THE

PHYSICAL REVIEW

A journal of experimental and theoretical physics established by E. L. Nichols in 1893

SECOND SERIES, VOL. 108, NO. 3 NOVEMBER 1, 1957

Correlation Energy of an Electron Gas at High Density: Plasma Oscillations

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(Received May 29, 1957)

The contribution from zero-point plasma oscillations to the correlation energy of an electron gas at high density is considered, using the exact high-density theory of Gell-Mann and Brueckner and of Sawada. The plasmon energy is determined as a function of q by an eigenvalue equation identical with the dispersion relation of Bohm and Pines. The plasma solutions are stable only below the energy-momentum values at which they merge with the continuum spectrum arising from particle excitation, thus introducing a natural cutoff into the theory. At high density, however, it is shown that this cutoff can be allowed to become infinite without affecting the correlation energy.

The contribution from the plasma energy is exactly re-expressed in terms of the contribution from the scattering states by making use of the analytic properties of the scattering amplitudes. This transformation also establishes the connection between the Gell-Mann-Brueckner and Sawada results.

Some remarks are finally made on the relation between these results and those of Bohm and Pines.

I. INTRODUCTION

IN two previous papers[1,2] the exact correlation energy of an electron gas has been determined at high density. This was done first by Gell-Mann and Brueckner[2] who showed by examination of the structure of the perturbation series that the infrared divergence appearing in this series could be removed by formal summation of the most divergent terms of the series, the summed series then giving correctly the screening of the long range Coulomb interaction. In its original form this theory did not exhibit explicitly the well-known features of the collective or plasma degrees of freedom of the electron gas. This led to some questions concerning the contribution from the excited bound states (plasma oscillations) to the correlation energy since this might be overlooked in the perturbation theoretic approach.

Following this work, one of us (K. Sawada)[1] showed that the selective series summation of G-B was equivalent to the solution for the eigenvalues of a reduced form of the Coulomb Hamiltonian. It was further noted that the identity in structure of this reduced Hamiltonian to that of scalar-pair meson theory made it possible to diagonalize the Hamiltonian directly following closely the methods used by Wentzel[3] in his solution of the pair theory. The significance of the plasma solutions in Sawada's result was later pointed out by one of us (R. Brout); the discussion of the plasma properties forms the principal content of this paper.

In Sec. II, the eigenvalues and eigenfunctions of the reduced Hamiltonian corresponding to plasma oscillations are obtained and their contributions to the correlation energy is discussed. The high-momentum cutoff of the plasma degrees of freedom is naturally derived from the theory. In Sec. III the correspondence between the present results and those obtained in G-B is demonstrated directly by making use of the Wentzel transformation. It is shown at the same time that the reason that the perturbation theoretic approach of G-B includes the contribution from the excited bound states (plasma oscillations) is due to the analytic behavior of the scattering amplitudes. In Sec. IV some comments are made on the Bohm-Pines theory[4] of plasma oscillation.

* On leave of absence from the Tokyo University of Education.

[1] K. Sawada, Phys. Rev. **106**, 372 (1957), hereafter referred to as (I).

[2] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957), hereafter referred to as G-B.

[3] G. Wentzel, Helv. Phys. Acta **15**, 111 (1942).

[4] D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953); D. Pines, in *Solid State Physics* (Academic Press, Inc., New York, 1955), Vol. 1, p. 367, hereafter referred to as B-P.

II. PLASMA SOLUTIONS AND PLASMA ZERO POINT ENERGY

The reduced Hamiltonian considered by Sawada is

$$H=H_0+H_c, \tag{1}$$

where

$$H_0=\sum_k (p_k^2/2m)(a_k^*a_k-b_k^*b_k), \tag{2}$$

$$H_c=\sum_q \frac{2\pi\hbar^2e^2}{\Omega q^2}\sum_p (a_{p+q}^*b_p^*+b_{p+q}a_p)\times\sum_{p'}(a_{p'-q}^*b_{p'}^*+b_{p'-q}a_{p'}). \tag{3}$$

The approximations involved in obtaining this form are discussed in detail in I. A similar approximation is involved in the commutation rules, which are

$$[a_{p+q}^*b_p^*,H_c]_-=-\frac{4\pi\hbar^2e^2}{\Omega q^2}\sum_{p'}(a_{p'+q}^*b_{p'}^*+b_{p'+q}a_{p'}), \tag{4a}$$

$$[b_{p+q}a_p,H_c]_-=\frac{4\pi\hbar^2e^2}{\Omega q^2}\sum_{p'}(a_{p'+q}^*b_{p'}^*+b_{p'+q}a_{p'}). \tag{4b}$$

The terms discarded in reducing the original Hamiltonian and commutation rules to these forms, except certain obviously negligible terms, are those where the interactions corresponding to different momentum transfers are involved. These terms give a contribution which has been shown to vanish in the high-density limit (except the second order exchange energy defined as $\epsilon_{(b)}^{(2)}$ in G-B and I) compared to the leading terms retained. It is interesting to note that the so-called "random phase approximation" of Bohm and Pines is very similar to the approximations made in obtaining Eqs. (3) and (4) and is exact in the high-density region.

To proceed, we next consider the eigenvalue equation for the excitations. This is directly obtained by an application of the commutation rules of Eq. (4), as derived in (I). The result is

$$1=\frac{4\pi\hbar^2e^2}{\Omega q^2}\left\{\sum_{p,\ |\mathbf{p}|<p_F,\ |\mathbf{p}+\mathbf{q}|>p_F} - \sum_{p,\ |\mathbf{p}|>p_F,\ |\mathbf{p}+\mathbf{q}|<p_F}\right\}\times\frac{1}{E-E_0+E_{\mathbf{p}}^{(0)}-E_{\mathbf{p}+\mathbf{q}}^{(0)}}. \tag{5}$$

Writing $E-E_0=\hbar\omega$ and making the transformation $\mathbf{p}+\mathbf{q}\to-\mathbf{p}$ in the second term, we have[5]

$$1=\frac{8\pi\hbar^2e^2}{\Omega q^2}\sum_{|\mathbf{p}|<p_F,\ |\mathbf{p}+\mathbf{q}|>p_F}\frac{(\mathbf{p}\cdot\mathbf{q}/m)+(q^2/2m)}{(\hbar\omega)^2-(\mathbf{p}\cdot\mathbf{q}/m+q^2/2m)^2}. \tag{6}$$

This eigenvalue equation has two types of solutions; the simplest are those for which the eigenvalues lie in the continuum of solutions for which

$$\hbar\omega=(\mathbf{p}\cdot\mathbf{q}/m)+(q^2/2m);\quad |\mathbf{p}|<p_F,\quad |\mathbf{p}+\mathbf{q}|>p_F. \tag{7}$$

These correspond to the energies of free pair excitation and may be called scattering solutions. These scattering solutions are given explicitly in I. They are of a standard form, i.e., an incoming wave together with a scattered wave. The continuum of solutions resulting from pair excitations terminates at the maximum value of energy possible, which for a given value of q is $\hbar\omega_{\max}=(p_Fq/m)+(q^2/2m)$. Another type of solution lies above this continuum; this solution is of the plasma type, as we show in more detail below.

Integration of Eq. (6) gives the relationship between the plasma frequency $\omega_{\rm pl}(q)$ and r_s as follows:

$$1=\frac{\alpha r_s}{4\pi}\frac{p_F(2m)^2}{q^5}\left[\left\{\left(\frac{q^2}{2m}\right)^2+(\hbar\omega)^2-\left(\frac{qp_F}{m}\right)^2\right\}\times\ln\left\{\frac{[(q^2/2m)+(qp_F/m)]^2-(\hbar\omega)^2}{[(q^2/2m)-(qp_F/m)]^2-(\hbar\omega)^2}\right\}+2\frac{q^2}{2m}\hbar\omega\ln\left\{\frac{(q^2/2m)^2-(\hbar\omega+qp_F/m)^2}{(q^2/2m)^2-(\hbar\omega-qp_F/m)^2}\right\}-4\frac{q^2}{2m}\frac{qp_F}{m}\right], \tag{8}$$

where

$$\alpha=(4/9\pi)^{\frac{1}{3}}.$$

It is easy to obtain from this equation the values of $q_{\max}$ and $\omega_{\rm pl}(q_{\max})$ at which the plasma solutions cross over into the continuum; this occurs at $\hbar\omega_{\rm pl}(q_{\max})=(q_{\max}^2/2m)+(q_{\max}p_F/m)$, which gives[6]

$$\frac{q_{\max}^2}{p_F^2}=\frac{\alpha r_s}{\pi}\left[\left(2+\frac{q_{\max}}{p_F}\right)\ln\left(1+2\frac{p_F}{q_{\max}}\right)-2\right]. \tag{9}$$

For momenta above this value, the plasma solutions are unstable and quickly transfer their energy into particle excitation. Such strongly-damped solutions do not contribute to the high density energy. Consequently, a characteristic high-momentum cutoff for the plasma oscillations appears in the theory.

We next consider the properties of the plasma solutions and their contributions to the energy. The first result of interest is the explicit form of the wave function for a plasma oscillation or "plasmon" of momentum q and energy $\hbar\omega_{\rm pl}(q)$; this is

$$\Psi_{\rm pl}(q)=N_q\sum_p\left[\frac{a_{p+q}^*b_p^*}{\hbar\omega_{\rm pl}(q)-E_{p+q}^{(0)}+E_p^{(0)}}+\frac{b_{p+q}a_p}{\hbar\omega_{\rm pl}(q)-E_{p+q}^{(0)}+E_p^{(0)}}\right]\Psi_0, \tag{10}$$

[5] By a simple transformation this can also be rewritten as

$$1=\frac{4\pi e^2\hbar^2}{m}\sum_{\mathbf{p},\ |\mathbf{p}|<p_F}\frac{1}{(\hbar\omega-\mathbf{q}\cdot\mathbf{p}/m)^2-(q^2/2m)^2}$$

similar to the B-P dispersion formula, except that p's are c numbers here instead of operators.

[6] This equation has been independently derived by R. Ferrell, Bull. Am. Phys. Soc. Ser. II, 2, 146 (1957).

where N_q is the normalization constant determined in the Appendix. This form of the plasmon wave function exhibits the simplicity of the particle excitations which give rise to the plasma oscillations, these being simply pair excitations with a fixed momentum transfer, summed with proper phase relations.

The contribution of the plasma zero-point oscillations to the correlation energy is now easily obtained using a method similar to that used in I in obtaining the scattering-states contribution.

The details are given in the appendix. The result is

$$E_{\rm pl}=\sum_q \frac{1}{2}\int_0^{e^2}\frac{\partial\hbar\omega_{\rm pl}(q)}{\partial e'^2}d(e'^2)$$
$$=\tfrac{1}{2}\sum_q[\hbar\omega_{\rm pl}(q)-\hbar\omega_{\rm pl}(q)_{(e^2=0)}]. \quad (11)$$

Thus the correlation energy arising from the plasma oscillation is given as the difference between the zero-point energy of this oscillation and the value this energy approaches as the coupling is switched off.[7] This value is simply

$$\hbar\omega_{\rm pl}(q)_{e^2=0}=(q^2/2m)+(qp_F/m), \quad (12)$$

which is the upper limit of the continuum of pair excitation energy (at given q). One consequence of the appearance of this difference of energies is that in the high density limit the plasma cutoff $q_{\rm max}$ can be allowed to become infinite without affecting the contribution from the plasma energy, since the plasma energy $\hbar\omega_{\rm pl}(q)$ lies very close to the continuum limit for large q and small r_s. This is shown in Fig. 1.

We make use of this result to obtain explicitly the plasma energy in the high density limit. In this limit the dispersion relation [Eq. (8)] becomes, neglecting everywhere q/p_F compared to unity,

$$1=\frac{2\alpha r_s}{\pi}\frac{p_F^2}{q^2}f(x), \quad (13)$$

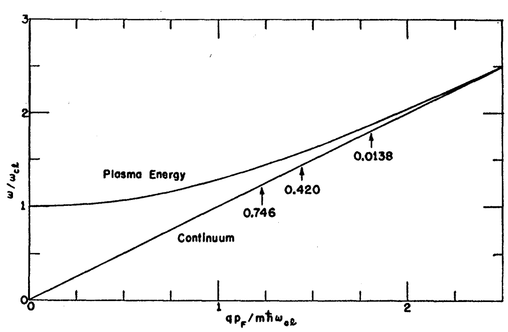

FIG. 1. Variation of plasma energy with momentum at very high density. Also shown are the cutoff momenta at the indicated values of r_s.

[7] In B-P, on the other hand, not the difference but the zero point energy alone appears explicitly in the result. Our result is more natural, as also seen in reference 3.

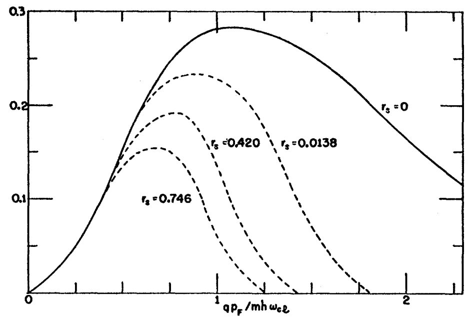

FIG. 2. Variation of the integrand of Eq. (15) determining the plasma energy. The function shown as a solid curve is the high-density limit of $\{[\hbar\omega_{\rm pl}(q)-qp_F/m]/\hbar\omega_{\rm cl}\}(qp_F/m\hbar\omega_{\rm cl})^2$. Also shown are approximate curves giving the above function at the indicated values of r_s.

where $x=qp_F/m\hbar\omega_{\rm cl}$ and

$$f(x)=\frac{1}{x}\ln\frac{1+x}{1-x}-2. \quad (14)$$

The plasma energy then is, summing over all momentum transfer q up to $q_{\rm max}$,

$$E_{\rm pl}=\frac{1}{2}\frac{4\pi\Omega}{(2\pi\hbar)^3}\int_0^{q_{\rm max}}q^2dq[\hbar\omega_{\rm pl}(q)-(qp_F/m)]. \quad (15)$$

To show precisely from what values of q the plasma energy arises, we give the integrand of Eq. (15) in Fig. 2, measuring the plasma energy in units of the classical plasma frequency

$$\omega_{\rm cl}=\lim_{q\to 0}\omega_{\rm pl}(q)=\frac{1}{\hbar}\left(\frac{4\alpha r_s}{3\pi}\frac{p_F^4}{m^2}\right)^{\frac{1}{2}}=(4\pi\rho e^2/m)^{\frac{1}{2}}, \quad (16)$$

and the momentum in units of $m\hbar\omega_{\rm cl}/p_F$. Figure 2 shows that the contribution comes largely from $(qp_F/m\hbar\omega_{\rm cl})$ of the order of or larger than unity, which corresponds to

$$(q/p_F)\gtrsim[(4/3\pi)\alpha r_s]^{\frac{1}{2}}=0.470r_s^{\frac{1}{2}}. \quad (17)$$

It is interesting to notice that the correlation energy at high density arising from the plasma oscillations comes mainly from value of (q/p_F) much larger than the limit obtained by Bohm and Pines,[4] which is

$$(q_{\rm max}/p_F)=0.353r_s^{\frac{1}{2}}. \quad (18)$$

We return to a discussion of this discrepancy in more detail in a later section.

Now returning to Eq. (15), we use the relation

$$(2qdq/p_F^2)=(2\alpha r_s/\pi)f'(x)dx, \quad (19)$$

and get

$$E_{\rm pl}=\frac{1}{2}\frac{4\pi\Omega}{(2\pi\hbar)^3}\int_0^1\frac{\alpha r_s}{\pi}f'(x)\left(\frac{1}{x}-1\right)\frac{p_F^5}{m}\frac{2\alpha r_s}{\pi}f(x)dx. \quad (20)$$

In the conventional notation, we measure the energy in Rydbergs and express it per particle; the result is

$$\epsilon_{\rm pl}=E_{\rm pl}/(me^2N/2\hbar^2)$$
$$=\frac{3}{\pi^2}\int_0^1 f(x)f'(x)\left[\frac{1}{x}-1\right]dx=\frac{3}{2\pi^2}\int_0^1\left[\frac{f(x)}{x}\right]^2 dx. \quad (21)$$

This integral cannot be evaluated analytically but numerical evaluation yields

$$\epsilon_{\rm pl}=0.133, \quad (22)$$

which, when combined with the scattering contribution

$$\epsilon_{\rm sc}=-0.229+0.0622\ \ln r_s, \quad (23)$$

gives as the total correlation energy

$$\epsilon_{\rm corr}=-0.096+0.0622\ \ln r_s. \quad (24)$$

This agrees with the result given in G-B.†

III. USE OF THE WENTZEL TRANSFORMATION

The correspondence between the results of the last section and those obtained by G-B can be demonstrated directly by using a transformation introduced by Wentzel in his treatment of the scalar pair theory. The total correlation energy (neglecting second order exchange) corresponding to a momentum transfer q is now given by (see appendix)

$$\frac{\partial E_{\rm corr}(q)}{\partial e^2}=\frac{1}{2}\frac{\partial\hbar\omega_{\rm pl}(q)}{\partial e^2}+\frac{2\pi\hbar^2}{\Omega q^2}\sum_{\mathbf{p},\,|\mathbf{p}|<p_F,\,|\mathbf{p}+\mathbf{q}|>p_F}\times\left(\frac{1}{|1+f(\omega_p+i\epsilon)|^2}-1\right), \quad (25)$$

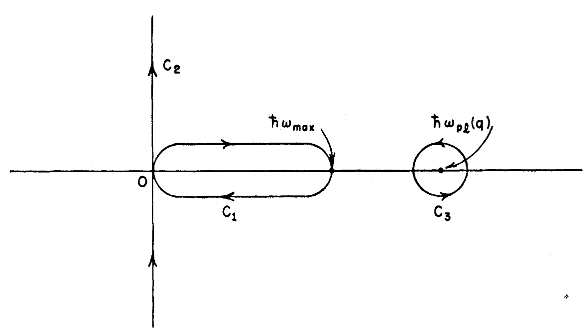

FIG. 3. Contours for analytic continuation. C_1 and C_3 circle around the continuum and the plasma energy, respectively. C_2 runs along the imaginary axis from $-i\infty$ to $+i\infty$.

† *Note added in proof.*—The integral in Eq. (21) has been evaluated by Professor Lars Onsager, who obtains the result for the plasma energy (in Rydbergs)

$$\epsilon_{\rm pl}=\frac{1}{3}-\frac{2}{\pi^2}=0.130691.$$

Re-evaluation of the scattering contribution, which must be done by numerical integration, gives $\epsilon_{\rm sc}=-0.227+0.0622\ \ln r_s$ so that the correlation energy is unchanged. We are indebted to Professor Onsager for informing us of his result.

where

$$f(\omega_p+i\epsilon)=\frac{4\pi\hbar^2e^2}{\Omega q^2}\sum_{p'}\left(\frac{1}{\omega_{p'}-\omega_p-i\epsilon}+\frac{1}{\omega_{p'}+\omega_p+i\epsilon}\right), \quad (26)$$

and

$$\omega_p=E_{p+q}^{(0)}-E_p^{(0)};\quad |\mathbf{p}|<p_F,\quad |\mathbf{p}+\mathbf{q}|>p_F. \quad (27)$$

We have added for the sake of convenience $+i\epsilon$ in the second denominator of f.

Making use of the identity[8]

$$\mathrm{Im}f(\omega_p+i\epsilon)=\pi\frac{4\pi\hbar^2e^2}{\Omega q^2}\sum_{p'}\delta(\omega_p-\omega_{p'}), \quad (28)$$

the 2nd term of Eq. (25) which is denoted by J is transformed into

$$J=\frac{1}{2\pi e^2}\int d\omega_p\,\mathrm{Im}f(\omega_p+i\epsilon)\left(\left|\frac{1}{1+f(\omega_p+i\epsilon)}\right|^2-1\right)$$
$$=\frac{1}{2\pi e^2}\,\mathrm{Im}\int d\omega_p\left(\frac{f(\omega_p+i\epsilon)}{1+f(\omega_p+i\epsilon)}-f(\omega_p+i\epsilon)\right). \quad (29)$$

The integral over ω_p runs from zero up to the upper bound of the continuous spectrum given by Eq. (7). We can write the above expression as the contour integral along C_1 shown in Fig. 3:

$$J=\frac{1}{4\pi e^2 i}\int_{C_1}dz\left(\frac{f(z)}{1+f(z)}-f(z)\right). \quad (30)$$

Now, using the analytic property of $f(z)$, it is easily shown, that

$$\int_{C_1}=\int_{C_2}+\int_{C_3}=\int_{C_2}+\text{Residue at }[z=\hbar\omega_{\rm pl}(q)], \quad (31)$$

where the contour C_2 runs along the imaginary z axis from $-i\infty$ to $+i\infty$. The residue at $\hbar\omega_{\rm pl}(q)$ is

$$\mathrm{Res}=2\pi i\lim_{z\to\hbar\omega_{\rm pl}(q)}\left[\frac{f(z)}{1+f(z)}-f(z)\right][z-\hbar\omega_{\rm pl}(q)]$$
$$=-2\pi i\frac{1}{(\partial/\partial z)f(z)}\bigg|_{z=\hbar\omega_{\rm pl}(q)}=-2\pi ie^2\frac{\partial\hbar\omega_{\rm pl}(q)}{\partial e^2}, \quad (32)$$

where use is made of Eq. (A-18) in the appendix and

[8] The scattering amplitude, or the T matrix introduced in I, [Eq. (A-3) in I], is given by

$$T_{p'+q,p';p+q,p}=\frac{4\pi\hbar^2e^2}{\Omega q^2}[1+f(\omega_{p'}+i\epsilon)]^{-1}.$$

Then the unitarity condition for the S matrix given in terms of this T matrix

$$\mathrm{Im}T_{p+q,p;p+q,p}=\pi\sum_{p'}|T_{p'+q,p';p+q,p}|^2\delta(\omega_p-\omega_{p'}),$$

is essentially identical with the identity, Eq. (28).

the eigenvalue equation

$$f(\omega_{\rm pl})+1=0. \tag{33}$$

Then, we get

$$\frac{\partial E_{\rm corr}(q)}{\partial e^2}=\frac{1}{4\pi e^2 i}\int_{C_2}dz\left(\frac{f(z)}{1+f(z)}-f(z)\right).$$

Putting $z=iv$ and integrating over e^2, we find

$$E_{\rm corr}=\sum_q\frac{1}{4\pi}\int_{-\infty}^{\infty}dv\left[\ln\left(1+\frac{8\pi\hbar^2e^2}{\Omega q^2}\sum_p\frac{\omega_p}{\omega_p{}^2+v^2}\right)-\frac{8\pi\hbar^2e^2}{\Omega q^2}\sum_p\frac{\omega_p}{\omega_p{}^2+v^2}\right]. \tag{34}$$

Now, to compare this result with that given by G-B, we make the change in variable

$$v=2u\frac{q}{p_F}\frac{p_F{}^2}{2m},\quad\left(\frac{p_F{}^2}{2m}=\frac{1}{\alpha^2r_s{}^2}\text{ Rydbergs}\right), \tag{35}$$

and then use the function $Q_q(u)$ defined in G-B (Eq. 18). We find

$$\frac{8\pi\hbar^2e^2}{\Omega q^2}\sum_p\frac{\omega_p}{\omega_p{}^2+v^2}=\frac{\alpha r_s}{\pi^2q^2}Q_q(u), \tag{36}$$

in dimensionless unit. In this unit $\sum_q$ is equal to $(3/8\pi)N\int d\mathbf{q}$, N being the number of electrons. Hence the correlation energy per electron becomes

$$\epsilon_{\rm corr}=\frac{E_{\rm corr}}{N}=\frac{3}{4\pi}\int_0^{\infty}q^3dq\int_{-\infty}^{\infty}\left[\ln\left(1+\frac{\alpha r_s}{\pi^2q^2}Q_q(u)\right)-\frac{\alpha r_s}{\pi^2q^2}Q_q(u)\right]du\frac{1}{\alpha^2r_s{}^2}\text{ Rydbergs}, \tag{37}$$

which gives just the same expression as obtained by G-B as a series [Eq. (19) in G-B]. This shows that the result obtained by G-B includes automatically the effect of bound states or plasma oscillations.

IV. COMPARISON WITH THE BOHM-PINES THEORY

The theory of Bohm and Pines has in the past been the only theory of the electron gas which has attempted to determine both the correlation energy and the collective properties of the system. As for the first point the B-P theory was quite successful since the correlation energy obtained agreed approximately with that obtained earlier by Wigner[9] and also with experiment. The plasma properties predicted also were highly reasonable since they were closely connected with the classical behavior of an ionized medium and experimentally confirmed. In spite of these successes which showed the soundness of the underlying physical concepts of the theory, it seems to us that the accurate quantitative aspects of the theory have been still somewhat in question. The uncertainties of the B-P results arose from certain approximations essential to their procedure, namely

(*a*) the random phase approximation,
(*b*) the perturbation theoretic treatment of the electron-plasma coupling,
(*c*) the determination of the cutoff momentum for the plasma oscillations,
(*d*) the neglect of the subsidiary conditions on the wave function.

We shall discuss these approximations and attempt to cast some light on their validity, making use of the results of the exact high-density theory given by the techniques of this and earlier papers.

The first approximation essential to the B-P theory is the random phase approximation which neglects the coupling between the excitations corresponding to different momentum transfers q and q'. As we have seen in our theory, this approximation is *in fact exact* in the high-density limit and is the *only approximation* required to obtain an *exact* high density result.

The validity of the perturbation treatment of the electron-plasma coupling is most readily examined by actually considering the structure of the B-P results in comparison with ours. Our result (taken in the G-B form),[10] disregarding $\epsilon_{(b)}{}^{(2)}$ and δ which are independent of r_s, is

$$\epsilon_{\rm corr}=-\frac{3}{4\pi}\int_0^1 q^3dq\int_{-\infty}^{\infty}\left[\frac{4\alpha r_s}{\pi q^2}R(u)-\ln\left(1+\frac{4\alpha r_s}{\pi q^2}R(u)\right)\right]du\frac{1}{\alpha^2r_s{}^2}\text{ Rydbergs}. \tag{38}$$

The B-P result is separated into two parts, that arising from long wavelengths ($q/p_F\leqslant\beta$):

$$\begin{aligned}\epsilon_{\rm L.R.}&=\frac{0.866}{r_s^{\frac{3}{2}}}\beta^3-\frac{0.458}{r_s}\beta^2+\frac{0.019}{r_s}\beta^4\text{ ry},\\ \Delta\epsilon_{\rm L.R.}&=\frac{0.708}{r_s{}^{5/2}}\beta^5\left(1+\frac{3}{10}\beta^2\right)-\frac{0.517}{r_s{}^2}\beta^4-\frac{0.058}{r_s{}^2}\beta^6\text{ ry}.\end{aligned} \tag{39}$$

and that given in second order perturbation theory applied to the screened Coulomb interaction[11] ($q/p_F\geqslant\beta$),

$$\epsilon_{\rm S.R.}=-(0.0254-0.0626\ln\beta+0.00637\beta^2)\text{ ry}. \tag{40}$$

In the exact theory the sum $\epsilon_{\rm L.R.}+\Delta\epsilon_{\rm L.R.}+\epsilon_{\rm S.R.}$ should be independent of β. This is not only manifestly not so

[9] E. P. Wigner, Phys. Rev. 46, 1002 (1934).

[10] Here $4\pi R(u)$ is the value of $Q_q(u)$ at $q=0$ and is given by $R(u)=1-u\tan^{-1}(1/u)$.

[11] The parallel spin correlation energies are omitted. See G-B, footnote 4.

for the B-P result, but also the polynomial expansion of $\epsilon_{\text{L.R.}}$ in powers of β is incompatible with the appearance of the term $\ln\beta$ in $\epsilon_{\text{S.R.}}$. In fact, the appearance of this term shows that a polynomial expansion for the long range part of the G-B-S energy, cutting off the integral at $q=\beta$ is not possible as is obvious from Eq. (38) since a direct expansion in powers of β^2 diverges at the term β^4.

The problems encountered above in the power series expansion in terms of β also cast some doubt on the B-P determination of the cut-off momentum $q_{\max}=\beta p_F$. This is evaluated by them by minimizing the energy given by part of their transformed Hamiltonian [$\epsilon_{\text{L.R.}}$ of Eq. (39)], assuming all the remaining terms dependent on β to be neglected. This procedure seems to us for several reasons to be only a semiquantitative procedure. First, since the actual correlation energy is independent of β, it is not possible to decouple a *small part* of the Hamiltonian giving a β-dependent energy and to minimize it with respect to β, neglecting the variation of the remaining larger terms. This criticism is equivalent to the statement that it is not possible to decouple the various terms in the Hamiltonian in such a way as to treat the β variation of $\epsilon_{\text{L.R.}}$ separately from that of much larger terms in $\Delta\epsilon_{\text{L.R.}}$ and $\epsilon_{\text{S.R.}}$. Even if such a decoupling could be qualitatively justified by physical rather than mathematical argument, the value of β so determined can give at best only a rough approximation to the actual magnitude of $\Delta\epsilon_{\text{L.R.}}$ and $\epsilon_{\text{S.R.}}$.

The actual value of the cutoff obtained by B-P, $\beta=0.353r_s^{\frac{1}{2}}$, is considerably below the point at which the plasma solutions start to merge with the pair excitation continuum, which occurs for values of q/p_F larger than $\beta=0.470r_s^{\frac{1}{2}}$, particularly at high density. Consequently an important part of the plasma oscillations (important since the contribution to the energy varies roughly as β^3) is omitted if the B-P cutoff is used. It is to be emphasized that the plasma solutions lying above the low B-P cutoff have a perfectly real physical meaning since the plasma can in fact oscillate stably for these frequencies, particularly at high density.

We finally wish to comment briefly on the question of the B-P neglect of the subsidiary condition. We believe, although we have not been able to prove this in detail, that the B-P subsidiary condition is equivalent to our definition of the ground state of the system. As shown in the Appendix, the ground state can be defined as that state in which no plasmons are present, i.e., it satisfies the condition

$$A\Psi_0=0, \tag{41}$$

where A is the annihilation operator for plasmon defined by Eq. (A-10) and Ψ_0 is the exact ground-state wave function. Written explicitly in terms of the particle creation and annihilation operators, this condition is

$$\sum_p\left[\frac{b_pa_{p+q}}{\hbar\omega_{\text{pl}}(q)-E_{p+q}^{(0)}+E_p^{(0)}}+\frac{a_p^*b_{p+q}^*}{\hbar\omega_{\text{pl}}(q)-E_{p+q}^{(0)}+E_p^{(0)}}\right]\Psi_0=0, \tag{42}$$

which is reminiscent of the B-P subsidiary condition

$$\sum_i\frac{\omega^2}{\omega^2-[(\mathbf{k}\cdot\mathbf{p}_i/m)-(\hbar k^2/2m)]^2}\Psi=0,\quad k<kc\quad (k=q/\hbar). \tag{43}$$

We wish here to emphasize that our condition stated in Eq. (41) or Eq. (42) is exactly satisfied at high density where our solution is exact; the B-P subsidiary condition will therefore also be exactly satisfied at high density by our ground-state wave function. The actual techniques used by B-P in obtaining their solution lead to some violation of the subsidiary condition, but almost certainly, as B-P emphasized, no serious error arises from this aspect of their approximations.

In conclusion we would like to say that the differences between our results and those of B-P are only in techniques and mathematical detail and that the latter theory, although it seems to be only semiquantitative in nature, provides an excellent physical insight into the properties of the electron gas.

ACKNOWLEDGMENTS

The authors wish to express their thanks to Dr. P. Nozières, Professor R. Ferrell, and particularly to Professor D. Pines for many stimulating discussions on this work.

APPENDIX A: CORRELATION ENERGY ARISING FROM PLASMA OSCILLATION

We first determine the plasma wave function. Since this is a one-pair state as discussed in Sec. II of I, it must have the form

$$\Psi_{\text{pl}}(q)=A_q^*\Psi_0, \tag{A-1}$$

where

$$A_q^*=\sum_p(\alpha_pa_{p+q}^*b_p^*+\beta_pb_{p+q}a_p). \tag{A-2}$$

The constants α_p and β_p must be chosen so that $\Psi_{\text{pl}}(q)$ is a properly normalized eigenfunction of the Hamiltonian, i.e.,

$$(H_0+H_c)\Psi_{\text{pl}}(q)=[E_0+\hbar\omega_{\text{pl}}(q)]\Psi_{\text{pl}}(q), \tag{A-3}$$

where

$$(H_0+H_c)\Psi_0=E_0\Psi_0. \tag{A-4}$$

This can also be written as an operator equation

$$[(H_0+H_c),A^*]_-=\hbar\omega_{\text{pl}}A^*. \tag{A-5}$$

Once this is satisfied it then follows that

$$[(H_0+H_c),A]_-=-\hbar\omega_{\text{pl}}A, \tag{A-6}$$

so that

$$(H_0+H_c)A\Psi_0=(E_0-\hbar\omega_{\rm pl})A\Psi_0. \qquad \text{(A-7)}$$

Since Ψ_0 is the state of lowest energy, this equation can be satisfied only if

$$A\Psi_0=0. \qquad \text{(A-8)}$$

This condition allows us to fix the normalization since

$$(\Psi_{\rm pl},\Psi_{\rm pl})=(\Psi_0,AA^*\Psi_0)=(\Psi_0,[A,A^*]_-\Psi_0)=\textstyle\sum_p(|\alpha_p|^2-|\beta_p|^2)=1. \qquad \text{(A-9)}$$

The coefficients α_p and β_p may now be determined by making use of the commutation rules given in Eq. (4); the result is that

$$\alpha_p=\frac{1}{\hbar\omega_{\rm pl}-E_{p+q}{}^{(0)}+E_p{}^{(0)}}\times\text{const}\quad \text{for } |\mathbf{p}|<p_F,\quad |\mathbf{p}+\mathbf{q}|>p_F;$$

$$\beta_p=\frac{1}{\hbar\omega_{\rm pl}-E_{p+q}{}^{(0)}+E_p{}^{(0)}}\times\text{const.}\quad \text{for } |\mathbf{p}|>n_F,\quad |\mathbf{p}+\mathbf{q}|<p_F. \qquad \text{(A-10)}$$

Combining this result with Eq. (A-9), we find

$$\Psi_{\rm pl}(q)=N_q\sum_p\left[\frac{a_{p+q}{}^*b_p{}^*}{\hbar\omega_{\rm pl}-E_{p+q}{}^{(0)}+E_p{}^{(0)}}+\frac{b_{p+q}a_p}{\hbar\omega_{\rm pl}-E_{p+q}{}^{(0)}+E_p{}^{(0)}}\right]\Psi_0, \qquad \text{(A-11)}$$

where

$$\{|N_q|^2\}^{-1}=\Bigg(\sum_{\substack{|\mathbf{p}|<p_F\\|\mathbf{p}+\mathbf{q}|>p_F}}{}_p-\sum_{\substack{|\mathbf{p}|>p_F\\|\mathbf{p}+\mathbf{q}|<p_F}}{}_p\Bigg)\times\frac{1}{(\hbar\omega_{\rm pl}(q)-E_{p+q}{}^{(0)}+E_p{}^{(0)})^2}. \qquad \text{(A-12)}$$

We now determine the plasma energy. Since the eigenvalue equation has a bound-state plasma solution, Eq. (9) in I should be modified to become

$$\textstyle\sum_p(a_{p+q}{}^*b_p{}^*+b_{p+q}a_p)=\text{scattering solutions}+C_{\rm pl}(q)\Psi_{\rm pl}(q), \qquad \text{(A-13)}$$

where $\Psi_{\rm pl}(q)$ is the normalized plasma solution given above. The plasma contribution to the energy then is

$$e^2\frac{\partial E_{\rm pl}}{\partial e^2}=\frac{2\pi\hbar^2e^2}{\Omega}\sum_q\frac{1}{q^2}|C_{\rm pl}(q)|^2. \qquad \text{(A-14)}$$

To obtain the expansion coefficient $C_{\rm pl}(q)$, we take the scalar product of Eq. (A-13) with $\Psi_{\rm pl}(q)$, obtaining

$$C_{\rm pl}(q)=(\Psi_{\rm pl}(q),\textstyle\sum_p(a_{p+q}{}^*b_p{}^*+b_{p+q}a_p)\Psi_0). \qquad \text{(A-15)}$$

Using Eqs. (A-1), (A-3), and (A-8), this becomes

$$C_{\rm pl}(q)=(\Psi_0,[A,\textstyle\sum_p(a_{p+q}{}^*b_p{}^*+b_{p+q}a_p)]_-\Psi_0)=\sum_p(\alpha_p-\beta_p).$$

Using Eqs. (A-9) and (A-10) for α_p and β_p, this is

$$C_{\rm pl}(q)=N_q\Bigg(\sum_{\substack{|\mathbf{p}|<p_F\\|\mathbf{p}+\mathbf{q}|>p_F}}{}_p-\sum_{\substack{|\mathbf{p}|>p_F\\|\mathbf{p}+\mathbf{q}|<p_F}}{}_p\Bigg)\times\frac{1}{\hbar\omega_{\rm pl}(q)-E_{p+q}{}^{(0)}+E_p{}^{(0)}}=\left(\frac{4\pi\hbar^2e^2}{\Omega q^2}\right)^{-1}N_q, \qquad \text{(A-16)}$$

where we have used the dispersion formula to eliminate the sum over p. To bring this to final form, we differentiate the dispersion relation with respect to e^2, which gives

$$0=1-\frac{4\pi\hbar^2e^2}{\Omega q^2}\Bigg(\sum_{\substack{|\mathbf{p}|<p_F\\|\mathbf{p}+\mathbf{q}|>p_F}}{}_p-\sum_{\substack{|\mathbf{p}|>p_F\\|\mathbf{p}+\mathbf{q}|<p_F}}{}_p\Bigg)\times\frac{1}{(\hbar\omega_{\rm pl}-E_{p+q}{}^{(0)}+E_p{}^{(0)})^2}e^2\frac{\partial\hbar\omega_{\rm pl}}{\partial e^2}, \qquad \text{(A-17)}$$

i.e., from (A-12),

$$|N_q|^2=\left(\frac{4\pi\hbar^2e^2}{\Omega q^2}\right)e^2\frac{\partial\hbar\omega_{\rm pl}(q)}{\partial e^2}. \qquad \text{(A-18)}$$

Thus we find

$$C_{\rm pl}(q)=\left(\frac{4\pi\hbar^2e^2}{\Omega q^2}\right)^{-\frac{1}{2}}\left(e^2\frac{\partial\hbar\omega_{\rm pl}(q)}{\partial e^2}\right)^{\frac{1}{2}}, \qquad \text{(A-19)}$$

so that Eq. (A-14) can be written as the simple result

$$\frac{\partial E_{\rm pl}}{\partial e^2}=\frac{1}{2}\sum_q\frac{\partial\hbar\omega_{\rm pl}(q)}{\partial e^2}. \qquad \text{(A-20)}$$

which is the desired answer.

Finally it is interesting to note that the plasma energy is expressed in terms of the contributions from the scattering states alone. To this end, we make use of the Chew-Low-Wick[12] equation for the T matrix introduced in Eq. (A-3) of I, from which a term arising from the bound state (plasma state) is separated. It turns out that this equation becomes a differential equation [by means of (A-19)] to determine the plasma energy in terms of the scattering amplitudes, which has the

[12] G. F. Chew and F. E. Low, Phys. Rev. **101**, 1570 (1956); G. C. Wick, Revs. Modern Phys. **27**, 339 (1955).

solution

$$\hbar\omega_{\rm pl}(q)=\left\{\left(\frac{qp_F}{m}+\frac{q^2}{2m}\right)^2+4\int_0^{e^2}\frac{2\pi\hbar^2}{\Omega q^2}\sum_{\substack{|\mathbf{p}|<p_F\\|\mathbf{p}+\mathbf{q}|>p_F}}\times\left(1-\frac{1}{|1+f(\omega_p+ie)|^2}\right)\omega_p de^2\right\}^{\frac{1}{2}},$$

which f defined in (26).

APPENDIX B

In order to exhibit the formal correspondence of our calculation with that of B-P, we may write our result as

$$E=E_{\rm ex}+E_{\rm pl}+E_{\rm sc}, \tag{B-1}$$

where $E_{\rm ex}$ is the exchange energy given by

$$E_{\rm ex}=-\sum_{\substack{p<p_F\\|\mathbf{p}+\mathbf{q}|<p_F}}\sum_q\frac{2\pi\hbar^2e^2}{\Omega q^2}+E_b^{(2)}. \tag{B-2}$$

$E_{\rm sc}$ as given in I, Eq. (19), is of the form

$$E_{\rm sc}=\sum_{\substack{p<p_F\\|\mathbf{p}+\mathbf{q}|>p_F}}\sum_q\frac{2\pi\hbar^2e^2}{\Omega q^2}[F_q(p)-1], \tag{B-3}$$

and $E_{\rm pl}$ is the plasma energy. In the perturbation limit, $E_{\rm sc}$ is simply the (divergent) second order interaction energy. For small q the nonperturbation function $F_q(p)$ varies as q^2 and hence the low-momentum transfers in the scattering are screened out. Thus, in some sense, Eq. (B-3) represents a screened Coulomb interaction term.

To make the correspondence with B-P more apparent, we arrange the terms in (B-1) in a different fashion. First, we note that the first term in $E_{\rm ex}$ and the second term of $E_{\rm sc}$ combine. We next make the replacement in the sum of the first term of Eq. (B-3):

$$\sum_{\substack{p<p_F\\|\mathbf{p}+\mathbf{q}|>p_F}}\sum_q\rightarrow\sum_{p<p_F}\sum_q-\sum_{\substack{p<p_F\\|\mathbf{p}+\mathbf{q}|<p_F}}\sum_q.$$

We thus can rearrange Eq. (B-1) into the form

$$E=E_{\rm pl}-\sum_{p<p_F}\sum_q\frac{2\pi\hbar^2e^2}{\Omega q^2}+\sum_{p<p_F}\sum_q\frac{2\pi\hbar^2e^2}{\Omega q^2}F_q(p)-\sum_{\substack{p<p_F\\|\mathbf{p}+\mathbf{q}|>p_F}}\sum_q\frac{2\pi\hbar^2e^2}{\Omega q^2}F_q(p)+E_b^{(2)}. \tag{B-4}$$

As it stands, the second and third terms in Eq. (B-4) each diverge at large q. However, the sum converges since $F_q(p)\rightarrow 1$ for large q. On the other hand, the two terms behave differently for small q, the $1/q^2$ behavior in the third term being cut off at small q. This suggests that the high-q part of the second term be separated and combined with the third. It also is convenient to choose the point of separation, which we denote as $q_{\rm max}$, to approximate as well as possible to the natural cutoff in $F_q(p)$. We thus are led to the final ordering:

$$E=\left[E_{\rm pl}-\sum_{p<p_F}\sum_{q<q_{\rm max}}\frac{2\pi\hbar^2e^2}{\Omega q^2}\right]-\left[\sum_{\substack{p<p_F\\|\mathbf{p}+\mathbf{q}|<p_F}}\sum_q\frac{2\pi\hbar^2e^2}{\Omega q^2}F_q(p)\right]+\left[\sum_{p<p_F}\sum_q\frac{2\pi\hbar^2e^2}{\Omega q^2}F_q(p)-\sum_{p<p_F}\sum_{q>q_{\rm max}}\frac{2\pi\hbar^2e^2}{\Omega q^2}\right]+E_b^{(2)}. \tag{B-5}$$

These terms are now in complete correspondence with the structure of the B-P result. The first bracketed terms correspond to the plasma energy of B-P, the second to the screened Coulomb exchange energy, and the third to Pines' screened short-range correlation energy.