

seems doubtful that one will find a simple result as suggested in Ref. 1.

The last condition, finally, depends on the value of  $H_1$  and of  $T_1$ , and also on the lattice-lattice relaxation times which will become a factor of importance in paramagnetic salts at low temperatures.

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## Energy of the Many-Fermion Normal System\*

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Perturbation theoretic equations for several properties of the zero-temperature many-fermion normal system are rederived from general considerations. Though none of the equations are new, some of the derivations are, and taken together they form a brief and simple summary of many-fermion relations and a basis for further investigation of the basic perturbation description of the many-fermion normal system: the Brueckner-Goldstone expansion. A "change-of-parameter" technique is then developed and employed to investigate the possible use of the true momentum density instead of the unperturbed Fermi distribution in the Brueckner-Goldstone expansion and in the Brueckner  $K$ -matrix approximation. The result is a simpler, approximate perturbation series for the interaction energy, whose accuracy for nuclear matter is estimated to be approximately  $\pm 2$  MeV. The new approximation is exact to the fourth order.

### I. INTRODUCTION

THE theory of the many-fermion system has been the object of intense study for many years. This paper is limited to a small portion of the over-all field, the study of the perturbation theory of the zero-temperature "normal" state—that state in which there is no binding which would lead to a phenomenon such as superconductivity. The basic theory for the perturbation treatment has been developed, and is presented briefly in the next section as the basic tool on which the remainder of this investigation depends. This basic tool is the Brueckner-Goldstone linked-cluster expansion<sup>1</sup> (BG expansion), the perturbation theoretic expression for the ground-state energy of the system described above. With the BG expansion as a basis, the properties of a many-fermion system are then analyzed and several general relations are developed. These have previously been derived with the framework of Green's function theory, but the equations developed here are expressed as explicit perturbation series in contrast to some of the original derivations.

A "change-of-parameter" technique is then developed and employed to derive an approximation to the BG

expansion in terms of the true momentum densities instead of the Fermi step function unperturbed distribution. It is shown that the above replacement, coupled with the neglect of the "self-energy" terms in the expansion, yields an approximation which is exact through fourth order and whose accuracy is estimated to be approximately  $\pm 2$  MeV for nuclear matter. This approximation further leads to a modified form of the Brueckner  $K$  matrix approximation in which the self-consistent energy denominators are replaced by free kinetic energies and the Fermi distributions by the (self-consistent) momentum densities. An application to nuclear matter calculations in which the momentum densities are calculated to low order in perturbation theory, avoiding the self-consistency restriction, is discussed in another paper.<sup>2</sup>

### II. THE BRUECKNER-GOLDSTONE LINKED-CLUSTER EXPANSION

The heart of the perturbation theory of the normal state of zero-temperature many-fermion systems is the Brueckner-Goldstone linked-cluster expansion (BG expansion).<sup>1</sup> It is briefly reviewed in this section because of its importance in the following sections and in order to establish notation.

The Schrödinger equation for the system is

$$(H_0 + H_I)\Psi = E\Psi = (E_0 + \Delta E)\Psi, \quad (2.1)$$

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<sup>1</sup> K. A. Brueckner, Phys. Rev. **97**, 1353 (1955); **100**, 36 (1955); *The Many-Body Problem* (John Wiley, & Sons, Inc., New York, 1959); J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

<sup>2</sup> K. S. Masterson, Jr. (to be published).

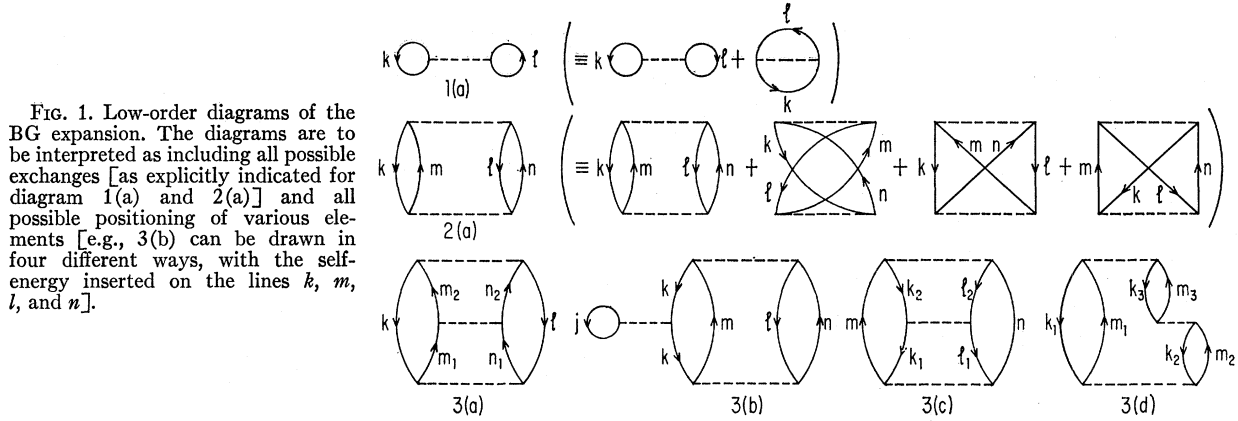


FIG. 1. Low-order diagrams of the BG expansion. The diagrams are to be interpreted as including all possible exchanges [as explicitly indicated for diagram 1(a) and 2(a)] and all possible positioning of various elements [e.g., 3(b) can be drawn in four different ways, with the self-energy inserted on the lines  $k$ ,  $m$ ,  $l$ , and  $n$ ].

with

$$H_0 = \sum_k \epsilon_k \hat{n}_k \quad (2.2)$$

satisfying

$$H_0 \Phi_0 = E_0 \Phi_0, \quad (2.3)$$

and

$$H_I = \frac{1}{2} \sum_{kl; mn} v_{kl; mn} a_l^* a_k^* a_m a_n \quad (2.4)$$

satisfying

$$(\Phi_0 H_I \Psi) = \Delta E (\Phi_0 \Psi). \quad (2.5)$$

In the equations above, and in those to follow, the states with which we are concerned are the momentum states, and the indices represent the vector quantities. In (2.2),  $\epsilon_k$  is the energy of the single-particle state with momentum  $\mathbf{k}$ , and for a spherically symmetric system is equal to the familiar  $k^2/2M$ . The number operator,  $\hat{n}_k$ , is the usual  $a_k^* a_k$ . For discrete states, the above summations are taken over all occupied states. For continuous states, they become integrals over occupied states, the integrals being over both magnitudes and angles of momentum. The system usually discussed is the spherical Fermi sea, in which the unperturbed system is a sphere (in momentum space) in which all states whose momentum is less than or equal to  $k_F$  in magnitude are occupied and all others vacant. For this case, the angular integration yields a constant, and the remaining integral is over all magnitudes of  $\mathbf{k}$  from 0 to  $k_F$ . In the equations to follow we will use the notation for the spherical, completely filled unperturbed Fermi sea, so that the region of the summations will be indicated as, e.g.,  $k \leq k_F$ . However, one should bear in mind that most of the equations derived in the following sections apply to more general discrete and continuous cases (even with a discontinuously filled unperturbed Fermi sea), including non-spherical states. Dependence of the Fermi energy (or momentum) on the spin or isotopic spin of the particles in the system (as, e.g., in a system with different neutron and proton densities) does not alter the basic conclusions of the following sections either.

The expectation value in the unperturbed ground

state of the number operator  $n_k = a_k^* a_k$  is just the Fermi step function

$$(\Phi_0, \hat{n}_k \Phi_0) \equiv n_k = \begin{cases} 1 & k \leq k_F \\ 0 & k > k_F. \end{cases}$$

The Fermi momentum,  $k_F$ , is determined by the condition

$$\sum_{k \leq k_F} n_k = N.$$

This equation indicates that each summation in our equations will introduce a factor proportional to  $N$ , the total number of particles in the system.

The BG expansion for the ground-state wave function is, in the notation of Goldstone,<sup>1</sup>

$$\Psi_0 = \lim_{\alpha \rightarrow 0} \sum_L \frac{1}{E_0 - H_0 + i\alpha} H_I \cdots H_I \frac{1}{E_0 - H_0 + 2i\alpha} \times H_I \frac{1}{E_0 - H_0 + i\alpha} H_I \Phi_0, \quad (2.6)$$

and the BG expansion for the interaction energy,  $\Delta E(n, \epsilon)$ , is

$$\Delta E = \lim_{\alpha \rightarrow 0} \sum_c \left( \Phi_0, H_I \frac{1}{E_0 - H_0 + i\alpha} H_I \cdots \times H_I \frac{1}{E_0 - H_0 + i2\alpha} H_I \frac{1}{E_0 - H_0 + i\alpha} H_I \Phi_0 \right), \quad (2.7)$$

where  $\sum_c$  means summation over all connected graphs leading from  $\Phi_0$  to  $\Phi_0$ , i.e., over all linked graphs with no external lines. In terms of the two-body interaction, the BG expansion is given by

$$E = \sum_k \epsilon_k n_k + \Delta E(n, \epsilon) = \sum_k \epsilon_k n_k + \frac{1}{2} \sum_{kl} v_{kl; (kl)} n_k n_l + \lim_{\alpha \rightarrow 0} \frac{1}{2} \sum_{kl; mn} v_{kl; mn} \times \frac{(1-n_m)(1-n_n)n_k n_l}{(\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n + i\alpha)} v_{mn; (kl)} + O(v^3), \quad (2.8)$$

where

$$v_{kl;(kl)} = v_{kl;kl} - v_{kl;lk}.$$

The rules for expressing the terms of any order in the BG expansion (2.7) in terms of all possible connected graphs of that order ("linked clusters"—see Fig. 1) are the same as those used by most authors,<sup>1,4</sup> with one exception. The restrictions on various summations to states above or below the Fermi sea are replaced in (2.8) by expressions involving the expectation values of the number operator,  $\hat{n}_k$ , which values are, in turn, obtained by (1) indicating explicitly the creation and annihilation operators associated with each  $v$  interaction, (2) reducing them to expectation values of the number operator by using the customary prescriptions

$$\begin{aligned} a_k^* a_k &= \hat{n}_k, \\ a_k a_k^* &= (1 - a_k^* a_k) = (1 - \hat{n}_k), \end{aligned} \quad (2.9)$$

and, (3) simplifying the resulting expansion through the use of the identities

$$\hat{n}_k^n = \hat{n}_k$$

and

$$(1 - \hat{n}_k)^n = (1 - \hat{n}_k). \quad (2.10)$$

The BG expansion is exact for a "normal" system with a spherically symmetric Fermi surface and characterized by an isotropic interaction. In particular, it has been proven<sup>3</sup> to apply in all orders in  $v$  to spin  $\frac{1}{2}$  Fermions interacting through central forces. Further, through second order it is known to apply to tensor forces,<sup>2</sup> but the proof has not yet been extended to all others. By a "normal" system we mean a system in which BCS correlations (leading to superfluidity) are absent. At present it appears that the BG expansion is applicable to nuclear matter and perhaps to zero-temperature helium-three. Even if it turns out that the normal state is not the ground state for these systems, it is probable that it will not be far above the true ground state and that the calculation of its properties will still be of considerable interest and usefulness. Furthermore, most of the equations we shall derive in the first few sections are applicable in general to any Fermion system, though some of the quantities in these equations may be undefined for other states. For the normal state, however, all of these quantities can be completely defined in terms of functional derivatives of the BG expansion, and are therefore formally calculable from first principles.

### III. MANY-FERMION SYSTEM PROPERTIES

In this section, fundamental formulas for the true momentum density and the single-particle energy are

<sup>3</sup> W. Kohn and J. M. Luttinger, Phys. Rev. **118**, 41 (1960); J. M. Luttinger and J. C. Ward, *ibid.* **118**, 1417 (1960).

<sup>4</sup> A. Klein and R. E. Prange, Phys. Rev. **112**, 994 (1958).

developed from the Brueckner-Goldstone expansion. Explicit perturbation series are exhibited. Then several zero-temperature forms of the equations of the Landau theory are derived more concisely than by previous derivations using Green's function theory (e.g., Klein and Prange<sup>4</sup> and Nozières and Luttinger<sup>5</sup>). Many of the relations so developed are then used in the development of the new approximation in Sec. IV of this paper.

#### A. True Momentum Density

The expectation value of the number operator,  $\hat{n}_p = a_p^* a_p$ , is the Fermi step-function when evaluated between the unperturbed states,  $\Phi_0$ . When evaluated between the states of the interacting system,  $\Psi$ , it yields the momentum density,  $\rho_p$ . From

$$E = [\Psi, (\sum_k \epsilon_k \hat{n}_k + v) \Psi] / (\Psi, \Psi), \quad (3.1)$$

we then show that  $\rho_p = (\Psi, \hat{n}_p \Psi) / (\Psi, \Psi)$  is equal to

$$\frac{\delta}{\delta \epsilon_p} E = \frac{\delta}{\delta \epsilon_p} \{ [\Psi(\epsilon_1 \epsilon_2 \dots), (\sum_k \epsilon_k \hat{n}_k + v) \Psi(\epsilon_1 \epsilon_2 \dots)] / (\Psi, \Psi) \}. \quad (3.2)$$

The only dependence of the wave functions which is indicated above is their implicit dependence on the single-particle energies as, e.g., given by (2.6). To prove that (3.2) is  $(\Psi, \hat{n}_p \Psi) / (\Psi, \Psi)$ , we must show that the functional derivative on the wave functions vanishes. If we write that derivative as

$$\frac{\delta}{\delta \epsilon_{p'}} [(\Psi(\dots \epsilon_{p'} \dots), (\sum_k \epsilon_k \hat{n}_k + v) \Psi(\dots \epsilon_{p'} \dots))] / (\Psi(\dots \epsilon_{p'} \dots), \Psi(\dots \epsilon_{p'} \dots)) \Big|_{\epsilon_{p'} = \epsilon_p} \quad (3.3)$$

and, if  $\epsilon_{p'}$  is regarded as a variational parameter, then the expectation value is stationary at the true wave function (where  $\epsilon_{p'} = \epsilon_p$ ), and the above derivative vanishes for  $\epsilon_{p'} = \epsilon_p$ . Thus (3.2) reduces to  $(\Psi, \hat{n}_p \Psi) / (\Psi, \Psi) = \rho_p$  (since  $v$  has no explicit dependence on the  $\epsilon_k$ ), and one obtains the well-known formula<sup>6</sup>:

$$\rho_p = (\delta / \delta \epsilon_p) E = n_p + (\delta / \delta \epsilon_p) \Delta E(n, \epsilon) \equiv n_p + \Delta n_p. \quad (3.4)$$

We remark here that the momentum indices are *vector indices*, and refer to both angle and magnitude of the momenta.

In (3.4) and throughout this discussion, the functional derivative is defined as operating on every  $\epsilon_p$  which occurs in the expression which follows it, including those  $\epsilon_p$  which occur under a summation (i.e., the single term in each sum for which the summation variable equals  $\epsilon_p$  in the example above).

<sup>5</sup> P. Nozières and J. M. Luttinger, Phys. Rev. **127**, 1423 (1962); J. M. Luttinger and P. Nozières, *ibid.* **127**, 1431 (1962).

<sup>6</sup> E. Daniel and S. H. Vosko, Phys. Rev. **120**, 2041 (1960).

From the BG equation for  $E$ , (2.8), we obtain

$$\rho_p(n, \epsilon) = n_p \left\{ 1 - \sum_{lmn} v_{pl; mn} \frac{n_l(1-n_m)(1-n_n)}{(\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n)^2} \right. \\ \left. \times v_{mn; (pl)} + \dots \right\} + (1-n_p) \left\{ \sum_{kln} v_{kl; pn} \right. \\ \left. \times \frac{n_k n_l (1-n_n)}{(\epsilon_k + \epsilon_l - \epsilon_p - \epsilon_n)^2} v_{pn; kl} + \dots \right\}. \quad (3.5)$$

We have used a change of summation indices to combine terms with identical structure arising from (2.8), thus cancelling the factors  $\frac{1}{2}$  in that equation. For example,

$$\frac{1}{2} n_p \sum_{lmn} v_{pl; mn} \frac{n_l(1-n_m)(1-n_n)}{(\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n)^2} v_{mn; (pl)} \\ + \frac{1}{2} n_p \sum_{kmn} v_{kp; mn} \frac{n_k(1-n_m)(1-n_n)}{(\epsilon_k + \epsilon_p - \epsilon_m - \epsilon_n)^2} v_{mn; (kp)} \\ = n_p \sum_{lmn} v_{pl; mn} \frac{n_l(1-n_m)(1-n_n)}{(\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n)^2} v_{mn; (pl)}. \quad (3.6)$$

Similar changes of summation indices to combine terms are employed throughout this dissertation without further comment.

The term not multiplied by  $n_p$  in (3.5) is the "tail" of the density distribution, extending beyond the Fermi sphere. It is readily verified that this equation for  $\rho_p$  can be truncated at any order in  $v$  and will still satisfy the identity<sup>7</sup>

$$\sum_p \rho_p = \sum_p n_p = N. \quad (3.7)$$

Equation (3.5) can be inverted to yield an equation for  $n_p$  in terms of  $\rho_p$ <sup>8</sup>:

$$n_p = \rho_p \left\{ 1 + \sum_{lmn} v_{pl; mn} \frac{\rho_l(1-\rho_m)(1-\rho_n)}{(\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n)^2} v_{mn; (pl)} + \dots \right\} \\ - (1-\rho_p) \left\{ \sum_{kln} v_{kl; pn} \frac{\rho_k \rho_l (1-\rho_n)}{(\epsilon_k + \epsilon_l - \epsilon_p - \epsilon_n)^2} \right. \\ \left. \times v_{pn; (kl)} + \dots \right\}. \quad (3.8)$$

## B. Single-Particle Energy

The "single-particle" energy may be obtained from the perturbation expression for the total energy in a fashion analogous to that employed for the density. The energy of an added particle of momentum  $\mathbf{p}$  is

<sup>7</sup> This identity is valid because all terms except the zero-order term ( $n_p$ ) cancel upon summation over  $p$ . This can be seen in second order by using (3.5) for  $\rho_p$ .

<sup>8</sup> The structure of this equation differs radically from (3.5) in third and higher orders; however, only the second-order expansion is required for subsequent discussions.

the difference

$$\omega_p = E(n_p', \epsilon) - E(n, \epsilon), \quad (3.9)$$

where  $E(n_p', \epsilon)$  means that in the expression (2.8) we take  $n_k$  as follows:

$$n_{k,p}' = 1 \quad \text{for } |\mathbf{k}| \leq k_F, \\ = 0 \quad \text{for } |\mathbf{k}| > k_F \text{ and } \mathbf{k} \neq \mathbf{p}, \\ = 1 \quad \text{for } |\mathbf{k}| > k_F \text{ and } \mathbf{k} = \mathbf{p}. \quad (3.10)$$

which corresponds to the change of occupied state in Goldstone's paper<sup>1</sup>, and we can see from (2.8) the energy thus obtained is in general complex, the imaginary part being related to the lifetime of the state. Similarly, the energy of an additional hole is

$$\omega_p = E(n, \epsilon) - E(n_p'', \epsilon), \quad (3.11)$$

with same meaning to  $E(n_p'', \epsilon)$ , where

$$n_{k,p}'' = 1 \quad |\mathbf{k}| \leq k_F \text{ and } \mathbf{k} \neq \mathbf{p}, \\ = 0 \quad |\mathbf{k}| < k_F \text{ and } \mathbf{k} = \mathbf{p}, \\ = 0 \quad |\mathbf{k}| > k_F. \quad (3.12)$$

It is apparent from the above expressions that the single-particle energy can be written as

$$\omega_p = \pm (E_p - E) = (\delta/\delta n_p) E(n, \epsilon) \\ = \epsilon_p + (\delta/\delta n_p) \Delta E(n, \epsilon) \\ = \epsilon_p + \Delta \epsilon_p; \quad \Delta \epsilon_p = (\delta/\delta n_p) \Delta E(n, \epsilon). \quad (3.13)$$

The definition of  $\delta/\delta n_p$  is similar to that of  $\delta/\delta \epsilon_p$ . It is known that  $E(n, \epsilon)$  is proportional to the total number,  $N$ ; therefore,  $\omega_p$  is of order unity compared to  $N$  because  $\delta/\delta n_p$  removes one summation of  $E(n, \epsilon)$ . Rigorously, (3.13) should contain terms with the higher derivatives  $\delta^2/\delta n_p^2$ ,  $\delta^3/\delta n_p^3$ , etc. However, each such derivative will remove one or more other summations and will thus introduce a factor of  $1/N$  or smaller. Such terms may be discarded in the normal system (for which we take the limit  $\Omega \rightarrow \infty$ , with the ratio  $N/\Omega$  remaining constant,  $\Omega$  being the volume).<sup>9</sup> From (2.8) we obtain the following expansion of (3.13).

$$\omega_p(\epsilon_p) = \epsilon_p + \sum_l v_{pl; (pl)} n_l + \lim_{\alpha \rightarrow 0} \sum_{lmn} v_{pl; mn} \\ \times \frac{n_l(1-n_m)(1-n_n)}{\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n + i\alpha} v_{mn; (pl)} \\ - \lim_{\alpha \rightarrow 0} \sum_{kln} v_{kl; pn} \frac{n_k n_l (1-n_n)}{\epsilon_k + \epsilon_l - \epsilon_p - \epsilon_n + i\alpha} \\ \times v_{pn; (kl)} + \dots \quad (3.14)$$

The imaginary terms from the Brueckner-Goldstone expansion, (2.7), are related to the lifetimes of the hole and particle states. In the subsequent discussions we shall not exhibit the imaginary terms explicitly. We should remember, however, that  $\omega_{k_F}$  has no imaginary part. The original BG series for the ground-state energy (of the normal system) contains no poles, and

<sup>9</sup> This technique is used without further comment in the remainder of this paper.

since (3.14) for  $p=k_F$  is just the upper or lower limit of one summation in the equation for the ground-state energy, it must also be real.

If we define an "effective interaction" matrix  $U(k,l)$  such that

$$\Delta E(n,\epsilon) = \frac{1}{2} \sum_{k,l} U(k,l) n_k n_l, \quad (3.15)$$

then (3.13) becomes

$$\omega_p = \epsilon_p + \sum_l U(p,l) n_l + \frac{1}{2} \sum_{k,l} n_k n_l (\delta/\delta n_p) U(k,l), \quad (3.16)$$

which is a restricted form of the Landau equation, with all the quantities in (3.15) completely specified by the BG expansion [which is an equation for  $U(k,l)$ ]. For example, to second order in  $v$ ,

$$U(k,l) = v_{kl;(kl)} + \sum_{m,n} v_{kl;mn} \frac{(1-n_m)(1-n_n)}{\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n} v_{mn;(kl)}, \quad (3.17)$$

and (3.14) is obviously obtained when this equation is substituted into (3.16). The third term in the equation for  $\omega_p$  is the so-called "rearrangement energy."<sup>10,11</sup> It represents the difference in the energy to remove a particle to infinity "quickly" (with no change in the states of the rest of the system) and the energy required to remove the particle adiabatically (the rest of the system "rearranging" itself to the ground state of the  $N-1$  particle system as the removed particle goes to infinity). If one identifies  $U(k,l)$  with Brueckner's  $K$  matrix,  $K_{kl;(kl)}$ , then (3.16) is identical to the equation derived by Brueckner and Goldman in their analysis of the rearrangement energy.<sup>10</sup> The rearrangement energy is sometimes cited as the reason for the failure of reaction-matrix calculations to satisfy the Bethe-Hugenholtz-Van Hove theorem<sup>12</sup> that the single-particle energy at the Fermi surface should equal the mean system energy. However, the actual situation was that, as is well known, this theorem is not applicable to reaction matrix calculations because the single-particle energies which were used in such calculations are computed "off-energy-shell" when singular energy denominators are involved. Therefore, they are not the energies defined in this section (e.g., for  $p=p_F$ , the separation energy) and need not satisfy the theorem. See Brueckner and Gammel<sup>13</sup> for further discussion.

### C. Discontinuity in Momentum Density at the Fermi Surface

The possibility that a Fermi surface might exist for zero-temperature interacting fermions was pointed out

<sup>10</sup> K. A. Brueckner and D. T. Goldman, Phys. Rev. **112**, 994 (1958).

<sup>11</sup> K. A. Brueckner, Phys. Rev. **110**, 597 (1958); K. A. Brueckner and D. T. Goldman, *ibid.* **116**, 424 (1959); D. J. Thouless, *ibid.* **112**, 906 (1958).

<sup>12</sup> H. A. Bethe, Phys. Rev. **103**, 1353 (1956); N. M. Hugenholtz and L. Van Hove, Physica **24**, 363 (1958).

<sup>13</sup> K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958). Referred to as BG. This paper gives extensive references to previous work.

by Migdal,<sup>14</sup> who noticed that under some circumstances it could be so that the *mean* occupation number of different single-particle momentum states in the true ground state is discontinuous. Luttinger<sup>15</sup> has examined the conditions for its existence and rederived the equation for the discontinuity. A calculation for the electron gas has been reported by Daniel and Vosko.<sup>6</sup> We present here still another derivation, which is based on the assumption that a valid perturbation expansion for the system energy exists.

From expression (3.5) for the momentum density,  $\rho_p$ , it is evident that  $\rho_p$  can be separated into two parts, one multiplied by  $n_p$  and the other having no explicit dependence on  $n_p$ :

$$\begin{aligned} \rho_p &= (\delta/\delta \epsilon_p) E(n,\epsilon) \\ &= n_p + n_p (\delta/\delta \epsilon_p) \left( \frac{\delta}{\delta n_p} \Delta E(n,\epsilon) \right) + \frac{\delta'}{\delta \epsilon_p} \Delta E(n,\epsilon). \end{aligned} \quad (3.18)$$

Henceforth  $\delta'/\delta \epsilon_p$  will indicate differentiation of those terms not multiplied by  $n_p$ . Thus the leading terms of the last two elements on the right-hand side of (3.15) are

$$\begin{aligned} & n_p \frac{\delta}{\delta \epsilon_p} \left( \frac{\delta}{\delta n_p} \Delta E(n,\epsilon) \right) \\ &= n_p \left\{ - \sum_{lmn} v_{pl;mn} \frac{n_l(1-n_m)(1-n_n)}{(\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n)^2} v_{mn;(pl)} - \right. \\ & \quad \left. - \sum_{kln} v_{kl;pn} \frac{n_k n_l (1-n_n)}{(\epsilon_k + \epsilon_l - \epsilon_p - \epsilon_n)^2} v_{pn;(kl)} + \dots \right\}, \end{aligned} \quad (3.19)$$

and

$$\begin{aligned} \frac{\delta'}{\delta \epsilon_p} \Delta E(n,\epsilon) &= + \sum_{kln} v_{kl;pn} \frac{n_k n_l (1-n_n)}{(\epsilon_k + \epsilon_l - \epsilon_p - \epsilon_n)^2} \\ & \quad \times v_{pn;(kl)} + \dots \end{aligned} \quad (3.20)$$

By using the definition of the single-particle energy change  $\Delta \epsilon_p(n,\epsilon)$  from (3.13), we can write (3.18) as

$$\begin{aligned} \rho_p &= n_p [1 + (\delta/\delta \epsilon_p) \Delta \epsilon_p] + \frac{\delta'}{\delta \epsilon_p} \Delta E(n,\epsilon) \\ &= n_p (\delta/\delta \epsilon_p) \omega_p(\epsilon_p) + (\delta'/\delta \epsilon_p) \Delta E(n,\epsilon). \end{aligned} \quad (3.21)$$

It can be seen that  $\delta/\delta \epsilon_p$  operates not only on the explicit  $\epsilon_p$  in  $\omega_p(\epsilon_p)$  but also on the single term in each sum for which the index of summation equals  $p$ . Because these latter operations yield terms of order  $(1/N)$  (because of the removal of one sum), they may be neglected and the functional derivative may be replaced by the partial derivative,  $\partial/\partial \epsilon_p$ . The density is then

<sup>14</sup> A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **32**, 399 (1957) [English transl.: Soviet Phys.—JETP **5**, 333 (1957)].

<sup>15</sup> J. M. Luttinger, Phys. Rev. **119**, 1153 (1960).

given by

$$\rho_p = n_p (\partial/\partial \epsilon_p) \omega_p(\epsilon_p) + (\delta'/\delta \epsilon_p) \Delta E(n, \epsilon). \quad (3.22)$$

Usually  $(\delta/\delta \epsilon_p) \omega_p$  is denoted as  $Z_p$ . Its physical meaning can be seen in the following way. For  $\epsilon_p > \epsilon_F$ , we have from the definition of  $\omega_p$  and from (3.4)

$$\begin{aligned} Z_p &= (\delta/\delta \epsilon_p) \omega_p = (\delta/\delta \epsilon_p) (E_p - E) \\ &= (\Psi_p, \hat{n}_p \Psi_p) - (\Psi, \hat{n}_p \Psi), \end{aligned} \quad (3.23)$$

where  $\Psi_p$  is the state with one extra particle of momentum  $\mathbf{p}$ . If we introduce the creation and annihilation operators,  $a_p^*$  and  $a_p$  ( $\hat{n}_p = a_p^* a_p$ ), and the complete set of unperturbed states,  $\Phi_i$ , we obtain

$$Z_p = \sum_i | (a_p^* \Phi_i, \Psi_p) |^2 - \sum_i | (a_p^* \Phi_i, \Psi) |^2. \quad (3.24)$$

A similar equation is obtained for  $\epsilon_p \leq \epsilon_F$ . Thus  $Z_p$  is the difference between the total probabilities of finding in  $\Psi_p$  and  $\Psi$  *unperturbed states* which contain a particle in state  $\mathbf{p}$ . If the state  $\mathbf{p}$  has a finite lifetime,  $\Psi_p$  must be replaced by an appropriate wave packet, and only the real part of  $Z_p$  can be interpreted in this manner. Because  $\omega_{k_F}$  contains no imaginary part [see below (3.14)], the above formulation is exact at the Fermi surface.

From (3.21) it is apparent that the discontinuity across  $\epsilon_p = \epsilon_F$  is given by

$$(\delta/\delta \epsilon_p) \omega_p |_{\epsilon_p = \epsilon_F} = Z_p |_{\epsilon_p = \epsilon_F} = N \rightarrow \infty (\partial/\partial \epsilon_p) \omega_p |_{\epsilon_p = \epsilon_F}. \quad (3.25)$$

Using the formalism developed in this section, we are now able to cast (3.22) into a different form. If we solve (3.14) for  $\epsilon_p$  as a function of  $\omega_p$ , we can write  $\Delta \epsilon_p$  of (3.13) in terms of  $\omega_p$  and obtain a new function,  $V(\omega_p)$ ,

which is numerically equal to  $\Delta \epsilon_p$ .  $V(\omega_p)$  is the "self-consistent" potential, since from (3.13)

$$\omega_p = \epsilon_p + V(\omega_p). \quad (3.26)$$

To obtain an expression for  $\rho_p$ , we operate on the above expression with  $\partial/\partial \epsilon_p$ , obtaining

$$(\partial/\partial \epsilon_p) \omega_p = 1 + (\partial/\partial \epsilon_p) \omega_p \cdot (\partial/\partial \omega_p) V(\omega_p). \quad (3.27)$$

This can be solved for  $\partial/\partial \epsilon_p(\omega_p)$ :

$$\frac{\partial}{\partial \epsilon_p} \omega_p = \frac{1}{1 - (\partial/\partial \omega_p) V(\omega_p)}. \quad (3.28)$$

From (3.21) we then obtain

$$\rho_p = \frac{n_p}{1 - (\partial/\partial \omega_p) V(\omega_p)} + (\delta'/\delta \epsilon_p) \Delta E(n, \epsilon). \quad (3.29)$$

The first term on the right in (3.29) corresponds to the density obtained by Puff and Martin<sup>16</sup> [see also Falk and Wilets,<sup>17</sup> Eq. (21)]. The smooth part in (3.29), which is neglected in their approximation, can be seen from (3.5) to be of order  $v^2$ .

#### D. Effective Mass Equation

We shall now derive the effective mass equation which was first obtained semiphenomenologically by Landau<sup>18</sup> and later from perturbation theory by Luttinger and Nozières.<sup>5</sup>

By taking derivatives of  $\omega_p$  [Eqs. (3.13) and (3.14)] with respect to  $p_x$ , we get

$$\begin{aligned} \frac{d}{dp_x} \omega_p &= \frac{p_x}{m} + \frac{d}{dp_x} \left( \frac{\delta}{\delta n_p} \Delta E(n, \epsilon) \right) \\ &= \frac{p_x}{m} + \frac{d}{dp_x} \left( \sum_l v_{pl}; (pl) n_l + \sum_{lmn} v_{pl}; mn \frac{n_l(1-n_m)(1-n_n)}{\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n} v_{mn}; (pl) + \dots \right) \\ &= \frac{p_x}{m} + \lim_{\Delta p_x \rightarrow 0} \left\{ \left( \sum_l v_{p+\Delta p_x, l}; (p+\Delta p_x, l) n_l + \sum_{lmn} v_{p+\Delta p_x, l}; mn \frac{n_l(1-n_m)(1-n_n)}{\epsilon_{p+\Delta p_x} + \epsilon_l - \epsilon_m - \epsilon_n} v_{mn}; (p+\Delta p_x, l) + \dots \right) \right. \\ &\quad \left. - (\Delta p_x = 0) \right\} \frac{1}{\Delta p_x}. \end{aligned} \quad (3.30)$$

We next change all the momentum variables under the summations by an amount  $\Delta p_x$ , and observe that in a Galilean invariant system

$$v_{p+\Delta p_x, l+\Delta p_x; m+\Delta p_x, n+\Delta p_x} = v_{pl; mn}$$

and due to conservation of total momentum

$$\epsilon_{p+\Delta p_x} + \epsilon_{l+\Delta p_x} - \epsilon_{m+\Delta p_x} - \epsilon_{n+\Delta p_x} = \epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n + 0((\Delta p_x)^2). \quad (3.31)$$

<sup>16</sup> R. D. Puff and P. C. Martin, Bull. Am. Phys. Soc. **5**, 30 (1960); R. D. Puff, Ann. Phys. (N. Y.) **13**, 317 (1961).

<sup>17</sup> D. S. Falk and L. Wilets, Phys. Rev. **124**, 1887 (1961).

<sup>18</sup> J. S. Langer, Phys. Rev. **120**, 714 (1960).

The result is

$$\frac{d}{d\phi_x} \omega_p = \frac{\phi_x}{m} + \lim_{\Delta p_x \rightarrow 0} \left\{ \left( \sum_l v_{pl}; (pl) n_l + \sum_{lmn} v_{pl; mn} \frac{n_l(1-n_m)(1-n_n)}{\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n} v_{mn; (pl)} + \dots \right) - (\Delta p_x = 0) \right\} \frac{1}{\Delta \phi_x}. \quad (3.32)$$

The second term on the right can be identified with

$$\sum_l v \frac{dn_l}{dl_x} \frac{\delta}{\delta n_l} \left( \sum_l v_{pl}; (pl) n_l + \sum_{lmn} v_{pl; mn} \frac{n_l(1-n_m)(1-n_n)}{\epsilon_p + \epsilon_l - \epsilon_m - \epsilon_n} v_{mn; (pl)} + \dots \right) = \sum_l \frac{dn_l}{dl_x} \frac{\delta}{\delta n_l} \left( \frac{\delta}{\delta n_p} \Delta E(n, \epsilon) \right). \quad (3.33)$$

Since  $n_l$  is a step-function,  $dn_l/dl_x$  is zero except at the Fermi surface, where its magnitude is  $-l_x/l$ . Thus,

$$\frac{d}{d\phi_x} \omega_p = \frac{\phi_x}{m} - \sum_l \frac{l_x}{l} \delta(l - k_F) \frac{\delta^2}{\delta n_l \delta n_p} \Delta E(n, \epsilon). \quad (3.34)$$

This equation is identical to that obtained by Landau, except now, by virtue of the BG expansion for  $\Delta E(n, \epsilon)$ , we have an explicit expression for every term in it.

If we take  $\omega_p|_{|p|=k_F} = \phi^2/2m^*$  and operate with  $(1/\phi^2) \sum_{xyz} \phi_x d/d\phi_x$  on  $\omega_p$ , we obtain

$$\begin{aligned} \frac{1}{m^*} &= \frac{1}{m} \frac{1}{k_F} \sum_l \cos(\mathbf{p}, \mathbf{l}) \delta(l - k_F) \frac{\delta^2}{\delta n_l \delta n_p} \Delta E(n, \epsilon) \Big|_{p=k_F} \\ &= \frac{1}{m} + \frac{\Omega}{(2\pi)^3} k_F \int d\Omega_l \cos(\mathbf{p}, \mathbf{l}) (-) \frac{\delta^2}{\delta n_l \delta n_p} \Delta E(n, \epsilon) \Big|_{p=k_F}. \end{aligned} \quad (3.35)$$

The quantity  $(-)\delta^2 E(n, \epsilon)/\delta n_l \delta n_p = f_{l;p}$  was interpreted by Landau<sup>19</sup> as (minus) the forward scattering amplitude of two particles,  $\mathbf{l}$  and  $\mathbf{p}$ , in the system. We reach the same identification by following the procedure by which we derived Eq. (3.13) for  $\omega_p$ .

### E. Bethe-Hugenholtz-Van Hove Separation Energy Theorem

With our formalism we can easily derive the Bethe-Hugenholtz-Van Hove<sup>12</sup> theorem which states that the energy of a particle on the Fermi surface is the negative of the energy required to remove the particle adiabatically to infinity (the separation energy) and equals the average energy of all the particles in the system. Alternately, the separation energy is the negative of the energy the system acquires when one particle is added at constant volume whereas the average energy is the energy acquired when a single particle is added at constant density. A somewhat more involved derivation has also been given by Brueckner.<sup>11</sup>

The proof begins with the observation that the total

energy  $E$  is a function of two parameters,  $N$  and  $\rho$ , where the density  $\rho$  is related to the total number of particles,  $N$ , and to the volume,  $\Omega$ , by the following equation (neglecting spin which gives a constant):

$$\rho = \frac{N}{\Omega} = \frac{1}{\Omega} \sum_k n_k = \frac{1}{(2\pi)^3} \int_0^{p_F} d\mathbf{k} = p_F^3/6\pi^2. \quad (3.36)$$

Further, since  $E$  is proportional to  $N$ ,<sup>1</sup> it may be written as  $E = Nf(\rho)$  where  $f(\rho)$  denotes the (unknown) functional dependence on the density. From the definition of the average energy, it is easily seen that  $E_{Av} = E/N$ . For a free system, the pressure,  $P$ , must be zero, and therefore at zero temperature

$$P \sim (\partial/\partial \rho)(E/N)_{\Omega} = 0 \quad (3.37)$$

(since the average energy,  $E/N$ , is a function of density alone). We can then expand the derivative of  $E = Nf(\rho)$  to obtain

$$(\partial/\partial N)(E)_{\Omega} = f(\rho) + N[\partial f(\rho)/\partial \rho](\partial \rho/\partial N), \quad (3.38)$$

to show that the separation energy equals the negative of the average energy, viz.:

$$E_s = -\frac{\partial}{\partial N}(E)_{\Omega} = -\frac{E}{N} - \rho \frac{\partial}{\partial \rho} \left( \frac{E}{N} \right)_{\Omega} = -\frac{E}{N}. \quad (3.39)$$

We can now apply the techniques of previous sections to obtain another equality involving  $E/N$ . Expanding (3.37), we obtain

$$\begin{aligned} -\frac{E}{N^2} \frac{\partial}{\partial \rho} (N)_{\Omega} + \frac{1}{N} \frac{\partial}{\partial \rho} (E)_{\Omega} \\ = -\frac{E}{N^2} \Omega + \frac{1}{N} \frac{\partial}{\partial \rho} (E)_{\Omega} = 0. \end{aligned} \quad (3.40)$$

Thus

$$E/N = 1/\Omega (\partial/\partial \rho)(E)_{\Omega}. \quad (3.41)$$

Using (3.36), we can rewrite (3.41) as

$$\begin{aligned} \frac{E}{N} &= \frac{1}{\Omega} \frac{2\pi^2}{\phi_F^2} \frac{\partial}{\partial \phi_F} (E) \\ &= \frac{2\pi^2}{\Omega \phi_F^2} \sum_k \left\{ \frac{\partial n_k}{\partial \phi_F} \frac{\delta}{\delta n_k} E + \frac{\partial \epsilon_k}{\partial \phi_F} \frac{\delta}{\delta \epsilon_k} E \right\}. \end{aligned} \quad (3.42)$$

<sup>19</sup> L. D. Landau, Zh. Eksperim. i Teor. Fiz. **30**, 1058 (1956); **32**, 59 (1957); **35**, 97 (1958) [English transl.: Soviet Phys.—JETP **3**, 920 (1957); **5**, 101 (1957); **8**, 70 (1959)].

The kinetic energy,  $\epsilon_k$ , is unchanged by an infinitesimal increase,  $\eta$ , in the magnitude of the Fermi momentum, but  $n_k$  will increase by unity for  $k = p_F + \eta$  if  $p_F$  increases by  $\eta$ . Therefore,  $\partial \epsilon_k / \partial p_F = 0$  and  $\partial n_k / \partial p_F = \delta(k - p_F)$ . Using

$$\sum_k \rightarrow \frac{\Omega}{(2\pi)^3} \int d\mathbf{k}, \quad (3.43)$$

and identifying  $\delta / \delta n_k(E)$  with  $\omega_k$  (3.6), we obtain

$$\frac{E}{N} = \frac{1}{4\pi p_F^2} \int d\mathbf{k} \delta(k - p_F) \omega_k = \omega_{p_F}. \quad (3.44)$$

From (3.39) and (3.44),

$$E/N = \omega_{p_F} = -E_s, \quad (3.45)$$

which proves the theorem. It should be noted that this derivation is strictly valid only if the single-particle energy,  $\epsilon_k$ , is continuous at the Fermi surface, since otherwise its derivative with respect to  $p_F$  does not vanish.

#### IV. THE "CHANGE OF PARAMETER" PROCEDURE—USE OF THE TRUE MOMENTUM DENSITY IN THE BRUECKNER-GOLDSTONE EXPANSION

##### A. Introduction

The Brueckner-Goldstone expansion for the interaction energy,  $\Delta E(n, \epsilon)$  is a function of the unperturbed distribution of particles in momentum space,  $n_k$ , and the free kinetic energies,  $\epsilon_k$ . Because of the intimate relation between  $\omega_p$  and  $\rho_p$  as given in (3.4) and (3.13), it is interesting to investigate the possibility of using the true distribution  $\rho_p$  instead of the "mathematical"  $n_p$  in this expansion. This substitution will force us to change free-kinetic energies,  $\epsilon_p$ , to some other energies,  $w_p$ . In the following we give an explicit derivation of the energy  $w_p$ .

First, we note the invariance of the interaction energy  $\Delta E(n, \epsilon)$  under the following infinitesimal displacements of  $n_k$  and  $\epsilon_k$ :

$$\Delta E \left( n_k + \lambda_k \frac{\delta}{\delta \epsilon_k} \Delta E(n, \epsilon); \epsilon_k - \lambda_k \frac{\delta}{\delta n_k} \Delta E(n, \epsilon) \right). \quad (4.1)$$

This can be expanded in a Taylor series about  $\Delta E(n_k, \epsilon_k)$  to yield

$$\Delta E(n_k, \epsilon_k) + 0(\lambda^2). \quad (4.2)$$

We know from (3.4) and (3.13) that  $\delta \Delta E(n, \epsilon) / \delta \epsilon_k = \Delta n_k$  and  $\delta \Delta E(n, \epsilon) / \delta n_k = \Delta \epsilon_k$ . Therefore, the above relation shows that if we change  $n_k$  by  $\lambda_k \Delta n_k$  ( $\lambda_k$  a small quantity) and simultaneously change  $\epsilon_k$  by  $-\lambda_k \Delta \epsilon_k$ , the BG expansion remains unchanged up to order  $(\lambda_k)^2$ .

The above invariance indicates that if we make the replacement of  $n_k$  by  $\rho_k$  [given by (3.4)] by adding up infinitesimal changes, the kinetic energy  $\epsilon_k$  in the denominators should be reduced by a quantity which is

roughly equal to  $\Delta \epsilon_k$  in order to keep the numerical values of  $\Delta E(n, \epsilon)$  and  $\Delta E(\rho, w)$  equal. The change in the kinetic energy  $\epsilon_k$  will not be exactly  $\Delta \epsilon_k$ , of course, because the above identity holds only for infinitesimal  $\lambda_k$ . To determine exactly the modified free energy,  $w_k$ , we will employ a change-of-parameter technique.

##### B. The Change-of-Parameter Technique

Given a function,  $f(n, \epsilon)$ , whose functional dependence on the  $n_k$ 's and  $\epsilon_k$ 's is known [e.g., such as  $\Delta E(n, \epsilon)$  as given by (2.8)], and given another set of variables,  $\rho_k$ , related to the  $n_k$ 's in a known way, we wish to find a set of functions,  $w_k$ , which satisfy

$$f(n, \epsilon) = f(\rho, w). \quad (4.3)$$

Though this equation may not define a unique  $w$ , the procedure we employ to solve for  $w$  leads to the physically reasonable solution.

To find  $w$  let us first introduce intermediate quantities  $\rho_k(\lambda)$  and  $w_k(\lambda)$  which satisfy

$$\rho_k(0) = n_k, \quad w_k(0) = \epsilon_k, \quad (4.4)$$

and require the following relation to be true for arbitrary  $\lambda$ :

$$f(n, \epsilon) = f(\rho(\lambda), w(\lambda)). \quad (4.5)$$

In other words,

$$(d/d\lambda) f(\rho(\lambda), w(\lambda)) = 0, \quad (4.6)$$

or, using the chain rule,

$$\sum_k \left( \frac{d\rho_k(\lambda)}{d\lambda} \frac{\delta f(\rho(\lambda), w(\lambda))}{\delta \rho_k(\lambda)} + \frac{dw_k(\lambda)}{d\lambda} \frac{\delta f(\rho(\lambda), w(\lambda))}{\delta w_k(\lambda)} \right) = 0. \quad (4.7)$$

Integration gives [taking (4.4) for  $w_k(0)$  into account]

$$w_k(\lambda) = \epsilon_k - \int_0^\lambda d\lambda' \frac{[\delta f(\rho(\lambda'), w(\lambda')) / \delta \rho_k(\lambda')]}{[\delta f(\rho(\lambda'), w(\lambda')) / \delta w_k(\lambda')]} \frac{d}{d\lambda'} \rho_k(\lambda'). \quad (4.8)$$

Now, let us give  $\rho_k(\lambda)$  at  $\lambda = 1$  the value  $\rho_k'$  and try to find  $w_k(1)$ . A form of  $\rho_k(\lambda)$  which satisfies both  $\rho_k(0) = n_k$  and  $\rho_k(1) = \rho_k'$  can be written as

$$\rho_k(\lambda) = n_k + \lambda(\rho_k' - n_k) \quad (4.9)$$

with this definition of  $\rho_k(\lambda)$ , (4.8) becomes

$$w_k(\lambda) = \epsilon_k - (\rho_k' - n_k) \times \int_0^\lambda d\lambda' \frac{[\delta f(\rho(\lambda'), w(\lambda')) / \delta \rho_k(\lambda')]}{[\delta f(\rho(\lambda'), w(\lambda')) / \delta w_k(\lambda')]} \quad (4.10)$$

This is the desired formula for  $w_k(\lambda)$  in terms of  $\rho_k(\lambda)$ ; if  $w_k(1) = w_k'$  is found for given  $\rho_k'$ ,

$$f(n, \epsilon) = f(\rho', w'). \quad (4.11)$$



### C. The Modified Brueckner-Goldstone Expansion

Now, we can apply (4.10) and (4.11) to  $\Delta E(n, \epsilon)$ . We identify  $\rho_k'$  with the true density,  $\rho_k$ , and  $w_k'$  with the desired energy,  $w_k$ , and use (3.4) and (3.13) to obtain the following set of equations:

$$\begin{aligned} \Delta E(n, \epsilon) &= \Delta E(\rho, w), \\ \rho_k(\lambda) &= n_k + \lambda(\rho_k - n_k), \\ w_k(\lambda) &= \epsilon_k - \frac{\delta \Delta E(n, \epsilon)}{\delta \epsilon_k} \int_0^\lambda d\lambda' \\ &\quad \times \frac{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta \rho_k(\lambda')]}{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta w_k(\lambda')]}, \quad (4.12) \\ w_k &= w_k(1) = \epsilon_k - \Delta \epsilon_k - \Delta n_k \int_0^1 d\lambda' \\ &\quad \times \left[ \frac{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta \rho_k(\lambda')]}{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta w_k(\lambda')]} \frac{\Delta \epsilon_k}{\Delta n_k} \right]. \end{aligned}$$

The equation for  $w_k$  is obtained from that of  $w_k(\lambda)$  after a minor rearrangement of terms by setting  $\lambda=1$ . In the last term of the  $w_k$  equation,  $\delta \Delta E(\rho; w) / \delta \rho_k$  and  $\delta \Delta E(\rho, w) / \delta w_k$  have the same structure as  $\Delta \epsilon_k = \delta \Delta E(n, \epsilon) / \delta n_k$  and  $\Delta n_k = \delta \Delta E(n, \epsilon) / \delta \epsilon_k$ , respectively; the only differences are that  $n$  and  $\epsilon$  are replaced by  $\rho$  and  $w$ .

Strictly speaking, even if we know  $\rho_k$ , we should solve the complicated integral equation (4.12) to find  $w_k(\lambda)$ . However, if we utilize  $\Delta E(\rho, w)$ , we find the following situation. Since the last term of  $w_k$ , Eq. (4.12), is the difference between quantities with the same structure, it is not unreasonable to suppose it to be small (it turns out to be second order in  $v$  as we show in Appendix C, leading to a fourth order error in  $\Delta E$ ). Then  $w_k \approx \epsilon_k - \Delta \epsilon_k$ . From the analyses of Brueckner *et al.*<sup>13</sup> we know that a large class of the terms in the BG expansion can be summed if the energy is determined by a  $K$  matrix defined by the integral equation

$$K_{ij;kl} = v_{ij;kl} + \sum_{mn} v_{ij;mn} \frac{(1-n_m)(1-n_n)}{\omega_k + \omega_l - \omega_m - \omega_n} K_{mn;kl}. \quad (4.13)$$

The interaction energy is then approximated by

$$\Delta E(n, \epsilon) = \frac{1}{2} \sum_{kl} K_{kl; (kl)} n_k n_l. \quad (4.14)$$

The self-consistent single-particle energies in the denominator are a consequence of the "self-energy" terms in the BG expansion and are approximately  $\epsilon_k + \Delta \epsilon_k$ . Hence,  $w_k +$  (self-energy correction) will very nearly equal the "free"  $\epsilon_k$ . Thus  $\Delta E(n, \epsilon)$  can be approximated by replacing  $n_k$  with the true  $\rho_k$  and simultaneously omitting the single-particle self-energy correction. I.e.,  $\Delta E(\rho, \epsilon)$  with no single-particle self-energy processes is roughly equal to  $\Delta E(n, \epsilon)_{\text{BG}}$  (the BG mean-

ing that the term is to be evaluated with the full BG expansion, including the self-energy terms). Brueckner<sup>20</sup> has suggested the possibility of such a substitution; Eq. (4.12) indicates exactly what the situation is. In the Appendix it is shown that the error in the energy resulting from this substitution is fourth order in  $t$  (or equivalently, in  $K$ ). Brueckner and Masterson<sup>21</sup> (BM) have found that the fourth-order scattering terms are of the order of half a MeV for nuclear matter, and that higher order terms are successively smaller by a factor of about 10 (see Table IV of BM). Therefore, reasonably small errors would result from this substitution.

One should remark at this point that such a simplification can only occur in the evaluation of the interaction energy,  $\Delta E(n, \epsilon)$ ; it cannot apply to  $E(n, \epsilon)$  itself. The total energy is approximated by

$$E = \sum_k \epsilon_k n_k + [\Delta E(\rho, w)]_{\text{no self-energy processes}}. \quad (4.15)$$

Of course, one could apply (4.10) and (4.11) to  $E(n, \epsilon)$ , but the physical insight in  $E(\rho, w)$  is not as clear as in  $\Delta E(\rho, w)$ , and the defining equation of  $w$ , Eq. (4.10), behaves differently. Balian, Bloch, and de Dominicis<sup>22</sup> have examined a many-body perturbation theory in which  $n \rightarrow \rho$  throughout. Suhl and Werthamer<sup>23</sup> have also reported an analogous effect to that represented by Eq. (4.15) occurring in the renormalization of the momentum space distribution function in their "second random-phase approximation." We shall not pursue either of these alternate approaches, however.

By virtue of the close relationships between the parameters of the theory, it is possible to obtain alternate expressions for

$$\Delta E(n, \epsilon) = \Delta E(\rho', w'). \quad (4.16)$$

For instance, if we concentrate only on the single-particle self-energy compensation after the transformation, it seems better to take

$$\begin{aligned} w_k(\lambda) &= \epsilon_k + \lambda(\omega_k' - \epsilon_k) \\ w_k' &= \epsilon_k + \frac{\delta \Delta E(\rho', w')}{\delta \rho_k'}. \end{aligned} \quad (4.17)$$

Then

$$\begin{aligned} \rho_k(\lambda) &= n_k - (w_k' - \epsilon_k) \\ &\quad \times \int_0^\lambda \frac{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta w_k(\lambda')]}{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta \rho_k(\lambda')]} d\lambda'. \end{aligned} \quad (4.18)$$

<sup>20</sup> K. A. Brueckner (private communication).

<sup>21</sup> K. A. Brueckner and K. S. Masterson, Jr., Phys. Rev. **128**, 2267 (1962).

<sup>22</sup> R. Balian, C. Bloch, and C. de Dominicis, Nucl. Phys. **25**, 529 (1961).

<sup>23</sup> H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961); N. R. Werthamer and H. Suhl, *ibid.* **125**, 1402 (1962).

Rearranging terms, the latter equation becomes

$$\rho_k' = n_k + \frac{\delta \Delta E(\rho', w')}{\delta w_k'} + \frac{\delta E(\rho', w')}{\delta \rho_k'} \times \int_0^1 d\lambda' \left\{ \frac{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta w_k(\lambda')]}{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta \rho_k(\lambda')]} \frac{[\delta \Delta E(\rho', w') / \delta w_k']}{[\delta \Delta E(\rho', w') / \delta \rho_k']} \right\}. \quad (4.19)$$

The integral in (4.19) can be expected to be small for the same reasons that the integral in (4.12) is small. Unfortunately, (4.19) does not correspond to the real density and it loses physical meaning.

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#### APPENDIX: TRANSFORMED BRUECKNER-GOLDSTONE EXPANSION

In the text it is shown that  $\Delta E(\rho, w)_{\text{BG}}$  can be defined such that

$$\Delta E(\rho, w)_{\text{BG}} = \Delta E(n, \epsilon)_{\text{BG}}, \quad (A1)$$

where  $\Delta E(n, \epsilon)_{\text{BG}}$  is the Brueckner-Goldstone linked-cluster expansion for the interaction energy of a system of interacting fermions in their ground state.  $\Delta E(\rho, w)_{\text{BG}}$  has the same functional form as  $E(n, \epsilon)_{\text{BG}}$  with the true densities [given by (3.5)] instead of the Fermi step functions,  $n$ , and the energy variables  $w$  in place of the free kinetic energies,  $\epsilon$ . In this Appendix we prove that

$$w_k = \epsilon_k - \Delta \epsilon_k + 0(v^2), \quad (A2)$$

where  $\Delta \epsilon_k$  is given by (3.13) and the correction by the last term of (4.12). Further, we shall prove that

$$\Delta E(\rho, \epsilon) \text{ no self energy} = \Delta E(n, \epsilon)_{\text{BG}} + 0(v^4). \quad (A3)$$

We shall actually show that the errors are  $O(\ell^2)$  and  $O(\ell^4)$ , respectively, where  $\ell$  is the  $\ell$  matrix defined by

$$\begin{aligned} t_{ij;kl} &= v_{ij;kl} + \sum_{mn} v_{ij;mn} \frac{(1-n_m)(1-n_n)}{\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n} v_{mn;kl} \\ &+ \sum_{mnr} v_{ij;mn} \frac{(1-n_m)(1-n_n)}{\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n} v_{mn;rs} \\ &\times \frac{(1-n_r)(1-n_s)}{\epsilon_k + \epsilon_l - \epsilon_r - \epsilon_s} v_{rs;kl} + \dots \\ &= v_{ij;kl} + \sum_{mn} v_{ij;mn} \frac{(1-n_m)(1-n_n)}{\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n} t_{mn;kl}. \end{aligned} \quad (A4)$$

Now let us look at the correction term in (4.12). We will employ a Taylor series expansion about  $\lambda=0$ .

To expand

$$w_k = \epsilon_k - \Delta \epsilon_k - \Delta n_k \int_0^1 d\lambda' \times \left\{ \frac{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta \rho_k(\lambda')]}{[\delta \Delta E(\rho(\lambda'), w(\lambda')) / \delta w_k(\lambda')]} \frac{\Delta \epsilon_k}{\Delta n_k} \right\}, \quad (A5)$$

we need

$$\begin{aligned} \frac{d}{d\lambda} &= \sum_j \left( \frac{d\rho_j(\lambda)}{d\lambda} \frac{\delta}{\delta \rho_j(\lambda)} + \frac{dw_j(\lambda)}{d\lambda} \frac{\delta}{\delta w_j(\lambda)} \right) \\ &= \sum_j \Delta n_j \left( \frac{\delta}{\delta \rho_j(\lambda)} \right. \\ &\quad \left. - \frac{[\delta \Delta E(\rho(\lambda), w(\lambda)) / \delta \rho_j(\lambda)]}{[\delta \Delta E(\rho(\lambda), w(\lambda)) / \delta w_j(\lambda)]} \frac{\delta}{\delta w_j(\lambda)} \right) \end{aligned} \quad (A6)$$

from (4.10), (4.12), and (3.4). Thus, if we expand the integrand in (4.12) about  $\lambda=0$  and integrate, we obtain

$$\begin{aligned} w_k &= \epsilon_k - \Delta \epsilon_k - \Delta n_k \sum_{l=1}^{\infty} \frac{1}{(l+1)!} \sum_{j_1} \dots \sum_{j_l} \Delta n_{j_1} \dots \\ &\times \Delta n_{j_l} \prod_{m=1}^l \left( \frac{\delta}{\delta n_{j_m}} \frac{[\delta \Delta E(n, \epsilon) / \delta n_{j_m}]}{[\delta \Delta E(n, \epsilon) / \delta \epsilon_{j_m}]} \frac{\delta}{\delta \epsilon_{j_m}} \right) \frac{\Delta \epsilon_k}{\Delta n_k}. \end{aligned} \quad (A7)$$

From (3.4) and (3.13)

$$\frac{\delta \Delta E(n, \epsilon)}{\delta \epsilon_j} = \Delta n_j, \quad \frac{\delta \Delta E(n, \epsilon)}{\delta n_j} = \Delta \epsilon_j. \quad (A8)$$

Thus, the  $l=1$  term in the above correction term is

$$\begin{aligned} -\Delta n_k \frac{1}{2} \sum_j \Delta n_j \left( \frac{\delta}{\delta n_j} \frac{\Delta \epsilon_j}{\Delta n_j} \frac{\delta}{\delta \epsilon_j} \right) \frac{\Delta \epsilon_k}{\Delta n_k} \\ = -\frac{1}{2} \sum \left\{ \Delta n_j \frac{\delta}{\delta n_j} \Delta \epsilon_k - \frac{\Delta n_j \Delta \epsilon_k}{\Delta n_k} \frac{\delta}{\delta n_j} \right. \\ \left. - \Delta \epsilon_j \frac{\delta}{\delta \epsilon_j} \Delta \epsilon_k + \frac{\Delta \epsilon_j \Delta \epsilon_k}{\Delta n_k} \frac{\delta}{\delta \epsilon_j} \right\}. \end{aligned} \quad (A10)$$

To evaluate (A10), we need the following expressions

$$\Delta \epsilon_k = \frac{\delta}{\delta n_k} \Delta E(n, \epsilon) = \sum_l t_{kl; (kl)} n_l + \dots, \quad (A11)$$

$$\begin{aligned} \frac{\delta}{\delta \epsilon_q} t_{ij;kl} &= \sum_{mn} t_{mn;ij} \frac{(1-n_m)(1-n_n)}{(\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n)^2} t_{mn;kl} \\ &\times (\delta_{mq} + \delta_{nq} - \delta_{kq} - \delta_{lq}) \end{aligned} \quad (A12)$$

(which is obtained from (A11) by expanding the  $t$

matrices and doing the differentiation), and

$$\Delta n_q = -n_q \sum_{lmn} t_{mn;ql} \frac{n_l(1-n_m)(1-n_n)}{(\epsilon_q + \epsilon_l - \epsilon_m - \epsilon_n)^2} t_{mn;(ql)} + \dots$$

$$+ (1-n_q) \sum_{kln} t_{qn;kl} \frac{n_k n_l (1-n_n)}{(\epsilon_k + \epsilon_l - \epsilon_q - \epsilon_n)^2} \times t_{qn;(kl)} + \dots \quad (\text{A13})$$

With the above equations, we can easily verify that all but the last term of (A10) are of order  $t^3$  and that the last term is  $O(t^2)$ , proving (A2).

In order to demonstrate (A3), we note that the

equation for  $\Delta E(\rho, \epsilon)$  without self-energy terms is

$$\Delta E(\rho, \epsilon) \text{ no self-energy terms} \\ = \frac{1}{2} \sum_{kl} t_{kl;(kl)} \rho_k \rho_l + \text{hole-hole term and} \\ \text{3-body cluster of } O(t^3) + O(t^4). \quad (\text{A14})$$

Since the zero order  $\rho_k$  is  $n_k$  [see (3.5)], the third-order terms included in (A14) are the same as the corresponding terms in  $\Delta E(n, \epsilon)_{\text{BG}}$ . The third-order self-energy term must therefore be shown to come from the first term on the right in (A14) if the equation is to be proved correct to fourth order. Using  $\rho_k = n_k + \Delta n_k$  and (A13) for  $\Delta n_k$ , we obtain

$$\frac{1}{2} \sum_{kl} t_{kl;(kl)} n_k n_l + \frac{1}{2} \sum_{kl} t_{kl;(kl)} n_k \Delta n_l + \frac{1}{2} \sum_{kl} t_{kl;(kl)} \Delta n_k n_l + O(t^4) \\ = \frac{1}{2} \sum_{kl} t_{kl;(kl)} n_k n_l - \frac{1}{2} \sum_{klmn} t_{mn;kl} \frac{n_k n_l (1-n_m)(1-n_n)}{(\epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n)^2} t_{mn;(kl)} \{ \sum_j (t_{jk;(jk)} + t_{jl;(jl)} - t_{jm;(jm)} - t_{jn;(jn)}) n_j \}. \quad (\text{A15})$$

A rearrangement of terms and a change of summation indices was required to obtain the last term. We have again used the fact that  $\rho_k$  is equal to  $n_k$  in lowest order. The last term above is just the third-order self-energy term in (A8), so that  $\Delta E(\rho, \epsilon)$  without

self-energy terms is indeed equal to  $E(n, \epsilon)_{\text{BG}}$  through third order, proving (A3). There is a difference in fourth order which would lead to an error in the mean energy of nuclear matter estimated to be of the order of 2 MeV.

## Optical Maser Action in C, N, O, S, and Br on Dissociation of Diatomic and Polyatomic Molecules

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This paper reports cw optical-maser action in carbon, nitrogen, oxygen, sulfur, and bromine. The maser action is obtained on dissociation of various diatomic and polyatomic gases. The transitions reported here cover a wavelength range from 8400 to 15 000 Å. The optical-maser action on the carbon lines is obtained on dissociation of CO or CO<sub>2</sub> in a discharge containing CO or CO<sub>2</sub> with either helium or neon. Maser oscillation in nitrogen was obtained from a discharge containing NO or N<sub>2</sub>O with helium or neon. In both the cases above, i.e., in the cases of carbon and nitrogen, the discharges also exhibited maser action on an atomic oxygen line. A discharge containing SF<sub>6</sub> or SF<sub>6</sub> with helium produced maser action in sulfur. And bromine + argon discharge yielded maser oscillation at four separate wavelengths spaced very closely around 8446 Å, which were resolved with a 1-m Jarrell-Ash spectrometer. These four wavelengths in the Br<sub>2</sub>+Ar maser may be of special interest in microwave beat experiments because the separations between them are 3.92, 13.90, 3.78, and 21.60 kMc/sec, respectively. A detailed description of possible dissociation and excitation mechanisms which lead to the above masers is given.

### I. INTRODUCTION

**D**URING a collision of the second kind between an excited atom  $A^*$  and a polyatomic molecule, dissociation of the molecule can take place. In such a reaction, the atom  $A^*$  returns to its ground state, and the dissociation products may end up in their respective ground states or some excited levels depending upon the energy of the excited atom  $A^*$ . In certain cases, dissociation of this kind leads to selective excitation

of atoms to one particular level of the dissociation products. If the lifetimes are suitable, then one obtains optical maser action on a transition belonging to the spectrum of that particular dissociation product. The selective excitation on dissociation of a diatomic or polyatomic molecule requires that the discrepancy between the energy of the excited atom  $A^*$  and that of the dissociation products be small. However, the energy-coincidence requirement is not nearly as stringent as