mathbf{k}_1,\cdots,\mathbf{k}_j) \times M(\mathbf{k}_{j+1},\cdots\mathbf{k}_l)\cdots M(\mathbf{k}_p,\cdots k_m), \quad (3.1)$$

where the f are regular functions of k and the β^m factor comes from the β' integrations. From (B,4) we may write (3.1) as

$$\sum_{\mathbf{k}_1\cdots\mathbf{k}_m}f_1(\mathbf{k}_1)\cdots f_m(\mathbf{k}_m)\partial^j \times\ln Z_0/\partial[-\epsilon(\mathbf{k}_1)]\cdots\partial[-\epsilon(\mathbf{k}_j)]\cdots\partial^{(m-p)} \times\ln Z_0/\partial[-\epsilon(\mathbf{k}_p)]\cdots\partial[-\epsilon(\mathbf{k}_m)]. \quad (3.2)$$

These derivatives are singular on the unperturbed Fermi surface in the limit $\beta\rightarrow\infty$ so that in general the contribution of terms like (3.2) do not vanish in the limit $T=0$; these graphs are in fact the correction to the Brueckner-Goldstone perturbation expansion. However, when the unperturbed Fermi surface is a sphere (isotropic system) and when the interaction potential is spherically symmetric [so that $v(q)$ depends only on the magnitude of $\mathbf{q}$], we have $f_j(\mathbf{k}_j)=f_j(|\mathbf{k}_j|)$, a point due to Kohn and Luttinger,[2] on the unperturbed Fermi surface. The sum on $\mathbf{k}_j$ may then be performed in the semi-invariant since there is a nonvanishing contribution only on the unperturbed Fermi surface thereby allowing factorization of the $f(|\mathbf{k}_j|)$. Since $\sum n(\mathbf{k}_1)=N$ which is a number fixed in the averaging process, the semi-invariant is zero by the same argument as that given in Appendix C. We see then that the Brueckner-Goldstone expansion is valid in the case of isotropy. We notice, however, that this argument works only at $T=0$ so that at finite temperature, graphs with dashed lines will appear.

4. RANDOM-PHASE APPROXIMATION (RPA)

As discussed in a previous paper, RPA is equivalent to the selection of the ring diagrams only. This may be regarded as a consequence of a simplified commutation rule,

$$[\rho_q(\beta')\rho_q^{\dagger}(\beta'')]=0 \quad \text{for} \quad q\neq q', \quad (4.1)$$

where

$$\rho_q=\sum_{\mathbf{k}}a_{\mathbf{k}+q}^{\dagger}a_{\mathbf{k}}. \quad (4.2)$$

In the petit ensemble, those dotted line corrections which connect rings with the same fixed q contribute $O(1)$ to the free energy, because of the lack of summation on different q. Thus, they may be neglected in the infinite limit. This shows that in RPA the perturbation series are identical in the grand and in the petit canonical ensembles. Thus the perturbed and unperturbed chemical potentials must be set equal in each term of the perturbation series in order to obtain consistent results.

ACKNOWLEDGMENT

One of us (R.B.) should like to thank Professor W. Kohn and Professor J. M. Luttinger for pointing out the difficulty in passing to the zero-temperature limit in the grand ensemble, as a consequence of the anomalous graphs. In fact their analysis was the entire stimulus of the present work.

APPENDIX A

We shall prove that the expectation value of a product of creation-destruction operator pairs with identical indices is equal to the sum of the expectation value of all sets of operators obtained by pairing in all possible ways the creation-destruction operators into number operators. The demonstration is identical to that of the Bloch-De Dominicis theorem[5] so that we simply recall the steps of the argument.

(a) If the theorem is true for all products of $2(p-1)$ operators and for one particular product of $2p$ operators, it is true for all products of $2p$ operators. This is a consequence of the identity

$$\langle A a_k a_k^\dagger B\rangle_0 = -\langle A a_k^\dagger a_k B\rangle_0 + \langle AB\rangle_0,$$

where A and B contain products of $a_k^\dagger$ and a_k.

(b) It is true for the particular product

$$\langle a_k^{\dagger p} a_k^p\rangle_0,$$

because this product gives zero for $p>1$.

APPENDIX B

We shall identify the p-order semi-invariant of the number operator with the p-order partial differentiation of the logarithm of the unperturbed partition function.

We define the semi-invariants $M^{(n)}(\mathbf{k}_1\cdots\mathbf{k}_n)$ as in (2.15) but in terms of the n (not in the n'); thus

$$\begin{aligned}&\langle n(\mathbf{k}_1)\rangle_0 = M^{(1)}(\mathbf{k}_1),\\ &\langle n(\mathbf{k}_1)n(\mathbf{k}_2)\rangle_0 = M^{(2)}(\mathbf{k}_1,\mathbf{k}_2)+M^{(1)}(\mathbf{k}_1)M^{(1)}(\mathbf{k}_2).\end{aligned}\quad (B.1)$$

This gives the $M^{(\nu)}(\mathbf{k}_1,\cdots,\mathbf{k}_\nu)$ as a function of the moments in the following way. The rule which expresses the M in terms of the $\langle\ \rangle_0$, are the same as the reciprocal relations (B.1) except for a coefficient $(-1)^{k-1}(k-1)!$, where k is the number of groups into which the p particles are divided.[7] For example,

$$\begin{aligned}M(\mathbf{k}_1,\mathbf{k}_2) &= \langle n(\mathbf{k}_1)n(\mathbf{k}_2)\rangle_0 - \langle n(\mathbf{k}_1)\rangle_0\langle n(\mathbf{k}_2)\rangle_0,\\ M(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3) &= \langle n(\mathbf{k}_1)n(\mathbf{k}_2)n(\mathbf{k}_3)\rangle_0\\ &\quad -\langle n\,\mathbf{k}_1)n(\mathbf{k}_2)\rangle\langle n(\mathbf{k}_3)\rangle_0\\ &\quad -\langle n(\mathbf{k}_1)n(\mathbf{k}_3)\rangle_0\langle n(\mathbf{k}_2)\rangle_0\\ &\quad -\langle n(\mathbf{k}_2)n(\mathbf{k}_3)\rangle_0\langle n(\mathbf{k}_1)\rangle_0\\ &\quad +2\langle n(\mathbf{k}_1)\rangle_0\langle n(\mathbf{k}_2)\rangle\langle n(\mathbf{k}_3)\rangle_0.\end{aligned}\quad (B.2)$$

The unperturbed partition function is

$$Z_0 = \mathrm{tr}\exp[-\beta\textstyle\sum n(\mathbf{k})\epsilon(\mathbf{k})],$$

from which it is immediately found that the pth order moment is given by

$$\langle n(\mathbf{k}_1)\cdots n(\mathbf{k}_p)\rangle = (1/Z_0)\partial^n Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)]\cdots \partial[-\beta\epsilon(\mathbf{k}_p)]. \quad (B.3)$$

The function $\mathfrak{M}^{(p)}(\mathbf{k}_1\cdots\mathbf{k}_p)$, defined by

$$\mathfrak{M}^{(p)}(\mathbf{k}_1\cdots\mathbf{k}_p) = \partial_p \ln Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)]\cdots \partial[-\beta\epsilon(\mathbf{k}_p)], \quad (B.4)$$

is identical with the p-order semi-invariant

$$M^{(p)}(\mathbf{k}_1,\cdots\mathbf{k}_p),$$

as seen by straightforward differentiation:

$$\begin{aligned}\mathfrak{M}^{(1)}(\mathbf{k}_1) &= \partial\ln Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)] = (1/Z_0)\partial Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)] = \langle n(\mathbf{k}_1)\rangle_0 = M^{(1)}(\mathbf{k}_1),\\ \mathfrak{M}^{(2)}(\mathbf{k}_1,\mathbf{k}_2) &= \{\partial/\partial[-\beta\epsilon(\mathbf{k}_2)]\}(1/Z_0)\partial Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)] + (1/Z_0)\partial^2 Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)]\partial[-\beta\epsilon(\mathbf{k}_2)]\\ &= -(1/Z_0^2)\{\partial Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)]\}\{\partial Z_0/\partial[-\alpha\epsilon(\mathbf{k}_2)]\} + (1/Z_0)\{\partial^2 Z_0/\partial[-\beta\epsilon(\mathbf{k}_1)]\partial[-\beta\epsilon(\mathbf{k}_2)]\}\\ &= M^{(2)}(\mathbf{k}_1,\mathbf{k}_2).\end{aligned}\quad (B.5)$$

For higher orders we obtain all combinations (B.2) and the coefficient of a term separated in k groups comes from

$$\partial^{k-1}\left(\frac{1}{Z_0}\right) = \frac{1}{Z_0^k}(-1)(-2)\cdots(-k+1)\partial Z_0 = \frac{1}{Z_0^k}(-1)^{k-1}(k-1)!\,\partial Z_0;$$

this is exactly the coefficient occurring in (B.2).

We now prove that the order of magnitude of $M^{(\nu)}(\mathbf{k}_1,\cdots\mathbf{k}_\nu)$ is given by

$$M^{(\nu)}(\mathbf{k}_1\cdots\mathbf{k}_\nu) = O(1/N^{p-1}),$$

where p is the number of distinct $\mathbf{k}_i$ in $\mathbf{k}_i\cdots\mathbf{k}_\nu$. For simplicity of notation $\mathbf{k}_i$ will be abbreviated by the index i. We begin with $M^{(2)}$:

$$M_{1,2}{}^{(2)} = \frac{\partial^2 \log Z_0}{\partial(-\beta\epsilon_1)\partial(-\beta\epsilon_2)} = \frac{\partial\langle n_1\rangle_0}{\partial(-\beta\epsilon_2)}. \quad (B.6)$$

Notice that Z_0 may be considered a function of $-\beta\epsilon_i$ and $\beta\mu_0$ which are connected by the relation

$$\textstyle\sum_i\langle n_i\{\beta\epsilon_i,\beta\mu_0\}\rangle_0 = N, \quad (B.7)$$

which we write $f(\beta\epsilon_1\cdots\beta\epsilon_i\cdots;\beta\mu_0)=0$ and note that

$$\partial f/\partial(-\beta\epsilon_i) = O(1);\quad \partial f/\partial\beta\mu_0 = O(N). \quad (B.8)$$

In these terms we have from (2.12)

$$M_{12}{}^{(2)} = \frac{\partial\langle n_1\rangle_0}{\partial\beta\mu_0}\frac{\partial\beta\mu_0}{\partial(-\beta\epsilon_2)} = \frac{-\partial\langle n_1\rangle_0}{\partial\beta\mu_0}\frac{\partial f/\partial(-\beta\epsilon_2)}{\partial f/\partial\beta\mu_0} = O(1/N). \quad (B.9)$$

Equation (B.9) is easily generalized as follows. Define

$$M_{12\ldots n}{}^{(n)} = \frac{\partial^n \ln Z_0}{\partial(-\beta\epsilon_1)\cdots\partial(-\beta\epsilon_n)}. \quad (B.10)$$

We now prove that

$$M_{12\ldots n}{}^{(n)} = O(1/N^{n-1}),\quad \mathbf{k}_1\neq\mathbf{k}_2\cdots\neq\mathbf{k}_n. \quad (B.11)$$

We proceed by induction. $M_{12\ldots n}{}^{(n)}$ is an explicit function of $(-\beta\epsilon_1)$, $\cdots(-\beta\epsilon_n)$; $\beta\mu_0$ as is evident for

$n=2$ from (B.9). Thus

$$\frac{\partial}{\partial(-\beta\epsilon_n)}M_{12\cdots n-1}{}^{(n-1)}(-\beta\epsilon_1,\cdots;\beta\mu_0)$$

$$=\frac{\partial M_{12\cdots n-1}{}^{(n-1)}}{\partial\beta\mu_0}\frac{\partial\beta\mu_0}{\partial(-\beta\epsilon_n)}=O(1/N)$$

$$\times O(M_{12\cdots n-1}{}^{(n-1)})=O(1/N^{n-1}). \quad \text{(B.12)}$$

Finally in (B.12) we note that rather than differentiation with respect to a different $\beta\epsilon_n$ in (B.12) we could have taken $[\partial/\partial(-\beta\epsilon_i)]M_{1\cdots n-1}{}^{(1)}$, $i=1,\cdots n-1$. In this case, the dependence of μ_0 on ϵ_i is unimportant since the direct functional dependence on ϵ_i plays the key role.

We thus find

$$\frac{\partial}{\partial(-\beta\epsilon_i)}M_{12\cdots n-1}{}^{(n-1)}(-\beta\epsilon_1,\cdots;\beta\mu_0)$$

$$=O(1/N^{n-2}). \quad \text{(B.13)}$$

APPENDIX C

The semi-invariant defined by (2.15) are the same for $\nu>1$ than the semi-invariants defined by (B.2). This is evident if all the n' correspond to "hole" lines because then $n'=n$; if some n' comes from particle lines, $n'=n-1$ and some n_k in (B.2) have to be replaced by n_k-1. The contribution of the factor -1 is, however, zero because it factorizes out of the correlation functions and so is always cancelled by other terms in the semi-invariant expansion (B.2).

APPENDIX D

Connection with Bloch-De Dominicis Expansion

Our expansion is also valid for the grand partition function: In that case all semi-invariants (dashed lines) may be removed except those connecting identical indices. However, these dashed lines do not appear in Bloch-De Dominicis Expansion; this is due to another interpretation of the theorem demonstrated in Appendix A which amount to interpret in their expansion our operator graphs as c-number graphs; this gives rise to a different evaluation of Pauli exclusion violating graphs and to nonvanishing anomalous graphs. For instance we have the following equivalence between Bloch-De Dominicis graphs and ours in the grand partition function (Fig. 6).

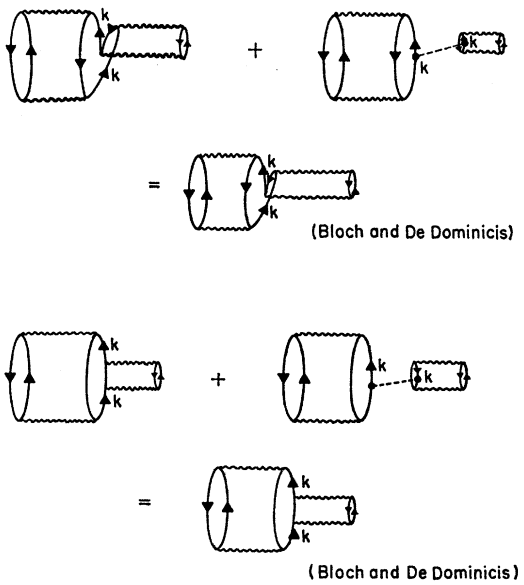

FIG. 6. Correspondence with the graphs of Bloch and De Dominicis in the grand ensemble.

We notice also that use of (2.1) is equivalent to a reduction by means of the cyclic invariance of the trace. This is due to the fact, that when perturbation expansion is valid (2.1) may be obtained by using this invariance.[10] This is the reason of the factor $1/n$ which appears in the evaluation of the graph; the contribution of one graph is equivalent to the sum of all contributions from the n graph obtained from the first one by cyclic permutation of the wavy lines.

[10] M. L. Goldberger and E. N. Adams, Chem. Phys. **20**, 240 (1952).