Influence of Correlations on the Dielectric Behavior of an Electron Gas.* Nonperturbative Approach to the Many-Fermion System

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Starting with the equation of motion for the density matrix operator of an electron gas in second quantization, a system of matrix equations is derived for matrix elements connecting states with various numbers of electron-hole pairs. Allowing up to n electron-hole pairs and neglecting all states with more than n pairs yields a set of $(n+1)^2$ coupled equations for the various amplitudes in close analogy to the nth order Tamm-Dancoff approximation. The starting point of this approximation, in which all matrix elements connecting the Fermi vacuum with any pair states are neglected (zero-order Tamm-Dancoff approximation), is an equation for the self-consistent field rather than for free particles as in the usual Tamm-Dancoff method. Correlation effects are therefore automatically taken into account when pair states are included. In a certain sense the approximation scheme given here can be thought of as being an expansion in the deviation of the Fermi surface from the sharp edge of the free-particle ground state, the deviation being caused by the Coulomb interaction among the particles. In this paper, we present calculations based on the first Tamm-Dancoff approximation (taking into account only one electron-hole pair). An expression for the dielectric constant will be derived and applied to a determination of the effects of correlations on the wavelength dependence of plasma oscillations. The theory will be compared with the experiments by Watanabe on the energy loss of fast electrons in metal foils and it will be seen that the agreement with experiment is good considering the inherent simplicity of the theory.

1. INTRODUCTION

In recent years much work has been devoted to and much understanding has been gained of the many-fermion system.[1] However, most investigations refer to the high-density limit with a few notable exceptions.[2] It is well known that in the high-density limit the random-phase approximation (RPA) becomes exact and correlation effects are, therefore, absent in this limit.[3] Strictly speaking, the correlation energy, if understood as being the difference between the energy calculated with the exact wave functions and the energy calculated within the self-consistent field approximation, vanishes in the high-density limit. Of course, what is usually known as correlation energy has been defined by Wigner[4] as the difference between the true energy and the sum of kinetic energy of a free Fermi gas plus the expectation value of the potential energy in the ground state of a free electron gas. Unfortunately, in real metals the electron density in the conduction band is in many cases by no means large enough to warrant confidence in the applicability of the results of the RPA. However, in some cases the predictions of the RPA are surprisingly good. This is particularly the case for the energy loss spectrum of high-energy electrons passing through metal foils.[5] In other cases the agreement is less conspicious. Of the correlation energy in the Wigner sense, for instance, only the high-density limit is reproduced.[6]

Most methods of dealing with the many-fermion system consider an expansion with respect to the coupling constant e^2 if they do not stay in the RPA right away. An exception is the work of Werthamer and Suhl,[7] but of course an expansion parameter is not known in their case and it is difficult to estimate the quality of the approximations. In this paper, we are going to present a method which is based on an expansion in electron-hole pair states. The starting point of the theory is the equation of motion for the density-matrix operator ρ in second quantization. Taking matrix elements of this operator equation between all possible states, one obtains an infinite set of coupled equations for the various unknown matrix elements of ρ. Truncating this set by neglecting all pair states with more than a given number, say n pairs, yields a closed system of equations in analogy to the Tamm-Dancoff method. In Sec. 2, the method will be applied to an electron gas under the influence of a weak external potential. The positive ions are treated as a smeared out background without any degrees of freedom of their own. In Sec. 3, the longitudinal dielectric constant ϵ will be derived. Subsequently, the resonance of ϵ^{-1}

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[1] K. A. Brueckner, Phys. Rev. **100**, 36 (1955); J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957); M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957); K. Sawada, *ibid.* **106**, 372 (1957); D. F. Du Bois, Ann. Phys. (New York) **7**, 174 (1959); J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1958). For a fairly exhaustive review see also T. D. Schultz, lecture notes, Space Technology Laboratories Report STL/TR-60-0000-GR-332 (unpublished).

[2] P. A. Wolff, Phys. Rev. **116**, 544 (1959); D. F. Du Bois, V. Gilinsky and M. G. Kivelson, Rand Report RM-3050-PR March, 1962 (unpublished); H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961). See also D. F. Du Bois, footnote 1.

[3] It should be kept in mind that correlation effects are due to deviations from the Hartree self-consistent field approximation which in its linearized form is just the RPA.

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

[5] D. Pines, Revs. Modern Phys. **28**, 184 (1956).

[6] K. Sawada, K. A. Brueckner, N. Fukuda, and R. Brout, Phys. Rev. **108**, 507 (1957). See also, J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1958).

[7] See footnote 2.

which determines the shift in plasmon energy and the dependence of the energy loss of a beam of electrons scattered in metal foils on the scattering angle will be determined and compared with the experimental values of Watanabe.[8]

During the preparation of the manuscript of this work, a paper by Osaka appeared[9] in which also the dispersion coefficient for the plasmon energy has been determined. Osaka uses essentially Du Bois' diagram technique, summing up diagrams which hitherto had been neglected, and so improves on the high-density limit. Although his results for the dispersion coefficient are substantially in agreement with ours in the cases of higher densities (Be and Al), this is not the case for lower densities (Mg, for instance). Although the experimental evidence is rather skimpy, it does indicate, however, that our values for the dispersion coefficient are superior at low densities ($r_s>2.5$).

Concluding this introduction, we should like to point out that methods similar to ours have been used recently by some authors[10] dealing with certain aspects of the many-body problem.

2. DEVELOPMENT OF THE THEORY

The starting point of our investigations is the Hamiltonian of a nonrelativistic electron gas contained in a volume V subject to external forces:

$$H(t)=\frac{\hbar^2}{2m}\sum_{s,\mathbf{k}}k^2a_s^\dagger(\mathbf{k})a_s(\mathbf{k})-\frac{2\pi e^2}{V}\sum_{\mathbf{k},\mathbf{k}'}\sum_{s,s'\mathbf{p}\neq 0}p^{-2}\times a_s^\dagger(\mathbf{k}+\mathbf{p})a_{s'}^\dagger(\mathbf{k}'-\mathbf{p})a_s(\mathbf{k})a_{s'}(\mathbf{k}')+\frac{1}{V}\sum_{s,\mathbf{k},\mathbf{k}'}\phi(\mathbf{k}',t)a_s^\dagger(\mathbf{k})a_s(\mathbf{k}-\mathbf{k}'). \quad (1)$$

$a_s(\mathbf{k})$ and $a_s^\dagger(\mathbf{k})$ are the usual destruction and creation operators of an electron with spin S momentum $\hbar\mathbf{k}$ satisfying the anticommutation relations:

$$\{a_s(\mathbf{k});a_{s'}^\dagger(\mathbf{k}')\}=\delta_{ss'}\delta(\mathbf{k}|\mathbf{k}'). \quad (2)$$

All other anticommutators vanish. $\phi(\mathbf{k},t)$ is the Fourier transform of the potential energy of a given external field:

$$\phi(\mathbf{k},t)=\int d^3r\,\phi_{\mathrm{ex}}(\mathbf{r},t)e^{-i\mathbf{k}\cdot\mathbf{r}}. \quad (3)$$

Since $H(t)$ commutes with $H(t')$ (the interactions are instantaneous) the Heisenberg operator for the density matrix is simply given by

$$\rho(\mathbf{K},\mathbf{K}',t)=\exp\left[-\frac{i}{\hbar}\int_0^t H(\tau)d\tau\right]\times\sum_s a_s^\dagger(\mathbf{K}')a_s(\mathbf{K})\exp\left[\frac{i}{\hbar}\int_0^t H(\tau)d\tau\right]. \quad (4)$$

Here, we have already taken the trace in spin space since spin-dependent forces are absent in our basic Hamiltonian (1). The equation of motion for ρ is now obtained from (1) and (4) after a little algebra and reads[11]:

$$i\hbar\frac{\partial}{\partial t}\rho(\mathbf{K},\mathbf{K}',t)=\frac{\hbar^2}{2m}(K'^2-K^2)\rho(\mathbf{K},\mathbf{K}',t)+\frac{1}{V}\sum_{\mathbf{k}}[\phi(\mathbf{k}-\mathbf{K}',t)\rho(\mathbf{K},\mathbf{k},t)-\phi(\mathbf{k}-\mathbf{K},t)\rho(\mathbf{k},\mathbf{K}',t)]+\frac{2\pi e^2}{V}\sum_{\mathbf{k},\mathbf{p}\neq 0}p^{-2}\{\rho(\mathbf{k},\mathbf{k}+\mathbf{p},t);[\rho(\mathbf{K},\mathbf{K}'-\mathbf{p},t)-\rho(\mathbf{K}+\mathbf{p},\mathbf{K}',t)]\}. \quad (5)$$

Let us now introduce the complete set of states $|\alpha\rangle$ which diagonalizes the Hamiltonian (1). Since the Hamiltonian (1) commutes with the number operator, let us immediately select the subset belonging to a fixed number of electrons N. Within this set Eq. (5) can be written as a coupled system of equations for the matrix elements $\langle\alpha|\rho|\beta\rangle$ which is of course completely equivalent to the operator equation (5). This infinite system of equations is still exact, and in order to be able to attack it approximations have to be introduced. We first write

$$\langle\alpha|\rho(\mathbf{K},\mathbf{K}',t)|\beta\rangle=\langle\alpha_0|\rho_0(\mathbf{K},\mathbf{K}',t)|\beta_0\rangle+g_{\alpha\beta}(\mathbf{K},\mathbf{K}',t), \quad (6)$$

where $|\alpha_0\rangle$ and ρ_0 are the free-particle values of the corresponding state $|\alpha\rangle$ and operator ρ. The functions $g_{\alpha\beta}$ are unknown. Since we ultimately want an expression for the dielectric constant of the electron gas which is only a useful concept for weak external fields, we replace the matrix elements of ρ by their free-particle values in all terms containing the external potential ϕ. This has the effect of making the equations for the $g_{\alpha\beta}$ inhomogeneous, as a glance at Eq. (5) shows. But this entails immediately another simplification. We are looking for solutions of the $g_{\alpha\beta}$ which vanish if the external potential is switched off.[12] The $g_{\alpha\beta}$ will, therefore, be proportional to ϕ and terms quadratic in the $g_{\alpha\beta}$ may be neglected (linearization).[13] The final and most important approximation we are going to

[8] H. Watanabe, J. Phys. Soc. Japan **11**, 112 (1956).
[9] Y. Osaka, J. Phys. Soc. Japan **17**, 547 (1962).
[10] H. Kummel, Z. Physik **166**, 243 (1962); H. Mitter and K. Yamasaki, Nuclear Phys. **30**, 683 (1962).
[11] Equation (5) has also been derived by Ehrenreich and Cohen [H. Ehrenreich and M. H. Cohen, Phys. Rev. **115**, 786 (1959)], Eq. (17) of their paper. The term due to the Coulomb interaction in their equation is in error.
[12] Strictly speaking, this constitutes another approximation. According to Eq. (6) the vanishing of $g_{\alpha\beta}$ is tantamount to assuming free-particle values for the matrix elements. That this is a good approximation may be inferred from the work of Werthamer and Suhl [N. R. Werthamer and H. Suhl, Phys. Rev. **125**, 1402 (1962)].
[13] Although simplifying the calculations considerably, the linearization in the $g_{\alpha\beta}$'s is not essential for this theory in contrast to the method of Werthamer and Suhl (see footnote 12). As will be apparent later on, keeping the nonlinear terms in the $g_{\alpha\beta}$'s is tantamount to starting with the Hartree approximation rather than with the RPA.

make consists of the following prescription: Matrix elements of the interaction term in Eq. (5), which may be written as

$$\langle\alpha|\rho\rho'|\beta\rangle=\sum_\delta\langle\alpha|\rho|\delta\rangle\langle\delta|\rho'|\beta\rangle, \tag{7}$$

where the sum runs over the complete set of state vectors, are approximated by a finite sum over only a finite number of intermediate states $|\delta\rangle$.

It is easy to see that if we allow n intermediate states we have exactly n^2 coupled equations for the quantities $g_{\alpha\beta}$. The states we are dealing with are the Fermi vacuum $|0\rangle$, the one-electron hole pair states $|\mathbf{K}_1,\mathbf{K}_2\rangle$, the two-electron hole pair states $|\mathbf{K}_1,\mathbf{K}_1';\mathbf{K}_2,\mathbf{K}_2'\rangle$, etc. Allowing up to n pairs yields at set of $(n+1)^2$ coupled linear equations from (5) which is the analog of the nth order Tamm-Dancoff approximation. We will presently see that the zero-order approximation which disregards all pair states already yields the equations for the self-consistent field. All correlation contributions are, therefore, contained in the higher order pair approximations. In what follows we will never go beyond the first-order approximation allowing, besides the Fermi vacuum, only one-electron hole pair states.

Zeroth Tamm-Dancoff Approximation

In this approximation we only deal with the ground state and have from Eq. (6)

$$\langle 0|\rho(\mathbf{K},\mathbf{K}',t)|0\rangle=2F(K)\delta(\mathbf{K}|\mathbf{K}')+2g_{00}(\mathbf{K},\mathbf{K}',t), \tag{8}$$

where $F(K)$ is the Fermi function

$$\begin{aligned} F(K)&=1 \quad \text{if} \quad K\leq k_F,\\ &=0 \quad \text{if} \quad K>k_F, \end{aligned} \tag{9}$$

with the normalization

$$\sum_{\mathbf{K}} F(K)=\tfrac{1}{2}N/V. \tag{10}$$

$\hbar k_F$ is the momentum of an electron at the Fermi surface. From Eq. (7) we see that in the sum over intermediate states only one term remains and that the zeroth Tamm-Dancoff approximation is equivalent to replacing the ground-state expectation value of a product of operators by the product of expectation values. This is just the approximation adopted by Ehrenreich and Cohen,[11] and, therefore, in the zeroth approximation we obtain identical results. Indeed, taking the expectation value of Eq. (5), we obtain after a little algebra the following equation:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}g_{00}(\mathbf{K},\mathbf{K}',t)&=\frac{\hbar^2}{2m}(K'^2-K^2)g_{00}(\mathbf{K},\mathbf{K}',t)\\ &+V^{-1}\phi(\mathbf{K}-\mathbf{K}')[F(K)-F(K')]+\frac{8\pi e^2}{V}|\mathbf{K}-\mathbf{K}'|^{-2}\\ &\times\sum_{\mathbf{k}} g_{00}(\mathbf{k},\mathbf{k}+\mathbf{K}'-\mathbf{K},t)[F(K)-F(K')], \end{aligned} \tag{11}$$

an equation which can readily be identified as the equation for the density matrix in the RPA. We will not deal further with Eq. (11) here, since this has been done elsewhere.[11,14]

First Tamm-Dancoff Approximation

In this case we also consider the pair states $|\mathbf{K}_1,\mathbf{K}_2\rangle$. $-\hbar\mathbf{K}_1$ is the momentum of the hole; $\hbar\mathbf{K}_2$ is the momentum of the electron above the Fermi surface. There are now four matrix elements. One of them is given by Eq. (8). Here, we are listing the remainder:

$$\begin{aligned} &\langle 0|\rho(\mathbf{K},\mathbf{K}',t)|\mathbf{K}_1,\mathbf{K}_2\rangle\\ &=F(K_1)\bar{F}(K_2)\delta(\mathbf{K}|\mathbf{K}_2)\delta(\mathbf{K}'|\mathbf{K}_1)\\ &\quad\times\exp\left[-\frac{i\hbar t}{2m}(K'^2-K^2)\right]+g_0(\mathbf{K},\mathbf{K}',\mathbf{K}_1,\mathbf{K}_2,t), \end{aligned} \tag{12}$$

$$\begin{aligned} &\langle\mathbf{K}_1,\mathbf{K}_2|\rho(\mathbf{K},\mathbf{K}',t)|0\rangle\\ &=F(K_1)\bar{F}(K_2)\delta(\mathbf{K}|\mathbf{K}_1)\delta(\mathbf{K}'|\mathbf{K}_2)\\ &\quad\times\exp\left[-\frac{i\hbar t}{2m}(K'^2-K^2)\right]+\bar{g}_0(\mathbf{K},\mathbf{K}',\mathbf{K}_1,\mathbf{K}_2,t), \end{aligned} \tag{13}$$

$$\begin{aligned} &\langle\mathbf{K}_1',\mathbf{K}_2'|\rho(\mathbf{K},\mathbf{K}',t)|\mathbf{K}_1,\mathbf{K}_2\rangle\\ &=[2-\delta(\mathbf{K}|\mathbf{K}_1)]F(K_1)\bar{F}(K_2)F(K)\\ &\quad\times\delta(\mathbf{K}|\mathbf{K}')\delta(\mathbf{K}_1'|\mathbf{K}_1)\delta(\mathbf{K}_2'|\mathbf{K}_2). \end{aligned} \tag{14}$$

In the above formulas, $\bar{F}$ is defined as

$$\bar{F}(K)=1-F(K), \tag{15}$$

with $F(K)$ from Eq. (9). The explicit dependence on spin of the matrix elements (12) to (14) has been suppressed. In the ensuing equations the functions g_0 and $\bar{g}_0$ have to be understood as traces in spin space. We also neglected the g function corresponding to the matrix element (14). As seen from Eq. (14), it would be a six-momentum function and belongs really to the next higher (two-pair) approximation.

If we now take matrix elements of Eq. (5) between the Fermi vacuum and a one-pair state, keeping in mind the approximations outlined above, using Eqs. (12)–(14), introduce a Fourier transformation in time:

$$g_{00}(\mathbf{K},\mathbf{K}',t)=\int dw\, e^{-iwt}g_{00}(\mathbf{K},\mathbf{K}',w), \tag{16}$$

$$\begin{aligned} g_0(\mathbf{K},\mathbf{K}',\mathbf{K}_1,\mathbf{K}_2,t)&=\int dw\, e^{-iwt}g_0(\mathbf{K},\mathbf{K}',\mathbf{K}_1,\mathbf{K}_2,w)\\ &\quad\times\exp\left[\frac{i\hbar t}{2m}(K_2^2-K_1^2)\right], \end{aligned} \tag{17}$$

[14] See also O. von Roos, Phys. Rev. **119**, 1174 (1960), where Eq. (11) has been derived using a quantum mechanical distribution function. In that paper, electron exchange was taken into account. In other words, instead of the Hartree self-consistent field method the Hartree-Fock scheme was used. Equation (11) of this paper does not contain any exchange contributions. But since the underlying theory takes exchange fully into account we conclude that exchange effects will show up in the higher approximations automatically.

with a similar equation for $\bar{g}_0$ and finally let the volume V go to infinity, we obtain the following equations for g_0 and $\bar{g}_0$:

$$\left[\hbar w+\frac{\hbar^2}{2m}(K_1^2-K_2^2+K^2-K'^2)\right]g_0(\mathbf{K},\mathbf{K}',\mathbf{K}_1,\mathbf{K}_2,w)$$
$$=F(K_1)\bar{F}(K_2)[\phi(\mathbf{K}_1-\mathbf{K}',w)\delta(\mathbf{K}-\mathbf{K}_2)$$
$$-\phi(\mathbf{K}_2-\mathbf{K},w)\delta(\mathbf{K}'-\mathbf{K}_1)]+\frac{e^2}{2\pi^2}|\mathbf{K}'-\mathbf{K}|^{-2}$$
$$\times[F(K)-F(K')][1+F(K_1)\bar{F}(K_2)]$$
$$\times\int d^3k\, g_0(\mathbf{k},\mathbf{k}+\mathbf{K}'-\mathbf{K},\mathbf{K}_1,\mathbf{K}_2,w)$$
$$+\frac{e^2}{2\pi^2}|\mathbf{K}_2-\mathbf{K}_1|^{-2}F(K_1)\bar{F}(K_2)$$
$$\times[g_{00}(\mathbf{K},\mathbf{K}'-\mathbf{K}_1+\mathbf{K}_2,w)$$
$$-g_{00}(\mathbf{K}+\mathbf{K}_1-\mathbf{K}_2,\mathbf{K}',w)]+2\pi e^2F(K_1)\bar{F}(K_2)$$
$$\times\Big\{\delta(\mathbf{K}-\mathbf{K}_2)|\mathbf{K}'-\mathbf{K}_1|^{-2}$$
$$\times\int d^3k\, g_{00}(\mathbf{k},\mathbf{k}+\mathbf{K}'-\mathbf{K}_1,w)$$
$$-\delta(\mathbf{K}'-\mathbf{K}_1)|\mathbf{K}-\mathbf{K}_2|^{-2}$$
$$\times\int d^3k\, g_{00}(\mathbf{k},\mathbf{k}+\mathbf{K}_2-\mathbf{K},w)\Big\},\quad(18)$$

and the equation for $\bar{g}_0$ follows from Eq. (18) if K_1 is interchanged with K_2 and also F with $\bar{F}$ or

$$\text{equation for }\bar{g}_0=\text{Eq. (18)}\{\mathbf{K}_1\leftrightarrow\mathbf{K}_2,F\leftrightarrow\bar{F}\}.\quad(19)$$

Now taking the ground-state expectation value of Eq. (5) and using the same procedure which led to Eqs. (18) and (19), we obtain the third equation necessary for the determination of the g functions:

$$\left[-\hbar w+\frac{\hbar^2}{2m}(K'^2-K^2)\right]g_{00}(\mathbf{K},\mathbf{K}',w)$$
$$=\frac{2}{(2\pi)^3}\phi(\mathbf{K}-\mathbf{K}',w)[F(K')-F(K)]$$
$$+\frac{e^2}{\pi^2}|\mathbf{K}-\mathbf{K}'|^{-2}[F(K')-F(K)]$$
$$\times\int d^3k\, g_{00}(\mathbf{k},\mathbf{k}+\mathbf{K}'-\mathbf{K},w)$$
$$-\frac{e^2}{(2\pi)^2}\int d^3p d^3k\, p^{-2}\{F(|\mathbf{k}+\mathbf{p}|)$$
$$\times\bar{F}(k)[\bar{g}_0(\mathbf{K},\mathbf{K}'-\mathbf{p},\mathbf{k}+\mathbf{p},\mathbf{k},w)$$
$$-\bar{g}_0(\mathbf{K}+\mathbf{p},\mathbf{K}',\mathbf{k}+\mathbf{p},\mathbf{k},w)]$$
$$+F(k)\bar{F}(|\mathbf{k}+\mathbf{p}|)[g_0(\mathbf{K},\mathbf{K}'-\mathbf{p},\mathbf{k},\mathbf{k}+\mathbf{p},w)$$
$$-g_0(\mathbf{K}+\mathbf{p},\mathbf{K}',\mathbf{k},\mathbf{k}+\mathbf{p},w)]$$
$$+F(\mathbf{K})\bar{F}(|\mathbf{K}'-\mathbf{p}|)g_0(\mathbf{k},\mathbf{k}+\mathbf{p},\mathbf{K},\mathbf{K}'-\mathbf{p},w)$$
$$-F(|\mathbf{K}+\mathbf{p}|)\bar{F}(K')g_0(\mathbf{k},\mathbf{k}+\mathbf{p},\mathbf{K}+\mathbf{p},\mathbf{K}',w)$$
$$+F(|\mathbf{K}'-\mathbf{p}|)\bar{F}(K)\bar{g}_0(\mathbf{k},\mathbf{k}+\mathbf{p},\mathbf{K}'-\mathbf{p},\mathbf{K},w)$$
$$-F(K')\bar{F}(|\mathbf{K}+\mathbf{p}|)$$
$$\times\bar{g}_0(\mathbf{k},\mathbf{k}+\mathbf{p},\mathbf{K}',\mathbf{K}+\mathbf{p},w)\}.\quad(20)$$

Equations (18), (19), and (20) constitute the basis for our further investigations.

3. THE DIELECTRIC CONSTANT AND THE DISPERSION RELATION FOR PLASMA OSCILLATIONS

An expression for the dielectric constant of the electron gas valid to all orders of the Tamm-Dancoff approximation is the following:

$$[\epsilon(K,w)]^{-1}=1+\frac{4\pi e^2}{K^2\phi(\mathbf{K},w)}\int d^3k\, g_{00}(\mathbf{k},\mathbf{k}+\mathbf{K},w).\quad(21)$$

This is easily proved noting that the integral on the right-hand side of Eq. (21) is nothing but the Fourier transform of the expectation value of the particle number density induced by the external field; an assertion which follows from the definitions (4) and (12). All we have to do now is to determine the integral in (21) from Eqs. (18), (19), and (20). To do so, we proceed in the following way. We know from experiment that the correlation contributions are not too large.[8] We, therefore, split g_{00} into two parts:

$$g_{00}=g_{00}^0+g_{00}^1.\quad(22)$$

The first part g_{00}^0 is to satisfy Eq. (20) without the terms containing g_0 and $\bar{g}_0$, i.e., without the last integral on the right-hand side of Eq. (20) the part which represents the correlation corrections. Once g_{00}^0 is determined, it is inserted into the equations for g_0 and $\bar{g}_0$ [Eqs. (18) and (19)]. Subsequently, g_0 and $\bar{g}_0$ are determined and inserted back into Eq. (20). Finally, g_{00}^1 is obtained from Eq. (20) with the correlation corrections now being known functions of their arguments. In order to execute the above program, we first determine g_{00}^0. But this is very easy; in fact it has been done before.[11,15] We therefore merely quote the result:

[15] J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **28**, 8 (1954).

With the definition

$$A(K,w')=\frac{e^2}{\pi^2 m}\int\frac{F(k)d^3k}{[w'-(\hbar/m)\mathbf{K}\cdot\mathbf{k}]^2-[(\hbar/2m)K^2]^2}, \quad (23)$$

and

$$w'=w+i\epsilon,$$

the small positive imaginary constant being due to the choice of a retarded Green's function, we have

$$g_{00}{}^0(\mathbf{K},\mathbf{K}+\mathbf{K}',w)=\frac{1}{4\pi^3}\phi(\mathbf{K}',w)[1-A(K,w')]^{-1}\times\frac{F(|\mathbf{K}+\mathbf{K}'|)-F(K)}{-\hbar w'+(\hbar^2/m)\mathbf{K}\cdot\mathbf{K}'+(\hbar^2/2m)K'^2}, \quad (24)$$

and

$$\int d^3k\, g_{00}{}^0(\mathbf{k},\mathbf{k}+\mathbf{K},w)=\frac{K^2\phi(\mathbf{K},w)}{4\pi e^2}\frac{A(K,w')}{1-A(K,w')}. \quad (25)$$

Equation (25) yields, incidentally, with the help of Eq. (21) for ϵ just Lindhard's expression[15]:

$$\epsilon(K,w')=1-A(K,w'). \quad (26)$$

We are now in a position to evaluate g_0 and $\bar{g}_0$ by merely inserting Eqs. (24) and (25) into Eqs. (18) and (19) and solving for g_0 and $\bar{g}_0$ with exactly the same method as the one which was used to obtain expression (24). The calculations are tedious but straightforward. Inserting the now determined functions g_0 and $\bar{g}_0$ into the right-hand side of Eq. (20) results in an equation for $g_{00}{}^1$ which again is easily solved using the same method as before. The result of all these lengthy but trivial calculations is eventually the following:

$$\int d^3k\, g_{00}{}^1(\mathbf{k},\mathbf{k}+\mathbf{K},w)=\frac{\phi(\mathbf{K},w)}{[1-A(K,w')]^2}\sum_{n=1}^{7}A_n(K,w'), \quad (27)$$

where the expressions A_n are certain well-defined integrals which are listed in Appendix I. We see now from Eqs. (21), (25), and (27) that the longitudinal dielectric constant is given by

$$\epsilon(K,w')=\frac{1-A}{1+4\pi e^2\sum A_n/K^2(1-A)}=1-A(K,w')-\frac{4\pi e^2}{K^2}\sum_{n=1}^{7}A_n(K,w'), \quad (28)$$

since the denominator is close to unity. Some caution has to be exerted in the derivation of the last expression of Eq. (28) near a resonance. A resonance occurs when the real part of the dielectric constant vanishes. This is the case for the dielectric constant in the RPA, Eq. (26), if

$$1=\mathrm{Re}A(K,w'). \quad (29)$$

But from a comparison between expression (25) and (27), we see that

$$4\pi e^2\sum A_n/K^2(1-A)\ll 1, \quad (30)$$

even near a resonance since $g_{00}{}^1\ll g_{00}{}^0$.

We are now in a position to proceed with an actual determination of the dispersion relation for plasma oscillations. This we do in the long-wavelength limit since it is in this limit that plasmons tend to be stable or, in our picture, that the imaginary part of ϵ tends to be small. Our task is then to find the zeros of

$$\lim_{K=0}\mathrm{Re}\epsilon(K,w')=0. \quad (31)$$

Now, the real parts of A and the integrals A_n are simply given by replacing w' with w and defining the integrals as principal values, if need be, according to the well-known relation

$$\frac{1}{x+i\epsilon}=\frac{P}{x}-i\pi\delta(x).$$

From Appendix I, we know that there are two types of integrals A_n. One type is multiplied with $1-A$, the other with $1-\frac{1}{2}A$. In the long-wavelength limit we have[15]

$$1-A(K,w)=1-\frac{w_p{}^2}{w^2}-\frac{3}{5}\frac{v_F{}^2w_p{}^2}{w^4}K^2, \quad (32)$$

where w_p is the classical plasma frequency and v_F the velocity of an electron at the Fermi surface. In the correction terms $\sum A_n$, we may replace w by w_p since we know that the true plasma frequency deviates only slightly from w_p. If we then expand the integrals A_n for small K and keep only terms up to order K^2, we arrive at a result of the form

$$0=1-A(K,w)-\frac{4\pi e^2}{K^2}\sum_{1}^{7}A_n(K,w_p), \quad (33)$$

an expression in which all terms have been expanded about $K=0$. The derivation will be sketched in Appendix II. It is then easy to solve for w (Appendix II). The result is

$$w=w_p+\delta w+\tfrac{3}{10}(v_F{}^2/w_p)AK^2, \quad (34)$$

where

$$\frac{\delta w}{w_p}=\frac{e^4k_F{}^6}{24\pi^2m^2w_p{}^4}I_1(\alpha)+\frac{e^6k_F{}^5}{24\pi^3\hbar^2mw_p{}^4}I_2(\alpha), \quad (35)$$

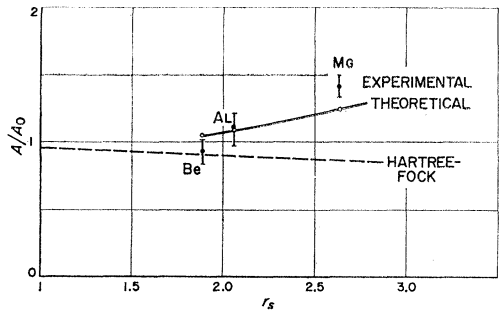

FIG. 1. A comparison between the experimental values for the dispersion coefficient as measured by Watanabe (reference 8) and calculated values using the present theory (solid line). The dashed line represents the exchange correction alone as obtained from a Hartree Fock self-consistent field calculation [O. von Roos and J. Zmuidzinas, Phys. Rev. 12, 941 (1961)]. $A_0=1$ is the value from the RPA.

$$A-1=\frac{e^4k_F{}^6}{12\pi^2m^2w_p{}^4}I_1(\alpha)+\frac{e^6k_F{}^5}{12\pi^3\hbar^2mw_p{}^4}I_2(\alpha)$$
$$-\frac{e^8mk_F{}^2}{6\pi^4\hbar^5w_p{}^3}I_3(\alpha)-\frac{e^6k_F{}^3}{6\pi^3\hbar^3w_p{}^3}$$
$$\times\frac{1+(\frac{1}{2}-\alpha)^{-1}}{1-A(k_F,w_p)}I_4(\alpha). \quad (36)$$

Equation (36) defines the dispersion coefficient [according to Eq. (34) $A=1$ and of course $\delta w=0$ is just the result of the RPA] and Eq. (35) defines the energy shift of the plasma oscillations at infinite wavelengths. The expressions I_1 to I_4 are double integrals defined in Appendix II. They are functions of the dimensionless parameter α given by

$$\alpha=mw_p/\hbar k_F{}^2. \quad (37)$$

The integrals I_1 to I_4 have been computed numerically. Figure 1 shows a comparison between the experimental values obtained by Watanabe[8] and the values obtained from Eq. (36). In Table I, the experimental and theoretical values for the shift in plasmon energy in units of $\hbar w_p$ are given. It is seen that the agreement between theory and experiment is fair. Certainly more experiments have to be done, in particular, in the low-density region ($r_s>3$) with metals in which the free-electron model is a very good approximation (alkalis) and higher pair approximations have to be considered, before it can be shown conclusively that indeed the electron-electron interaction is alone responsible for the long-wavelength behavior of the collective modes of a metal plasma.

TABLE I. A comparison between the experimental values of the shift in plasmon energy (reference 8) and the theoretical values from Eq. (35).

Metal	$(\delta w/w_p)_{\text{experimental}}$	$(\delta w/w_p)_{\text{theoretical}}$
Be	0	−0.03
Al	−0.06	−0.04
Mg	−0.05	−0.05

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APPENDIX A

Here, we quote the quantities A_n which appear in the expression (28) for the dielectric constant. With the definitions:

$$D_\pm(\mathbf{K},\mathbf{K}')=[-w'+(\hbar/m)\mathbf{K}\cdot\mathbf{K}'\pm(\hbar/2m)K'^2]^{-1}, \quad (A1)$$

$$G(k,k')=F(k)\bar{F}(k')+F(k')\bar{F}(k), \quad (A2)$$

$$B_\pm(\mathbf{K},\mathbf{K}_1,\mathbf{K}_2,w')=\frac{e^2}{2\pi^2m}[1+F(K_1)\bar{F}(K_2)]\int d^3k\frac{F(k)}{[-w'+(\hbar/m)\mathbf{k}\cdot\mathbf{K}\pm(\hbar/2m)(K_2{}^2-K_1{}^2)]^2-[(\hbar/2m)K^2]^2}, \quad (A3)$$

the various A_n are listed below.

$$A_1=-\left(\frac{e}{2\pi\hbar}\right)^2[1-\tfrac{1}{2}A(K,w')]\int d^3kd^3p\,p^{-2}G(|\mathbf{k}+\mathbf{p}|,k)\{[D_-(\mathbf{k}+\mathbf{p},\mathbf{K})-D_-(\mathbf{k},\mathbf{K})]D_-(\mathbf{k}+\mathbf{p},\mathbf{K})$$
$$-[D_+(\mathbf{k}+\mathbf{p},\mathbf{K})-D_+(\mathbf{k},\mathbf{K})]D_+(\mathbf{k},\mathbf{K})\}, \quad (A4)$$

$$A_2=\left(\frac{e}{2\pi\hbar}\right)^2[1-\tfrac{1}{2}A(K,w')]\int d^3kd^3p\,p^{-2}G(|\mathbf{k}+\mathbf{K}-\mathbf{p}|,k)[1-B_+(\mathbf{p},\mathbf{k},\mathbf{k}+\mathbf{K}-\mathbf{p},w')]^{-1}$$
$$\times[D_+(\mathbf{k},\mathbf{K})-D_+(\mathbf{k}-\mathbf{p},\mathbf{K})][D_+(\mathbf{k},\mathbf{K})-D_+(\mathbf{k}-\mathbf{p},\mathbf{K})], \quad (A5)$$

$$A_3=-\frac{e^4}{4\pi^4\hbar^3}[1-\tfrac{1}{2}A(K,w')]\int d^3kd^3k'd^3p\,p^{-2}|\mathbf{K}-\mathbf{p}|^{-2}G(|\mathbf{k}+\mathbf{p}|,\mathbf{k})[1-B_-(\mathbf{K}-\mathbf{p},\mathbf{k}+\mathbf{p},\mathbf{k},w')]^{-1}$$
$$\times[F(|\mathbf{k}'-\mathbf{p}+\mathbf{K}|)-F(k')][D_+(\mathbf{k}',K)-D_+(\mathbf{k}'-\mathbf{p},\mathbf{K})][D_-(\mathbf{k}+\mathbf{p},\mathbf{K})-D_+(\mathbf{k},\mathbf{K})]$$
$$\times\left(-w'+\frac{\hbar}{2m}[(\mathbf{k}+\mathbf{p})^2-k^2+2\mathbf{k}'\cdot(\mathbf{K}-\mathbf{p})+(\mathbf{K}-\mathbf{p})^2]\right)^{-1}, \quad \text{(A6)}$$

$$A_4=-\frac{e^2}{2^6\pi^7\hbar^3}[1-A(K,w')]\int d^3kd^3k'd^3p\,p^{-4}G(|\mathbf{k}+\mathbf{p}|,k)[F(|\mathbf{k}'-\mathbf{p}+\mathbf{K}|)-F(|\mathbf{k}'-\mathbf{p}|)]$$
$$\times[1-A(|\mathbf{k}'-\mathbf{p}|,w')]^{-1}D_+(\mathbf{k}'-\mathbf{p},\mathbf{K})[D_+(\mathbf{k}',\mathbf{K})-D_+(\mathbf{k}'-\mathbf{p},\mathbf{K})]$$
$$\times\left(-w'+\frac{\hbar}{2m}[(\mathbf{k}+\mathbf{p})^2-k^2+2\mathbf{k}'\cdot(\mathbf{K}-\mathbf{p})+(\mathbf{K}-\mathbf{p})^2]\right)^{-1}, \quad \text{(A7)}$$

$$A_5=\frac{e^4}{2^6\pi^7\hbar^3}[1-A(K,w')]\int d^3kd^3k'd^3p\,p^{-4}G(|\mathbf{k}+\mathbf{p}|,k)[1-A(k',w')]^{-1}[F(|\mathbf{k}'+\mathbf{K}|)-F(k')]D_+(\mathbf{k}',\mathbf{K})$$
$$\times[D_+(\mathbf{k}',\mathbf{K})-D_+(\mathbf{k}'-\mathbf{p},\mathbf{K})]\left(-w'+\frac{\hbar}{2m}[(\mathbf{k}+\mathbf{p})^2-k^2+2\mathbf{k}'\cdot(\mathbf{K}-\mathbf{p})+(\mathbf{K}-\mathbf{p})^2]\right)^{-1}, \quad \text{(A8)}$$

$$A_6=-\frac{e^4}{2^6\pi^7\hbar^3}[1-A(K,w')]\int d^3kd^3k'd^3p\,p^{-2}|\mathbf{p}-\mathbf{K}|^{-2}[1-B_+(\mathbf{p},\mathbf{k}',\mathbf{k}'-\mathbf{p}+\mathbf{K},w')]^{-1}[1-A(k,w')]^{-1}$$
$$\times[F(|\mathbf{k}+\mathbf{K}|)-F(k)]G(|\mathbf{k}-\mathbf{p}+\mathbf{K}|,k')D_+(\mathbf{k},\mathbf{K})[D_+(\mathbf{k}',K)-D_+(\mathbf{k}'-\mathbf{p},\mathbf{K})]$$
$$\times\left\{\left(-w'+\frac{\hbar}{2m}[(\mathbf{k}'-\mathbf{p}+\mathbf{K})^2-k'^2-p^2+2(\mathbf{k}+\mathbf{K})\cdot\mathbf{p}]\right)^{-1}\right.$$
$$\left.-\left(-w'+\frac{\hbar}{2m}[(\mathbf{k}'-\mathbf{p}+\mathbf{K})^2-k'^2+p^2+2\mathbf{k}\cdot\mathbf{p}]\right)^{-1}\right\}, \quad \text{(A9)}$$

$$A_7=-\frac{e^6}{2^6\pi^9\hbar^4}[1-A(K,w')]\int d^3kd^3k'd^3pd^3l\,p^{-4}|\mathbf{K}-\mathbf{p}|^{-2}G(|\mathbf{k}+\mathbf{p}|,\mathbf{k})[1-A(l,w')]^{-1}$$
$$\times[1-B_-(\mathbf{K}-\mathbf{p},\mathbf{k}+\mathbf{p},\mathbf{k},w')]^{-1}[F(|\mathbf{l}+\mathbf{K}|)-F(l)][F(|\mathbf{k}'-\mathbf{p}+\mathbf{K}|)-F(k')]D_+(\mathbf{l},\mathbf{K})$$
$$\times[D_+(\mathbf{k}',\mathbf{K})-D_+(\mathbf{k}'-\mathbf{p},\mathbf{K})]\left[\left(-w'+\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p}+\mathbf{l}\cdot\mathbf{p}-\mathbf{l}\cdot\mathbf{K})+\frac{\hbar}{2m}K^2\right)^{-1}\right.$$
$$\left.-\left(-w'+\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p}+\mathbf{l}\cdot\mathbf{K}-\mathbf{l}\cdot\mathbf{p}-\mathbf{K}\cdot\mathbf{p})+\frac{\hbar}{m}(p^2+\tfrac{1}{2}K^2)\right)^{-1}\right]$$
$$\times\left(-w'+\frac{\hbar}{m}(\mathbf{k}\cdot\mathbf{p}+\mathbf{k}'\cdot\mathbf{K}-\mathbf{k}'\cdot\mathbf{p}-\mathbf{K}\cdot\mathbf{p})+\frac{\hbar}{m}(p^2+\tfrac{1}{2}K^2)\right)^{-1}. \quad \text{(A10)}$$

APPENDIX B

Here we sketch the derivation leading from Eq. (33) to Eqs. (35) and (36) in the text. Since the expressions A_n are all treated in the same manner, we will concentrate in this sketch on only a few of them as a typical example. So let us take A_1 and A_2. One notices from Eqs. (A4) and (A5) of Appendix A, that A_1 and A_2 diverge separately for large p. The sum converges, however. If we now expand the integrands about $K=0$, we obtain

$$\lim_{K=0}(A_1+A_2)=\frac{e^2}{(2\pi)^2m^2w_p{}^4}[1-A(K,w_p)]\int d^3kd^3pG(|\mathbf{k}+\mathbf{p}|,k)\frac{(\mathbf{p}\cdot\mathbf{K})^2}{p^2}\times\frac{B_+(-\mathbf{p},\mathbf{k},\mathbf{k}+\mathbf{p},w_p)}{1-B_+(-\mathbf{p},\mathbf{k},\mathbf{k}+\mathbf{p},w_p)}. \quad \text{(B1)}$$

Expression (B1) is further reduced by noting that the integrand depends only on the magnitudes p, k and the angle between p and k, i.e., $\mathbf{p}\cdot\mathbf{k}$, in a nontrivial manner. The integral B_+ as defined in (A3) can readily be integrated exactly. Noting that it differs only slightly from the integral A, Eq. (23) of the text, we can use Lindhard's results[15]

directly. Now writing everything dimensionless, i.e., measuring all wave vectors in units of k_F, all energies in units of the Fermi energy, using Eq. (32) of the text, and substituting $k\cdot p=Z$, we obtain the following formula for A_1+A_2:

$$A_1+A_2\rightarrow\frac{e^4k_F{}^6}{3(2\pi)^2m^2w_p{}^4}\left[\frac{1}{2}-\frac{3}{5}\frac{v_F{}^2k_F{}^2}{w_p{}^2}K^2\right]I_1(\alpha), \tag{B2}$$

where

$$I_1(\alpha)=\int_0^{10}pdp\int_{-p}^{+p}dZ\left[\max(1;1+p^2+2Z)-\max\left(1;\frac{Z^2}{p^2}+p^2+2Z\right)\right]\frac{2B(\alpha,Z,p)}{1-2B(\alpha,Z,p)}$$
$$+\int_0^{10}pdp\int_{-10p}^{10p}dZ\left[\min(1;100+p^2+2Z)-\min(1;\max(1;Z^2/p^2)+p^2+2Z)\right]\frac{B(\alpha,Z,p)}{1-B(\alpha,Z,p)}. \tag{B3}$$

Here, we used the definitions

$$\begin{aligned}\max(\alpha;\beta)&=\alpha \quad \text{if} \quad \alpha>\beta,\\ &=\beta \quad \text{if} \quad \alpha<\beta,\\ \min(\alpha;\beta)&=-\max(-\alpha;-\beta),\end{aligned} \tag{B4}$$

and B is given by

$$B(\alpha,Z,p)=-(3\alpha^2/p^2)f(\tfrac{1}{2}p,\ |\alpha-Z-\tfrac{1}{2}p^2|/p), \tag{B5}$$

with

$$\alpha=mw_p/\hbar k_F{}^2, \tag{B6}$$

and

$$f(x,y)=\tfrac{1}{2}+1/8x[1-(x-y)^2]\ln|x-y+1/x-y-1|+1/8x[1-(x+y)^2]\ln|x+y+1/x+y-1|. \tag{B7}$$

In the integral I_1, Eq. (B3), we have taken the upper limit of the p integration as $p_{\max}=10k_F$. The integral converges rapidly and the error is, therefore, small; also for numerical calculations an upper cutoff is necessary anyway. Numerical calculations showed subsequently that the error is indeed small. Treating the other integrals A_n of Appendix B in the same way, we arrive at the Eqs. (35) and (36) of the text. Here, we list the remaining terms I_2 to I_4.

$$I_2(\alpha)=\int_0^{10}\frac{dp}{p}\int_{-p}^{+p}dZ\,S_1(Z,p)\frac{A(\alpha,Z,p)}{1-2B(\alpha,Z,p)}+\int_0^{10}\frac{dp}{p}\int_{-10p}^{+10p}dZ\,S_2(Z,p)\frac{A(\alpha,Z,p)}{1-B(\alpha,Z,p)}, \tag{B8}$$

where

$$A(\alpha,Z,p)=-2+\frac{1}{p}\left[1-\frac{(\alpha-p^2-Z)^2}{p^2}\right]\ln\left|\frac{\alpha-p^2-Z+p}{\alpha-p^2-Z-p}\right|-\frac{1}{p}\left[1-\frac{(\alpha-Z)^2}{p^2}\right]\ln\left|\frac{\alpha-Z+p}{\alpha-Z-p}\right|, \tag{B9}$$

and

$$\begin{aligned}S_1&=\max(1;1+p^2+2Z)-\max(1;Z^2/p^2+p^2+2Z),\\ S_2&=\min(1;100+p^2+2Z)-\min(1;\max(1;Z^2/p^2)+p^2+2Z),\end{aligned} \tag{B10}$$

$$I_3(\alpha)=\int_0^{10}dp\int_{-p}^{+p}dZ\,S_1(Z,p)\frac{A(\alpha,Z,p)(C\alpha,Z,p)}{1-2B(\alpha,Z,p)}+\int_0^{10}dp\int_{-10p}^{10p}dZ\,S_2(Z,p)\frac{A(\alpha,Z,p)(C\alpha,Z,p)}{1-B(\alpha,Z,p)}, \tag{B11}$$

where

$$(C\alpha,Z,p)=(Z-\alpha)\ln\left|\frac{Z-\alpha-p}{Z-\alpha+p}\right|-(Z-\alpha+p^2)\ln\left|\frac{Z-\alpha+p^2-p}{Z-\alpha+p^2+p}\right|, \tag{B12}$$

$$I_4(\alpha)=\int_0^{10}\frac{dp}{p^4}\int_{-p}^{+p}dZ\,S_1(Z,p)D(\alpha,Z,p)+\int_0^{10}\frac{dp}{p^4}\int_{-10p}^{+10p}dZ\,S_2(Z,p)D(\alpha,Z,p), \tag{B13}$$

where

$$D(\alpha,Z,p)=(Z+\alpha)\ln\left|\frac{Z+\alpha-p}{Z+\alpha+p}\right|-(Z+\alpha-p^2)\ln\left|\frac{Z+\alpha-p^2-p}{Z+\alpha-p^2+p}\right|. \tag{B14}$$