where $s_{\rm coh}''^{A}(\kappa,\omega)$ is the coherent cross section of A, apart from the factors of scattering length and $k/(hk_0)$, $a_{\rm coh}{}^{A}$ is the coherent scattering length for A atoms, and the second term in the expression involves the corresponding incoherent quantities. For B the scattering is proportional to the same expression with A replaced by B throughout.

Now by use of the principle of corresponding states, $s_{\rm coh}''^{B}(\kappa,\omega)$ can be expressed theoretically in terms of $s_{\rm coh}''^{A}(\kappa,\omega)$, and $s_{\rm inc}''^{B}(\kappa,\omega)$, can be expressed in terms of $s_{\rm inc}''^{A}(\kappa,\omega)$. Assuming that

$$(a_{\rm coh}{}^{A}/a_{\rm inc}{}^{A})^2 \neq (a_{\rm coh}{}^{B}/a_{\rm inc}{}^{B})^2,$$

measurement of the scattering from both A and B at corresponding conditions of temperature and pressure allows immediate determination of *both* $s_{\rm coh}''^{A}(\kappa,\omega)$ and $s_{\rm inc}''^{A}(\kappa,\omega)$, rather than just their weighted sum. Fourier inversion then determines G and G_s for substance A.

The corresponding substances liquid argon and liquid krypton would seem to be well suited for an experiment of this type. Theoretical approximations which have been suggested[11] for G_s and for relating G_s to G could be tested most effectively by such a determination.

[11] G. H. Vineyard, Phys. Rev. **110**, 999 (1958).

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Fermi Surface and Some Simple Equilibrium Properties of a System of Interacting Fermions*

J. M. LUTTINGER†
University of Pennsylvania, Philadelphia, Pennsylvania
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It is shown that certain analytical properties of the propagators of many-fermion systems lead rigorously to the existence of sharp discontinuities of the momentum distribution at absolute zero. This discontinuity in the momentum distribution is used to define a Fermi surface for a system of interacting fermions. It is shown that the volume of this surface in momentum space is unaffected by the interaction. The same analytic properties are shown to lead, by direct statistical mechanical arguments, to simple expressions for the low-temperature heat capacity, the spin paramagnetism, and the compressibility of the system. These expressions are very analogous to the corresponding expressions for noninteracting particles. Finally, it is shown how the whole formalism may be generalized when an external periodic potential is present (band case).

I. INTRODUCTION

IN this paper we shall be concerned with the existence and characteristics of the Fermi surface (FS) for a system of interacting fermions, as well as some simple equilibrium properties of such a system. Usually such a surface is introduced into momentum space only for a system of noninteracting fermions. In that case this surface represents the limit of occupation of the different single-particle momentum states in the ground state of the system. All the states with momentum contained within this surface are occupied, all those with momentum outside this surface are unoccupied. As soon as one considers interaction between the particles the above definition of the FS becomes meaningless. None the less, we shall show that with a suitable definition, and under certain conditions, such a surface can be given a rigorous meaning for a system of interacting fermions. This possibility was first pointed out by Migdal,[1] 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 still possesses a discontinuity. Migdal's argument can certainly not be general, i.e., it cannot be valid for all systems of interacting fermions. Consider, for example, a collection of interacting deuterium atoms. These obey Fermi statistics. However, the ground state of this system is certainly a molecular crystal made up of D_2 molecules, and has no trace of a FS in its momentum distribution. Therefore the existence of a FS depends on the nature of the forces between the fermions. We shall investigate the problem here under the assumption that the forces between particles are such as to allow a power series expansion in their strength to give a good representation of certain properties of the system. We cannot expect that such a power series will be truly convergent, but rather that it is at most an asymptotic expansion. This was already clear from the difficulties which arise in the theory of superconductivity when one has even arbitrarily weak attractive forces. More recently Van Hove[2] has indicated how

* This work was supported in part by the Office of Naval Research.
† Now at: Dept. of Physics, Columbia University, New York 27, N. Y.
[1] A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R.) **32**, 399 (1957) [translation: Soviet Phys.—JETP **5**, 333 (1957)]. See also V. M. Galitsky and A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 139 (1958) [translation: Soviet Phys.—JETP **7**, 96 (1958)].
[2] L. Van Hove, Physica **25**, 849 (1959).

terms which cannot be represented by a power series may be found in the ground-state energy, even in the case of very weak repulsive forces. These terms are, however, exponentially small (for weak repulsive forces) so that in a case like this we would expect the power series to give an excellent asymptotic representation. Whether or not such expansions are good representations for practical cases (say He^3, or electrons in metals) is an open question.

We shall deal with this expansion by means of a propagator formalism introduced earlier.[3] In Sec. II it is shown that certain analytic properties of these propagators (which may be established by means of a power series expansion) lead to the Migdal result. The result is obtained not only for the case where the FS is a sphere in momentum space, but also for the situation (nonisotropic situation) where the FS is distorted by the interaction between the particles. It is also shown that the volume (in momentum space) of the FS is conserved. That is, the true FS has the same volume as the FS for the particles without interaction. In Sec. III, it is shown that the same analytic properties of the propagators lead to an expression for the low-temperature heat capacity of the system which is quite analogous to the expression for noninteracting particles. In Sec. IV, a similar treatment is given for the spin paramagnetism. Finally, in Sec. V, these results are all generalized for the case where in addition to the interaction between the particles there is also the external periodic potential of a lattice present. This is the case of interest for electrons in solids.

In a later publication we shall show (in collaboration with W. Kohn) that the FS as defined here is the same as the one obtained from studying the response of the system to external electric fields ("Kohn effect"). Similarly the response to a homogeneous external magnetic field (de Haas-van Alphen effect) also indicates the presence of the same FS.

II. DISCONTINUITY IN THE MOMENTUM DISTRIBUTION

In order to avoid complications we shall assume initially that we are dealing with spinless fermions. Therefore our single-particle states are labelled only by a momentum $\mathbf{k}$. (We choose units such that $\hbar=1$.) Now the momentum distribution function is defined as the mean occupation number of the state $\mathbf{k}$. This is[4]

$$\bar{n}_{\mathbf{k}}=\mathrm{Tr}\{a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\exp[\beta(\Omega-\mathcal{H}+\mu N)]\}. \tag{1}$$

It is easy to see that $\bar{n}_{\mathbf{k}}$ may be expressed in terms of the propagator $S_{\mathbf{k}}'(\zeta_l)$ previously defined. From the definition of the thermodynamic potential Ω we have

$$\bar{n}_{\mathbf{k}}=\partial\Omega/\partial\epsilon_{\mathbf{k}}. \tag{2}$$

Using the expression (LW 55) for Ω, and remembering that Ω is stationary with respect to first order changes in $G_{\mathbf{k}}(\zeta_l)$, we get at once

$$\bar{n}_{\mathbf{k}}=-\frac{1}{\beta}\sum_l \exp(\zeta_l 0^+)\frac{1}{\zeta_l-\epsilon_{\mathbf{k}}-G_{\mathbf{k}}(\zeta_l)}. \tag{3}$$

(This expression may also be established immediately from the expression for the propagator in terms of Green's functions.)

We shall only be interested in $\bar{n}_{\mathbf{k}}$ in the zero-temperature limit (it is only there that a discontinuity can occur). In this limit we have

$$\bar{n}_{\mathbf{k}}=\frac{1}{2\pi i}\int_{\mu-i\infty}^{\mu+i\infty}d\zeta\exp(\zeta 0^+)\frac{1}{\zeta-\epsilon_{\mathbf{k}}-G_{\mathbf{k}}(\zeta)}. \tag{4}$$

In what follows we shall again assume the analytic properties of $G_{\mathbf{k}}(\zeta)$ which are summarized in (LW 58, 59, 60, 61).[5] Then (4) may be written (by closing the contour to the left)

$$\bar{n}_{\mathbf{k}}=\frac{1}{2\pi i}\int_{-\infty}^{\mu}dx\left\{\frac{1}{x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(x)-iJ_{\mathbf{k}}(x)}-\text{c.c.}\right\}. \tag{5}$$

There is no reason not to expect $K_{\mathbf{k}}$ and $J_{\mathbf{k}}$ to be smooth functions of $\mathbf{k}$. If this is so, then any discontinuous behavior of the $\bar{n}_{\mathbf{k}}$ as a function of $\mathbf{k}$ can only come from a singularity of the integrand. Since $J_{\mathbf{k}}(x)$ approaches zero only in the neighborhood of $x=\mu$, any possible discontinuous behavior must come from the neighborhood of $x=\mu$. Now consider the $\mathbf{k}$ values which satisfy the equation

$$\mu-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(\mu)=0. \tag{6}$$

In general, they lie on a surface in momentum space. If there is no interaction between the particles $K_{\mathbf{k}}$ is zero, and (6) clearly becomes the equation for the FS in the usual sense. *We shall call the surface defined by (6) the FS of the interacting system.*[6] We next show that the momentum distribution has a discontinuity as we cross the FS so defined.

Let us consider values of $\mathbf{k}$ near the FS. Then the equation

$$x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(x)=0, \tag{7}$$

will in general have a solution $x=E_{\mathbf{k}}$, with $E_{\mathbf{k}}$ near μ. We shall call $E_{\mathbf{k}}$ the *true single-particle excitation energy* of the system. Call $\mathbf{k}_0$ the point on the FS closest to $\mathbf{k}$. Then

$$\mathbf{k}=\mathbf{k}_0+\boldsymbol{\delta},$$

where $\boldsymbol{\delta}$ is perpendicular to the FS at $\mathbf{k}_0$, and is small. We

[3] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

[4] Unless otherwise specified we follow the notation of reference 3. We shall refer to this paper as LW in the future.

[5] In a latter publication we shall give the explicit proof of these expressions, at least for the power series expansion of $G_{\mathbf{k}}(\zeta_l)$.

[6] If the interaction and the $\epsilon_{\mathbf{k}}$ are isotropic, then $K_{\mathbf{k}}$ is a function of the magnitude of $\mathbf{k}$ alone. In this case the FS will be a sphere or several concentric spheres. We are not assuming isotropy, however, so that in general the FS will not be spherical in shape.

may write for such values of $\mathbf{k}$

$$x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(x)=Z_{\mathbf{k}}^{-1}(x-E_{\mathbf{k}})+b_{\mathbf{k}}(x-E_{\mathbf{k}})^2+\cdots, \quad (8)$$

if x is near $E_{\mathbf{k}}$. The coefficient $Z_{\mathbf{k}}^{-1}$ is given by

$$Z_{\mathbf{k}}^{-1}=\frac{\partial}{\partial x}[x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(x)]\Big|_{x=E_{\mathbf{k}}}=1-\left[\frac{\partial K_{\mathbf{k}}(x)}{\partial x}\right]_{x=E_{\mathbf{k}}}. \quad (9)$$

Thus for x near μ and $\mathbf{k}$ near $\mathbf{k}_0$, we can write the denominator in the integrand of (5) as

$$x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(x)-iJ_{\mathbf{k}}(x) =Z_{\mathbf{k}}^{-1}(x-E_{\mathbf{k}})-iC_{\mathbf{k}}(\mu-x)^2+\cdots, \quad (10)$$

on making use of (LW 62). Let us write the integrals in (5) in two parts

$$\int_{-\infty}^{\mu}=\int_{\mu-\eta}^{\mu}+\int_{-\infty}^{\mu-\eta}. \quad (11)$$

For small but fixed η the second term cannot give rise to discontinuous behavior for $\bar{n}_{\mathbf{k}}$ since the integrand is never singular. Writing

$$\bar{n}_{\mathbf{k}}=\bar{n}_{\mathbf{k}}'+\bar{n}_{\mathbf{k}}'', \quad (12)$$

corresponding to (11), we have that $\bar{n}_{\mathbf{k}}''$ cannot have a discontinuity. For small η we may use (10) so that we have

$$\bar{n}_{\mathbf{k}}'=\frac{1}{2\pi i}\int_{\mu-\eta}^{\mu}dx\left\{\frac{1}{Z_{\mathbf{k}}^{-1}(x-E_{\mathbf{k}})-iC_{\mathbf{k}}(x-\mu)^2}-\text{c.c.}\right\}. \quad (13)$$

Putting

$$E_{\mathbf{k}}=\mu-\Delta_{\mathbf{k}}, \quad (14)$$

and using

$$E_{\mathbf{k}}=E_{\mathbf{k}_0+\delta}=E_{\mathbf{k}_0}\pm|\nabla_{\mathbf{k}_0}E_{\mathbf{k}_0}|\,\delta=\mu\pm|\nabla_{\mathbf{k}_0}E_{\mathbf{k}_0}|\,\delta, \quad (15)$$

where the plus obtains if $\boldsymbol{\delta}$ is parallel to the normal to the FS at $\mathbf{k}_0$, the minus if $\boldsymbol{\delta}$ is antiparallel to the normal to the FS at $\mathbf{k}_0$. We have

$$\Delta_{\mathbf{k}}=\mp|\nabla_{\mathbf{k}_0}E_{\mathbf{k}_0}|\,\delta. \quad (16)$$

Writing $y=\mu-x$, (13) becomes

$$\bar{n}_{k}'=\frac{1}{2\pi i}\int_{0}^{\eta}dy\left\{\frac{1}{Z_{\mathbf{k}}^{-1}(\Delta_{\mathbf{k}}-y)-iC_{\mathbf{k}}y^2}-\text{c.c.}\right\}. \quad (17)$$

Let us put

$$t=|\Delta_{\mathbf{k}}|/y. \quad (18)$$

Then (17) becomes

$$\bar{n}_{\mathbf{k}}'=\int_{|\Delta_k|/\eta}^{\infty}dt\frac{(\alpha_{\mathbf{k}}/\pi)}{(Z_{\mathbf{k}}^{-1})^2t^2(t\mp1)^2+\alpha_{\mathbf{k}}^2}, \quad (19)$$

where

$$\alpha_{\mathbf{k}}=C_{\mathbf{k}}|\Delta_{\mathbf{k}}|>0, \quad (20)$$

and the minus sign in (19) goes with $\Delta_{\mathbf{k}}>0$, the plus sign with $\Delta_{\mathbf{k}}<0$.

Now as we approach the FS, δ approaches zero, and therefore $\alpha_{\mathbf{k}}$ approaches zero. The integrand in (19) then approaches a δ function so that

$$\bar{n}_{\mathbf{k}}'=\int_0^{\infty}dt\,\delta[|Z_{\mathbf{k}}^{-1}|\,(t\mp1)]. \quad (21)$$

(It is easily seen that the small values of t near the lower limit give us no contribution as δ approaches zero. This is because the $\alpha_{\mathbf{k}}^2$ term in the denominator is negligible compared to the first term in the denominator.) For the minus sign the argument of the δ function vanishes at a point in the range of integration, for the plus sign it does not. Therefore we obtain

$$\bar{n}_{\mathbf{k}}'=|Z_{\mathbf{k}}^{-1}|, \quad (22)$$

for $\mathbf{k}$ differing infinitesimally from $\mathbf{k}_0$, but in the direction opposite to the normal to the FS at $\mathbf{k}_0$, and

$$\bar{n}_{\mathbf{k}}'=0, \quad (23)$$

for $\mathbf{k}$ differing infinitesimally from $\mathbf{k}_0$, but in the direction parallel to the normal to the FS at $\mathbf{k}_0$. Finally, therefore, we may state the result that as we cross the FS at $\mathbf{k}_0$ in the direction of the normal at $\mathbf{k}_0$ the function $\bar{n}_{\mathbf{k}}'$ has a discontinuous drop of magnitude $|Z_{\mathbf{k}_0}|$. Since $\bar{n}_{\mathbf{k}}''$ is continuous, this shows that the entire momentum distribution function has the discontinuous drop $|Z_{\mathbf{k}_0}|$.

Another way of stating this result is to write

$$\bar{n}_{\mathbf{k}}=|Z_{\mathbf{k}}|\theta(\mu-E_{\mathbf{k}})+g_{\mathbf{k}}. \quad (24)$$

In (24) $\theta(x)$ is the step-function

$$\theta(x)=1 \quad x>0$$
$$=0 \quad x<0, \quad (25)$$

and $g_{\mathbf{k}}$ has no discontinuities as a function of the momentum $\mathbf{k}$.

Since the integrand in (5) is positive both $\bar{n}_{\mathbf{k}}'$ and $\bar{n}_{\mathbf{k}}''$ must be. Further from its definition $\bar{n}_{\mathbf{k}}$ must be between zero and one. Therefore it follows that the discontinuity must satisfy

$$|Z_{\mathbf{k}_0}|<1. \quad (26)$$

We shall next show that the FS defined as above has the same volume in momentum space as the original unperturbed FS. Let us consider first the unperturbed FS. This is defined by the equation

$$\epsilon_{\mathbf{k}}=\mu_0, \quad (27)$$

where μ_0 is the unperturbed chemical potential. The volume of this surface in momentum space (V_{FS}^0) may be written

$$V_{\mathrm{FS}}^0=\int d\mathbf{k}\,\theta(\mu_0-\epsilon_{\mathbf{k}}). \quad (28)$$

On the other hand, the mean number of particles is given by

$$\bar{N}=\sum_{\mathbf{k}}\theta(\mu_0-\epsilon_{\mathbf{k}})=\frac{V}{(2\pi)^3}\int d\mathbf{k}\,\theta(\mu_0-\epsilon_{\mathbf{k}}), \quad (29)$$

where V is the volume of the fermion system. Therefore

$$\bar{N}=VV_{\mathrm{FS}}{}^{0}/(2\pi)^{3}. \tag{30}$$

In order to show that (30) still holds when we replace $V_{\mathrm{FS}}{}^{0}$ by V_{FS} (the volume of the new FS), we shall transform the general expression for $\bar{N}$. The discussion is identical with that of (LW 57), no use having been made of isotropy in the argument. Therefore we have [from (LW 69)]

$$\bar{N}=\sum_{\mathbf{k}}\theta(\mu-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(\mu))$$
$$=\frac{V}{(2\pi)^{3}}\int d\mathbf{k}\,\theta(\mu-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(\mu)). \tag{31}$$

Since the surface

$$\mu-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(\mu)=0,$$

is by definition the FS, we may also write[7] (31) as

$$\bar{N}=VV_{\mathrm{FS}}/(2\pi)^{3}. \tag{32}$$

From (30) and (32) we have

$$V_{\mathrm{FS}}=V_{\mathrm{FS}}{}^{0}, \tag{33}$$

which is the desired theorem. The interaction may deform the FS, but it cannot change its volume. In the isotropic case, where symmetry requires the FS to remain a sphere, its radius must then remain k_F (the Fermi momentum of the unperturbed system).

III. HEAT CAPACITY

We now consider the problem of finding the heat capacity of a system of interacting fermions at low temperatures. Consider the thermodynamic potential $\Omega=\Omega(\mu,V,T)$. The entropy is given by

$$S=-(\partial\Omega/\partial T)_{\mu,V}, \tag{34}$$

and the heat capacity at constant volume

$$C_V=T(\partial S/\partial T)_V. \tag{35}$$

In (35) it is understood that not μ but the number of particles is being held fixed. As we shall see below, at low temperatures we may expand Ω in even powers of the temperature

$$\Omega=\Omega(\mu,V,0)-\tfrac{1}{2}\gamma(\mu,V)T^{2}+\cdots. \tag{36}$$

Then

$$S=\gamma(\mu,V)T+\cdots. \tag{37}$$

The quantity μ is the chemical potential at the temperature T. Writing

$$\mu=\mu^{0}+\mu'+\cdots, \tag{38}$$

where μ^{0} is the chemical potential of the interacting system at $T=0$, μ' is of order T^{2}, etc., we have

$$S=\gamma(\mu^{0},V)T+\cdots. \tag{39}$$

Therefore, since μ^{0} is a function of $\bar{N}$ and V alone,

$$C_V=\gamma(\mu^{0},V)T+\cdots. \tag{40}$$

The heat capacity will therefore be a linear function of temperature at low temperatures, just as for the ideal Fermi gas. It remains to evaluate the coefficient $\gamma(\mu^{0},V)$.

The expansion of Ω in powers of T is obtained most directly from the expression (47, 48, 55) for Ω given in LW. This is

$$\Omega=-\frac{1}{\beta}\sum_{\mathbf{k}}\sum_{l}\exp(\zeta_l 0^{+})\{\ln[\epsilon_{\mathbf{k}}+G_{\mathbf{k}}(\zeta_l)-\zeta_l]$$
$$+G_{\mathbf{k}}(\zeta_l)S_{\mathbf{k}}'(\zeta_l)\}+\Omega', \tag{41}$$

$\Omega'=$[Contribution of a closed linked skeleton diagrams but with $S_{\mathbf{k}}(\zeta_l)$ replaced by $S_{\mathbf{k}}'(\zeta_l)$]. (42)

We also know that the expression (41) for Ω is stationary with respect to changes in the proper self-energy part $G_{\mathbf{k}}(\zeta_l)$. Therefore if we are just interested in the first correction to Ω, we can neglect the explicit temperature dependence of the $G_{\mathbf{k}}(\zeta_l)$ and replace them by $G_{\mathbf{k}}{}^{0}(\zeta_l)$, which is the value calculated at $T=0$. Thus the first correction to the $T=0$ value of (41) comes only from the difference between the l sums in (41) and what we would get if we replaced them by integrals according to (LW 62).

Consider Ω'. Since each line of a skeleton diagram contains an l sum, the total first correction to Ω' is obtained by correcting the computation in each diagram for a single line, using (LW 62) for the other l sums of the diagram, and finally summing over every line. This will clearly give us for Ω' correct to the first order

$$\Omega'=-\frac{1}{\beta}\sum_{\mathbf{k}}\sum_{l}\frac{1}{\zeta_l-\epsilon_{\mathbf{k}}-G_{\mathbf{k}}{}^{0}(\zeta_l)}G_{\mathbf{k}}{}^{0}(\zeta_l), \tag{43}$$

since in a νth-order skeleton diagram opening up the 2ν lines just gives the proper self-energy part to the νth order.

From (43) and (41) we get, to first order,

$$\Omega=-\frac{1}{\beta}\sum_{\mathbf{k}}\sum_{l}\exp(\zeta_l 0^{+})\{\ln[\epsilon_{\mathbf{k}}+G_{\mathbf{k}}(\zeta_l)-\zeta_l]\}. \tag{44}$$

Using the technique of reference 3, Appendix A, we may write the l sum as an integral

$$\Omega=-\sum_{\mathbf{k}}\frac{1}{2\pi i}\int_{\Gamma_0}d\zeta\,\exp(\zeta 0^{+})\ln[\epsilon_{\mathbf{k}}+G_{\mathbf{k}}(\zeta)-\zeta]$$
$$\times\frac{1}{e^{\beta(\zeta-\mu)}+1}, \tag{45}$$

[7] The FS divides momentum space into two parts: those regions for which $\mu-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}(\mu)$ is greater than zero, and those regions for which it is less than zero. We define the former region as the *interior* of the FS.

where Γ_0 is a contour which goes from $+\infty$ to $-\infty$ immediately above the real axis, and from $-\infty$ to $+\infty$ immediately below the real axis. Therefore we may write

$$\Omega=-\sum_{\mathbf{k}}\frac{1}{2\pi i}\int_{-\infty}^{\infty}dx\{\ln[\epsilon_{\mathbf{k}}+K_{\mathbf{k}}{}^0(x)-x+iJ_{\mathbf{k}}{}^0(x)] -\text{c.c.}\}\frac{1}{e^{\beta(x-\mu)}+1}. \quad (46)$$

The term in (46) proportional to T^2 is obtained by the usual Sommerfeld technique

$$\int f(x)\frac{dx}{e^{\beta(x-\mu)}+1}=\int f(x)\theta(\mu-x)dx +\frac{\pi^2}{6}(kT)^2f'(\mu)+\cdots. \quad (47)$$

Combining (47), (46), and (36) we have at once

$$\gamma(\mu^0,V)=\frac{1}{2\pi i}\frac{\pi^2}{3}k^2\sum_{\mathbf{k}}\frac{\partial}{\partial x}\{\ln[\epsilon_{\mathbf{k}}+K_{\mathbf{k}}{}^0(x) -x+iJ_{k}{}^0(x)]-\text{c.c.}\}\Big|_{x=\mu^0}. \quad (48)$$

From (LW 68) one has [since x is near μ^0, $J_{\mathbf{k}}{}^0(x)$ is a positive infinitesimal]

$$(1/2\pi i)\{\ln[\epsilon_{\mathbf{k}}+K_{\mathbf{k}}{}^0(x)-x+iJ_{\mathbf{k}}{}^0(x)]-\text{c.c.}\} =\theta(x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}{}^0(x)). \quad (49)$$

Again, since the solution of the equation

$$x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}{}^0(x)=0,$$

is just the true single-particle excitation energy $E_{\mathbf{k}}$, we may write

$$\theta(x-\epsilon_{\mathbf{k}}-K_{\mathbf{k}}{}^0(x))=\theta(x-E_{\mathbf{k}}). \quad (50)$$

Finally, therefore, we obtain

$$\gamma(\mu^0,V)=\frac{\pi^2}{3}k^2\sum_{\mathbf{k}}\frac{\partial}{\partial x}\theta(x-E_{\mathbf{k}})\Big|_{x=\mu^0} =\frac{\pi^2}{3}k^2\sum_{\mathbf{k}}\delta(\mu^0-E_{\mathbf{k}}). \quad (51)$$

The expression (51) for the coefficient of the linear term in the heat capacity is to be compared with the result

$$\gamma_0=\frac{\pi^2}{3}k^2\sum_{\mathbf{k}}\delta(\mu_0{}^0-\epsilon_{\mathbf{k}}), \quad (52)$$

for the unperturbed system of fermions. All one need do to obtain the correct result is to replace the unperturbed chemical potential by the true chemical potential and the original single-particle energies by the "true" single-particle excitation energies. The expression (51) has been suggested and semi-intuitive grounds by Gell-Mann[8] and by Landau,[9] but we are not aware of any derivation which proceeds from the general principles of statistical mechanics.

IV. SPIN PARAMAGNETISM

We must consider the zero-temperature paramagnetic susceptibility arising from the spins of the fermions. We leave out of consideration the effect of the external magnetic field on their orbital motion. Strictly speaking, this applies to a collection of uncharged fermions (like He^3) and not to electrons in metals. However, even for electrons in metals it will be part of susceptibility, and actually it can be measured approximately under some circumstances.

We now have to discuss the effect of introducing spin into our formalism. For simplicity we limit ourselves to spin $\frac{1}{2}$ fermions. The single-particle states must be labelled by an index r which gives the momentum $\mathbf{k}$ and the spin direction σ ($\sigma=\pm1$). We imagine that there is an external magnetic field H in the Z direction, and take the axis of quantization of the spins also to be in this direction. Let the particles have an intrinsic magnetic moment p. Then the unperturbed single-particle energy is

$$\epsilon_r=\epsilon_{\mathbf{k}}-pH\sigma. \quad (53)$$

We now use (41) with the index $\mathbf{k}$ replaced by r. A word of justification is necessary, however. In the derivation of (41) given in LW we made use of the isotropy of the situation. This was used only in order to establish the fact that in a propagator diagram the entering line and the emerging line must represent the same state. (See the discussion at the beginning of Sec. III of LW.) In order to preserve this simplicity we shall again assume isotropy for the interactions and the $\epsilon_{\mathbf{k}}$. Total isotropy cannot be present, however, because of the magnetic field. Still, for spin $\frac{1}{2}$ fermions the emerging line of a propagator diagram must represent the same state as the entering line. One sees this as follows. Represent all possibilities of changing the spin state by a two by two matrix, which must be linear in the Pauli spin matrices σ_i. By isotropy this matrix must be a rotational invariant, if we also rotate the magnetic field. The only invariants involving σ_i that we can construct from the vectors which are available ($\boldsymbol{\sigma}$,$\mathbf{k}$,$\mathbf{H}$) are $\boldsymbol{\sigma}\cdot\mathbf{k}$, $(\boldsymbol{\sigma}\times\mathbf{H})\cdot\mathbf{k}$ and $\boldsymbol{\sigma}\cdot\mathbf{H}$. The first of these is not possible by space inversion, the second is eliminated by time inversion. This leaves us only with the third, which is diagonal if we take the direction of quantization to be along the field.

In order to calculate the susceptibility we need to know the mean magnetic moment M. This is given by

$$M=-\partial\Omega(\mu,V,T,H)/\partial H. \quad (54)$$

[8] M. Gell-Mann, Phys. Rev. **106**, 369 (1959).
[9] L. Landau, J. Exptl. Theoret. Phys. (U.S.S.R.) **30**, 1058 (1956) [translation: Soviet Phys.—JETP **3**, 920 (1956)].

Differentiating the expression (41) for Ω and making use of its stationary property with respect to variations in $G_r(\zeta_l)$ we have at once

$$M=-\frac{1}{\beta}\sum_r\sum_l \exp(\zeta_l 0^+)\left(-\frac{\partial\epsilon_r}{\partial H}\right)\frac{1}{\zeta_l-\epsilon_r-G_r(\zeta_l)}$$
$$=-\frac{1}{\beta}\sum_r\sum_l \exp(\zeta_l 0^+)\frac{p\sigma}{\zeta_l-\epsilon_r-G_r(\zeta_l)}. \quad (55)$$

(This expression may also be written down at once by noting that the magnetic moment is p times the mean number of spins up minus the mean number of spins down.)

It is convenient to rewrite (55) as follows

$$M=-\frac{1}{\beta}\sum_r\sum_l p\sigma\exp(\zeta_l 0^+)\frac{\partial}{\partial\zeta_l}\ln[\epsilon_r+G_r(\zeta_l)-\zeta_l]+J, \quad (56)$$

$$J\equiv-\frac{1}{\beta}\sum_r p\sigma\sum_l \exp(\zeta_l 0^+)\frac{\partial G_r(\zeta_l)}{\partial\zeta_l}\frac{1}{\zeta_l-\epsilon_r-G_r(\zeta_l)}. \quad (57)$$

We now discuss J. In (57) we can pass to the zero-temperature limit in the usual way (LW 62). [In fact the discussion which follows here is very closely related to the one in LW for $\bar{N}$, leading to (LW 69).]

$$J=\frac{1}{2\pi i}\sum_r p\sigma\int_C d\zeta\exp(\zeta 0^+)\left(\frac{\partial G_r(\zeta)}{\partial\zeta}\right)\frac{1}{\zeta-\epsilon_r-G_r(\zeta)}. \quad (58)$$

Dropping the $\exp(\zeta 0^+)$ factor (which is not necessary for convergence in this term) and integrating by parts we obtain

$$J=-\frac{1}{2\pi i}\sum_r p\sigma\int_C d\zeta\, G_r(\zeta)\frac{\partial}{\partial\zeta}\frac{1}{\zeta-\epsilon_r-G_r(\zeta)}. \quad (59)$$

If we were simply summing on r without the weighting factor σ, then this would be identically zero by the argument immediately following (LW 63). We have to be a little more careful in the present case because of the factor σ. First we note that all diagrams for $G_{\mathbf{k}\sigma}(\zeta)$ may be obtained by "opening" any line of the closed, linked irreducible skeleton diagrams (Ω'), which bears the index σ, and then taking the sum of all these contributions. Therefore we may write

$$\frac{1}{2\pi i}\sum_{\mathbf{k}}\int_C d\zeta\, G_{\mathbf{k}\sigma}(\zeta)\frac{\partial}{\partial\zeta}\frac{1}{\zeta-\epsilon_{\mathbf{k}\sigma}-G_{\mathbf{k}\sigma}(\zeta)}$$
$$=[\text{derivative of the integrand of }\Omega'\text{ with respect to the }\zeta\text{ in every propagator which bears the index }\sigma]. \quad (60)$$

For any propagator which contains a ζ which is integrated over independently, we get no contribution to (60), since we may integrate by parts. We therefore have to consider those ζ's which are connected by the "energy conservation" condition (LW 30). This gives rise to a term in (61), the ζ integrations of which have the form

$$\int_C d\zeta_1 d\zeta_2 d\zeta_3 d\zeta_4\,\delta(\zeta_1+\zeta_2-\zeta_3-\zeta_4)\left(\sum_{i=1}^{4}{}'\frac{\partial}{\partial\zeta_i}\right)$$
$$\times S_{\mathbf{k}_1\sigma_1}'(\zeta_1)S_{\mathbf{k}_2\sigma_2}'(\zeta_2)S_{\mathbf{k}_3\sigma_3}'(\zeta_3)S_{\mathbf{k}_4\sigma_4}'(\zeta_4), \quad (61)$$

where the prime on the summation means that we are only to take a derivative if the corresponding S' bears the index σ. If all the $\sigma_i=\sigma$ then (61) gives nothing by the same argument as (LW 64). If three of the σ_i's were σ and the other one was not, then (61) will certainly not vanish by itself. To avoid this complication, we shall assume that the interaction is spin independent. Then $\sigma_1=\sigma_3$, $\sigma_2=\sigma_4$. The only case left to study is where (say) $\sigma_1=\sigma_3=\sigma$, $\sigma_2=\sigma_4\neq\sigma$. Then we have

$$\sum_{i=1}^{4}\frac{\partial}{\partial\zeta_i}=\frac{\partial}{\partial\zeta_1}+\frac{\partial}{\partial\zeta_3}.$$

Integrating (61) by parts with respect to ζ_1 and ζ_3, and using

$$\left(\frac{\partial}{\partial\zeta_1}+\frac{\partial}{\partial\zeta_3}\right)\delta(\zeta_1+\zeta_2-\zeta_3-\zeta_4)=0,$$

we again obtain zero.

For the case of spin-independent forces we have shown that $J=0$ and therefore that

$$M=-\frac{1}{\beta}\sum_r\sum_l p\sigma\exp(\zeta_l 0^+)\frac{\partial}{\partial\zeta_l}\ln[\epsilon_r+G_r(\zeta_l)-\zeta_l]. \quad (62)$$

Passing to the zero-temperature limit in (62) we have at once (LW 65–69)

$$M=p\sum_{\mathbf{k}\sigma}\sigma\theta(\mu-\epsilon_{\mathbf{k}\sigma}-K_{\mathbf{k}\sigma}(\mu)). \quad (63)$$

Just as in the spinless case, we define "true single-particle excitation energies" $E_{\mathbf{k}\sigma}$ by

$$E_{\mathbf{k}\sigma}-\epsilon_{\mathbf{k}\sigma}-K_{\mathbf{k}\sigma}(E_{\mathbf{k}\sigma})=0. \quad (64)$$

There will be two Fermi surfaces defined by $E_{\mathbf{k}\sigma}=\mu$ for $\sigma=\pm 1$, and discontinuities in the momentum distribution will occur at each. In terms of $E_{\mathbf{k}\sigma}$ (64) becomes

$$M=p\sum_{\mathbf{k}\sigma}\sigma\theta(\mu-E_{\mathbf{k}\sigma}). \quad (65)$$

To calculate the susceptibility we need the term proportional to H. Let us write

$$E_{\mathbf{k}\sigma}=E_{\mathbf{k}}-p\gamma(\mathbf{k})H\sigma+O(H^2), \quad (66)$$

where $E_{\mathbf{k}}$ is the true single-particle energy without the field (it is spin independent under our assumptions), and

$\gamma(\mathbf{k})$ is a measure of the modification of the effective magnetic moments of the particles due to interaction between them. It is to be calculated from (64). Inserting (66) in (65) and expanding, we obtain for the susceptibility[10]

$$\chi=\frac{M}{VH}=\frac{2p^2}{V}\sum_{\mathbf{k}}\gamma(\mathbf{k})\delta(\mu-E_{\mathbf{k}}), \tag{67}$$

where μ is the chemical potential of the system in the absence of the field.

Thus the low-temperature spin susceptibility like the low-temperature heat capacity depends only on the true single-particle excitation energies. As a result of the factor $\gamma(\mathbf{k})$, however, these two quantities are no longer simply related as they are in the case of noninteracting fermions. In this connection we may mention that the zero-temperature compressibility (K) of the system may also be put in a similar form. We start with the thermodynamic identity

$$K=-\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T=\frac{V}{\bar{N}^2}\left(\frac{\partial \bar{N}}{\partial \mu}\right)_{V,T}. \tag{68}$$

From our old work, at zero temperature,

$$\bar{N}=\sum_{\mathbf{k}}\theta(\mu-E_{\mathbf{k}}(\mu)), \tag{69}$$

(here we drop spin indices for simplicity and also indicate explicitly that the true single-particle excitation energies will depend on μ). Therefore

$$\left(\frac{\partial \bar{N}}{\partial \mu}\right)_{V,T}=\sum_{\mathbf{k}}\left[1-\left(\frac{\partial E_{\mathbf{k}}(\mu)}{\partial \mu}\right)_V\right]\delta(\mu-E_k(\mu)). \tag{70}$$

We thus have

$$K=\frac{V}{\bar{N}^2}\sum_{\mathbf{k}}\left[1-\left(\frac{\partial E_{\mathbf{k}}(\mu)}{\partial \mu}\right)_V\right]\delta(\mu-E_{\mathbf{k}}). \tag{71}$$

The zero-temperature compressibility therefore may also be written a function of $E_{\mathbf{k}}$. However, because of the factor $\{1-[\partial E_{\mathbf{k}}(\mu)/\partial\mu]_V\}$ it is not simply related to the spin paramagnetism or heat capacity, as it is for a system of noninteracting fermions. Related formulas for the spin paramagnetism and compressibility of a system of interacting fermions have also been discussed by Landau[9] from the point of view of his semiphenomenological theory of Fermi liquids.

V. THE BAND CASE

We now want to generalize the previous results to the case where in addition to the interaction between the particles, each moves in an external periodic potential (of a lattice, say). The unperturbed single-particle energies will then be labelled with a band index n, a quasi-momentum $\mathbf{k}$ (which ranges over the first Brillouin zone of the lattice), and finally a spin index σ. Let us again denote all these quantum numbers by r. The general formalism of LW is unchanged, up to the point where we introduce propagators. The difference comes because general conservation rules no longer tell us that the entering line of a propagator diagram represents the same state as the emerging line. Even if there is sufficient isotropy so that the spin index does not change, the band index will change in general. (The translational symmetry of the interaction between the fermions insures conservation of $\mathbf{k}$.) The most general propagator diagram then has the form given in Fig. 1(a). Let us call a diagram of the type in Fig. 1(b) a proper diagram. We denote the contributions of all proper diagrams by

$$\frac{1}{\zeta_l-\epsilon_r}G_{rr'}(\zeta_l)\frac{1}{\zeta_l-\epsilon_{r'}},$$

the quantity $G_{rr'}(\zeta_l)$ again being referred to as the proper self-energy part. The total contribution of all propagator diagrams will be denoted by $S_{rr'}(\zeta_l)$. Then clearly

$$S_{rr'}(\zeta_l)=\frac{1}{\zeta_l-\epsilon_r}\delta_{rr'}+\frac{1}{\zeta_l-\epsilon_r}G_{rr'}(\zeta_l)\frac{1}{\zeta_l-\epsilon_{r'}}+\sum_{r''}\frac{1}{\zeta_l-\epsilon_r}\times G_{rr''}(\zeta_l)\frac{1}{\zeta_l-\epsilon_{r''}}G_{r''r'}(\zeta_l)\frac{1}{\zeta_l-\epsilon_{r'}}+\cdots. \tag{72}$$

Introducing the matrices $\boldsymbol{\epsilon}$, $\mathbf{G}(\zeta)$, $\mathbf{S}'(\zeta)$ defined by their

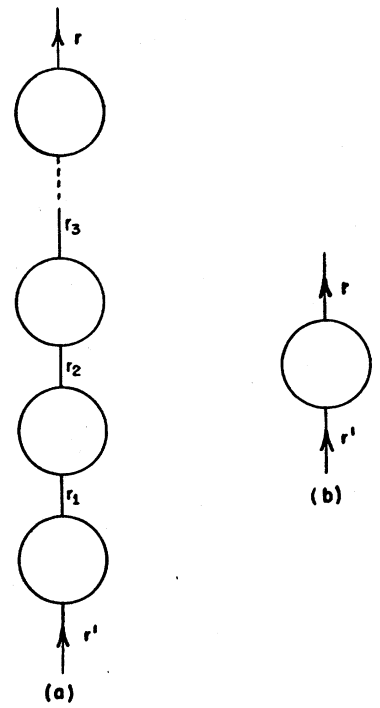

FIG. 1. (a) The general structure of a propagator diagram. (b) A proper propagator diagram.

[10] We wish to emphasize that this formula has only been derived here under the assumption of spin $\frac{1}{2}$ fermions, isotropy, and spin-independent interactions between the particles.

matrix elements

$$(\boldsymbol{\varepsilon})_{rr'}=\epsilon_r\delta_{rr'},$$
$$(\mathbf{G})_{rr'}=G_{rr'}, \tag{73}$$
$$(\mathbf{S}')_{rr'}=S_{rr'}',$$

we may write (72) as

$$\mathbf{S}'(\zeta_l)=\frac{1}{\zeta_l-\boldsymbol{\varepsilon}-\mathbf{G}(\zeta_l)}. \tag{74}$$

Since $\mathbf{G}$ and $\mathbf{S}'$ have nondiagonal matrix elements the expression for Ω [Eq. (41) of this paper] upon which most of our work has been based is no longer valid. It is easy to see what takes its place, however. We shall show that Ω is given by

$$\Omega=-\frac{1}{\beta}\sum_l \mathrm{Tr}\{\ln[\boldsymbol{\varepsilon}+\mathbf{G}(\zeta_l)-\zeta_l] +\mathbf{S}'(\zeta_l)\mathbf{G}(\zeta_l)\}\exp(\zeta_l 0^+)+\Omega', \tag{75}$$

$\Omega'=$[contribution of all closed linked skeleton diagrams, but with $S_r(\zeta_l)\delta_{rr'}$ replaced by $S_{rr'}'(\zeta_l)$]. (76)

In (75), Tr means the trace with respect to the matrix indices r, r'. The definition (76) is best illustrated by an example. Consider the skeleton diagram of Fig. 2. Apart from numerical factors (the same ones which would appear if the particle lines were free propagators) this gives a contribution

$$\sum_{\substack{r_1r_2r_3r_4\\ r_1'r_2'r_3'r_4'}}\sum_{l_1l_2l_3l_4}\delta_{l_1+l_2,\,l_3+l_4}(r_1r_2|v|r_3r_4)(r_3'r_4'|v|r_1'r_2') \times S_{r_1'r_1'}(\zeta_{l_1})S_{r_2'r_2'}(\zeta_{l_2})S_{r_3r_3'}(\zeta_{l_3})S_{r_4r_4'}(\zeta_{l_4}). \tag{77}$$

That is, the rules for computing Ω' are just the same as those given before except that each line is provided with *two* indices (an initial and a final one) which tell what matrix element of $\mathbf{S}'(\zeta_l)$ to take.

We proceed with an outline of the proof of (75), which follows that of the analogous expression in LW almost exactly. We note first that in analogy to (LW 40) we may write

$G_{rr'}(\zeta_l)=$[contribution for all possible skeleton diagrams for $G_{rr'}(\zeta_l)$, but with $S_{r_1}(\zeta_l)\delta_{r_1r_2}$ replaced by $S_{r_1r_2}'(\zeta_l)$, just as in (76)]. (78)

This is simply because there is a unique way, for the self-energy part, of making the reduction to skeleton diagrams.

Regarding Ω, as defined by (75), as a function of all the $G_{rr'}(\zeta_l)$, we next show that it is stationary around the correct value of $G_{rr'}(\zeta_l)$. Consider

$$\frac{\partial\Omega}{\partial G_{r'r}(\zeta_l)}=-\frac{1}{\beta}\sum_{r_1r_2}\frac{\partial S_{r_1r_2}'(\zeta_l)}{\partial G_{r'r}(\zeta_l)}G_{r_2r_1}(\zeta_l)+\frac{\partial\Omega'}{\partial G_{r'r}(\zeta_l)}. \tag{79}$$

In (79) we have used the identity (valid for two not necessarily commuting matrices A and B).

$$\frac{\partial}{\partial A_{r'r}}\mathrm{Tr}f(A+B)=[f'(A+B)]_{rr'}. \tag{80}$$

Now from the definition of Ω', and making use of exactly the same reasoning that went into the derivation of (LW 51) we have

$$\frac{\partial\Omega'}{\partial G_{r'r}(\zeta_l)}=\frac{1}{\beta}\sum_{r_1r_2}\frac{\partial S_{r_1r_2}'(\zeta_l)}{\partial G_{r'r}(\zeta_l)}G_{r_2r_1}(\zeta_l). \tag{81}$$

Therefore, the right-hand side of (79) vanishes, and we have the required stationary property

$$\partial\Omega/\partial G_{r'r}(\zeta_l)=0. \tag{82}$$

Next consider $\lambda\partial\Omega/\partial\lambda$, μ held fixed. Then by the stationary property (82) we can ignore the dependence of the $G_{rr'}$ on λ, and the only contribution comes from the explicit λ dependence of the interactions in Ω'. This gives, just as in LW,

$$\lambda\frac{\partial\Omega}{\partial\lambda}=\frac{1}{2\beta}\sum_l\mathrm{Tr}[\mathbf{S}'(\zeta_l)\mathbf{G}(\zeta_l)]. \tag{83}$$

On the other hand from (LW 41) we have

$$\Omega=\frac{1}{\beta}\sum_n\sum_r\sum_l\frac{1}{2n}\frac{1}{\zeta_l-\epsilon_r}[G_{rr'}(\zeta_l)]_n, \tag{84}$$

where $[G_{rr'}(\zeta_l)]_n$ is the rr element of the total reducible propagator of nth order in λ. Differentiating with respect to λ we have

$$\begin{aligned}\lambda\frac{\partial\Omega}{\partial\lambda}&=\frac{1}{2\beta}\sum_n\sum_r\sum_l\frac{1}{\zeta_l-\epsilon_r}[G_{rr'}(\zeta_l)]_n\\ &=\frac{1}{2\beta}\sum_r\sum_l\frac{1}{\zeta_l-\epsilon_r}G_{rr'}(\zeta_l)\\ &=\frac{1}{2\beta}\sum_r\sum_l\frac{1}{\zeta_l-\epsilon_r}\Big\{G_{rr}(\zeta_l)+\sum_{r'}G_{rr'}(\zeta_l)\frac{1}{\zeta_l-\epsilon_{r'}}G_{r'r}(\zeta_l)+\cdots\Big\}\\ &=\frac{1}{2\beta}\sum_l\sum_{r,r'}\Big\{\frac{1}{\zeta_l-\epsilon_r}\delta_{rr'}+\frac{1}{\zeta_l-\epsilon_r}G_{rr'}(\zeta_l)\frac{1}{\zeta_l-\epsilon_{r'}}+\cdots\Big\}G_{r'r}(\zeta_l)\\ &=\frac{1}{2\beta}\sum_l\mathrm{Tr}[\mathbf{S}'(\zeta_l)\mathbf{G}(\zeta_l)].\end{aligned} \tag{85}$$

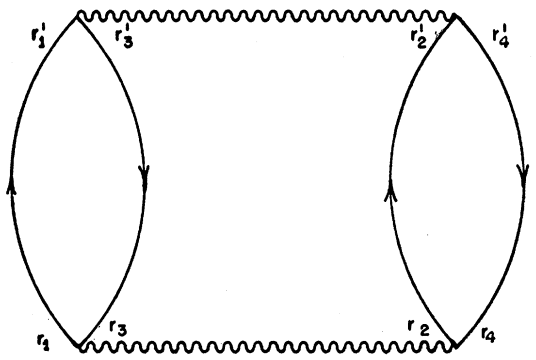

FIG. 2. A skeleton diagram corresponding to Ω'.

Therefore we have proved that the derivative of (75) with respect to λ gives the correct result. The proof that (75) is correct for $\lambda=0$ is identical with that in LW. Therefore we have established (75) in general.

Although we have had the band case in mind in deriving this formalism, it is of course quite generally valid. It is necessary in any problem where the interaction is such that the propagator is not automatically diagonal. Other examples where it is necessary are the case of particles of arbitrary spin when there is no isotropy, and that of an external magnetic field acting on the orbital motion of charged interacting particles.

The same derivation that led to (3) now gives for the mean occupation number of state r ($\bar{n}_r$)

$$\bar{n}_r=-\frac{1}{\beta}\sum_l \exp(\zeta_l 0^+)\left(\frac{1}{\zeta_l-\boldsymbol{\varepsilon}-\mathbf{G}(\zeta_l)}\right)_{rr}. \tag{86}$$

For the band case $\boldsymbol{\varepsilon}$ and $\mathbf{G}$ are diagonal in $\mathbf{k}$. Let us write $r=\mathbf{k}$, ν, ν being a discrete index which labels band and spin.

$$\epsilon_{rr'}=\epsilon_{\nu\mathbf{k}}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\nu\nu'}\equiv(\boldsymbol{\varepsilon}_{\mathbf{k}})_{\nu\nu'}\delta_{\mathbf{k},\mathbf{k}'}, \tag{87}$$

$$G_{rr'}=G_{\mathbf{k}\nu,\nu'\delta_{\mathbf{k},\mathbf{k}'}}=(\mathbf{G}_{\mathbf{k}})_{\nu\nu'}\delta_{\mathbf{k},\mathbf{k}'}. \tag{88}$$

Therefore

$$\bar{n}_{\nu\mathbf{k}}=-\frac{1}{\beta}\sum_l \exp(\zeta_l 0^+)\left(\frac{1}{\zeta_l-\boldsymbol{\varepsilon}_{\mathbf{k}}-\mathbf{G}_{\mathbf{k}}(\zeta_l)}\right)_{\nu\nu}. \tag{89}$$

The "momentum" distribution will be given by

$$\bar{n}_{\mathbf{k}}=\sum_\nu \bar{n}_{\nu k}=-\frac{1}{\beta}\sum_l \exp(\zeta_l 0^+)\,\mathrm{Tr}\left[\frac{1}{\zeta_l-\boldsymbol{\varepsilon}_{\mathbf{k}}-\mathbf{G}_{\mathbf{k}}(\zeta_l)}\right]. \tag{90}$$

We now take advantage of the fact that the trace of a function of a matrix is just the sum of the values of the function at the characteristic values of the matrix.[11] This is true whether or not the matrix is diagonalizable by a similarity transformation or not. [It will only be in very exceptional cases, however, that a similarity transformation will not exist which will diagonalize $\boldsymbol{\varepsilon}_{\mathbf{k}}+\mathbf{G}_{\mathbf{k}}(\zeta_l)$.] It is not surprising that the problem of finding the characteristic values of a new matrix still exists in the theory. Even in the usual Hartree-Fock approximation, new bands are defined by the new effective potential which arises from the average effect of all the other particles on one of them. In Appendix A, we will show how the Hartree-Fock in fact arises naturally as a very simple first step in our formulation. Let us write the characteristic values of $\boldsymbol{\varepsilon}_{\mathbf{k}}+\mathbf{G}_{\mathbf{k}}(\zeta_l)$ as $L_{\mathbf{k}\rho}(\zeta_l)$. The discrete index ρ is what replaces our former band and spin indices. We shall refer to ρ as the "true" band index. From (90)

$$\bar{n}_{\mathbf{k}}=-\frac{1}{\beta}\sum_l\sum_\rho \exp(\zeta_l 0^+)\frac{1}{\zeta_l-L_{\mathbf{k}\rho}(\zeta_l)}. \tag{91}$$

Going to the zero-temperature limit, and closing the resulting contour to the left, we have (η an infinitesimal positive number)

$$\bar{n}_{\mathbf{k}}=\frac{1}{2\pi i}\sum_\rho\int_{-\infty}^{\mu}dx\left\{\frac{1}{x-i\eta-L_{\mathbf{k}\rho}(x-i\eta)}-\frac{1}{x+i\eta-L_{\mathbf{k}\rho}(x+i\eta)}\right\}. \tag{92}$$

Let us write

$$L_{\mathbf{k}\rho}(x-i\eta)=Q_{\mathbf{k}\rho}(x)+iJ_{\mathbf{k}\rho}(x). \tag{93}$$

The quantity $Q_{\mathbf{k}\rho}$ plays the same role here that $\epsilon_r+K_r(x)$ played in earlier work. The quantity $J_{\mathbf{k}\rho}(x)$ plays exactly the same role as $J_r(x)$ did previously. If we again assume the analytic properties that we did formerly (they follow in an analogous fashion), then results just like our former ones are clearly still valid. For example, discontinuities will occur in $\mathbf{k}$ space at the values of $\mathbf{k}$ satisfying

$$\mu-Q_{\mathbf{k}\rho}(\mu)=0. \tag{94}$$

We shall again call this collection of surfaces the FS of the system. In general for a metal (94) will only have solutions for a few ρ values; these will play the role of the "unfilled bands" in conventional metal theory. For an insulator or semiconductor there will be no values of ρ which enable us to find solutions of (94), so that no FS and no metallic properties can exist.

The discussion of the volume of the FS also proceeds as before. Analogously to (31), we have

$$\bar{N}=\sum_{\rho\mathbf{k}}\theta(\mu-Q_{\mathbf{k}\rho}(\mu)). \tag{95}$$

We now divide the band indices ρ into three classes:

(1) Equation (94) is never satisfied, and $\mu-Q_{\mathbf{k}\rho}(\mu)>0$. We call these the "filled" bands.

[11] See, for example, P. R. Halmos, *Finite Dimensional Vector Spaces* (Princeton University Press, Princeton, New Jersey, 1942), pp. 80–85. The required result follows for finite matrices and polynomial functions from the last sentence of that section. The characteristic values are defined in the case of nondiagonalizability as just the roots of the secular equation.

(2) Equation (94) is satisfied on certain surfaces in $\mathbf{k}$ space. We call these the "conduction" bands.

(3) Equation (94) is never satisfied, and $\mu-Q_{\mathbf{k}\rho}(\mu)<0$. We call these the "empty" bands.

Each filled band contributes to (95) an amount N_b, where N_b is the number of $\mathbf{k}$ states in a band. This is determined only by the geometry of the crystal and is the same as for the noninteracting particle problem. It is equal to the number of unit cells of the crystal. The empty bands contribute nothing. Therefore we have

$$N_c=\sum_{\rho\mathbf{k}}{}'\,\theta(\mu-Q_{\mathbf{k}\rho}(\mu)), \tag{96}$$

where N_c is the total number of particles present minus the number of filled bands times N_b. We may call it the "number of particles in the conduction band." The prime on the summation means that it only extends over the conduction bands. This gives[12]

$$N_c=\sum_{\rho}{}'\frac{V}{(2\pi)^3}\int d\mathbf{k}\,\theta(\mu-Q_{\mathbf{k}\rho}(\mu))$$
$$=VV_{\mathrm{FS}}/(2\pi)^3. \tag{97}$$

For the noninteracting case we have,

$$N_c=VV_{\mathrm{FS}}{}^0/(2\pi)^3, \tag{98}$$

so that

$$V_{\mathrm{FS}}=V_{\mathrm{FS}}{}^0, \tag{99}$$

once more.

The low-temperature heat capacity also is easily found. By reasoning exactly analogous to that which led to (48) we obtain

$$C_V=\frac{\pi^2}{3}k^2T\sum_{\mathbf{k}}\frac{\partial}{\partial x}$$
$$\times\{\mathrm{Tr}[\ln(\boldsymbol{\varepsilon}_{\mathbf{k}}+\mathbf{G}_{\mathbf{k}}(x-i\eta)-x)]-\mathrm{c.c.}\}\Big|_{x=\mu}. \tag{100}$$

Since (100) only contains the trace, we can again introduce the characteristic values $L_{\mathbf{k}\rho}(\zeta)$. This gives

$$C_V=\frac{\pi^2}{3}k^2T\sum_{\mathbf{k}\rho}\frac{\partial}{\partial x}$$
$$\times\{\ln[Q_{\mathbf{k}\rho}(x)-x+iJ_{\mathbf{k}\rho}(x)]-\mathrm{c.c.}\}\Big|_{x=\mu}. \tag{101}$$

Let us again define a true single-particle excitation energy $E_{\mathbf{k}\rho}$ by

$$Q_{\mathbf{k}\rho}(E_{\mathbf{k}\rho})-E_{\mathbf{k}\rho}=0. \tag{102}$$

These $E_{\mathbf{k}\rho}$ are only meaningful for those ρ for which (94) has solutions, so that there are solutions of (102) with $E_{\mathbf{k}\rho}$ near μ. Then the identical reasoning that led to (51) from (48) now gives

$$C_V=\frac{\pi^2}{3}k^2T\sum_{\mathbf{k}\rho}{}'\,\delta(\mu-E_{\mathbf{k}\rho}), \tag{103}$$

once more identical in form with the noninteracting particle case.

[12] By V_{FS} here we mean of course the sum of the volume contained in the FS of each conduction band.

ACKNOWLEDGMENT

I would like to thank Professor W. Kohn and Professor J. C. Ward for many discussions of the material of this paper.

APPENDIX A. HARTREE-FOCK APPROXIMATION

In terms of the formalism of this paper the Hartree-Fock approximation has a very simple interpretation. Let us consider the contribution to $G_{rr'}(\zeta_l)$ [as given by (78)] of the lowest order skeleton diagrams. Call this $G_{rr'}{}^{(1)}(\zeta_l)$. Then one sees at once (the diagrams are given in Fig. 3) that

$$G_{rr'}{}^{(1)}(\zeta_l)=\tfrac{1}{2}\sum_{r'',r'''}\{(rr'''|v|r'r'')+(r'''r|v|r''r')$$
$$-(r'''r|v|r'r'')-(rr'''|v|r''r')\}$$
$$\cdot\frac{1}{\beta}\sum_{l'}\exp(\zeta_{l'}0^+)S_{r''r'''}{}'(\zeta_{l'}). \tag{A.1}$$

In (A.1)

$$(r_1r_2|v|r_3r_4)$$
$$=\int\int d^3x_1d^3x_2\psi_{r_1}{}^*(1)\psi_{r_2}{}^*(2)v(12)\psi_{r_3}(1)\psi_{r_4}(2), \tag{A.2}$$

where $v(12)$ is the interaction between any pair of particles 1 and 2, and the integration also implies any spin summations necessary. The ψ_r are the single-particle basis functions.

Clearly $G_{rr'}{}^{(1)}$ is independent of ζ_l, and it is easily seen to be Hermitian. Therefore, if we work to this order it is possible to choose the basic functions ψ_r so that $\boldsymbol{\varepsilon}+\mathbf{G}^{(1)}$ is diagonal. Imagine that this has been done, then

$$(\boldsymbol{\varepsilon}+\mathbf{G}^{(1)})_{rr'}=\tilde{\epsilon}_r\delta_{rr'}, \tag{A.3}$$

where the $\tilde{\epsilon}_r$ are the characteristic values of $\boldsymbol{\varepsilon}+\mathbf{G}^{(1)}$. Call the propagator to this order and in this representation

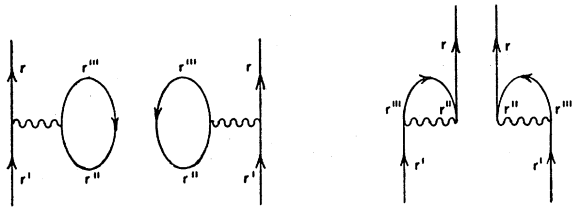

FIG. 3. First-order skeleton diagrams for proper self-energy part.

$S_{rr'}^{(1)}(\zeta_l)$. Then by (74)

$$S_{rr'}^{(1)}(\zeta_l)=\frac{1}{\zeta_l-\tilde{\epsilon}_r}\delta_{rr'}. \tag{A.4}$$

Further,

$$\frac{1}{\beta}\sum_{l'}\exp(\zeta_{l'}0^+)S_{rr'}^{(1)}(\zeta_{l'})=\delta_{rr'}\frac{1}{\exp[\beta(\tilde{\epsilon}_r-\mu)]+1}. \tag{A.5}$$

Going over to the zero-temperature limit (A.1) becomes

$$G_{rr'}^{(1)}=\tfrac{1}{2}\sum_{\substack{r''\\ \tilde{\epsilon}_{r''}<\mu}}\{(rr''|v|r'r'')+(r''r|v|r''r') -(r''r|v|r'r'')-(rr''|v|r''r')\}. \tag{A.6}$$

The condition (A.3) on the basis ψ_r then becomes

$$\int\psi_r^*(1)\tilde{\mathfrak{H}}\psi_{r'}(1)d^3x_1=\tilde{\epsilon}_r\delta_{rr'}, \tag{A.7}$$

where

$$\tilde{\mathfrak{H}}=h+V_H-A. \tag{A.8}$$

In (A.8), h is the unperturbed single-particle Hamiltonian of the problem, V_H is the Hartree potential

$$V_H=\sum_{\substack{r''\\ \tilde{\epsilon}_{r''}<\mu}}\int\psi_{r''}^*(2)\bar{v}(12)\psi_{r''}(2)dx_2^3, \tag{A.9}$$

$$\bar{v}(12)=\tfrac{1}{2}[v(12)+v(21)], \tag{A.10}$$

and A is the Dirac exchange operator defined by

$$A\psi_{r'}(1) =\sum_{\substack{r''\\ \tilde{\epsilon}_{r''}<\mu}}\int\left(d^3x_2\psi_{r''}^*(2)\bar{v}(12)\psi_{r'}(2)\right)\psi_{r''}(1). \tag{A.11}$$

$\tilde{\mathfrak{H}}$ is easily seen to be Hermitian, so that (A.7) is satisfied by taking

$$\tilde{\mathfrak{H}}\psi_r=\tilde{\epsilon}_r\psi_r, \tag{A.12}$$

which is exactly the Hartree-Fock equation for the determination of the ψ_r. The $\tilde{\epsilon}_r$ are therefore just the Hartree-Fock single-particle energies.

Using $G^{(1)}$ and $S^{(1)}$ in the expression (75) for Ω, [including the first-order skeleton diagrams for Ω' given in Fig. 1(b) of (LW)], we obtain

$$\Omega=\sum_{\substack{r\\ \tilde{\epsilon}_r<\mu}}(\tilde{\epsilon}_r-\mu) -\tfrac{1}{2}\sum_{\substack{r,r'\\ \tilde{\epsilon}_r,\tilde{\epsilon}_{r'}<\mu}}[(rr'|v|rr')-(rr'|v|r'r)]. \tag{A.13}$$

One can obtain the equation for the chemical potential directly from this by differentiating with respect to μ (and remembering $\tilde{\epsilon}_r$ depends on μ). However, it is easier to use the matrix generalization of (LW 74), namely

$$\bar{N}=\frac{1}{\beta}\sum_l\exp(\zeta_l0^+)\,\mathrm{Tr}\left(\frac{1}{\zeta_l-\boldsymbol{\epsilon}-\mathbf{G}(\zeta_l)}\right). \tag{A.14}$$

In our approximation this becomes simply

$$\bar{N}=\frac{1}{\beta}\sum_r\sum_l\exp(\zeta_l0^+)\frac{1}{\zeta_l-\tilde{\epsilon}_r}=\sum_{\substack{r\\ \tilde{\epsilon}_r<\mu}}1. \tag{A.15}$$

Therefore the expression for the ground-state energy (LW 9) becomes

$$E_0=\Omega+\mu\bar{N}=\sum_{\substack{r\\ \tilde{\epsilon}_r<\mu}}\tilde{\epsilon}_r -\tfrac{1}{2}\sum_{\substack{r,r'\\ \tilde{\epsilon}_r,\tilde{\epsilon}_{r'}<\mu}}\{(rr'|v|rr')-(rr'|v|r'r)\}. \tag{A.16}$$

The expression (A.16) is just the usual expression for the energy in the Hartree-Fock theory. It would not be difficult to push this type of approximation a step further by taking into account all skeleton diagrams for which the interaction occurs explicitly twice, but we shall not enter into this kind of generalized Hartree-Fock theory here. We also wish to remark that the passage to the zero-temperature limit was not at all necessary, and that our equations form a convenient basis for defining a Hartree-Fock procedure for finite temperatures.