wave function, it must not be considered as localized on any one negative ion. It is clear that to interpret the data uniquely simple models such as we have used[37] are not adequate but that accurate positron and electron wave functions are required.

[37] Another form is given in reference 21.

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Momentum Distribution of an Interacting Electron Gas*

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The momentum distribution of an interacting electron gas at zero temperature is studied in the high-density region. Numerical computations are made for the graphs corresponding to the excitation of pairs, which are known to be equivalent to the random phase approximation of Bohm and Pines. Exchange graphs are discussed. The numerical results, extrapolated to actual electronic densities in metals, show that a large discontinuity in the momentum distribution still remains at the Fermi level.

1. INTRODUCTION

IN a noninteracting Fermi gas at zero temperature, the occupation probability of the individual particle energy levels is one for levels below the Fermi energy and zero for energies above the Fermi level. It is of interest to know to what extent the Fermi surface remains well defined in a real electron gas when the interaction between the particles is taken into account. Recently, Migdal[1] has shown that the characteristic discontinuity in the momentum distribution may still exist. In this paper, the momentum distribution is studied by perturbation theory. Since a discontinuity exists in zeroth order of the interaction, it is clear that it will persist. However, since the convergence of the expansion is questionable, this does not prove that the true ground state of the system will have such a discontinuity. The purpose of this paper is to estimate the magnitude of the discontinuity by a perturbation expansion, assuming that such an expansion has some validity.

Experimentally, the sharpness of the Fermi surface is strongly suggested by the de Haas-van Alphen effect, cyclotron resonance in metals and the existence of long-range interactions in metals and alloys through oscillating densities of the conduction electrons.[2]

It is clear that the Fermi surface is the more sharply defined the higher the electronic density. The reason for this is that the average kinetic energy of the electrons increases as the square of their inverse average spacing, while their Coulomb energy increases only as the inverse of this spacing. As we consider the Coulomb interaction as a perturbation, we are justified in starting from a high-density case. Our calculation follows the same lines as Gell-Mann and Brueckner's calculation of the correlation energy of an electron gas.[3]

2. THE FICTIVE INTERACTION

We consider an electron gas in a very large volume Ω. Let k_F be the radius of the Fermi sphere for the noninteracting gas. Without Coulomb interactions, the normalized wave function for an electron with momentum $\mathbf{p}k_F$ and spin $s=\pm\frac{1}{2}$ would be[4]

$$\psi_{\mathbf{p},s}=(1/\Omega^{\frac{1}{2}})\chi_s e^{i(\mathbf{p}\cdot\mathbf{r})k_F}.$$

χ_s is the spin wave function and $\mathbf{r}$ gives the spatial coordinates of the electron.

The density of states in the $\mathbf{p}$ vector space is $\Omega k_F^3/8\pi^3$ for each direction of spin. At zero temperature, all the states with $p<1$ would be occupied, and all the states with $p>1$ would be empty. Using the second quantization formalism, we define this configuration as the vacuum for the interacting gas. We introduce the following creation and annihilation operators:

$a_{\mathbf{p},s}^*$, which creates an electron with momentum $\mathbf{p}k_F$ and spin s if $p>1$ (it destroys a hole with momentum $-\mathbf{p}k_F$ and spin $-s$ if $p<1$); and $a_{\mathbf{p},s}$, which annihilates an electron with momentum $\mathbf{p}k_F$ and spin s if $p>1$ (it creates a hole with momentum $-\mathbf{p}k_F$ and spin $-s$

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[1] A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R.) **32**, 399 (1957) [translation: Soviet Phys.—JETP **5**, 333 (1957)].
[2] M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954); A. Blandin, E. Daniel, and J. Friedel, Phil. Mag. **4**, 180 (1959); J. S. Langer and S. H. Vosko, J. Phys. Chem. Solids **12**, 196 (1959); W. Kohn and S. H. Vosko, Phys. Rev. **119**, 912 (1960).
[3] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).
[4] The reduced Planck constant $\hbar$ and the electron mass are set equal to one throughout this paper.

if $p<1$). These operators obey the usual anticommutation relations. Let $\mathbf{k}$ be the momentum of an electron, measured in units of k_F. We want to compute the probability $P(\mathbf{k})$ for an electron to be found in a state of momentum $\mathbf{k}$, with $|\mathbf{k}|>1$ or for a hole to be found for $|\mathbf{k}|<1$, as a result of the Coulomb interaction between electrons. In other words, we are looking for the expectation value of the operator $a_{\mathbf{k},s}{}^*a_{\mathbf{k},s}$ in the ground state of the interacting electron gas.

It is possible and convenient to reduce the problem to the calculation of the ground-state energy of the system by including an appropriate fictive interaction besides the Coulomb interaction between electrons. This allows us to make use of the linked-cluster expansion of Goldstone.[5]

To this end, we introduce the following fictive interaction into the Hamiltonian:

$$\lambda k_F{}^2 \sum_{\mathbf{p},s} \delta_{|\mathbf{p}|,k} a_{\mathbf{p},s}{}^* a_{\mathbf{p},s}.$$

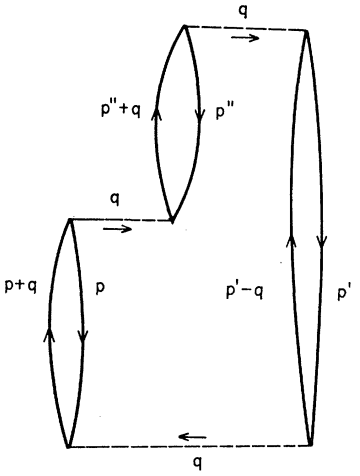

FIG. 1. Third-order graph for electron-hole pair excitations.

This operator selects the particles with $|\mathbf{p}|=k$. The numerical factor λ is an infinitesimal parameter and $\delta_{|\mathbf{p}|,k}$ is the usual Kronecker symbol: $\delta_{|\mathbf{p}|,k}=1$ if $|\mathbf{p}|=k$, and $\delta_{|\mathbf{p}|,k}=0$ if $|\mathbf{p}|\neq k$.

The effective total Hamiltonian can then be written as $k_F{}^2H$, where

$$H=\sum_{|\mathbf{p}|>1,s}(\tfrac{1}{2}\mathbf{p}^2+\lambda\delta_{|\mathbf{p}|,k})a_{\mathbf{p},s}{}^*a_{\mathbf{p},s} - \sum_{|\mathbf{p}|<1,s}(\tfrac{1}{2}\mathbf{p}^2+\lambda\delta_{|\mathbf{p}|,k})a_{\mathbf{p},s}a_{\mathbf{p},s}{}^* + \frac{2\pi^3}{\Omega k_F{}^3}\alpha\sum_{\mathbf{q}\neq 0}\sum_{\mathbf{p},\mathbf{p}',s,s'}\frac{1}{q^2}a_{\mathbf{p}+\mathbf{q},s}{}^*a_{\mathbf{p}'-\mathbf{q},s'}{}^*a_{\mathbf{p}',s'}a_{\mathbf{p},s}.$$

The condition $\mathbf{q}\neq 0$ takes into account the positive background needed for electrical neutrality; α is the dimensionless quantity

$$\alpha=e^2/\pi^2k_F,$$

which characterizes the strength of the Coulomb interaction between electrons with respect to the density of the gas.

Now, in the expectation value of H in the ground state of the system, the coefficient of λ just gives the probability $P(k)$ for having an electron above the Fermi level (for $k>1$) or having a hole below this level (for $k<1$). Thus, the computation of $P(k)$ is now reduced to calculating the ground-state energy of a system described by the effective Hamiltonian H, to all orders in α, but to first order only in λ.

3. CONTRIBUTION OF THE ELECTRON-HOLE PAIR EXCITATIONS

As shown by Gell-Mann and Brueckner,[3] in the high-density limit, the correlation energy of an electron gas is obtained from the electron-hole pair excitations. This is equivalent to the "random phase approximation" of Bohm and Pines. An example of the corresponding graphs is shown in Fig. 1 for third order. In this paragraph, we limit ourselves to the same type of graphs and use Gell-Mann and Brueckner's technique for summing up their total contribution. The main difference between their calculation and ours arises from the introduction of the λ term; also, we do not restrict ourselves to small values of the momentum transfer $\mathbf{q}$. As the summation on both directions of spin is most easily done at each interaction line for this kind of graph, we can drop the spin subscripts in H.

In order to apply Gell-Mann and Brueckner's technique of summation, it is most convenient to include the λ terms in the Hamiltonian for the unperturbed system and to consider the Coulomb interaction, that is to say the α term in H, as a perturbation. Corresponding to Eq. (19) in their paper,[3] we now get for the total contribution of the electron-hole pair excitations to the correlation energy the following quantity:

$$\epsilon(\lambda)=-\frac{1}{2}\frac{\Omega k_F{}^3}{8\pi^3}\frac{1}{2\pi}\int_{|\mathbf{p}+\mathbf{q}|>1}q\,d\mathbf{q} \times\sum_{n=2}^{\infty}\frac{(-1)^n}{n}\int_{-\infty}^{\infty}\left[\frac{\alpha Q(u)}{q^2}\right]^n du, \quad (1)$$

where

$$Q(u)=\int_{p<1}d\mathbf{p}\int_{-\infty}^{\infty}dt\,e^{ituq}\exp\{-|t|[\tfrac{1}{2}q^2+\mathbf{q}\cdot\mathbf{p} +\lambda(\delta_{|\mathbf{p}+\mathbf{q}|,k}-\delta_{|\mathbf{p}|,k})]\}. \quad (2)$$

To first order in λ, we may write

$$Q=Q_0+\lambda Q_1,$$

[5] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

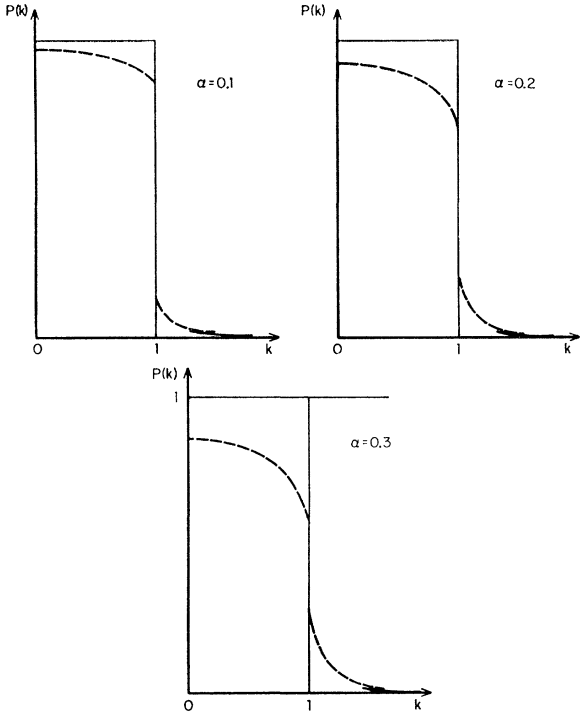

FIG. 2. Momentum distribution for several electronic densities. Dotted lines: computed from electron-hole pair graphs only; solid line: with exchange graphs included for large k.

with

$$Q_0=\int_{p<1} d\mathbf{p}\int_{-\infty}^{\infty} dt\, e^{itu}\exp[-|t|(\tfrac{1}{2}q^2+\mathbf{q}\cdot\mathbf{p})]$$

$$=2\pi\Big[1+\frac{1}{2q}(1-\tfrac{1}{4}q^2+u^2)\ln\frac{(1+\frac{1}{2}q)^2+u^2}{(1-\frac{1}{2}q)^2+u^2}$$

$$-u\tan^{-1}\Big(\frac{1+\frac{1}{2}q}{u}\Big)-u\tan^{-1}\Big(\frac{1-\frac{1}{2}q}{u}\Big)\Big], \quad (3)$$

and

$$Q_1=-\int_{p<1} d\mathbf{p}(\delta_{|\mathbf{p}+\mathbf{q}|,k}-\delta_{|\mathbf{p}|,k})\int_{-\infty}^{\infty} dt|t|e^{itu}$$

$$\times\exp[-|t|(\tfrac{1}{2}q^2+\mathbf{q}\cdot\mathbf{p})].$$

For $k<1$:

$$Q_1=-\frac{4\pi k}{q^2}\Big[\frac{k+\frac{1}{2}q}{(k+\frac{1}{2}q)^2+u^2}-\frac{kx_0+\frac{1}{2}q}{(kx_0+\frac{1}{2}q)^2+u^2}\Big], \quad (4)$$

where $x_0=-1$ if $q>1+k$, and $kx_0+\frac{1}{2}q=(1-k^2)/2q$ if $q<1+k$. For $k>1$:

$$Q_1=\frac{4\pi k}{q^2}\Big[\frac{k-\frac{1}{2}q}{(k-\frac{1}{2}q)^2+u^2}-\frac{(k^2-1)/2q}{[(k^2-1)/2q]^2+u^2}\Big]. \quad (5)$$

Writing now

$$\epsilon(\lambda)=\epsilon_0+\lambda\epsilon_1(k),$$

we get

$$\epsilon_1(k)=\frac{1}{2}\frac{\Omega k_F^3}{8\pi^3}\frac{1}{2\pi}\int_{|\mathbf{p}+\mathbf{q}|>1}\frac{d\mathbf{q}}{q}\int_{-\infty}^{\infty}du\,\alpha Q_1\sum_{n=1}^{\infty}\Big(\frac{-\alpha Q_0}{q^2}\Big)^n,$$

and performing the sum over n gives

$$\epsilon_1(k)=2\frac{\Omega k_F^3}{8\pi^3}\int_{|\mathbf{p}+\mathbf{q}|>1} qdq\int_0^{\infty}\alpha Q_1\Big[\frac{q^2}{q^2+\alpha Q_0}-1\Big]du, \quad (6)$$

when one takes into account the fact that Q_0 and Q_1 are even functions of u.

Now, recalling that the density of states in $\mathbf{p}$ space is just $\Omega k_F^3/8\pi^3$, and that ϵ_1 is built up of all the electronic states in a shell of radius k in $\mathbf{p}$ space, with both directions of spin included, we see that

$$\epsilon_1(k)=\frac{\Omega k_F^3}{8\pi^3}\times 2\times 4\pi k^2P(k)=\frac{\Omega k_F^3}{\pi^2}k^2P(k). \quad (7)$$

If $k>1$, we get in this way for the probability for an electron to be excited to a state of momentum $\mathbf{k}$ above the Fermi level:

$$P(k)=\frac{\alpha}{k}\int_{k-1}^{k+1} qdq\int_0^{\infty}\Big[\frac{k-\frac{1}{2}q}{(k-\frac{1}{2}q)^2+u^2}$$

$$-\frac{(k^2-1)/2q}{[(k^2-1)/2q]^2+u^2}\Big]\frac{du}{q^2+\alpha Q_0}. \quad (8)$$

Subtracting from unity the probability of finding a hole in a given state below the Fermi level, that is to say with $k<1$, we get for the probability for this state

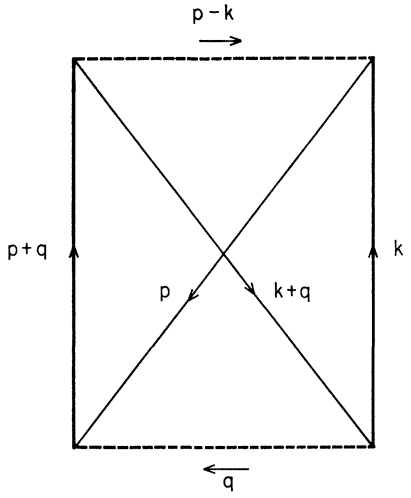

FIG. 3. Second-order exchange graph.

to be occupied by an electron:

$$P(k)=1-\frac{\alpha}{k}\Big\{\int_{1-k}^{1+k}qdq\int_0^\infty\Big[\frac{k+\frac{1}{2}q}{(k+\frac{1}{2}q)^2+u^2}-\frac{(1-k^2)/2q}{[(1-k^2)/2q]^2+u^2}\Big]\frac{du}{q^2+\alpha Q_0}+\int_{1+k}^\infty qdq\int_0^\infty\Big[\frac{k+\frac{1}{2}q}{(k+\frac{1}{2}q)^2+u^2}-\frac{\frac{1}{2}q-k}{(\frac{1}{2}q-k)^2+u^2}\Big]\frac{du}{q^2+\alpha Q_0}\Big\}. \quad (9)$$

For $k=0$, only the last integral contributes, giving

$$P(0)=1-2\alpha\int_1^\infty qdq\int_0^\infty\frac{u^2-(\frac{1}{2}q)^2}{[u^2+(\frac{1}{2}q)^2]^2}\frac{du}{q^2+\alpha Q_0}. \quad (10)$$

The integrals (8), (9), and (10) have been computed numerically for the following values of α: $\alpha=0.1$, $\alpha=0.2$, and $\alpha=0.3$. The results are represented by dotted lines in Fig. 2. These values of α correspond in fact to electronic densities occurring actually in metals: $\alpha=0.1$ corresponds approximately to Al, $\alpha=0.2$ to Na and $\alpha=0.3$ to Cs. So, the curves shown in Fig. 2 are extrapolations of results valid in the high-density limit ($\alpha\ll1$).

For large values of k, the value of $P(k)$ given by Eq. (8) turns out to be equivalent to the result of second order perturbation theory, that is to say,

$$P(k)\rightarrow(8\pi^2/9)(\alpha^2/k^8).$$

Finally, it can easily be seen from Eqs. (8) and (9) that the slopes of the curves are finite on both sides of their discontinuities at $k=1$.

Right at the Fermi surface, in the high-density limit, integration of Eq. (8) gives

$$\lim_{\alpha\rightarrow0}P(1+0)\simeq1.7\alpha,$$

while Eq. (9) gives

$$\lim_{\alpha\rightarrow0}P(1-0)\simeq1-1.7\alpha.$$

4. EXCHANGE GRAPHS

The first-order exchange graph gives no term in λ. In order to discuss the next order corrections, let us first write the contribution to $P(k)$ given by the second-order electron-hole pair graph; for $k>1$, for instance, it can be written as

$$P_2(k)=\frac{\alpha^2}{2}\int_{|\mathbf{p}+\mathbf{q}|>1}\frac{d\mathbf{q}}{q^4}\int_{p<1}\frac{d\mathbf{p}}{[\mathbf{q}\cdot(\mathbf{p}-\mathbf{k})]^2}. \quad (11)$$

It is easily seen that it diverges as $1/q^2$ for small values of q. The divergence is removed only through the summation of all the electron-hole pair graphs.

Let us consider now the second-order exchange term. The corresponding graph is shown in Fig. 3. Its contribution can be written as

$$P_2^{\rm ex}(k)=-\frac{\alpha^2}{4}\int_{|\mathbf{p}+\mathbf{q}|>1}\frac{d\mathbf{q}}{q^2}\int_{p<1}\frac{d\mathbf{p}}{[\mathbf{q}\cdot(\mathbf{p}-\mathbf{k})]^2(\mathbf{p}-\mathbf{k})^2}. \quad (12)$$

It diverges only logarithmically for small values of q. In higher orders, it can be seen in the same way that, for small values of q, exchange and more complicated graphs become negligibly small compared with the corresponding electron-hole pair excitation graphs. So, we expect the latter to give the exact value of $P(k)$ right at the Fermi surface, where small values of q become dominant.

Even though the high-density limit does not strictly apply to the conduction electron in metals, the dotted curves in Fig. 2 indicate that a large discontinuity still occurs at the Fermi surface. That is to say, the Fermi surface remains well defined for the interacting electron gas and the discontinuity is closer to unity the higher the density.

For $k\neq1$, the second order electron-hole pair graph and the second-order exchange graph give the leading contribution (of order α^2) in the high-density limit. However, only for $k\gg1$ was it possible for us to evaluate the exchange term. In this region, it subtracts just one half from the electron-hole pair graph. This result is indicated by the solid lines in Fig. 2.

We plan in a subsequent paper to use these results as a starting point for a discussion of the annihilation of positrons in metals.

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