Perturbation Theory for an Infinite Medium of Fermions. II*

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New forms of the linked cluster expansion for the ground-state energy of a normal spherical system are given in terms of the exact single-particle propagator and of the associated self-energy operator. These forms are shown to be stationary with respect to variations of the latter quantities. A new concise proof of the Hugenholtz-Van Hove theorem on single-particle energies is then possible. The variational principle also explains the insensitivity of recent binding energy calculations to the choice of single-particle energies. It is shown how all results may be extended to systems with anisotropic features.

I. INTRODUCTION

THIS paper is intended as an extension of the results of a previous paper[1] with the same title. Its essential limitation is the same as that of the previous work, namely the restriction to normal systems at zero temperature. Most candidly, a system is to be defined as normal with respect to those properties which can be described adequately by a power series in the coupling strength or suitable partial resummation thereof. Though the experimental and theoretical evidence runs strongly counter to the existence of such systems, at least where the forces are suitably attractive,[2] the justification for our investigations is twofold: they are preliminary to a report of an investigation of similar systems at finite temperatures[3] where they appear to be applicable to normal metals and to liquid He^3; even for superconducting and similar systems the bulk properties here under investigation are largely given by normal system theory, as has been assumed in previous theoretical treatments,[4] and as we shall attempt to show more cogently in later papers of this series.

We work with the same Hamiltonian as in I, which in momentum space is

$$H=H_0+\lambda H_1 =\sum_{\mathbf{p}} a^\dagger(\mathbf{p})a(\mathbf{p})p^2 +\frac{\lambda}{2\Omega}\sum_{\mathbf{p},\mathbf{p}',\mathbf{q}} a^\dagger(\mathbf{p}+\mathbf{q})a^\dagger(\mathbf{p}'-\mathbf{q})v(\mathbf{q})a(\mathbf{p}')a(\mathbf{p}), \quad (1)$$

and follow the notation of I where applicable. Except in the last section we take $v(\mathbf{q})=v(|\mathbf{q}|)$. Throughout we shall be concerned essentially with new forms of the linked cluster expansion (LCE). In Sec. II we obtain a new expression for the latter in terms of the exact propagator, $G(\mathbf{p},p_0)$ and the exact self-energy operator $M(\mathbf{p},p_0)$, where these are related as usual by the equation

$$[-p_0+p^2-M(\mathbf{p},p_0)]G(\mathbf{p},p_0)=1. \quad (2)$$

This new form of the LCE is shown to be stationary with respect to arbitrary variations of either M or G.[5] In Sec. III this property is used to yield a concise proof of the theorem of Hugenholtz and Van Hove[6] on single-particle energies. On the basis of this theorem, it is shown in Sec. IV how a concept of self-consistent potential different from the Hartree-Fock one or recent generalizations[7] can be introduced for binding energy calculations. A real potential, it can in principle be determined exactly because of its relation to the separation energy at an appropriate density. It is also shown how the LCE of Sec. II may be rewritten to incorporate it, at the same time preserving the variational property. It is seen that the unsensitivity of binding energy calculations[7] to the actual choice of single-particle energies is reflective of this variational property. Finally in Sec. V, it is shown how all results may be generalized to systems exhibiting anisotropic features.[8] This in-

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[1] A. Klein and R. E. Prange, Phys. Rev. **112**, 994 (1958), hereafter referred to as I. An improved version of this paper as well as some of the results of the present paper may be found in *Lectures at the International Spring School of Theoretical Physics, University of Naples*, **1960** [Nuovo cimento (to be published)].

[2] See, for instance, L. N. Cooper, Phys. Rev. **104**, 1353 (1956); K. Gottfried, CERN Report (unpublished); L. Van Hove, Physica **25**, 849 (1959); V. J. Emery, University of California Radiation Laboratory Report UCRL-9076 (unpublished); M. L. Mehta, Saclay (to be published); H. Kummel, University of Mainz (to be published).

[3] Related treatments have been developed by J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960); J. M. Luttinger, Phys. Rev. **119**, 1153 (1960); R. Balian, C. Bloch, and C. De Dominicis, *Lectures at the International Spring School of Theoretical Physics*, University of Naples, **1960** [Nuovo cimento (to be published)]; R. Balian, C. Bloch, and C. DeDominicis, Comp. rend **250**, 2850 (1960); and Nuclear Phys. (to be published); R. Balian and C. DeDominicis, Nuclear Phys. **16**, 502 (1960); Comp. rend. **250**, 3285, 4111 (1960).

[4] This is the philosophy of the reduced Hamiltonian. See J. Bardeen, L. Cooper, and J. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[5] A related variational principle, found in the work of Luttinger and Ward, reference 3, provided the original incentive for some of our investigations.

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

[7] See, for instance, K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958); R. E. Prange and A. Klein, Phys. Rev. **112**, 1008 (1958); R. E. Prange (private communication).

[8] A preliminary account of this part of the work appears in A. Klein, Phys. Rev. Letters **4**, 601 (1960).

volves the introduction of a generalized adiabatic assumption which incorporates the basic feature that infinite normal Fermi systems, by definition, exhibit a sharp Fermi surface.[9] The assumption requires that the exact state and its adiabatic transform (unperturbed state) be characterized by the same Fermi surface.

II. VARIATIONAL PRINCIPLE FOR THE GROUND-STATE ENERGY

The developments of this section are based on the following formula for the ground-state energy [see I-(9), (17), and (29)]:

$$\Delta E=E(N,0)-E_0(N,0)$$
$$=-\tfrac{1}{2}i\int_0^\lambda \frac{d\lambda'}{\lambda'}\int d\mathbf{r}d^4x'\, M(x;x')G(x';x). \quad (3)$$

By means of the generic Fourier transform

$$F(x;x')\equiv F(x-x')$$
$$=\frac{1}{2\pi}\int dp_0 \frac{1}{\Omega}\sum_{\mathbf{p}} F(\mathbf{p},p_0)$$
$$\times\exp[i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')-ip_0(t-t')], \quad (4)$$

and the passage to the continuous limit [$\Omega^{-1}\sum_{\mathbf{p}}\rightarrow(2\pi)^{-3}\int d\mathbf{p}$], Eq. (3) becomes

$$\Delta E=-\tfrac{1}{2}i\Omega\int_0^\lambda \frac{d\lambda'}{\lambda'}\int\frac{d\mathbf{p}}{(2\pi)^3}\oint\frac{dp_0}{(2\pi)}M(\mathbf{p},p_0)G(\mathbf{p},p_0)$$
$$=-\tfrac{1}{2}\Omega\int_0^\lambda\frac{d\lambda'}{\lambda'}\,\mathrm{tr}MG, \quad (5)$$

with the meaning of the operation "tr" defined by the equality in (5). If one traces Eq. (5) from its origins, one learns that in the event of an ambiguity in the evaluation of the p_0 integral (this can only arise in connection with the Hartree-Fock contributions to the energy) the contour is to be closed in the upper half plane.

In the present section we shall consider M as a functional of the exact G. The consequent diagrammatic representation has been described in I: M is the sum of all self-energy diagrams (one open line) with no self-energy insertions in any internal line. The quantity trMG is then a sum of all closed-loop diagrams obtained by closing in turn each diagram of M. We shall refer to M and E diagrams, respectively. We represent the series for M by the formal expression

$$M\equiv M[G]=\sum_1^\infty \lambda^n M^{(n)}[G], \quad (6)$$

where the factor λ^n exhibits the explicit dependence of the "nth-order" term on the potential, but we must remember that since particle lines are represented by the exact propagator, $G(p,p_0)$, there is additional implicit dependence on λ of any nth-order diagram.

To complete the review of the ingredients of our discussion, we recall that M and G are related through Eq. (2), and that the solution of this equation which is relevant to a normal spherical system is

$$G(\mathbf{p},p_0)$$
$$=\frac{\theta_+(p^2-p_F^2)}{-p_0+p^2-M(\mathbf{p},p_0)-i\eta}+\frac{\theta_-(p^2-p_F^2)}{-p_0+p^2-M(p,p_0)+i\eta}$$
$$=P\frac{1}{-p_0+p^2-M(\mathbf{p},p_0)}$$
$$+i\pi[\theta_+(p^2-p_F^2)-\theta_-(p^2-p_F^2)]$$
$$\times\delta(-p_0+p^2-M), \quad (7)$$

where $\theta_\pm$ are the step functions for above and below the Fermi surface and η is an infinitesimal positive quantity.

We now describe a property of E diagrams which is basic to the developments of this section. This is the concept of *equivalent* lines.[10] Consider a diagram of nth order with $2n$ particle lines, each of which is assigned a four-momentum $\mathbf{p}$, p_0. In general these are all distinct. (This is in contrast to the complete power series, where two or more lines can carry the same four-momentum. These are the so-called anomalous diagrams which arise from the series expansion of the particle propagators.) By removing any line of an E diagram we obtain an M diagram. Two lines are said to be equivalent if removing either of them yields the same (topologically equivalent) M diagram. The different M diagrams obtainable from a given E diagram then equals the number, $c(n^{(\alpha)})$ of classes of inequivalent lines in the diagram α in nth order. From (5) it also follows that $c(n^{(\alpha)})$ is the number of times the given E diagram occurs in the energy series. A more subtle, but equally true and vital fact is that each class of an E diagram contains the same number, $\nu(n^{(\alpha)})$, of lines. Though we have not attempted to construct a formal proof of this assertion, it can be induced from a study of the diagrams. We thus have the equation $2n=\nu(n^{(\alpha)})c(n^{(\alpha)})$, where $2n$ is now the total number of equivalent lines among the $c(n^{(\alpha)})$ identical E diagrams.

The basic result just given will find application in the typical formula

$$(\partial/\partial\lambda)\,\mathrm{tr}M^{(n)}[G]G=2n\,\mathrm{tr}M^{(n)}[G](\partial G/\partial\lambda), \quad (8)$$

for the factors to be differentiated are in turn solely the $2n$ particle propagators $G(\mathbf{p},p_0)$ associated with the $2n$ lines of each diagram. Equation (8) expresses the fact

[9] A. B. Migdal, Soviet Phys.-JETP **5**, 333 (1957); V. M. Galitsky and A. B. Migdal, Soviet Phys.-JETP **7**, 96 (1958); J. M. Luttinger, reference 3.

[10] This concept also appears in Luttinger and Ward, reference 3.

that the $2n$ *equivalent* lines each yield the same derivative.

With the help of Eqs. (6) and (8) we now transform the integral in Eq. (5). By integrating by parts, we find

$$(\Delta E/\Omega)=-\frac{1}{2}\int_0^\lambda \frac{d\lambda'}{\lambda'}\sum_1^\infty (\lambda')^n \operatorname{tr}M^{(n)}[G]G$$
$$=-\tfrac{1}{2}\sum_1^\infty \frac{\lambda^{2n}}{2n}\operatorname{tr}M^{(n)}G+\sum_1^\infty \int_0^\lambda d\lambda'(\lambda')^n \times\operatorname{tr}M^{(n)}(\partial G/\delta\lambda'). \quad (9)$$

The last term of (9) can in turn be written with the help of (7) as

$$\int_0^\lambda d\lambda' \operatorname{tr}M(\lambda')[\partial G(\lambda')/\partial\lambda']$$
$$=\operatorname{tr}MG-\operatorname{tr}\int_0^M dM(\lambda')G(\lambda')$$
$$=\operatorname{tr}MG-\operatorname{tr}P\int_0^M \frac{dM(\lambda')}{-p_0+p^2-M(p,p_0)}$$
$$-i\pi\operatorname{tr}[\theta_+(p^2-p_F{}^2)-\theta_-(p^2-p_F{}^2)]$$
$$\times\int_0^M dM(\lambda')\delta(-p_0+p^2-M(\lambda'))$$
$$=\operatorname{tr}MG+\operatorname{tr}\ln G^{(0)}G^{-1}. \quad (10)$$

Here the expression $\operatorname{tr}\ln G^{(0)}G^{-1}$ is a shorthand expression for the last two terms of the penultimate form of (10). We can also write as definition

$$\operatorname{tr}\ln G^{(0)}G^{-1}=\operatorname{tr}\ln\left|\frac{(-p_0+p^2-M(\mathbf{p},p_0)}{-p_0+p^2}\right|$$
$$-i\pi\operatorname{tr}[\theta_+(p^2-p_F{}^2)-\theta_-(p^2-p_F{}^2)]$$
$$\times\int_0^M dM(\lambda')\delta(-p_0+p^2-M(\lambda')). \quad (11)$$

We finally have, therefore

$$(\Delta E/\Omega)=-\sum_1^\infty \frac{\lambda^n}{2n}\operatorname{tr}M^{(n)}G+\operatorname{tr}MG+\operatorname{tr}\ln G^{(0)}G^{-1}. \quad (12)$$

The series (12) has the fundamental property that it is stationary with respect to arbitrary variations of the self-energy operator M. The hint that such a variational principle exists is seen by computing the λ derivative of this expression. The required result [from (5)], namely $(-2\lambda)^{-1}\operatorname{tr}MG$ arises completely from the explicit λ dependence in the first term of (12), and therefore the implicit dependence must somehow cancel. This can be verified by considering $(\Delta E/\Omega)$ as given by (12) to be a functional of the self-energy operator $M(\mathbf{p},p_0)$, since $M^{(n)}$ is a functional of G and G is in turn a *function* of M. We now study $[\delta/\delta M(\mathbf{p},p_0)]\times(\Delta E/\Omega)$. Differentiating in turn the three terms of (12), we find (except for unessential numerical factors)

$$[\delta/\delta M(\mathbf{p},p_0)]\left[-\sum_1^\infty \frac{\lambda^n}{2n}M^{(n)}G\right]$$
$$=-\sum_1^\infty \lambda^n M^{(n)}(G)^2=-G(\mathbf{p},p_0)M(\mathbf{p},p_0)G(\mathbf{p},p_0), \quad (13)$$

where we have used an equivalent of Eq. (8),

$$[\delta/\delta M(\mathbf{p},p_0)]\operatorname{tr}MG$$
$$=G(\mathbf{p},p_0)+G(\mathbf{p},p_0)M(\mathbf{p},p_0)G(\mathbf{p},p_0), \quad (14)$$

and

$$[\delta/\delta M(\mathbf{p},p_0)]\operatorname{tr}\ln G^{(0)}G^{-1}=-G(\mathbf{p},p_0). \quad (15)$$

Adding Eqs. (13), (14), and (15) affirms the result

$$[\delta/\delta M(\mathbf{p},p_0)](\Delta E/\Omega)=0. \quad (16)$$

It is equally true and sometimes more convenient to recognize that (12) is stationary also with respect to variations of $G(\mathbf{p},p_0)$. For this statement to obtain we must now consider $M^{(n)}$ as a functional of G and $M(\mathbf{p},p_0)$ to be defined as $[G^{(0)}(\mathbf{p},p_0)]^{-1}-[G(\mathbf{p},p_0)]^{-1}$. The property

$$[\delta/\delta G(\mathbf{p},p_0)](\Delta E/\Omega). \quad (17)$$

can then be verified directly. In deriving either (16) or (17) we have treated the ln term of (12) cavalierly. That we have not erred can be seen by studying the actual definition (11) or its antecedents.

Though we have established a variational principle, it does not appear to be true that we actually have an extremum. To see this we study the second variation with respect to G of (12). We find as a preliminary exact result

$$\{(\Delta E[G+\delta G]-\Delta E[G])/\Omega\}$$
$$=-\operatorname{tr}\sum_1^\infty \lambda^n M^{(n)}[G+\delta G]\delta G$$
$$+\operatorname{tr}M\delta G-\operatorname{tr}\delta G^{-1}\delta G. \quad (18)$$

In Eq. (18) we have deliberately left the summation in the first term to emphasize that in this term $M[G]$ is to be interpreted as a power series, whereas in the second term $M=(G^{(0)})^{-1}-G^{-1}$. We thus obtain

$$\delta^2(\Delta E/\Omega)=i(2\pi)^4\operatorname{tr}(\operatorname{tr})'[\delta M(\mathbf{p},p_0)/\delta G(\mathbf{p}',p_0')]$$
$$\times\delta G(\mathbf{p}',p_0')\delta G(\mathbf{p},p_0)-\operatorname{tr}\delta G^{-1}(\mathbf{p},p_0)\delta G(\mathbf{p},p_0), \quad (19)$$

an expression with apparently no definite sign.

We turn below to applications of the variational principle.

III. NEW PROOF OF THE HUGENHOLTZ-VAN HOVE THEOREM

We refer here to the statement that for a normal spherical system, the equation

$$\mu = p_F^2 - M(\mathbf{p}_F,\mu) \tag{20}$$

is satisfied, where μ is the chemical potential or separation energy, i.e.,

$$\mu = (\partial E/\partial N)_\Omega = (d/d\rho)(E/\Omega) = (2\pi^2/p_F^2)(d/dp_F)(E/\Omega) = (4\pi^2/p_F)(d/dp_F^2)(E/\Omega). \tag{21}$$

To avoid confusion, it is necessary to be quite explicit about what is assumed and what is to be proved. We assume our system to be normal over the entire range of coupling strengths, $0<|\lambda'|<|\lambda|$. By definition this means that we assume that the one-particle Green's function $G(\mathbf{p},p_0)$ has a pole (with finite residue) at the points $|\mathbf{p}|=|\mathbf{p}_F|$, $p_0=\epsilon_F(\mathbf{p}_F,\lambda)\equiv\mu(\mathbf{p}_F,\lambda)$ for all required values of λ. This is tantamount to (20) which expresses this assumption for the actual λ. The *theorem* to be proved is that formally, the series (12) and the definition (21) imply (20). Thus if the series converges, it represents the ground state of a normal system.

Our proof is now greatly simplified by the variational property of which we invoke the one expressing stationarity with respect to variations of G. In (12), the dependence of $(\Delta E/\Omega)$ on p_F^2 comes about almost solely through its occurrence in $G(\mathbf{p},p_0)$, whose exact form, Eq. (7), we must now remember. In carrying out the derivative required by Eq. (21), we can simply neglect *this* dependence. Examination then reveals that the only dependence on p_F^2 not thus accounted for is that exhibited in the $\theta_\pm$ factors of the last term of (11). Carrying out the differentiation here yields

$$\mu - p_F^2 = \frac{4\pi^2}{p_F}\,\mathrm{tr}\int_0^{M(\mathbf{p},p_0,\lambda)} dM(\mathbf{p},p_0,\lambda') \times 2\pi i\delta(p^2-p_F^2)\delta(-p_0+p^2-M(\mathbf{p},p_0,\lambda')). \tag{22}$$

If we now invoke our basic assumption for a normal system, that the equation

$$-p_0+p_F^2-M(\mathbf{p}_F,p_0,\lambda')=0 \tag{23}$$

has for every λ' a unique real solution $\epsilon_F(\mathbf{p}_F,\lambda')$, we can write

$$\delta(-p_0+p_F^2-M(\mathbf{p}_F,p_0,\lambda')) = \delta(-p_0+\epsilon_F(\mathbf{p}_F,\lambda'))[1+(\partial M/\partial p_0)]^{-1}|_{p_0=\epsilon_F}. \tag{24}$$

We also find with the help of (23) that

$$[\partial M(\mathbf{p}_F,\epsilon_F(\lambda'),\lambda')/\partial\lambda']|_{\epsilon_F} = [dM(\mathbf{p}_F,\epsilon_F(\lambda'),\lambda')/d\lambda'][1+(\partial M/\partial p_0)|_{p_0=\epsilon_F}]. \tag{25}$$

Writing Eq. (22) in the form

$$\mu = p_F^2 + \frac{4\pi^2}{p_F}\,\mathrm{tr}\int_0^\lambda d\lambda'[\partial M(\mathbf{p},p_0,\lambda')/\partial\lambda'] \times 2\pi i\delta(p^2-p_F^2)\delta(-p_0+p^2-M(\mathbf{p},p_0,\lambda')), \tag{26}$$

and making use of Eqs. (23), (24), and (25) permits us to carry out the integrations in (26), yielding the result

$$\mu = p_F^2 - M(\mathbf{p}_F,\epsilon_F(\mathbf{p}_F,\lambda),\lambda)\equiv\epsilon_F(\mathbf{p}_F,\lambda), \tag{27}$$

as required for a normal system.

IV. INTRODUCTION AND UTILITY OF THE SELF-CONSISTENT POTENTIAL

The theorem of the previous section suggests the introduction of a real self-consistent potential, different in purpose and meaning from the Hartree-Fock potential. We write

$$\mu = p_F^2 - M(\mathbf{p}_F,\mu(\mathbf{p}_F))\equiv p_F^2+\mathcal{U}(\mathbf{p}_F)\equiv\epsilon(\mathbf{p}_F), \tag{28}$$

where we again understand p_F or, dropping the subscript, p, to represent the density according to the standard equation $\rho=(p_F^3/6\pi^2)$. With the definitions (21), Eq. (28) may now be integrated yielding

$$E=\Omega\int_0^\rho \mu(\rho')d\rho' = \frac{\Omega}{(2\pi)^3}\int_0^{p_F}\epsilon(\mathbf{p})d\mathbf{p} = \sum_{\epsilon(\mathbf{p})<\mu}\epsilon(\mathbf{p}). \tag{29}$$

This equation, however, has an obvious physical significance, in that it provides us with a model Hamiltonian of independent particle character, such that when the single-particle levels are filled up to the unperturbed Fermi surface, we obtain thereby the *exact* ground-state energy of our system, if it is normal. Of course, the physically more fundamental way of expressing the content of Eq. (29) is to remark that $\epsilon(\mathbf{p})$ represents the chemical potential at a density corresponding to $|\mathbf{p}|$. Thus we start from zero density and volume Ω and add particles adiabatically until we reach the number N (thus slowly increasing the density from zero to its final value p_F). To previous assumptions we add the one that our system is normal over a whole range of densities.

The considerations above thus suggest the introduction of a model Hamiltonian, H_m, where

$$H_m = \sum_{\mathbf{p}} a^\dagger(\mathbf{p})a(\mathbf{p})\epsilon(\mathbf{p}) = \sum_{\mathbf{p}} a^\dagger(\mathbf{p})a(\mathbf{p})[p^2+\mathcal{U}(\mathbf{p},\lambda)]\equiv H_0+V(\lambda). \tag{30}$$

The ground state of H_m then yields the exact energy of the normal system, although the wave function is the model wave function belonging to the unperturbed Fermi sphere.

We now show that with the help of $H_m(\lambda)$ a novel formulation of the ground-state energy problem and of the associated variational principle may be found, whose worth will become increasingly apparent, not

only from the considerations to follow in this section, but also when we consider the generalization to nonspherical systems in the next section and to finite temperatures in a succeeding paper.

Toward this end, we consider the Hamiltonian $H(\lambda,\lambda')$ defined by the equation

$$H(\lambda,\lambda')=H_m(\lambda)+\lambda' H_1-V(\lambda'). \tag{31}$$

The expectation value of $H(\lambda,\lambda')$ in its exact ground state reduces in both limits $\lambda'=0$ and $\lambda'=\lambda$ to the exact ground-state energy. From the variational principle we find

$$(\partial/\partial\lambda')\langle H(\lambda,\lambda')\rangle_{N,\Omega}=\langle H_1\rangle+\langle\partial V(\lambda')/\partial\lambda'\rangle. \tag{32}$$

Integrating (32), we now have

$$E=\frac{\Omega}{(2\pi)^3}\int_0^{p_F} d\mathbf{p}[p^2+\mathcal{U}(\mathbf{p},\lambda)] + \int_0^{\lambda} d\lambda'\{\langle H_1(\lambda')\rangle-\langle\partial V(\lambda')/\partial\lambda'\rangle\}. \tag{33}$$

We shall also write E_m for the first term of (33).

To recast Eq. (33) into propagator form, we first introduce the model propagator $G_m(\lambda,\lambda')$, defined by the equation

$$G_m(\mathbf{p},p_0;\lambda,\lambda')=\frac{\theta_+(p^2-p_F^2)}{-p_0+\epsilon(\mathbf{p},\lambda)-\mathcal{U}(\lambda')-i\eta} + \frac{\theta_-(p^2-p_F^2)}{-p_0+\epsilon(\mathbf{p},\lambda)-\mathcal{U}(\lambda')+i\eta}, \tag{34}$$

and also the exact Green's function $G(\lambda,\lambda')$ for the Hamiltonian $(H\lambda,\lambda')$,

$$G(\mathbf{p},p_0,\lambda,\lambda')=\frac{\theta_+(p^2-p_F^2)}{-p_0+\epsilon(\mathbf{p},\lambda)-\mathcal{U}(\lambda')-M(\lambda,\lambda')-i\eta} + \frac{\theta_-(p^2-p_F^2)}{-p_0+\epsilon(\mathbf{p},\lambda)-\mathcal{U}(\lambda')-M(\lambda,\lambda')+i\eta}, \tag{35}$$

where $M(\lambda,\lambda')$ is term by term the same as for the actual Hamiltonian H, except that $G^{(0)}$ is everywhere replaced by $G_m(\lambda,\lambda')$. With the help of (35), (33) may be rewritten in analogy with (5) as

$$E=E_m-\tfrac{1}{2}\Omega\int_0^{\lambda}\frac{d\lambda'}{\lambda'} \times\mathrm{tr}\{M(\lambda,\lambda')G(\lambda,\lambda')+\lambda'[\partial\mathcal{U}(\lambda')/\partial\lambda']G(\lambda,\lambda')\}, \tag{36}$$

and

$$E_m=\mathrm{tr}\epsilon G_m(\lambda,0)=\mathrm{tr}(p^2+\mathcal{U})G_m(\lambda,0). \tag{37}$$

Equation (36) can be transformed into the analog of (12). We omit the detailed steps which are similar to those which led to the latter equation. We shall, however, verify below that the result attained is

$$(E/\Omega)=(E_m/\Omega)-\sum_1^{\infty}(\lambda^n/2n)\,\mathrm{tr}M^{(n)}G +\mathrm{tr}MG+\mathrm{tr}\ln G_m G^{-1}, \tag{38}$$

where the Green's functions are $G=G(\lambda,\lambda)$, $G_m=G_m(\lambda,0)$, respectively. That this result is correct can be verified by showing that

$$(E_m/\Omega)+\mathrm{tr}\ln G_m G^{-1}=(E_0/\Omega)+\mathrm{tr}\ln G^{(0)}G^{-1}, \tag{39}$$

which reduces (38) to (12). That (39) is true we see by computing

$$\mathrm{tr}\ln G^{(0)}G^{-1}-\mathrm{tr}\ln G_m G^{-1}=\mathrm{tr}\ln G^{(0)}G_m{}^{-1} =\mathrm{tr}\int_0^{\mathcal{U}(\lambda)} d^{\mathcal{U}}(\lambda')G_m(0,\lambda')=\frac{1}{(2\pi)^3}\int_0^{p_F} d\mathbf{p}\mathcal{U}(\mathbf{p}), \tag{40}$$

after performing the integral over p_0 in the operation "tr." This result reduces (39) to an identity.

It follows now that (38) is also stationary with respect to variations of either M or G, with the appropriate interpretations of $M[G]$ or $G[M]$ as given in connection with (12).

We conclude this section by indicating briefly how the variational principles (12) or (38) may be used in practice for normal systems. Let us choose the approximation

$$G(\mathbf{p},p_0)\cong G_m(\mathbf{p},p_0), \tag{41}$$

which in turn implies that

$$M(\mathbf{p},p_0)\cong-\mathcal{U}(\mathbf{p}). \tag{42}$$

Under this approximation the last two terms of (12) cancel exactly, as one easily verifies. We then have

$$(\Delta E/\Omega)\cong-\sum_1^{\infty}(\lambda^n/2n)\,\mathrm{tr}M^{(n)}[G_m]G_m. \tag{43}$$

Here the quantity $\mathcal{U}(p)$ or rather $\epsilon(p)=p^2+\mathcal{U}(p)$ has the physical meaning that it is the separation energy at a density corresponding to a Fermi momentum equal to the p in question. By means of the defining Eq. (21), utilized in conjunction with (43) or any further approximation to it, the quantities, $\epsilon(\mathbf{p})$, can in principle be determined completely self-consistently. The nonphysical question of "rearrangement energy" then never arises.

We may finally remark that the existence of a variational principle provides an explanation for the phenomenon observed both by Brueckner and collaborators and by those who have studied extensions of the Brueckner theory,[7] that the binding energy itself is insensitive to the choice of single-particle energies. As we have seen above the introduction of modified single-particle energies may be viewed as an approximation to the true self-energy operator $M(\mathbf{p},p_0)$. As a consequence

the stationary property of the binding energy with respect to variations of this quantity comes into play.

V. EXTENSION TO NONSPHERICAL SYSTEMS

All our previous considerations have been confined to the case of a Hamiltonian invariant under rotations. Recently Kohn and Luttinger[11] and Luttinger and Ward[3] have shown by using statistical mechanics that the linked cluster expansion must be modified if the system lacks spherical symmetry. The purpose of this section is to develop completely the altered form of the energy expansion for this case. For illustration it suffices to deal with the same form of Hamiltonian as hitherto with the single change that we now consider the potential function $v(\mathbf{q})$ to be nonspherically symmetric.

A "derivation" of the correct result has already been given in a previous publication.[8] There the emphasis was on the proper choice of an adiabatic transform of the ground-state wave function, i.e., of an unperturbed wave function which is "guaranteed" to be nonorthogonal to the actual ground state. It was argued that in general such a state has to differ from the unperturbed Fermi sphere, and indeed must be an unperturbed state bounded in momentum space sharply by the exact Fermi surface, a concept redefined below. In this section we shall develop a more complete version of the same basic argument.

Our previous results were entirely dependent upon the specific choice of the Green's function

$$G(\mathbf{p},t-t')=i\langle\Psi_0|T(a(\mathbf{p},t)a^\dagger(\mathbf{p},t'))|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle$$
$$=i\,\mathrm{Tr}\{T(a(\mathbf{p}t)a^\dagger(\mathbf{p}t'))\rho(0)\}, \quad (44)$$

where Tr represents the trace and $\rho(0)$ is the projection operator (not to be confused with the particle density for which the symbol ρ has been used) for the ground state Ψ_0,

$$\rho(0)=|\Psi_0\rangle\langle\Psi_0|/\langle\Psi_0|\Psi_0\rangle. \quad (45)$$

The class of *normal spherical* systems can be defined for present purposes as the class for which $\rho(0)$ is the adiabatic transform of $\rho_0(0)=|\Phi_0\rangle\langle\Phi_0|$, the projection operator for the filled Fermi sphere, according to the equation

$$\rho(0)=U(0,-\infty)\rho_0(0)U(\infty,0)/\mathrm{Tr}U(\infty,-\infty)\rho_0(0), \quad (46)$$

which is the same as the adiabatic assumption made, for instance, by Goldstone.[12] Here $U(t,t')$ is the time development operator in the interaction representation for the interaction λH_1, and $U(\infty,-\infty)$ is the S matrix. We then have the well-known form,

$$G(\mathbf{p},t-t')=i\langle\Phi_0|T(a_0(\mathbf{p}t)a_0^\dagger(\mathbf{p}t')S)|\Phi_0\rangle/\langle\Phi_0|S|\Phi_0\rangle, \quad (47)$$

where $a_0(pt)$ is the free-particle operator

$$a_0(\mathbf{p}t)=a(\mathbf{p})\exp(-ip^2t). \quad (48)$$

The Green's function (47) is precisely that given in Eq. (7). The essential connection between Φ_0 and Ψ_0 and the one that can be generalized to the nonspherical case is that the self-same Fermi surface $|\mathbf{p}|=|\mathbf{p}_F|$ which characterizes Φ_0 is also determined by Ψ_0 through the equation

$$\mu=p_F^2-M(\mathbf{p}_F,\mu), \quad (49)$$

which here is viewed as the equation which determines p_F, given μ.

We turn now to the nonspherical case. By the definition of a normal system we again have an equation of the form (49). To start with we may think of M as defined purely formally, for example with the help of the perfectly general spectral representation of the one-particle propagator. In the present instance for given μ, the solutions define the anisotropic Fermi surface $p_F(\omega)$, where ω denotes direction in momentum space. We write

$$\mu=\mu[p_F(\omega),\lambda]=\epsilon_F[p_F(\omega),\lambda], \quad (50)$$

to indicate that μ is a functional of the surface $p_F(\omega)$. In general, however, we must have

$$\mu=\mu(\rho,\lambda), \quad (51)$$

with ρ the particle density. Equation (51) is determined by adjoining to (50) a relation

$$\rho=\rho[p_F(\omega)]. \quad (52)$$

We confine ourselves to the case where the relation (52) is monotonic, i.e., $\rho=0$ corresponds to the origin and $\rho_1>\rho_2$ implies that $p_{F1}(\omega)$ lies outside $p_{F2}(\omega)$. Henceforth we drop the subscript F except when referring to the actual Fermi surface. The family of exact Fermi surfaces is now associated with a set of single-particle energies $\epsilon(\mathbf{p})=\mu(\mathbf{p})$ [Eq. (50)] exactly as in the spherical case, where

$$\epsilon(\mathbf{p})=p^2-M(\mathbf{p},\epsilon(\mathbf{p}))\equiv p^2\mathcal{U}+(\mathbf{p}). \quad (53)$$

In analogy with Eq. (29), the ground-state energy is given by the formula

$$E=\sum_{\epsilon<\mu}\epsilon(\mathbf{p})=\frac{\Omega}{(2\pi)^3}\int d\omega\int_0^{p_F(\omega)}\epsilon(\mathbf{p})\mathrm{p}^2d\mathrm{p}, \quad (54)$$

where

$$N=\sum_{\epsilon<\mu}1=\frac{\Omega}{(2\pi)^3}\int d\omega\int_0^{p_F(\omega)}p^2dp. \quad (55)$$

Again it is convenient to define a model Hamiltonian

$$H_m=\sum_{\mathbf{p}}a^\dagger(\mathbf{p})a(\mathbf{p})[\mathbf{p}^2+\mathcal{U}(\mathbf{p},\lambda)]$$
$$=H_0+V(\lambda), \quad (56)$$

[11] W. Kohn and J. M. Luttinger, Phys. Rev. **118**, 4 (1960).
[12] J. Goldstoné, Proc. Roy. Soc. (London) **A293**, 533 (1957).

whose ground state Φ_m has energy given by (54) and is bounded in momentum space by the actual Fermi surface.

All of the above is still purely formal. To actually obtain the LCE, we need an appropriate adiabatic assumption. In accordance with what has been suggested above we assume that the exact ground state $\Psi_0(\lambda)$ is the adiabatic transform of the model state Φ_m characterized by the same Fermi surface. With slightly greater generality yet we write

$$H(\lambda,\lambda')=H_m(\lambda)+\lambda' H_1-V(\lambda'), \tag{57}$$

and furthermore define an interpolating family of projection operators

$$\begin{aligned}\rho(\lambda,\lambda')&=|\Psi_0(\lambda,\lambda')\rangle\langle\Psi_0(\lambda,\lambda')|/\langle\Psi_0(\lambda,\lambda')|\Psi_0(\lambda,\lambda')\rangle\\&=U_{\lambda'}(0,-\infty)\rho_m U_{\lambda'}(\infty,0)/\mathrm{Tr}S_{\lambda'}\rho_m,\end{aligned} \tag{58}$$

where $U_{\lambda'}(t,t')$ is the evolution operator for the interaction $\lambda' H_1-V(\lambda')$, and $\rho_m=|\Phi_m\rangle\langle\Phi_m|$. For every value of λ, λ', $0<|\lambda'|<|\lambda|$, there is an interpolating set of Green's functions

$$G(\mathbf{p},t-t';\lambda,\lambda')=i\,\mathrm{Tr}\{T(a(\mathbf{p}t)a^\dagger(\mathbf{p}t')\rho(\lambda,\lambda'))\}, \tag{59}$$

with Fourier transform

$$\begin{aligned}&G(\mathbf{p},p_0;\lambda,\lambda')\\&\quad=\frac{\theta_+(p^2-p_F^2(\omega))}{-p_0+\epsilon(\mathbf{p},\lambda)-\mathcal{U}(\lambda')-M(\lambda,\lambda')-i\eta}\\&\qquad+\frac{\theta_-(p^2-p_F^2(\omega))}{-p_0+\epsilon(\mathbf{p},\lambda)-\mathcal{U}(\lambda')-M(\lambda,\lambda')+i\eta},\end{aligned} \tag{60}$$

which is the exact analog of Eq. (35), except that the boundary conditions refer to the exact Fermi surface which characterizes both Φ_m and $\Psi_0(\lambda,\lambda)$.

To derive a linked cluster expansion, we could, for example, apply the procedure of Goldstone starting from Φ_m. [For this of course, we do not require all of the above machinery, but only the connection between $\Psi_0(\lambda,\lambda)=\Psi_0$ and Φ_m.] We would then obtain a linked cluster expansion which differs from the spherical one which uses H_0 and Φ_0 as a starting point in three respects. (1) The momentum integrations are carried out above or below the exact Fermi surface. (2) The energy denominators involve the model single-particle energies, $\epsilon(p)$, which possess the symmetry appropriate to the actual Fermi surface at every density. This assures us, for example, that there are no vanishing energy denominators in the expansion. (3) The diagrams involve not only the two-particle potential, but, also, the model single-particle potential $\mathcal{U}(\mathbf{p})$.

This expansion is, of course, incomplete without a procedure for the codetermination of the self-consistent potential $\mathcal{U}(\mathbf{p})$. For this purpose we utilize the defining equation for μ which together with Eqs. (54) and (55) permit us to write

$$\begin{aligned}\mu=\epsilon(\mathbf{p}_F)&=p_F^2+\mathcal{U}(\mathbf{p}_F)=(\partial E/\partial N)_\Omega=(d/d\rho)(E/\Omega)\\&=[(2\pi)^3/p_F^2(\omega)][\delta/\delta p_F(\omega)](E/\Omega).\end{aligned} \tag{61}$$

Equation (61) and the linked cluster expansion can be used either iteratively or self-consistently to determine both the energy and the chemical potential. In contrast to previously suggested schemes, *exact* self-consistency is possible in principle.

Verification of the above scheme is, however, still lacking in one essential detail, and it is for this that the Green's function (60) and associated ideas will be utilized. It is still to be shown that the new expansion for E verifies Eq. (61). Aside from the more profound questions of convergence, which have been completely eschewed in this work, this verification provides the only test of self-consistency of our adiabatic assumption, i.e., the only test within the framework of the normal system hypothesis.

Toward this end we employ the methods of Secs. II–IV. We first outline our *modus operandi*. We shall show that the adiabatic assumption (58) results in equations which are the exact analogs of our basic results Eqs. (38) and (12), except that every reference to the spherical Fermi surface is replaced by the exactly corresponding reference to the anisotropic Fermi surface; i.e., everywhere $\theta_\pm(p^2-p_F^2)$ is replaced by $\theta_\pm(p^2-p_F^2(\omega))$. Assuming this, it then follows from the analog of (12) that Eq. (61) is indeed true, the proof being exactly the same as that given in Sec. III for the spherical case.

It remains to establish the equivalence of Eqs. (38) and (12). For this purpose, we utilize $H(\lambda,\lambda')$, Eq. (57) and follow a procedure like that associated with Eq. (32) and sequel. We study the quantity

$$E[\Omega,p_F(\omega);\lambda,\lambda']=\langle\Psi(\lambda,\lambda')|H(\lambda,\lambda')|\Psi(\lambda,\lambda')\rangle, \tag{62}$$

which by definition of $\Psi(\lambda,\lambda')$, Eq. (58), is characterized as a functional of $p_F(\omega)$. For the extrapolating set of energies (62), we have N constantly given by (55). In Sec. III the derivative $\partial E(\lambda,\lambda')/\partial\lambda'$ was taken at fixed N and Ω. Here we perform the same differentiation, but in a more restrictive manner, keeping Ω fixed and assuring the constancy of N by keeping the $p_F(\omega)$, i.e., Φ_m fixed. We are thus varying through the family of states (58). The reader may then convince himself that precisely this procedure yields all the analogs of the equations of Sec. IV, with the help of the Green's function (60) and of the associated model Green's function. In the first instance it yields Eq. (38). Then utilizing Eqs. (39) and (40) it leads to Eq. (12). Finally the latter yields the Hugenholtz-Van Hove theorem.

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