equations are

$$\partial_0[(-g_{00})T^{00}]=-\partial_k[(-g_{00})T^{0k}]+\tfrac{1}{2}T^{0k}\partial_k g_{00}$$

and

$$\partial_0[(-g_{00})^{1/2}T^{0k}]=-\partial_l[(-g_{00})^{1/2}T^{kl}]+\tfrac{1}{2}(-g_{00})^{1/2}T^{00}\partial_k g_{00},$$

where each form is chosen to avoid the explicit appearance of $\partial_0 g_{00}$. We confine our attention to the class of physical systems which are such that T^{kl} does not contain explicitly the time derivative of g_{00}, although it may be an explicit function of g_{00} at the same time.[2] It can be concluded that neither $(-g_{00})T^{00}$ nor $(-g_{00})^{1/2}T^{0k}$ are explicit functions of g_{00} for this distinguished class of material system, which is to say that these local quantities are the same functions of the fundamental dynamical variables as in the absence of an external gravitational field. The equation of motion for $(-g_{00})T^{00}$ now implies the equal-time commutator

$$-i\left[(-g_{00}T^{00})(x),\int(d\mathbf{x}')(-g_{00}T^{00})(x')\delta(-g_{00}(x'))^{1/2}\right]$$
$$=-\partial_k[(-g_{00})^{1/2}T^{0k}(x)\delta(-g_{00}(x))^{1/2}]-(-g_{00})^{1/2}T^{0k}(x)\partial_k\delta(-g_{00}(x))^{1/2},$$

where, it is noted, there is no explicit dependence upon $g_{00}(x)$, which indicates the consistency of the physical restriction. On setting $-g_{00}=1$, we obtain

$$-i[T^{00}(x),T^{00}(x')]=-[T^{0k}(x)+T^{0k}(x')]\partial_k\delta(\mathbf{x}-\mathbf{x}').$$

This derivation of the energy density commutator condition, for a class of physical systems, supplies a simple and general basis for what may well be considered the most fundamental equation of relativistic quantum field theory.

[2] In fact, T^{kl} must be an explicit local function of the second spatial derivatives of g_{00}.

PHYSICAL REVIEW VOLUME 130, NUMBER 1 1 APRIL 196

Zero-Temperature Properties of the Many-Fermion System*

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(Received 29 November 1962)

It is shown that the class of correlation graphs which arise in the calculation of thermodynamic properties in the canonical ensemble can be summed to give renormalized single-particle populations. In the limit of zero temperature the perturbation expansion of the energy then reduces to the adiabatic expansion of Goldstone about the *correct* model state. Arguments for the consistency of the expansion are developed for the case of the nonspherical Fermi surface.

I. INTRODUCTION

IT is the purpose of this article to explore the physical consequences of the correlation bond graphs introduced by two of us in a previous article.[1] In the latter, it was shown that the free energy could be expressed in terms of graphs which strongly resembled the graphs of Bloch and Dominicis[2] plus graphs which arose because of correlations in the single-particle state populations, $n(\mathbf{k})$. These correlations arise because of the restraint in the trace to a summation over states with fixed number of particles.

In the limit as the number of particles goes to infinity, it was found that the only correlation graphs which arise are those which are simply connected. In this article, we exploit this property to show that the elimination of correlation bonds by summation (which is possible because of the rule of simple connectivity) results in a renormalization of the populations $\langle n(\mathbf{k})\rangle_0$. In the limit of zero temperature, one then recovers for the energy a series of terms which involves the renormalized $\langle n(\mathbf{k})\rangle$. This series is precisely the usually adiabatic series of Goldstone.[3] It is, thus, shown that

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[2] C. Bloch and C. de Dominicis, Nucl. Phys. **7**, 459 (1958).
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elimination of the correlation bonds in the zero-temperature limit leads to the correct model wave function of Bethe.[4] It is also shown that the transformation to the new $\langle n(\mathbf{k})\rangle$ is volume conserving. The adiabatic expansion about this model state follows as a by-product.

This result is the same as obtained by Balian, Bloch, and de Dominicis using the grand ensemble.[5] There are two possible advantages of a formulation in the canonical ensemble. Firstly, the true chemical potential never appears at the final stage. Hence, in any given approximation to the complete series by selection of a particular set of graphs, the single-particle energies which occur in $\langle n(\mathbf{k})\rangle$ as well as the chemical potential are estimated to the same order of approximation, always in such a way as to automatically conserve the volume of the Fermi sea. Secondly, the present formalism can be studied for a finite number of particles. This condition invalidates the rule of simple connectivity. Hence, no longer does the theory reduce to an adiabatic expansion about some model state. We, thus, have a tool with which to study the validity of the nuclear shell model as a function of the number of nucleons in the system. This is proposed here as a problem for future study.

In Sec. 2, the main results of I are recapitulated. In Sec. 3, Hartree-Fock theory is derived as an example of population renormalization. In Sec. 4, the time-independent form of the theory is formulated in anticipation of the principal theorem of the paper which is announced, discussed, and proved in Sec. 5. In Sec. 6 the zero-temperature limit is shown to coincide with the Goldstone expansion.[3]

At first sight, if the interaction distorts the Fermi surface the theory might seem to be ambiguous as poles arise in the denominators of the adiabatic perturbation series. This is discussed in Sec. 7. In Hartree-Fock theory, this difficulty disappears upon single-particle energy renormalization arising from self-energy insertions. In general, the best one can do is to show that when the set of self-energy insertions on a propagator of a state at the true Fermi surface is summed, then these singularities go out for transitions in the neighborhood of the Fermi surface. In fact, the situation is the same as in the adiabatic theory for the spherical case where one essentially assumes the consistency of the calculation, i.e., the poles of the single-particle propagator on the real axis lie on the Fermi surface.

2. THE FREE-ENERGY EXPANSION

We are considering an N-particle system of interacting fermions whose Hamiltonian is

$$H=H_0+\xi V, \tag{2.1}$$

which for notational simplicity we take to be translationally invariant:

$$H=\sum \epsilon(\mathbf{k})a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}, \tag{2.2}$$

and

$$\xi V=\xi \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} [v(\mathbf{q})/\Omega]a_{\mathbf{k}+\mathbf{q}}^{+}a_{\mathbf{k}'-\mathbf{q}}^{+}a_{\mathbf{k}'}a_{\mathbf{k}}, \tag{2.3}$$

ξ being the coupling constant; we ignore spin indices except when they interest us. The free energy is given by

$$-\beta F=\ln \operatorname{tr}\exp[-\beta(H_0+\xi V)]=\ln Z, \tag{2.4}$$

where the partition sum is

$$Z=\operatorname{tr}\exp[-\beta(H_0+\xi V)]. \tag{2.5}$$

For expansion purposes there are two convenient forms in which the free energy can be written: (1) As in I, as an integral over the coupling constant of the canonical ensemble average of the interaction V.

$$F=F(\xi=0)+\int_0^{\xi} d\xi'\,\langle V\rangle_{\xi'}. \tag{2.6}$$

(2) Symbolically representing the series in interaction representation based on (imaginary) times

$$F=F_0-(1/\beta)\ln\left\langle T\exp\left[-\xi\int_0^{\beta} d\beta'\,V(\beta')\right]\right\rangle_0, \tag{2.7}$$

where T is the time-ordering operator arranging the β' in the expansion of the exponential in order of decreasing time from right to left. Operators in interaction representation are defined according to

$$O(\beta')=\exp(\beta' H_0)O\exp(-\beta' H_0). \tag{2.8}$$

$\langle O\rangle_0$ is an average of O in the unperturbed canonical ensemble of the N-particle system with Hamiltonian H_0. Thus referring to Eq. (2.7) we see that F_0 and $F(\xi=0)$ are identical. $F-F_0$ can be expanded in a semi-invariant expansion

$$F-F_0=\sum_{n=1}^{\infty}(-\xi)^n/n!M_n, \tag{2.9}$$

where

$$M_n=\partial^n F/\partial(-\xi)^n \tag{2.10}$$

are the time-ordered generalizations of semi-invariants. In I, $\langle V\rangle_{\xi}$ was similarly expanded

$$\langle V\rangle_{\xi}=-(1/\beta)\sum_{n=1}^{\infty}(-\xi)^{n-1}/(n-1)!M_n. \tag{2.11}$$

On inserting Eq. (2.11) into Eq. (2.6) and integrating, the result differs from Eq. (2.9) in that, in $\langle V\rangle_{\xi}$ one interaction is at zero and only $\beta_2\cdots\beta_n$ are integrated, and in (2.9) all the β_j are integrated. The equality of the two forms follows from the cyclic invariance of the trace. To obtain the zero-temperature limit we have found it convenient to work with the expansion (2.9).

[4] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).
[5] R. Balian, C. Bloch, and C. de Dominicis, Nucl. Phys. **25**, 529 (1961).

This point is expanded upon in Sec. 4. The results of I in view of the identity of Eqs. (2.9) and (2.11) can be transcribed directly into the expansion of Eq. (2.9).

The expansion in I was obtained by expanding the nth order term of Eq. (2.11) in diagrams. The distinctive feature of the C.E. (canonical ensemble) expansion is based on the fact that due to the restriction to fixed N, the correlation between populations of different states do not vanish even in the unperturbed C.E. average. Thus, for example,

$$\langle n_{\mathbf{k}} n_{\mathbf{k}'}\rangle_0 - \langle n_{\mathbf{k}}\rangle_0 \langle n_{\mathbf{k}'}\rangle_0 \neq 0, \quad k \neq k' \qquad (2.12)$$

in contrast to the analogous grand canonical ensemble (G.C.E.) case. This leads to the existence of an extra class of graphs involving this type of correlation. Diagrams which are unlinked in the usual sense remain in the C.E. expansion but to order N in the simple form of Cayley trees.

The unlinked diagrams are simply connected together by dashed lines; an nth semi-invariant associated with correlation of n different populations involves n dashed lines joined at a point, a correlation junction. Simple connectedness means that a cutting of any dashed line leaves the diagram divided into two disjoint pieces. It would be possible to represent the contribution of the C.E. graphs by the same rules as for the G.C.E. except for the junctions of the unlinked graphs just described. The derivation in I leads instead to a more symmetrical form in which the correlation junction can involve populations with the same as well as different indices. Figure 1(b) represents one diagram which vanishes for the G.C.E. case but not for the C.E. when $k \neq k'$; for $k = k'$ it is merely a regraphing of the G.C.E. ensemble linked graph [Fig. 1(a)]. The remaining contribution from linked parts must then differ from the G.C.E. rules. The operator graph convention, introduced for this purpose, is described below.

The central result of (2.1) was a set of rules for calculating the free energy or $\langle V\rangle_\xi$ in the nth order. We summarize the rules for the calculation of the nth order contribution to the free energy:

(1) Draw all diagrams linked and unlinked having n interactions in a specified time sequence; the unlinked diagrams are connected by means of correlations bonds into all simply connected structures. A line directed upwards (towards increasing β_i) is a particle line while a downwards directed line (towards decreasing β_i) is a hole line. Each interaction line (horizontal wavy line) represents a matrix element; the interaction lines occur at $\beta_1, \beta_2, \cdots \beta_n$. The latter variables are subsequently integrated from 0 to β maintaining the sequential order. Dashed lines join particle and/or hole lines to one junction point for each correlation function.

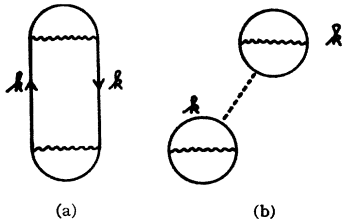


FIG. 1. Anomalous graphs in grand canonical and canonical ensembles.

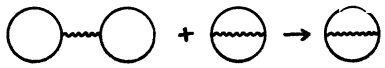


FIG. 2. Notation of HF graphs.

(2) A particle line propagating from β_1 to $\beta_2 (\beta_2 > \beta_1)$ is associated with a factor $(1-n_{\mathbf{k}}) \exp[-(\beta_2-\beta_1)\epsilon_{\mathbf{k}}]$; a hole line propagating from β_1 to $\beta_2 (\beta_1 > \beta_2)$ is associated with a factor $n_{\mathbf{k}} \exp[-(\beta_2-\beta_1)\epsilon_{\mathbf{k}}]$. The operator definition of the diagrams for the case of l_i hole (particle) lines in the state $\mathbf{k}_i$ results in $[n_{\mathbf{k}_i}]^{l_i}([1-n_{\mathbf{k}i}]^{l_i})$; while a combination of l_i hole lines and l_i' particles lines for the state $\mathbf{k}_i$ gives

$$[n_{\mathbf{k}_i}]^{l_i}[1-n_{\mathbf{k}_i}]^{l_i'} = 0, \quad l_i, l_i' \neq 0.$$

(3) A diagram with several unlinked parts, connected by correlated bonds may have one or more sets of correlated states, each set having a common correlation junction point. The contribution of a junction point joined by ν dashed lines with states with indices $\mathbf{k}_1 \cdots \mathbf{k}_\nu$ is the semi-invariant $M_\nu(\mathbf{k}_1 \cdots \mathbf{k}_\nu)$. Since

$$M_\nu = \prod_{i=1}^{\nu} [\partial/\partial(-\beta\epsilon_{\mathbf{k}_i})] \ln \operatorname{tr} \exp[-\beta \textstyle\sum n_{\mathbf{k}} \epsilon_{\mathbf{k}}],$$

we can also consider the junction point to represent $\ln \operatorname{tr} \exp[-\beta \sum n_{\mathbf{k}}\epsilon_{\mathbf{k}}] = \ln Z_0$ (Z_0 is the partition sum for the Hamiltonian H_0), and the dashed line joining a particle or hole state $\mathbf{k}_i$ to the junction point is $[\partial/\partial(-\beta\epsilon_{\mathbf{k}_i})]$.

(4) The value of the remaining lines on linked parts is to be evaluated on the operator basis of Rule 2. The contribution of a hole state $\mathbf{k}_i$ is $\langle n_{\mathbf{k}_i}\rangle$, a particle state $\mathbf{k}_i'$, $\langle 1-n_{\mathbf{k}_i'}\rangle$ for one or more particle or hole lines in each state. No state has both particle and hole lines. Thus, anomalous graphs do not appear.

(5) The sign of a diagram is $(-1)^{l+h+t}$ where l is the number of closed fermion loops, h is the total number of hole lines, and t is the number of dashed lines connected to particle states.

3. HARTREE-FOCK THEORY

In order to illustrate the nature of the results of the complete expansion, we first review what occurs when there are dotted line connections to Hartree-Fock (HF) graphs. For simplicity of notation we use one graph for both the direct and exchange term (Fig. 2).

Consider the second-order graph of Fig. 3(a) together with the HF dotted line insertions [Figs. 3(b) and 3(c)]. Because of the rule of simple connectivity, Fig. 3(d) does not arise. This simplification makes possible direct summation of the series. The factor that goes with the line indicated by an arrow in Fig. 3(a) is $\langle n_k\rangle_0 \exp(\beta'\epsilon_{\mathbf{k}})$, where β' is a temperature variable

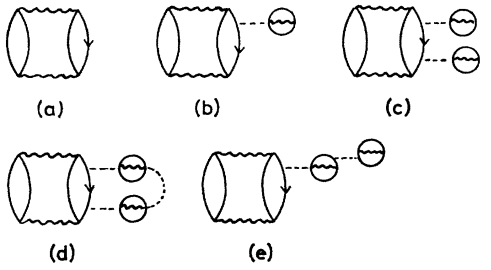


FIG. 3. Typical HF insertions.

which is eventually integrated from zero to β. The self-energy $V_{\mathrm{HF}}{}^0(\mathbf{k})$ is the value of the HF bubble for a given k as it appears in Fig. 3(a). This is given by

$$V_{\mathrm{HF}}{}^0(\mathbf{k})=\sum_{\mathbf{k}',\sigma'}\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}'\mathbf{k}\rangle\langle n_{\mathbf{k}'}\rangle_0 - \sum_{\mathbf{k}',\sigma'||\sigma}\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}'\mathbf{k}\rangle\langle n(\mathbf{k}')\rangle_0. \quad (3.1)$$

We have placed a superscript on $V_{\mathrm{HF}}{}^0(\mathbf{k})$ because of a subsequent renormalization to be introduced at a later stage.

Each of the insertions in Figs. 3(b), 3(c), $\cdots$, occur at independent times $\beta_1\cdots\beta_n$. These must be integrated in time-ordered sequence to give a factor of $(-1)^n\beta^n/n!$ Thus, the series of terms in question is

$$\exp(\beta'\epsilon_{\mathbf{k}})\Big[\langle n_{\mathbf{k}}\rangle_0-\beta\sum_{\mathbf{k}_1}V_{\mathrm{HF}}{}^0(\mathbf{k}_1)M_2(\mathbf{k}\mathbf{k}_1)+\cdots + \frac{(-\beta)^n}{n!}\sum_{\mathbf{k}_1\cdots\mathbf{k}_n}M_{n+1}(\mathbf{k}_1\cdots\mathbf{k}_n) \times V_{\mathrm{HF}}{}^0(\mathbf{k}_1)\cdots V_{\mathrm{HF}}{}^0(\mathbf{k}_n)+\cdots\Big]. \quad (3.2)$$

We now introduce the generating function introduced in connection with Rule 3 of the preceding section.

$$\begin{aligned}M_{n+1}(\mathbf{k},\mathbf{k}_1,\cdots,\mathbf{k}_n)&=[\partial^{n+1}/\partial(-\beta\epsilon_{\mathbf{k}})\partial(-\beta\epsilon_{\mathbf{k}_1})\cdots\partial(-\beta\epsilon_{\mathbf{k}_n})]Z_0\\&=[\partial^n/\partial(-\beta\epsilon_{\mathbf{k}_1})\cdots\partial(-\beta\epsilon_{\mathbf{k}_n})]\langle n_{\mathbf{k}}\rangle_0. \quad (3.3)\end{aligned}$$

Introducing this expression into (3.2) we have

$$\begin{aligned}&[\exp\beta'\epsilon_{\mathbf{k}}]\sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\Big[\sum_{\mathbf{k}'}V_{\mathrm{HF}}{}^0(\mathbf{k}')\frac{\partial}{\partial(-\beta\epsilon_{\mathbf{k}'})}\Big]^n \times[\exp\beta(\epsilon_{\mathbf{k}}-\mu_0)-1]^{-1}\\&=[\exp\beta'\epsilon_{\mathbf{k}}]\exp\Big[-\beta\sum_{\mathbf{k}'}V_{\mathrm{HF}}{}^0(\mathbf{k}')\frac{\partial}{\partial(-\beta\epsilon_{\mathbf{k}'})}\Big] \times[\exp\beta(\epsilon_{\mathbf{k}}-\mu_0)-1]^{-1}\\&=[\exp\beta'\epsilon_{\mathbf{k}}][\exp\beta(E_{\mathrm{HF}}{}^0(\mathbf{k})-\mu_{\mathrm{HF}}{}^0)-1]\\&=[\exp\beta'\epsilon_{\mathbf{k}}]\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}{}^0. \quad (3.4)\end{aligned}$$

We have introduced the unperturbed chemical potential

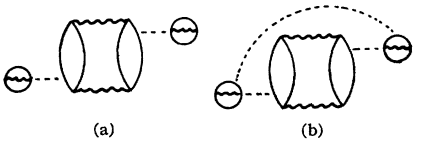


FIG. 4. Independent renormalization of propagator.

μ_0 defined according to

$$\sum\langle n_{\mathbf{k}}\rangle_0=N. \quad (3.5)$$

In Eq. (3.4), we have shown how the dotted line insertions sum to a finite displacement operator, the net effect of which is to change the single-particle energies occurring in $\langle n_{\mathbf{k}}\rangle_0$ from $\epsilon_{\mathbf{k}}$ to $E_{\mathrm{HF}}{}^0(\mathbf{k})$ where

$$E_{\mathrm{HF}}{}^0(\mathbf{k})=\epsilon_{\mathbf{k}}+V_{\mathrm{HF}}{}^0(\mathbf{k}). \quad (3.6)$$

At the same time the displacement operator also has acted on μ_0 which is to be considered as a function of the set $\{\epsilon_{\mathbf{k}}\}$ given by Eq. (3.5). In fact, we have

$$\mu_{\mathrm{HF}}{}^0=\mu^0(\{E_{\mathrm{HF}}{}^0(\mathbf{k})\}). \quad (3.7)$$

It is an easy matter to show that the transformation from $\langle n_{\mathbf{k}}\rangle_0$ to $\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}{}^0$ is volume conserving, i.e.,

$$\sum\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}{}^0=N, \quad (3.8)$$

which supplies an alternative equation for $\mu_{\mathrm{HF}}{}^0$. For the proof see Eq. (7.1).

The next stage in renormalization is to renormalize the $V_{\mathrm{HF}}{}^0(\mathbf{k})$ according to Fig. 3(e), for example. This converts the $\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}{}^0$ in (3.4) to $\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}$ which is given by

$$\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}=[\exp\beta(\epsilon_{\mathbf{k}}+V_{\mathrm{HF}}(\mathbf{k})-\mu_{\mathrm{HF}})-1]^{-1}, \quad (3.9)$$

where

$$V_{\mathrm{HF}}(\mathbf{k})=\sum\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}'\mathbf{k}\rangle\langle n(\mathbf{k}')\rangle_{\mathrm{HF}} - \sum_{\sigma||\sigma'}\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}'\mathbf{k}\rangle\langle n(\mathbf{k}')\rangle_{\mathrm{HF}}, \quad (3.10)$$

and again μ_{HF} is determined by

$$\sum\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}=N. \quad (3.11)$$

Because of the law of simple connectivity, any of the lines in a graph can be so renormalized, independently of any of the others, as indicated in Fig. 4(a). This would not be the case if non-simply-connected graphs [Fig. 4(b)] occurred. In this way all dotted line connections to HF graphs can be eliminated and $\langle n_{\mathbf{k}}\rangle_0$ replaced by $\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}$. We shall see that this procedure is general and all dotted line graphs are simply eliminated by renormalization of $\langle n_{\mathbf{k}}\rangle_0$.

It is a special feature of the Hartree-Fock theory that the factor $\exp(\beta'\epsilon_{\mathbf{k}})$ which goes with line $\mathbf{k}$ is renormalized in the same way as the factor $\langle n_{\mathbf{k}}\rangle_0$. In fact consider the set of insertions of Fig. 5. These insertions occur

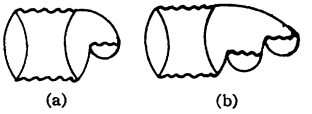
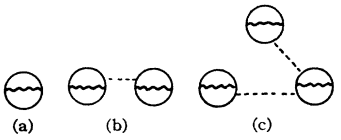


FIG. 5. Graphs which renormalize the $\exp(\beta'\epsilon_{\mathbf{k}})$ according to Eq. (3.12).

FIG. 6. Graphs contributing to the free energy in HF theory.



from zero to β' and, hence, contribute a factor

$$[\exp\beta'\epsilon_{\mathbf{k}}][1+\beta' V_{\mathrm{HF}}(\mathbf{k})+\cdots] = \exp\beta'(\epsilon_{\mathbf{k}}+V_{\mathrm{HF}}(\mathbf{k})). \quad (3.12)$$

The integrations over the times involving the insertions in this case is very simple since the HF insertion is independent of β'.

The complete HF theory for the free energy at zero temperature is the sum of the graphs the first few of which are illustrated in Fig. 6. Here the theory is complicated by the dilemma of overcounting, since one does not know which HF bubble normalizes which. It is a straightforward matter to prove that

$$\lim_{T\to 0} F_{\mathrm{HF}} = -\frac{1}{2}\sum_{\mathbf{k}\mathbf{k}'}[\langle \mathbf{k}\mathbf{k}'|v|\mathbf{k}\mathbf{k}'\rangle - \delta_{\sigma\sigma'}\langle \mathbf{k}\mathbf{k}'|v|\mathbf{k}\mathbf{k}'\rangle]\langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}\langle n_{\mathbf{k}'}\rangle_{\mathrm{HF}} + \sum \langle n_{\mathbf{k}}\rangle_{\mathrm{HF}}\epsilon_{\mathbf{k}}. \quad (3.13)$$

The first term is what would occur straightforwardly if, say, one of the bubbles was distinguished. The remaining term takes into account the overcounting. It simply counts the unperturbed energy in the right ground state. This point is proved in a more general context at the end of Sec. 6.

4. TIME-INDEPENDENT FORMALISM

A "time"-independent form of the free-energy expansion is most convenient for examining the zero-temperature limit. In this section we shall set up a formalism which will enable us first to make a non-adiabatic renormalization of the occupancy number $\langle n_{\mathbf{k}}\rangle_0$ and then to identify the remaining terms of the expansion as the usual adiabatic Goldstone theory.

As mentioned in Sec. 2 we have two equivalent forms for the free-energy expansion which may be written symbolically

$$F(1)=F(0)+\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\times\int_0^{\beta}\cdots\int_0^{\beta}\langle TV(\beta_n)\cdots V(\beta_1)V(0)\rangle_{0,\,\mathrm{linked}}\times d\beta_n\cdots d\beta_1, \quad (4.1)$$

$$F(1)=F(0)-\frac{1}{\beta}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\times\int_0^{\beta}\cdots\int_0^{\beta}\langle TV(\beta_n)\cdots V(\beta_1)\rangle_{0,\,\mathrm{linked}}\times d\beta_n\cdots d\beta_1. \quad (4.2)$$

The equivalence of these two forms may be seen as a consequence of the cyclic invariance of the trace. The second form leads more simply to the elimination of dotted line graphs in the zero-temperature expansion by a renormalization of the $\langle n_{\mathbf{k}}\rangle_0$. The reason for this will appear later on; thus for the moment we shall work with expansion (4.2).

Let us review the structure of the terms in the free energy expansion. From this point on, dotted line insertions on a propagator will be called C insertions and non-dotted-line insertions of the type of Fig. 7 will be called L insertions. For a given set of indices in a particular time sequence, there is, in general, a whole set of diagrams. Figure 7 illustrates sets of different diagrams corresponding to the same choice of indices. We can describe a set as follows: Beginning with the diagram linking all elements possible which do not vanish by operator graph rules, the remaining members of the set are obtained by converting in all ways L insertions into C insertions with the same time ordering.

Let us consider the contribution to the free energy of the two diagrams of Fig. 7:

$$F_\gamma=\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}B_\gamma(\mathbf{k},\mathbf{k}'\mathbf{q})A(\Delta), \quad (\gamma=a,b) \quad (4.3)$$

where the common factor containing the (integrated) time dependence is

$$A(\Delta)=\frac{1}{\beta}\int_0^{\beta}d\beta_3\int_0^{\beta_3}d\beta_2\int_0^{\beta_2}d\beta_1\{\exp[-(\beta_3-\beta_2)\Delta]\}\times\{\exp[-(\beta_2-\beta_1)\Delta]\}, \quad (4.4)$$

and the excitation energy

$$\Delta=\epsilon[_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}'-\mathbf{q}}-\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}] \quad (4.5)$$

is the sum of the particle (ascending) lines minus the sum of hole (descending) lines excited in both time intervals $\beta_3-\beta_2$ and $\beta_2-\beta_1$ between successive interactions. The time-independent factors are

$$B_a=C\langle n_{\mathbf{k}}\rangle_0, \quad (4.6)$$

and

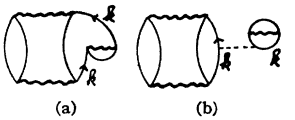
$$B_b=-CM_2(\mathbf{k}), \quad (4.7)$$

where

$$C=-\frac{[v(\mathbf{q})]^2}{\Omega^2}V_{\mathrm{HF}}{}^0(\mathbf{k})\langle n_{\mathbf{k}'}\rangle_0\langle 1-n_{\mathbf{k}+\mathbf{q}}\rangle_0\langle 1-n_{\mathbf{k}'-\mathbf{q}}\rangle_0. \quad (4.8)$$

$V_{\mathrm{HF}}{}^0(\mathbf{k})$ being the HF self-energy given by Eq. (3.1). B_a and B_b differ only in containing the factors $\langle n_{\mathbf{k}}\rangle_0$ and $M_2(\mathbf{k})$, respectively. Their sum is $\langle n_{\mathbf{k}}\rangle_0{}^2$, which is the contribution such a term would have in the usual

FIG. 7. Two diagrams corresponding to the same choice of indices.



G.C.E. representation. In this C.E. case there is, of course, an additional diagram like Fig. 7(b) with the hole line of the HF graph joined to the correlation bond having an index $\mathbf{k}_1 \neq \mathbf{k}$.

In general, the common time-dependent part of all members of a set of diagrams in the nth order consists of a product of exponentials $\exp(\omega_i \Delta_i)$ where the ω_i are time intervals $\omega_1=\beta_1$, $\omega_2=\beta_2-\beta_1$, $\cdots$ and the "excitation energy" in the ith interval is $\Delta_i=\sum_t \epsilon(n_t)-\sum_s \epsilon(m_s)$ where the n_t label the states of particle (ascending) lines and the m_s label the states of the hole (descending) lines traversing the ith interval. In the usual perturbation results ($T=0$) one has for the particle lines $\epsilon(n)>\mu_0$ and for the hole lines $\epsilon(m)<\mu_0$; consequently, the $\Delta_i>0$. At finite temperatures the Δ_i can be negative.

We thus obtain for the time-dependent contribution

$$A(\{\Delta_i\})=\frac{1}{\beta}\int_0^{\beta} d\beta_n \cdots \int_0^{\beta_2} d\beta_1 \prod_{i=1}^{n} \exp(-\omega_i \Delta_i). \quad (4.9)$$

This integrand depends only on the (positive) time intervals ω_i and so we can replace the integration variables β_i by ω_i and we obtain

$$A=\frac{1}{\beta}\int_0^{\infty} d\omega_n \cdots \int_0^{\infty} d\omega_1 \prod_{i=1}^{n} \exp(-\omega_i \Delta_i), \quad \sum_{i=1}^{n} \omega_i < \beta. \quad (4.10)$$

Following Bloch and de Dominicis,[2] we use the step function $\theta_-(\sum \omega_i-\beta)$ to replace the restriction on the integration; this becomes

$$A=\frac{1}{\beta}\int_0^{\infty} d\omega_n \cdots \int_0^{\infty} d\omega_1 \, \theta_-\Big(\sum_{i=1}^{n} \omega_i-\beta\Big) \times \prod_{i=1}^{n} \exp(-\omega_i \Delta_i). \quad (4.11)$$

Introducing the representation of the step function

$$\theta_-\Big(\sum_{i=1}^{n} \omega_i-\beta\Big)=\frac{1}{2\pi i}\int_C \frac{d\epsilon}{\epsilon} \exp\Big[\epsilon\Big(\sum_{i=1}^{n} \omega_i-\beta\Big)\Big], \quad (4.12)$$

where the contour C in the complex plane is parallel to the imaginary axis and to the left of all Δ_i, Eq. (4.11) becomes

$$A=\frac{1}{2\pi i \beta}\int_C \frac{d\epsilon}{\epsilon}[\exp(-\beta\epsilon)] \times \prod_{i=1}^{n} \int_0^{\infty} d\omega_i \exp[-\omega_i(\Delta_i-\epsilon)], \quad (4.13)$$

and integrating, we get

$$A=\frac{1}{2\pi i \beta}\int_C \frac{d\epsilon}{\epsilon}[\exp(-\beta\epsilon)] \prod_{i=1}^{n} \frac{1}{\epsilon-\Delta_i}. \quad (4.14)$$

Since in the interval ω_1 from 0 to β_1 there are no excitations, so that $\Delta_1=0$, we then arrive at the final form

$$A=\frac{1}{2\pi i \beta}\int_C \frac{d\epsilon}{\epsilon^2}[\exp(-\beta\epsilon)] \prod_{i=2}^{n} \frac{1}{\epsilon-\Delta_i} = R_0+\sum_{i=2}^{n} R_i. \quad (4.15)$$

Cauchy's theorem has been used to express the integral as the sum of the residues where we denote the residue from $\epsilon=0$ by R_0 and from $\epsilon=\Delta_i$ by R_i.

Expression (4.15) differs from the corresponding expression of Balian *et al.*[5] only by an extra factor of ϵ in the denominator and by a factor of $1/n$. This, in turn, comes from the extra integration in Eq. (4.2) as compared to (4.1). The two expressions are thus equivalent but as will be proven, expression (4.15) will contain in the limit $\beta \to \infty$ only contributions from the $\epsilon=0$ pole which will allow an immediate correspondence with the terms of the adiabatic theory. On the contrary, the reduction to these graphs using the alternate expression would be possible only by use of cyclic invariance (or an equivalent concept) at each step of the reasoning.

5. THE ZERO-TEMPERATURE LIMIT

We now prove the following theorem. The terms of the expansion of the free energy which remain in the limit $\beta \to \infty$ comprise:

(1) Linked graphs with positive excitation energies ($\Delta_i>0$). This implies descending lines contribute only for states less than and ascending lines only for states greater than the unperturbed Fermi energy μ_0. These terms arise from the residue at $\epsilon=0$ in Eq. (4.15).

(2) Correlation-connected unlinked graphs which do not overlap in time represent singular terms which renormalize the Fermi functions $\langle n_{\mathbf{k}} \rangle_0$. Overlapping correlation-connected graphs do not contribute. Finally, there are no contributions from residues $\epsilon=\Delta_i \neq 0$.

Discussion of proof. The complication of taking the zero-temperature limit primarily involves showing that overlapping C-linked graphs do not contribute. For the $\epsilon=\Delta_i$ residues with $\Delta_i<0$ this involves cancellation of a set of graphs rather than a single graph.

The determination of which diagrams vanish at zero temperature follows from the limiting temperature dependence of the function $\langle n_k \rangle_0$ and M_n. The Fermi function $\langle n_{\mathbf{k}} \rangle_0$ becomes a step function (independent of β)

$$\lim_{\beta \to \infty} \langle n_{\mathbf{k}} \rangle_0 = \theta(\mu_0-\epsilon_{\mathbf{k}}), \quad (5.1)$$

where the step function is

$$\theta(x)=0, \quad x<0 \qquad =1, \quad x>0. \quad (5.2)$$

Using the generating function definition of the M_n, we have

$$\beta^{n-1}M_n(\mathbf{k}_1\cdots\mathbf{k}_n) = (-1)^{n-1}[\partial^{n-1}/\partial\epsilon(\mathbf{k}_2)\cdots\partial\epsilon(\mathbf{k}_n)]\langle n_{\mathbf{k}_1}\rangle_0. \quad (5.3)$$

The quantities $\beta^{n-1}M_n$ are generalized functions (see Appendix A) related to δ functions and their derivatives which are singular on the Fermi surface, but their integrals are finite. On the other hand, for $m<n-1$ we have

$$\beta^m M_n = O(\beta^{-(n-1-m)}), \quad (5.4)$$

i.e., $\beta^m M_n$ (on integration) yields a result going to zero as $\beta^{-(n-1-m)}$. These statements are discussed and proved in Appendix A.

The proof of the theorem is divided into two parts. We first prove that the residue at $\epsilon=0$ gives all of the nonvanishing terms of the theorem. We then show that all other residues vanish in the limit of zero temperature.

Proof

For a graph consisting of n unlinked parts joined together by correlation bonds at a single junction there is a factor M_n. If no two of the n parts overlap in time, such a graph also carries a factor $[\epsilon]^{-n+1}$ in Eq. (4.15). This follows from the existence of $(n-1)$ intervals for which $\Delta_i=0$. The residue from $\epsilon=0$ then gives the nonvanishing $\beta^{n-1}M_n$. If two or more linked parts overlap, this residue decreases by one or more powers in β and hence vanishes by Eq. (5.4).

As for the contribution from the $\epsilon=0$ residue due to linked parts, the factor $1/\beta$ in front of the expression in Eq. (4.15) cancels and one is left with a contribution in which one propagates between two interactions times β_i and β_{i+1} with $[\Delta_i]^{-1}$ the reciprocal of the excitation energy.

The graphs with particle (hole) lines propagating in the forward (backward) direction give a residue of $[\Delta_i]^{-1}$ in the ith time interval. Graphs with particle (hole) lines propagating in the "wrong" direction are smaller than the previous class by $\exp(-\beta|\epsilon_{\mathbf{k}}-\epsilon_F|)$ and hence vanish in the zero-temperature limit. In this way the contribution to the $\epsilon=0$ residue from linked graphs with no dotted lines gives the conventional adiabatic result at zero temperature.

Let us now turn to the residues from $\epsilon=\Delta_i$. Since such a term is proportional to the factor $\exp(-\beta\Delta_i)$, it follows that for $\Delta_i>0$ such contributions clearly go to zero. For $\Delta_i<0$ the result would appear to diverge. Before proceeding to the general proof that this is not so, let us consider the example of the second-order graph (Fig. 8). The contribution is proportional to

$$\langle 1-n(\mathbf{k})\rangle_0\langle 1-n(\mathbf{k}_1)\rangle_0\langle n(\mathbf{k}')\rangle_0\langle n(\mathbf{k}_1')\rangle_0\int\frac{d\epsilon\, e^{-\beta\epsilon}}{\epsilon^2(\epsilon-\Delta)}, \quad (5.5)$$

where, for example, $\mathbf{k}$ and $\mathbf{k}_1$ are hole states, $\mathbf{k}'$ and $\mathbf{k}_1'$ particle states. This automatically insures $\Delta<0$ with

FIG. 8. A typical second-order graph.

$$\Delta=\epsilon(\mathbf{k})+\epsilon(\mathbf{k}_1)-\epsilon(\mathbf{k}')-\epsilon(\mathbf{k}_1'). \quad (5.6)$$

The $\epsilon=\Delta$ residue is

$$\frac{\exp(-\beta\Delta)}{\beta}\frac{\langle 1-n(\mathbf{k})\rangle_0\langle 1-n(\mathbf{k}_1)\rangle_0\langle n(\mathbf{k}')\rangle_0\langle n(\mathbf{k}_1')\rangle_0}{\Delta^2}. \quad (5.7)$$

Note that in this form we cannot pass to the zero-temperature limit since the hole and particle states contain the "wrong" statistical factors. However, we may use detailed balance to prepare for the limit operation. From

$$\langle n(\mathbf{k})\rangle_0=\exp[-\beta(\epsilon(\mathbf{k})-\mu_0)]\langle 1-n(\mathbf{k})\rangle_0, \quad (5.8)$$

we have

$$\langle 1-n(\mathbf{k})\rangle_0\langle 1-n(\mathbf{k}_1)\rangle_0\langle n(\mathbf{k}')\rangle_0\langle n(\mathbf{k}_1')\rangle_0 = \exp(\beta\Delta)\langle n(\mathbf{k})\rangle_0\langle n(\mathbf{k}_1)\rangle_0 \times\langle 1-n(\mathbf{k}')\rangle_0\langle 1-n(\mathbf{k}_1')\rangle_0, \quad (5.9)$$

whence the exponentially divergent factor in R_Δ is compensated and, in fact, the result goes to zero as $1/\beta$. In general, for the $\epsilon=\Delta_i$ residue, one simply applies detailed balance to the states in the time interval in question which eliminates the divergent exponential leaving the $\langle n(\mathbf{k})\rangle\langle 1-n(\mathbf{k}')\rangle$ finite at $T=0$. The factor $1/\beta$ remains from such a pole and linked and unlinked graphs vanish as $1/\beta$.

It remains to consider the case where $\epsilon=\Delta$ is a multiple pole. This arises when we have multiple L insertions or overlapping C insertions. Here one must group all terms with the same time integrand [the same function A of Eq. (4.9)]. In Fig. 9 a particular set of such graphs has been drawn. The special index singled out is the hole index k for which we write the semi-invariant combinations, which arise from C insertions on $\mathbf{k}$:

$$M_1-M_2 \quad (5.10a)$$

$$M_1-2M_2+M_3 \quad (5.10b)$$

$$M_1-\binom{n}{1}M_2+\binom{n}{2}M_3+\cdots\pm M_n. \quad (5.10c)$$

The nth order term can be written in the form

$$\sum_{r=1}^{n}\binom{n}{r-1}M_r=\sum_{r=0}^{n-1}\binom{n-1}{r}\left(\frac{\partial}{\partial\beta\epsilon_{\mathbf{k}}}\right)^r\langle n_{\mathbf{k}}\rangle_0 = (1+\partial/\partial\beta\epsilon_{\mathbf{k}})^{n-1}\langle n_{\mathbf{k}}\rangle_0. \quad (5.11)$$

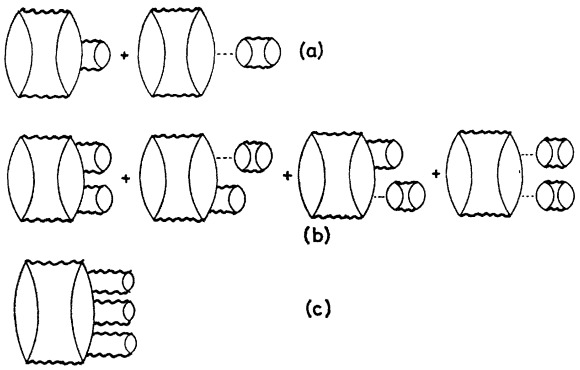


FIG. 9. The graphs which comprise the set of Eq. (5.10).

The contribution of the nth order term of Fig. 9 is proportional to

$$-(1/\beta)\int \frac{e^{-\beta\epsilon}}{\epsilon^2}\frac{\langle g\rangle}{(\epsilon-\Delta_1)^n(\epsilon-\Delta_1-\Delta_2)\cdots(\epsilon-\Delta_1-\Delta_n)} \times\left(1+\frac{\partial}{\partial\beta\epsilon_k}\right)^{n-1}\langle n_k\rangle d\epsilon. \quad (5.12)$$

$\langle g\rangle$ is the product of $\langle n_{k'}\rangle$ for particles and hole line other than the kth. Δ_1 is the energy denominator from the first interval and Δ_i is the energy denominator of the ith self-energy insertion. For $\Delta_1<0$ the residue from $\epsilon=\Delta_1$ is to leading order in β

$$\frac{1}{(n-1)!}(-\beta)^{n-2}\frac{(-1)^n e^{-\beta\Delta_1}\langle g\rangle}{\Delta_1^2\Delta_2\cdots\Delta_n}\left[1+\frac{\partial}{\partial\beta\epsilon_k}\right]^{n-1}M_1. \quad (5.13)$$

$\langle g\rangle$ contains the three remaining lines $\mathbf{k}'$, $\mathbf{k}_1$, $\mathbf{k}_1'$. The negative value of Δ_1 is due to some or all of the lines $\mathbf{k}$, $\mathbf{k}'$, $\mathbf{k}_1$, $\mathbf{k}_1'$ going the "wrong way." The argument of detailed balance is then applicable. For example, if all four lines go the wrong way,

$$\exp[\beta\Delta_1+\beta(\epsilon_k-\mu_0)]\langle(1-n(\mathbf{k}_1)\rangle_0\langle n(\mathbf{k}')\rangle_0\langle n(\mathbf{k}_1')\rangle_0 =\langle n(\mathbf{k}_1)\rangle_0\langle(1-n(\mathbf{k}')\rangle_0\langle(1-n(\mathbf{k}_1')\rangle_0, \quad (5.14)$$

all factors remaining finite in limit $\beta\to\infty$. One can show easily that, if not all the lines of a linked part are "wrong," the graph vanishes exponentially in the limit $\beta\to\infty$. However, for graphs with all lines "wrong" the group of terms in question vanishes as β^{-1} as shown below.

In Appendix B we prove that

$$\exp[\beta(\epsilon(\mathbf{k})-\mu_0)]\left[1+\frac{\partial}{\partial\beta\epsilon(\mathbf{k})}\right]^{n-1}M_1=M_n. \quad (5.15)$$

Putting Eq. (5.15) into Eq. (5.13) we see that the divergent exponential has again been eliminated, but there is one factor too few of β to leave a finite contribution. This result clearly does not depend on what the insertions are. It is thus seen that all contributions from $\epsilon=\Delta_i$ residues vanish at zero temperature. This completes the proof. We recall that all this is true only because of the use of expression (4.2) for the free energy. Had we used (4.1), "wrong graphs" would have to be included and dotted-line graphs would not have been eliminated by a simple "n_k renormalization." It should be noted that the proof in I on the reduction to the Brueckner-Goldstone theory in the isotropic case must be interpreted from the point of view of expansion (4.2) and not as was originally done, from expansion (4.1).

6. ELIMINATION OF DOTTED LINES—GROUND-STATE ENERGY

In the zero-temperature limit, we are thus left with (1) all the L graphs (linked graphs) and (2) all the nonoverlapping C insertions. All these graphs contain factors of $\langle n_k\rangle_0$ and $\langle(1-n_k)\rangle_0$ referring to the unperturbed Fermi distribution at $T=0$. We now sum all the C insertions.

Consider all possible linked graphs attached by a single dotted line to a given propagator characterized by $\langle n_{k'}\rangle_0$ or $\langle(1-n_{k'})\rangle_0$. This dotted line connects the propagator to a $\langle n_k\rangle_0$ or a $\langle(1-n_k)\rangle_0$. Except for the semi-invariant factor, the sum $W_0(\mathbf{k})$ of all the linked graphs connecting the $\langle n_k\rangle_0$ or the $\langle(1-n_k)\rangle_0$ propagator to the $\langle n_{k'}\rangle_0$ [or $\langle(1-n_{k'})\rangle_0$] is then given by

$$W_0(\mathbf{k})=\frac{\partial L_0}{\partial\langle n_k\rangle_0}-\frac{\partial L_0}{\partial\langle(1-n_k)\rangle_0}. \quad (6.1)$$

Here L_0 is the sum of all the linked graphs (without C insertions) considered as a function of $\langle n_k\rangle_0$ and $\langle 1-n_{k_0}\rangle_0$. Naturally, the derivative is to be interpreted at finite temperature and then the limit to $T=0$ is taken. The sum of all L graphs connected by dotted lines to a propagator is then carried out as in the Hartree-Fock case. Again the $W_0(\mathbf{k})$ for $\mathbf{k}\neq\mathbf{k}'$ renormalizes the chemical potential $\mu_0(\{\epsilon_k\})$ in $\langle n_{k'}\rangle$ to $\mu_0(\{\epsilon_k+W_0(\mathbf{k})\})=\mu$ and for $\mathbf{k}=\mathbf{k}'$ it renormalizes $\epsilon_{k'}$ to $\epsilon_{k'}+W_0(\mathbf{k}')$ in $\langle n_{k'}\rangle$. Again this procedure may then be repeated self-consistently by attaching dotted-line graphs to L_0 to give

$$W(\mathbf{k})=\frac{\partial L}{\partial\langle n_k\rangle}-\frac{\partial L}{\partial\langle(1-n_k)\rangle}; \quad (6.2)$$

$$\begin{aligned}&\langle n_k\rangle=1, \quad \epsilon_k+W(\mathbf{k})<\mu(\{\epsilon_{k'}+W(\mathbf{k}')\}),\\ &\langle n_k\rangle=0, \quad \epsilon_k+W(\mathbf{k})>\mu(\{\epsilon_{k'}+W(\mathbf{k}')\}).\end{aligned} \quad (6.3)$$

L is here the same function of $\langle n_k\rangle$ as L_0 was of the unrenormalized $\langle n_k\rangle_0$.

It would seem that the ground-state energy would then be given simply by L evaluated with the correct renormalized $\langle n_k\rangle$ and $\langle(1-n_k)\rangle$. However, as in HF theory, this would amount to overcounting the dotted-

line connections. As promised at the end of Sec. 3 we now present the solution of this problem. The method we use is to include in the unperturbed Hamiltonian H_0 a "counter-term" $W(\mathbf{k})$ given by (6.2), i.e., one writes

$$H_0=\sum_{\mathbf{k}}[\epsilon_{\mathbf{k}}+W(\mathbf{k})]a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}, \tag{6.4}$$

and

$$V=\sum_{\mathbf{k}_1\mathbf{k}',\mathbf{q}}\frac{v(\mathbf{q})}{\Omega}a_{\mathbf{k}+\mathbf{q}}^{+}a_{\mathbf{k}'-\mathbf{q}}^{+}a_{\mathbf{k}'}a_{\mathbf{k}}-\sum_{\mathbf{k}}W(\mathbf{k})a_{\mathbf{k}}^{+}a_{\mathbf{k}}. \tag{6.5}$$

We now have new graphs arising from the second term in the interaction. These occur both as L graphs and in C insertions. The L graphs, however, remain unchanged because insertion of all possible $W(\mathbf{k})$ interactions in the propagator which now is a function of $\epsilon_{\mathbf{k}}+W(\mathbf{k})$ simply restores the unperturbed $\epsilon_{\mathbf{k}}$. This can be seen immediately from Fig. 5 if one replaces a HF insertion by a $W(\mathbf{k})$ insertion. Further, the C graphs vanish because we have to add $-W(\mathbf{k})$ to the sum of all linked graphs connected to a propagator by a single dotted line; these indeed sum precisely to $W(\mathbf{k})$. Notice that the first-order term which arises from that part of the interaction due to $W(\mathbf{k})$ cancels the counter term in (6.4) so that the ground-state energy is simply

$$E=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}\langle n_{\mathbf{k}}\rangle+L. \tag{6.6}$$

We see that the effect of the overcounting is entirely included in the change of $\langle n_{\mathbf{k}}\rangle_0$ to $\langle n_{\mathbf{k}}\rangle$ in the unperturbed energy. The result (6.6) expresses the fact that once a model wave function corresponding to a new Fermi surface defined by the $\langle n_{\mathbf{k}}\rangle$ is chosen, adiabatic theory is valid. Note that $W(\mathbf{k})$ does not appear anywhere in (6.6) except for defining the new $\langle n_{\mathbf{k}}\rangle$. This means that the only relevant $W(\mathbf{k})$ of the theory at zero temperature are those evaluated at the modified Fermi surface. Indeed, this must be so because $W(\mathbf{k})$ acquires definition only on the Fermi surface at zero temperature.

7. DISCUSSION OF STABILITY PROBLEM

The first important point is to observe that the transformation of Fermi surface from that of the $\epsilon_{\mathbf{k}}$ representation to that of the $\epsilon_{\mathbf{k}}+W(\mathbf{k})$ representation is volume conserving, i.e.,

$$\sum\langle n_{\mathbf{k}}\rangle=\sum\langle n_{\mathbf{k}}\rangle_0=N. \tag{7.1}$$

The proof of (7.1) follows from

$$\langle n_{\mathbf{k}}\rangle=\sum_{n=0}^{\infty}\left[\frac{\beta^n}{n!}\sum_{\mathbf{k}_1\cdots\mathbf{k}_n}W(\mathbf{k}_1)W(\mathbf{k}_2)\cdots W(\mathbf{k}_n)\times M_{n+1}(\mathbf{k},\mathbf{k}_1,\cdots\mathbf{k}_n)\right]\langle n_{\mathbf{k}}\rangle_0. \tag{7.2}$$

Now sum over $\mathbf{k}$ and observe that

$$\sum_{\mathbf{k}}M_{n+1}(\mathbf{k},\mathbf{k}_1,\cdots\mathbf{k}_n)=0$$

for $n>0$, thereby proving Eq. (7.1). To prove this statement we notice that the sum $\sum_{\mathbf{k}}n_{\mathbf{k}}=N$ is kept constant in all members of the ensemble and the semi-invariants of order greater than one, containing a random variable which is a constant, vanish. From Eq. (7.1) it follows that the correct chemical potential μ is the same functional of $\epsilon_{\mathbf{k}}+W(\mathbf{k})$ as μ_0 is of $\epsilon_{\mathbf{k}}$, i.e.,

$$\mu=\mu_0(\{\epsilon_{\mathbf{k}}+W(\mathbf{k})\}). \tag{7.3}$$

The new Fermi surface is then determined by

$$E_{\mathbf{k}}=\epsilon_{\mathbf{k}}+W(\mathbf{k})=\mu \tag{7.4}$$

It must be remembered that $E_{\mathbf{k}}$ is a function of $\langle n(\mathbf{k})\rangle$ so that the self-consistent problems involved are formidable indeed. Nevertheless, the formalism provides a framework for an approximate determination of the Fermi surface. It is a particular advantage of the above formalism that approximate theories are easily accommodated since the chemical potential μ which arises is determined to the same accuracy as the approximate $E(\mathbf{k})$.

Let us now discuss the nature of the adiabatic expansion. If the Fermi surface is unchanged by the interaction, then the terms of the series are well defined and the Brueckner-Goldstone expansion follows in unmodified form.

If the interaction changes the form of the Fermi surface, then zero-energy denominators can occur due to interchange of particles and hole states. In Fig. 10 we illustrate a transition which can give rise to such a divergence. The question is whether such a divergence will persist when the adiabatic self-energy insertions are summed.

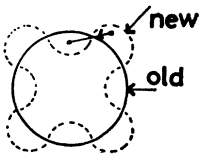


FIG. 10. Transition which might give rise to divergencies.

First observe that in HF theory that the self-energy insertions when summed convert the $\epsilon_{\mathbf{k}}$ to $(E_{\mathbf{k}})_{\mathrm{HF}}$. Thus, divergencies arising from deformation of the Fermi surface in HF theory are entirely spurious. The same is true of any static external potential such as a crystal field. In general, however, the self-energy insertions depend on the interactions in the remaining portions of the graph and a proof is much less evident. However we may conjecture that the most fruitful approach is probably in the single-particle propagator formalism.[6]

Our plan of attack on this problem is to first prove the identity of μ defined by Eq. (7.3) with the true chemical potential: $(\partial F/\partial N)_{V,T}$. It is most convenient to do this at finite temperature and then pass to the zero-temperature limit. After this is done we will recall the theorem of Hugenholtz and Van Hove[7] which

[6] See for example, V. Galitskii and A. Migdal, Zh. Eksperim. i Teor. Fiz. **34**, 139 (1958) [translation: Soviet Phys.—JETP **7**, 96 (1958).

[7] N. Hugenholtz and L. Van Hove, Physica **24**, 363 (1958).

proves that the pole of the single-particle propagator for $\mathbf{k}$ on the Fermi surface is also at μ. In this way we will have shown that poles arising from crossed transitions as in Fig. 10 are, in fact, spurious for transitions involving particles and holes in the neighborhood of the Fermi surface. We may then speculate on further conditions which are necessary to make the theory meaningful. The main point is that the theory of the nonspherical Fermi surface is brought to the same state of development as the spherical case.

To prove the identity of μ with $(\partial F/\partial N)_{V,T}$, we first generalize Eq. (6.6) to an equation for F at finite T. By the identical arguments that led to (6.6), it is clear that the overcounting problem is eliminated by the use of the model Hamiltonian (6.4). $W(\mathbf{k})$ is now a function of T. The result is then [*Note added in proof.* Equation (7.5) is valid only if $O(\exp-\beta\epsilon_F)$ may be neglected.]

$$F=F_0(\{E_\mathbf{k}\})-\textstyle\sum_\mathbf{k}\langle n_\mathbf{k}\rangle W_\mathbf{k}+L. \tag{7.5}$$

Here, F_0 is the free energy of an ideal gas whose single-particle energies are $E_\mathbf{k}=\epsilon_\mathbf{k}+W_\mathbf{k}$. It has the variational properties (the variations being taken along the minimum of F)

$$\delta F_0/\delta\langle n_\mathbf{k}\rangle=\mu,\quad \delta F_0/\delta W_\mathbf{k}=+\langle n_\mathbf{k}\rangle. \tag{7.6}$$

Using these results, we may vary F in Eq. (7.5) with respect to $W_\mathbf{k}$ and $\langle n_\mathbf{k}\rangle$ to give

$$\delta F=\sum_\mathbf{k}\Big[\mu\delta\langle n_\mathbf{k}\rangle+\langle n_\mathbf{k}\rangle\delta W_\mathbf{k}-\langle n_\mathbf{k}\rangle\delta W_\mathbf{k} -W_\mathbf{k}\delta\langle n_\mathbf{k}\rangle+\frac{\partial L}{\partial\langle n_\mathbf{k}\rangle}\delta\langle n_\mathbf{k}\rangle\Big]. \tag{7.7}$$

We now use the result of Eq. (6.2) which gives $\partial L/\partial\langle n_\mathbf{k}\rangle=W_\mathbf{k}$, since varying $\langle n_\mathbf{k}\rangle$ in (7.7) varies both $\langle n_\mathbf{k}\rangle$ and $\langle 1-n_\mathbf{k}\rangle$. Also we used the fact that L is an explicit function of $\langle n_\mathbf{k}\rangle$ only. Now use $\sum\delta\langle n_\mathbf{k}\rangle=\delta N$ so that (7.7) becomes

$$(\partial F/\partial N)_{V,T}=\mu. \tag{7.8}$$

The next point to prove is that at zero temperature the pole of the single propagator [$\bar{D}_\mathbf{k}(z)$ in the notation of reference 7] is at $\epsilon_\mathbf{k}+W_\mathbf{k}=\mu$ for $\mathbf{k}$ on the Fermi surface. This point is explicitly proved by Hugenholtz and Van Hove[7] (hereafter referred to as HV). These authors prove the following theorem: The form of the single-particle propagator is

$$\bar{D}_\mathbf{k}(z)=\frac{1}{\epsilon_\mathbf{k}-z-\Sigma_\mathbf{k}(z)}, \tag{7.9}$$

where $\Sigma_\mathbf{k}(z)$ is the proper self-energy insertion on a particle line of state $\mathbf{k}$, with (complex) energy z and is equal to

$$\Sigma_\mathbf{k}(z)=\partial G_0(z)/\partial\langle n_\mathbf{k}\rangle. \tag{7.10}$$

(We use G rather than the B of HV which differs from Σ by a factor of z^2. It is also convenient to set $\epsilon_0=0$.)

$G_0(z)$ is the sum of linked graphs where the propagator in intermediate states is $(H_0-z)^{-1}$. The equivalence of HV to (7.10) is contained in the paragraph following their Eq. (7) and the reasoning that leads to our Eq. (7.10) is the same as that which leads to their Eq. (8). In particular, for $z=0$, Eq. (7.10) reads

$$\Sigma_\mathbf{k}(0)=\partial L/\partial\langle n_k\rangle=W_k. \tag{7.11}$$

HV then point out that the analytic branch cut characteristics of the expectation value of the resolvent of the $(N+1)$ particle system with $\mathbf{k}$ added at the Fermi surface are the same as those of the N-particle system. Consequently, $\bar{D}_\mathbf{k}(\epsilon_\mathbf{k}+z)$, which shares the same analytic properties as $D_\mathbf{k}(\epsilon_\mathbf{k}+z)$ (the entire resolvent of the $N+1$ particle state), must have a pole on the real axis. As stressed by Hugenholtz, this "pole" is not a true pole in the mathematical sense, but the value of the branch discontinuity is sufficiently weak in the neighborhood of the pole to be able to calculate as if it were a true pole. The result is the $\bar{D}_\mathbf{k}(z)$ has a singularity on the real axis for $\mathbf{k}$ on the Fermi surface, at the point (in the notation of HV)

$$z=\epsilon_\mathbf{k}+\partial G_0(0)/\partial\langle n_\mathbf{k}\rangle=\epsilon_\mathbf{k}+W_\mathbf{k}=\mu. \tag{7.12}$$

In this way one sees that when the adiabatic diagrams of L are resummed and expressed all in terms of $\bar{D}_\mathbf{k}(z)$ that the series takes exactly the same form as for the spherical case. By this we mean that the usual adiabatic perturbation series for the spherical case takes on the same form as we have found when all self-energy insertions are summed and the series is expressed in terms of renormalized propagators only. The propagators which have pole singularities on the real axis are indeed at the Fermi surface. Those off the Fermi surface have only branch singularities if the series has meaning. This is the essential assumption of the validity of the adiabatic perturbation series.

We may then say that if the system does behave like a Fermi liquid at low temperature, then the present method will calculate all properties correctly. The problem of stability both for the spherical and nonspherical case is probably concerned with the singular structure of $\bar{D}_\mathbf{k}(z)$ about the Fermi surface. One may speculate that if $\mathrm{Re}\Sigma_\mathbf{k}(z)$ for z at the quasi-particle poles is ordered correctly through the Fermi surface, then the Fermi liquid will be stable since no further poles will arise in the structure of $\bar{D}_k(z)$.

If one finds the adiabatic formalism meaningless, then in the present theory one may envision two modifications. Firstly, one may go back to the finite-temperature result and resum in an alternative way to that of this paper. Secondly, certain terms of $O(1)$ may become of $O(N)$ because of a transition to an ordered phase. Such is the case in ferromagnetism[8] and

[8] See, for example, R. Brout, Phys. Rev. **118**, 1009 (1960).

has to some extent been investigated in the theory of superconductivity by Thouless.[9] *Note added in proof.* Recently one of us (R. B.) has shown how to recover the BCS theory of superconductivity by allowing the correlations between $n_{\mathbf{k}}$ and $n_{-\mathbf{k}}$ to be $O(1)$ rather than $O(1/N)$.

APPENDIX A

We first examine the functions $\beta^{n-1}M_n$. Since in the limit $\beta\to\infty$, $\langle n_{\mathbf{k}}\rangle_0$ is a step function, and since

$$\partial\theta_-(x)/\partial x=\delta(x), \tag{A1}$$

we expect βM_2 to be a δ function and, in general, $\beta^{n-1}M_n$ the $(n-2)$th derivative of a δ function, in the limit $\beta\to\infty$. Let us illustrate these results in terms of integrals.

$$-\beta M_2=\frac{\partial}{\partial\epsilon_{\mathbf{k}}}\langle n_{\mathbf{k}}\rangle_0(\epsilon_{\mathbf{k}}-\mu_0), \tag{A2}$$

and we have $(N\to\infty)$ for arbitrary F such that $F(0)=0$

$$I=\int_0^\infty d\epsilon_{\mathbf{k}}\,F(\epsilon_{\mathbf{k}})\beta M_{\mathbf{k}}{}^2=\int_0^\infty d\epsilon_{\mathbf{k}}\,F(\epsilon_{\mathbf{k}})\frac{\partial}{\partial\epsilon_{\mathbf{k}}}\langle n_{\mathbf{k}}\rangle_0, \tag{A3}$$

$$I=\int_0^\infty d\epsilon_{\mathbf{k}}\,F'(\epsilon_{\mathbf{k}})\langle n_{\mathbf{k}}\rangle_0\underset{\beta\to\infty}{=}\int_0^{\mu_0}F'(\epsilon)d\epsilon=F(\mu_0). \tag{A4}$$

If we had M_2 instead of βM_2, the result would have gone to zero as $1/\beta$. Similarly for $\beta^{n-1}M_n$ we would obtain

$$I=\int d\epsilon_{\mathbf{k}}\,F(\epsilon_{\mathbf{k}})\frac{\partial^{n-1}}{\partial\epsilon_{\mathbf{k}}{}^{n-1}}\langle n_{\mathbf{k}}\rangle_0=F^{n-2}(\mu_0), \tag{A5}$$

while any lower power in $\beta^m M_n$ will vanish as $(1/\beta)^{n-1-m}$.

The generalization to multivariate M_n follows from the factorization of M_n into similar functions of the separate variables. Thus, e.g.,

$$M_2(\mathbf{k},\mathbf{k}')=\frac{\partial\langle n_{\mathbf{k}}\rangle_0}{\partial(-\beta\epsilon_{\mathbf{k}'})}=\frac{\partial\langle n_{\mathbf{k}}\rangle_0}{\partial\mu_0}\frac{\partial\mu_0}{\partial\epsilon_{\mathbf{k}'}}=-\frac{M_2(\mathbf{k})M_2(\mathbf{k}')}{\Sigma_{\mathbf{k}''}M_2(\mathbf{k}'')}.$$

[9] D. J. Thouless, Ann. Phys. (N.Y.) **10**, 1342 (1960).

APPENDIX B

In this Appendix we prove the relationship

$$e^{-x}\left(1-\frac{\partial}{\partial x}\right)^n M_1(x)=(-1)^{n+1}M_{n+1}(x), \tag{B1}$$

where

$$M_n(x)=\frac{\partial^{n-1}}{\partial x^{n-1}}\langle n(x)\rangle_0, \tag{B2}$$

and

$$x=-\beta(\epsilon-\mu_0). \tag{B3}$$

The proof is by induction. We define

$$\phi_n(x)=\left(1-\frac{\partial}{\partial x}\right)^n,\quad M_1=\left(1-\frac{\partial}{\partial x}\right)\phi_{n-1}(x). \tag{B4}$$

We assume the result for n

$$e^{-x}\phi_n=(-1)^{n+1}M_{n+1}, \tag{B5}$$

and examine the equations for $n+1$.

From the definition of ϕ_n

$$e^{-x}\phi_{n+1}=e^{-x}\left(1-\frac{\partial}{\partial x}\right)\phi_n. \tag{B6}$$

Using Eq. (B5) this becomes

$$(-1)^{n+1}M_{n+1}-e^{-x}\left(\frac{\partial}{\partial x}\right)\phi_n, \tag{B7}$$

but

$$e^{-x}\left(\frac{\partial}{\partial x}\right)\phi_n=\left(\frac{\partial}{\partial x}\right)(e^{-x}\phi_n)-e^{-x}\phi_n$$
$$=(-1)^{n+1}\left(\frac{\partial}{\partial x}M_{n+1}-M_{n+1}\right), \tag{B8}$$

using Eqs. (B5) and (B6).

Thus combining (B6) and (B8) we obtain

$$e^{-x}\phi_{n+1}=(-1)^{n+2}M_{n+2}, \tag{B9}$$

and the relationship (B1) is established for $n+1$. If this is true for $n=1$, then the result is proved. We take $x=-\beta(\epsilon-\mu_0)$ and $M_1=\langle n\rangle$, then

$$e^{\beta(\epsilon-\mu_0)}\left(1-\frac{\partial}{\partial(-\beta\epsilon)}\right)\langle n\rangle=M_2. \tag{B10}$$