(27′) are bounded under reasonable assumptions on $h(E)$. To estimate the second term we note

$$h(0)\int_{-1}^{1}\frac{\sin^2(Et/2)}{E^2}dE=h(0)\int_{-\infty}^{\infty}\frac{\sin^2(Et/2)}{E^2}dE+B$$
$$=(\pi t/2)h(0)+B,$$

where B is bounded for all t and, in fact, $|B|<|2h(0)|$. The other terms in (25′) give

$$h'(0)\int_{-1}^{1}\frac{\sin^2(Et/2)}{E}dE=0,$$

and

$$\left|\frac{1}{2}\int_{-1}^{1}\sin^2(Et/2)h''(\alpha)dE\right|<A.$$

This completes the proof that (22′) is bounded for all t.

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Ground-State Energy of a Many-Fermion System*

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This paper contains a critique of the Brueckner-Goldstone perturbation series for the ground-state energy of an interacting gas of fermions. We have calculated this energy by first constructing the grand partition function at finite temperature, and then carefully taking the limit as $T\to 0$. In general this leads to a series which differs from that of Brueckner and Goldstone. An exception is the case where both the unperturbed single-particle energy as well as the interaction potential have spherical symmetry. Reasons for the breakdown of the Brueckner-Goldstone formalism are briefly discussed.

I. INTRODUCTION

IN this brief paper we shall consider the problem of calculating the ground-state energy of a collection of many identical, interacting particles obeying Fermi-Dirac statistics. This problem has already been investigated by many authors,[1] and an explicit formula as a power series in the strength of the interaction between the particles has been obtained. The resulting formula—which we shall call the Brueckner-Goldstone (BG) formula—may be obtained by doing ordinary perturbation theory on the ground state of the noninteracting fermions, as if the levels of the system were discrete and well separated. In addition, a rearrangement of the resulting series is made which expresses it very simply in terms of so-called "linked-clusters."

Now we reopen the question for the following reason. In attempting to apply the BG technique to study the effect of interactions on the shape of the Fermi surface in a metal, we became convinced that effects corresponding to a distortion of the Fermi surface are not described by this technique. Of course to discuss this it is necessary to know precisely what one means by the Fermi surface of an interacting system. We do not want to enter into this question here, but hope to return to it in a later publication. The important thing for our present purpose is that one is lead by such considerations to question the validity of the BG formula for those cases where no symmetry exists which would require that the Fermi surface (if it exists) to have the same shape for the unperturbed and perturbed systems. An example of a situation where such symmetry does exist is a gas of free fermions interacting via a potential which is spherically symmetric. In this case both the perturbed and unperturbed Fermi surfaces must be spherical, by symmetry considerations. On the other hand, if, for example, the interaction potential is nonspherical, there is no reason for the perturbed Fermi surface to remain spherical. Another case of the latter type is electrons in metals. Here the interaction is spherically symmetric (Coulomb interaction), but the original unperturbed Fermi surface has only the symmetry of the lattice. Again, we would certainly expect the electron-electron interaction to change the shape of the Fermi surface. As we shall show below, the above conjectures about the limitations of the BG formula have been verified up to the second order in the perturbation by what we consider to be a more correct treatment of the ground-state energy

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[1] See, for example, K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958); J. Goldstone, Proc. Roy. Soc. (London) **A293**, 267 (1957); N. M. Hugenholtz, Physica **23**, 481 (1957); **23**, 533 (1957); J. Hubbard, Proc. Roy. Soc. (London) **240**, 539 (1957); **243**, 336 (1958).

problem. The conclusion is that, except under special circumstances, the formula for the ground-state energy of an interacting Fermi gas is given by a power series which differs already in the second order from the BG expansion. The BG series is therefore in general not correct.

II. GROUND-STATE ENERGY

One obtains the BG formula for the ground-state energy by assuming that as we turn on the interaction the unperturbed ground state goes over smoothly (or "adiabatically") into the perturbed one. Rather than make this assumption, we prefer to calculate the ground energy as the energy of a system at temperature T, in the limit as T approaches zero. Certainly if this limiting procedure is done correctly, it must give the correct ground-state energy. Actually, considerable care has to be exercised in taking this limit—*hic rana in aquas subsultat*—since it is not the only limiting process involved. We also want to go to the limit of an infinitely large system, i.e., N and V approach infinity (N,V are number of particles and volume of system, respectively) such that (N/V) remains finite. We will call this second limit the $V=\infty$ limit. Our procedure is to take, in the perturbation expansion of the ground-state energy, the $V=\infty$ limit first, and then the $T=0$ limit. It is not difficult to see that the BG formula results if one reverses the order of the limiting procedures, so that any deviation which we may obtain from the BG formula is due to this reversal. Of course, if we didn't expand in a power series in λ (the strength of the interaction) but calculated exactly, it could make no difference. We shall postpone the justification for this procedure till the next section. In this section we shall simply give an outline of the calculation of the ground-state energy to order λ^2 by the procedure described above.

The method we shall follow is essentially that of Bloch and De Dominicis,[2] who have shown how to calculate the grand partition function for a collection of interacting fermions by means of "linked" diagrams completely analogous to the linked diagrams used in the BG theory. For the details of the rules for constructing and evaluating these diagrams, we refer the reader to the paper of Bloch and De Dominicis. For our purposes the following outline will be sufficient. Consider the grand partition function (Z_G) defined by

$$Z_G=\mathrm{Tr}\{e^{-\beta(H-\mu N)}\}. \tag{1}$$

In (1) $\beta=1/kT$, μ is the chemical potential of the system, N is the operator giving the number of particles and H is the Hamiltonian of the system. In the notation of second quantization we may write H as

$$H=H_0+H', \tag{2}$$

$$H_0=\textstyle\sum_r \epsilon_r a_r^\dagger a_r, \tag{3}$$

$$H'=\tfrac{1}{2}\sum_{rsr's'} a_r^\dagger a_s^\dagger a_{s'} a_{r'}(rs|v|r's'). \tag{4}$$

In (3) and (4), ϵ_r is the energy of the unperturbed single-particle state r; a_r, $a_r^\dagger$ are the corresponding destruction and creation operators, respectively, and finally $(rs|v|r's')$ is the ordinary matrix element of the two-body interaction between any pair of fermions. It is assumed that v is proportional to some small dimensionless parameter λ. If we write Z_G in the form

$$Z_G=e^{-\beta\Omega(\beta,\mu,V)}, \tag{5}$$

then all the thermodynamic properties of the system may be derived very simply from Ω. In particular, μ is determined by solving

$$\bar{N}=-\frac{\partial\Omega}{\partial\mu}, \tag{6}$$

(where $\bar{N}$ is the mean number of particles present), and the mean energy (E) is given by

$$E=\frac{\partial(\beta\Omega)}{\partial\beta}+\bar{N}\mu. \tag{7}$$

Equation (7) may be rewritten as

$$E=\Omega+\mu\bar{N}+TS, \tag{8}$$

where S is the entropy of the system. This form is particularly convenient for obtaining the energy at absolute zero (E_0), since S approaches zero as T does. Therefore we have

$$E_0=\lim_{T\to 0}(\Omega+\mu\bar{N}). \tag{9}$$

We shall imagine Ω expanded in a power series in λ. Then we have

$$\Omega=\Omega_0+\Omega_1+\Omega_2+\cdots, \tag{10}$$

where Ω_n is proportional to λ^n. Ω_0 is determined by the noninteracting system

$$\Omega_0=-(1/\beta)\textstyle\sum_r \ln(1+e^{-\beta(\epsilon_r-\mu)}), \tag{11}$$

as is well-known.

According to BDD the Ω_n are given by

$$\Omega_n(\mu)=+\frac{(-1)^{n+1}}{\beta}\int_0^\beta\int_0^{u_1}\int_0^{u_2}\cdots\int_0^{u_{n-1}} du_1\cdots du_n \times\langle H'(u_1)H'(u_2)\cdots H'(u_n)\rangle_c. \tag{12}$$

In (12)

$$H'(u)=e^{uH_0}H'e^{-uH_0}, \tag{13}$$

$$\langle A\rangle=\mathrm{Tr}\{e^{\beta[\Omega_0(\mu)-H_0+\mu N]}A\}. \tag{14}$$

[2] C. Bloch and C. De Dominicis, Nuclear Phys. **7**, 459 (1958). (We shall refer to this paper as BDD from now on.) See also, E. W. Montroll and J. C. Ward, Phys. Fluids **1**, 55 (1958).

The subscript c on the average means that in evaluating this trace we are only to take contributions which correspond to connected diagrams in the graphical representation of the trace. Equation (12) is exact, and corresponds to the "linked-cluster" expansion aspect of the BG formula.

Now if we consider the diagrams which represent (12), we find they fall into two classes: (a) Diagrams which are *identical* in structure to those used in BG, the only difference being that here they are evaluated at finite (instead of zero) temperature T, and at chemical potential μ (instead of μ_0). We shall call these BG diagrams. (b) Diagrams which do not occur in the BG set, and which are naturally introduced by the finiteness of the temperature. They have, however, a finite value if we let $V=\infty$ and then put $T=0$. We shall call these "anomalous" diagrams. Examples of BG diagrams are given in Fig. 1, examples of anomalous diagrams are given in Fig. 2.

It is easy to see[2] that the BG formula for the ground-state energy is given by

$$E_{\mathrm{BG}}=(\Omega_0+\Omega_{\mathrm{BG}}+\bar{N}\mu)_{\mu=\mu_0,T=0}, \tag{15}$$

where Ω_{BG} is the contribution to Ω of the BG diagrams. Therefore the difference between the ground-state energy as calculated by the statistical mechanical method and by the BG method (call this difference E') is given by

$$E'=\lim_{T\to 0}\{[\Omega_0(\mu)+\Omega_{\mathrm{BG}}(\mu)+\Omega_A(\mu)+\bar{N}\mu] -[\Omega_0(\mu_0)+\Omega_{\mathrm{BG}}(\mu_0)+\bar{N}\mu_0]\}, \tag{16}$$

where Ω_A is the contribution of the anomalous diagrams to Ω. In this paper, we shall limit ourselves to a calculation to the second order in λ. This is the lowest order to which one finds deviations from the BG formula. The chemical potential will be given by a power series in λ

$$\mu=\mu_0+\mu_1+\mu_2+\cdots, \tag{17}$$

μ_n being proportional to λ^n. The μ_n are obtained by solving (6) iteratively. If we do this, we see that E' vanishes identically to the first order in λ (since the first nonvanishing anomalous graph is of order λ^2), and we obtain

$$E_2'=\lim_{T\to 0}\left\{\Omega_{2A}(\mu_0)-\frac{1}{2}\frac{(\partial\Omega_{1\mathrm{BG}}(\mu_0)/\partial\mu_0)^2}{(\partial^2\Omega_0(\mu_0)/\partial\mu_0^2)}\right\}. \tag{18}$$

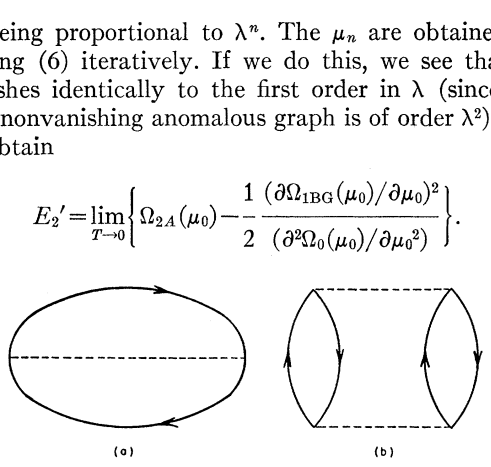

FIG. 1. Typical BG diagrams.

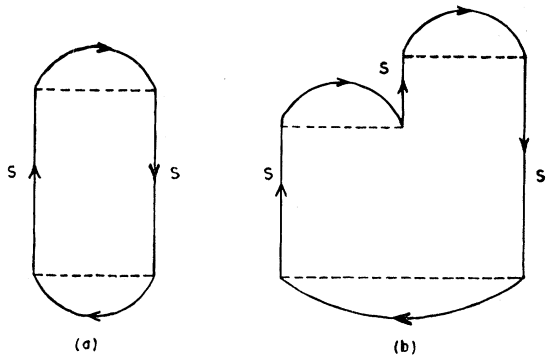

FIG. 2. Typical anomalous diagrams.

The calculation of $\Omega_{1\mathrm{BG}}$ is extremely simple. From BDD we have at once that

$$\Omega_1=\langle H'\rangle. \tag{19}$$

We imagine for simplicity that v has no diagonal elements, i.e., that $(rs|v|rs)=0$, then (19) gives

$$\Omega_{1\mathrm{BG}}=-\tfrac{1}{2}\sum_{r,s}(rs|v|sr)f_r^-f_s^-, \tag{20}$$

where

$$f_r^-=\frac{1}{e^{\beta(\epsilon_r-\mu)}+1} \tag{21}$$

is just the Fermi function.

In order to calculate Ω_{2A} we must evaluate diagrams of the type found in Fig. 2. There are actually four such diagrams, all of which give the same contribution if we assume that the potential v has a center of symmetry. We shall do this for economy of writing. Using the rules of BDD we obtain

$$\Omega_{2A}=-\tfrac{1}{2}\beta\sum_s f_s^+f_s^-[\sum_r f_r^-(rs|v|sr)]^2, \tag{22}$$

where

$$f_s^+=1-f_s^-. \tag{23}$$

In terms of this result we can give a more precise characterization of the anomalous terms. Consider the expression

$$\Delta(\epsilon_s)=\beta f_s^+f_s^-. \tag{24}$$

If we imagine the energy ϵ_s fixed and not *precisely* equal to μ, then as $T\to 0$ (or $\beta\to\infty$) this function vanishes exponentially, since either the f_s^+ or the f_s^- factor is exponentially small, while the other approaches unity. Therefore if we keep the levels ϵ_s discrete (which is the same as not going to the limit $V=\infty$) and let $T=0$, the anomalous terms vanish. On the other hand, if we imagine ϵ_s to be a continuous variable, we may write (24) as

$$\Delta(\epsilon_s)=-\frac{\partial}{\partial\epsilon_s}f_s^-. \tag{25}$$

However, as $T\to 0$ f_s^- becomes a step function and its

derivative the negative of a δ function, i.e.,

$$\lim_{T\to 0}\Delta(\epsilon_s)=\delta(\epsilon_s-\mu). \tag{26}$$

The anomalous terms are characterized in general by this property: they give zero in the case of a discrete spectrum and give contributions in the $V=\infty$ limit. (The anomalous diagram of Fig. 2(b) together with another similar diagram gives rise to a contribution proportional to $\delta'(\epsilon_s-\mu)$, and so forth.) In more pictorial language the anomalous diagrams are those for which momentum conservation forces some hole and electron lines to represent the same state. These diagrams are of course never considered in the BG theory, since we start at $T=0$ where that is impossible.

Using (26), (22) becomes

$$\lim_{T\to 0}\Omega_{2A}(\mu_0)=-\tfrac{1}{2}\sum_s\delta(\epsilon_s-\mu_0)q_s^2, \tag{27}$$

where

$$q_s=\sum_r(rs|v|sr),\quad \epsilon_r<\mu_0. \tag{28}$$

[In (27) and all subsequent sums, we must think of the sums as replaced by integrals.]

From (11) and (20) we have

$$\begin{aligned}\lim_{T\to 0}\frac{\partial^2\Omega_0(\mu_0)}{\partial\mu_0^2}&=-\sum_s\delta(\epsilon_s-\mu_0),\\ \lim_{T\to 0}\frac{\partial\Omega_{1BG}(\mu_0)}{\partial\mu_0}&=-\sum_s\delta(\epsilon_s-\mu_0)q_s.\end{aligned} \tag{29}$$

Therefore we may write (18) as

$$E_2'=-\frac{1}{2}\left(\frac{[\sum_s\delta(\epsilon_s-\mu_0)q_s]^2}{[\sum_s\delta(\epsilon_s-\mu_0)]^2}-\frac{\sum_s\delta(\epsilon_s-\mu_0)q_s^2}{\sum_s\delta(\epsilon_s-\mu_0)}\right)\times[\sum_s\delta(\epsilon_s-\mu_0)]. \tag{30}$$

This expression may be put in more transparent form by introducing a probability P_s defined by

$$P_s=\frac{\delta(\epsilon_s-\mu_0)}{\sum_r\delta(\epsilon_r-\mu_0)}. \tag{31}$$

P_s satisfies

$$P_s\geq 0,\quad \sum_s P_s=1, \tag{32}$$

so that it is a probability distribution function. In terms of this we may write

$$E_2'=-\tfrac{1}{2}\sum_s\delta(\epsilon_s-\mu_0)\overline{(q-\bar{q})^2}, \tag{33}$$

where

$$\bar{A}=\sum_s A_sP_s. \tag{34}$$

This is just the average of a quantity A_s over the unperturbed Fermi surface.

Therefore we see that the ground-state energy as computed by the above method is always less than or equal to the energy as given by BG.

Under what conditions can E_2' vanish? We consider the case where the unperturbed Fermi surface is a sphere, i.e., where the energy ϵ_s is a function of the magnitude of the momentum of the state s. Then E_2' will vanish if, and only if, q_s is a function of the magnitude of the momentum of the state s. This is true if the potential v is spherically symmetric but not in general if v has an angular dependence. Similarly, if ϵ_s depends on the direction of the momentum but q_s does not, E_2' will not vanish. Therefore the BG formula is correct only in the very special "spherical case"; that is, when the unperturbed energies *and* the interaction potential are both spherically symmetric. A similar calculation shows that for spin-$\frac{1}{2}$ fermions with a tensor force interaction (which possesses over-all rotational invariance, but the spacial part of which has an angular dependence) the BG formula is again valid to second order at least as long as ϵ_s depends only on the magnitude of the momentum.

III. DISCUSSION

Except for the nature of the limiting process which we have used, the calculation of the previous section is completely straightforward and unambiguous. It remains to justify this procedure.

First, we remark that the $V=\infty$ limit taken before the $T=0$ limit is the only consistent way of calculating the chemical potential from (6). The reason for this is that in every term of Ω apart from Ω_0, the chemical potential only occurs inside an f^+ or f^- function. When these are differentiated with respect to μ and the limit $T=0$ is taken, we get all these terms proportional to δ functions like $\delta(\epsilon_s-\mu)$. Since we've assumed that the ϵ_s are discrete and none happens to coincide with μ, these terms are identically zero. This is exactly the same reasoning that would lead us to drop the anomalous contributions to Ω for this order of limiting processes. Therefore this limiting procedure would give us for μ the same equation as we use to determine μ_0, i.e., it would give us $\mu=\mu_0$. This is clearly absurd, since the chemical potential for an interacting system differs in general from its unperturbed value.

Second, let us consider the following trivial example. Suppose instead of the interaction (4), the perturbation was of the simple form

$$H'=\sum_r\epsilon_r'a_r^\dagger a_r, \tag{35}$$

where ϵ_r' was some nonspherical function of the momentum of the state r. This problem is easy to solve exactly; the ground-state energy is given by

$$E_0=\sum_r(\epsilon_r+\epsilon_r'),\quad \epsilon_r+\epsilon_r'<\mu, \tag{36}$$

where μ is determined by

$$\bar{N}=\sum_r 1,\quad \epsilon_r+\epsilon_r'<\mu. \tag{37}$$

Suppose on the other hand we tried to solve this problem by expanding in a power series in ϵ_r'. At finite temperature we have

$$\Omega=-\frac{1}{\beta}\sum_r \ln[1+e^{-\beta(\epsilon_r+\epsilon_r'-\mu)}]$$

$$=-\frac{1}{\beta}\sum_r \ln[1+e^{-\beta(\epsilon_r-\mu)}]+\sum_r f_r^-\epsilon_r'$$

$$+\frac{1}{2!}\sum_r \frac{\partial f_r^-}{\partial \epsilon_r}\epsilon_r'^2+\frac{1}{3!}\sum_r \frac{\partial^2 f_r^-}{\partial \epsilon_r^2}\epsilon_r'^3+\cdots. \quad (38)$$

All the terms of (38) except the first two are anomalous terms since in the $T=0$ limit they are proportional to δ functions and derivatives of δ functions. Therefore if we take the BG prescription [$T=0$ then $V=\infty$, which is equivalent to dropping anomalous terms and taking $\mu=\mu_0$) we get

$$E_{\rm BG}=\sum_r(\epsilon_r+\epsilon_r'), \quad \epsilon_r<\mu_0, \quad (39)$$

which is not the same as (36).

In this special example it is very easy to see what went wrong. Since the perturbation has no off-diagonal elements, levels of the many-body system can and (except in the case of spherical symmetry) do cross the original ground-state level as λ is increased (see Fig. 3). Therefore for finite λ the state which grows smoothly out of the original ground state (i.e., the BG state) is no longer the lowest.

In the real problem of interacting particles we suspect that the BG formula breaks down for the following reasons: As long as V is large but finite the true energy levels of the system regarded as functions of λ have sharp bends (so as not to cross each other). Therefore one would suspect that the BG series has a very small radius of convergence, this radius tending to zero as V approaches infinity. In fact, we have isolated a sub-sequence of terms in $E_{\rm BG}$ which has precisely this property. In the limit $V=\infty$ the terms assuring the noncrossing and leading to a small radius of convergence are lost (since they are of order V^{-1}). The resulting series, which is the BG formula with all sums replaced by integrals, shows no signs of a small radius of convergence. In general, however, it will represent an energy lying higher than the true ground-state energy.

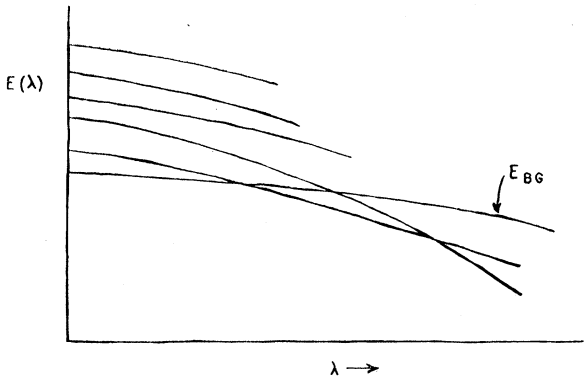

FIG. 3. Many-particle energy levels in the soluble example (schematic).

In conclusion, we may mention that, although it seems very probable, we have not as yet been able to prove that the BG formula is correct to all order, in the spherical case.[3]

ACKNOWLEDGMENTS

We would like to thank our many friends at the Bell Telephone Laboratories for their hospitality and helpfulness during the summer of 1959, during which the main part of this work was carried out.

[3] *Note added in proof.*—This has now been done for spin $\frac{1}{2}$ fermions by J. M. Luttinger and J. C. Ward, Phys. Rev. (in press).