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Plasma Frequency of the Electron Gas in Layered Structures

M. Apostol

Institute of Atomic Physics, Bucharest-Magurele, Romania

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Abstract. The plasma frequency of a complete degenerate electron gas in the layered model of Visscher and Falicov is calculated by means of both the Bohm-Pines canonical transformation method and the equation-of-motion method in the RPA. The dispersion equation for plasmons is obtained in a finite system of n planes with both the cyclic condition and free ends. It is shown that the thermodynamic limit ($n \to \infty$) of the plasma frequency is independent of the boundary conditions. The previous results obtained by various authors in different ways are shown to be certain limits of our result.

1. Introduction

Recently, there has been much interest in the rather unusual properties of layered structures. The static dielectric response of a layered electron gas has been calculated by Visscher and Falicov [1]. The model consists of a succession of parallel equally spaced planes of electrons. The electrons are allowed to move freely in each plane in a neutralizing rigid background of positive charge but tunneling between planes is completely forbidden. This very anisotropic model could be made more realistic by including the momentum component of the electron normal to the planes and also the potential function that localizes the electrons to the planes. An attempt was done in this direction by Grecu [2], who generalized the model to include the electron tunneling between adjacent planes.

This paper is intended to apply many body techniques to the anisotropic layered model of Visscher and Falicov in order to calculate the plasma frequency at zero temperature. The more realistic model including the electron tunneling will be treated in the same manner in a forthcoming paper.

Fetter [3] approximated the electrons in this system by a macroscopic charged fluid and wrote down the electro-hydrodynamic equations for the ideal case of an infinite succession of planes. The plasma frequency given by him is

$$\omega^2(\kappa, k) = \omega_p^2 \frac{a k}{2} \frac{\sinh a k}{\cosh a k - \cos a \kappa} + s^2 k^2, \qquad (1)$$

where κ and $\mathbf{k}$ are the perpendicular to the plane and in-plane components of the wave vector, respectively, $\omega_p^2 = 4\pi N e^2/M a$ is the usual bulk plasma frequency (e = electron charge, M = electron mass, a = distance between two neighbouring planes, N = the number of electrons per unit area in each plane) and s is the adiabatic speed of sound in the two-dimensional Fermi gas of electrons. The same plasma frequency was obtained by Fetter imposing periodic conditions on the boundaries of a sample of n planes, the length of periodicity being taken equal to $n a$ (cyclic condition). The component κ of the wave vector is given by $\kappa = (2\pi/n a)\, p$, p any integer, and restricted to the first Brillouin zone, $-\pi/a \leq \kappa < \pi/a$. In the thermodynamic limit κ becomes a continuous variable which runs over this range.

The work of Fetter rises two problems. First, it is necessary to give a dispersion relation like (1) by means of the many body techniques, treating the electrons as a set of quantum mechanical particles which interact through the Coulomb potential*. Secondly, it is known that the actual physical systems which are experimentally investigated consist of a finite number of planes and their boundaries are free planes, that is no special condition is imposed on the boundary planes. Therefore, we must consider a finite system of n planes with free ends. It will be verified that the mathematical cyclic condition leads to a plasma frequency which corresponds to the physical free-ends condition in the thermodynamic limit, as it might be expected from the translational invariance of these systems.

In order to apply many body techniques for calculating the plasma frequency at non-zero values of the wave vector it must be pointed out that at finite values of κ the plasmons which propagate in different planes are appreciably coupled together through the electric field of the in-plane charge and at finite values of $\mathbf{k}$ the coupling between electrons and plasmons in each plane becomes unnegligible. Therefore, it is essential for our purpose to regard this quantum system as electrons + field and to take into account both the plasmon-plasmon and electron-plasmon coupling. These two requirements are fulfilled by the canonical transformation method developed many years ago by Bohm and Pines [4] for the isotropic three-dimensional electron gas. This approach starts with a quantized Hamiltonian of electrons and field and succeeds in decoupling the electron-plasmon interaction in first order of a perturbative scheme. Besides, this approach provides us with the oscillatory part (collective component) of the electron density operator. We are able to apply the equation-of-motion method with this operator. Moreover, in the framework of the Bohm-Pines theory, the effects of both cyclic and free-ends condition can be easily emphasized. For these reasons the Bohm-Pines method is applied in the next sections to the layered electron gas**.

The plasmon dispersion relation (1) will be obtained in which the macroscopic parameter s is given explicitly in terms of the microscopic theory and an additional quantum-mechanical k^4-term will appear. It will be shown that this plasma frequency corresponds to both the free-ends system in the thermodynamic limit and the system with cyclic condition.

2. The Bohm-Pines Canonical Transformation Method

As we have already mentioned, the system consists of n parallel equally spaced electron planes, the distance between two neighbouring planes being a. Electrons move freely in each plane but tunneling between planes is forbidden. The number of electrons per unit area in each plane is N. A uniform rigid background of positive charge exists in each plane, whose density is equal to the average electron density, in order to ensure the stability of the system. The sample of n planes is confined to a prismatic box with the base of unit area in the (y, z) plane and the height equal to L along the x direction, so that $L \neq n a$. Periodic conditions are to be imposed on the boundaries of this prism. Then we shall take the boundaries of the prism to infinity, as it is usually done in the quantization of the electromagnetic field with sources. The plasma frequencies will be given as the characteristic roots of an eigenvalue equation, which is easy to solve in the thermodynamic limit $(n \to \infty)$.

The electron density is

$$\rho(x, \mathbf{r}) = -e \sum_{mi} \delta(x - m a)\, \delta(\mathbf{r} - \mathbf{r}_{mi}), \tag{2}$$

where $\mathbf{r} = (y, z)$, m labels the planes, $m = -(n-1)/2, \ldots, (n-1)/2$ (n odd) and i labels the electrons in each plane. The summation is extended over all electrons of the system. The Fourier expansion of the electron density (2) is

$$\rho(x, \mathbf{r}) = -e L^{-1} \sum_{\mathbf{K}} \Big[\sum_{mi} \exp(-i \kappa m a) \exp(-i \mathbf{k}\, \mathbf{r}_{mi})\Big] \cdot \exp(i \kappa x) \exp(i \mathbf{k}\, \mathbf{r}), \tag{3}$$

where the values of the wave vector $\mathbf{K} = (\kappa, \mathbf{k})$ lie inside the infinite Fermi cylinder $0 < k \leq k_F = (2 \pi N)^{1/2}$, $-\infty < \kappa < +\infty$, $\kappa = (2 \pi / L)\, p$, p runs over all integers.

The Hamiltonian of the system may be written as

$$H = \sum_{mi} \mathbf{p}_{mi}^2 / 2M + 2 \pi e^2 L^{-1} \sum_{\substack{mi, m'i' \\ \mathbf{K}}} K^{-2} \exp[i \kappa (m - m')\, a] \cdot \exp[i \mathbf{k} (\mathbf{r}_{mi} - \mathbf{r}_{m'i'})] - 2 \pi e^2 n N L^{-1} \sum_{\mathbf{K}} K^{-2}, \tag{4}$$

where $\mathbf{p}_{mi}$ is the momentum of the mi-th electron.

It is convenient to introduce the longitudinal vector potential of the electromagnetic field

$$\mathbf{A}(x, \mathbf{r}) = (4 \pi c^2 / L)^{1/2} \sum_{\mathbf{K}} q_{\mathbf{K}}\, \boldsymbol{\varepsilon}_{\mathbf{K}} \exp(i \kappa x) \exp(i \mathbf{k}\, \mathbf{r}), \tag{5}$$

with $\boldsymbol{\varepsilon}_{\mathbf{K}} = \mathbf{K}/K$ a unit vector in the $\mathbf{K}$ direction and c – the light velocity. The electric field is

$$\mathbf{E}(x, \mathbf{r}) = (4 \pi / L)^{1/2} \sum_{\mathbf{K}} p_{-\mathbf{K}}\, \boldsymbol{\varepsilon}_{\mathbf{K}} \exp(i \kappa x) \exp(i \mathbf{k}\, \mathbf{r}), \tag{6}$$

where $p_{-\mathbf{K}} = -\dot{q}_{\mathbf{K}}$, and $q_{\mathbf{K}} = -q_{-\mathbf{K}}^{+}$, $p_{\mathbf{K}} = -p_{-\mathbf{K}}^{+}$. The field is quantized by the commutation relation

$$[q_{\mathbf{K}}, p_{\mathbf{K}'}] = i \hbar\, \delta_{\mathbf{K}\mathbf{K}'}. \tag{7}$$

* The equation-of-motion method has been applied by Grecu [2]. The plasma frequency obtained by him is the long-wavelength limit ($\kappa \to 0$, $k \to 0$) of Eq. (1).

** As regards the theoretical foundations of the Bohm-Pines theory we refer to the recent work of N. Shevchik [5].

The field variables $q_{\mathbf{K}}$ and $p_{\mathbf{K}}$ will be proved to be a convenient means of describing the collective modes (plasmons). As is well known, the $\mathbf{k}$ component of the wave vector of these plasmons is restricted to $k<k_c$, where the cut-off momentum k_c can be determined by minimizing the ground state energy [4]. The $\mathbf{k}$ indices which are beyond k_c correspond to the individual electron degrees of freedom. In order to carry out this splitting the first Bohm-Pines canonical transformation is applied in the in-plane RPA. The Hamiltonian (4) becomes equivalent to the Hamiltonian

$$H=H_{\text{part}}+H_{\text{sr}}+H_{\text{field}}+H_{\text{int}}, \tag{8}$$

which is used in conjunction with a set of subsidiary conditions acting on the wave function of the system

$$\Omega_{\mathbf{K}}\,\psi=0 \quad \text{for } k<k_c, \tag{9}$$

$$p_{\mathbf{K}}\,\psi=0 \quad \text{for } k\geqq k_c, \tag{9'}$$

where

$$\Omega_{\mathbf{K}}=p_{-\mathbf{K}}-i(4\pi e^2/LK^2)^{1/2} \cdot \sum_{mi}\exp(-i\kappa m a)\exp(-i\mathbf{k}\,\mathbf{r}_{mi}). \tag{10}$$

The subsidiary conditions (9), (9′) originate in the Maxwell equation $\operatorname{div}\mathbf{E}(x,\mathbf{r})-4\pi\rho(x,\mathbf{r})=0$. It is easy to verify that the Bohm-Pines theorem, the exact lowest state wave function automatically satisfies the subsidiary conditions (9), is valid also in our case of the layered structure. The conditions (9′) are satisfied provided the wave function does not depend on the variables $q_{\mathbf{K}}$ for $k\geqq k_c$.

In the Hamiltonian (8) H_{part} contains the kinetic energy of all electrons from which the Coulomb self-energy corresponding to the plasma degrees of freedom is subtracted,

$$H_{\text{part}}=\sum_{mi}\mathbf{p}_{mi}^2/2M-2\pi e^2 n N L^{-1}\sum_{\substack{\kappa\mathbf{k}\\ k<k_c}}K^{-2}. \tag{11}$$

These electrons interact through the short range Coulomb potential

$$H_{\text{sr}}=2\pi e^2 L^{-1}\sum_{\substack{mi,\,m'i',\,\kappa\mathbf{k}\\ m\neq m',\,i\neq i',\,k\geq k_c}}K^{-2}\exp[i\kappa(m-m')a] \cdot\exp[i\mathbf{k}(\mathbf{r}_{mi}-\mathbf{r}_{m'i'})]. \tag{12}$$

The long range Coulomb interaction is responsible for the plasma oscillations which are described by

$$H_{\text{field}}=-\tfrac{1}{2}\sum_{\substack{\kappa\mathbf{k}\\ k<k_c}}\Big[p_{\kappa\mathbf{k}}\,p_{-(\kappa\mathbf{k})}+2\pi L^{-1}\sum_{\kappa'}\omega(\kappa,k)\,\omega(\kappa',k) \cdot g_n(\kappa-\kappa')\,q_{\kappa\mathbf{k}}\,q_{-(\kappa'\mathbf{k})}\Big], \tag{13}$$

where $\omega(\kappa,k)$ is given by

$$\omega(\kappa,k)=\omega_p\frac{k}{K} \tag{14}$$

and

$$g_n(\kappa-\kappa')=a(2\pi)^{-1}\sum_{m=-(n-1)/2}^{(n-1)/2}\exp[i(\kappa-\kappa')\,m a]. \tag{15}$$

H_{field} represents the Hamiltonian appropriate to a set of oscillators which are coupled together through the matrix $\omega(\kappa,k)\,\omega(\kappa',k)\,g_n(\kappa-\kappa')$. This plasmon-plasmon coupling comes from the fact that the plasmons propagate in a finite system of n planes and they are not allowed to leave the planes while the electromagnetic waves which generate them take any spatial direction. This plasmon Hamiltonian can be easily diagonalized, as it will be shown in the next section. In so doing, only the interaction between plasmons in different planes is taken into account. But, there is, in addition, another coupling between electrons and plasmons in each plane. It is given by

$$H_{\text{int}}=(4\pi/L)^{1/2}\,e\,M^{-1}\sum_{\substack{mi,\,\kappa\mathbf{k}\\ k<k_c}}\frac{\mathbf{k}}{K}\left(\mathbf{p}_{mi}-\frac{\hbar\mathbf{k}}{2}\right)q_{\mathbf{K}} \cdot\exp(i\kappa m a)\exp(i\mathbf{k}\,\mathbf{r}_{mi}). \tag{16}$$

In order to eliminate both the electron-plasmon coupling and the plasmon-plasmon coupling to a good degree of accuracy, not only in the Hamiltonian but also in the subsidiary conditions, the second Bohm-Pines canonical transformation is applied in the in-plane RPA. The extent to which we are successful in carrying out this decoupling is measured by the expansion parameter

$$\alpha=(k p_F/M\omega)^2, \tag{17}$$

where p_F is the Fermi momentum and ω is the plasma frequency. The condition $\alpha<1$ is fulfilled for sufficiently small values of k (as we shall see in the next section). Thus, the leading contributions are given by the first terms in the expansion of both the Hamiltonian and the subsidiary conditions performed by the second canonical transformation. It can be shown [4] that the effect of this transformation on H_{sr} (which act to damp the plasma oscillations) is small enough to be neglected here. Under these conditions the decoupling is accomplished up to the first power of α.

As it is usually, the plasmon creation and destruction operators of frequency ω are introduced by the relations

$$q_{\mathbf{K}}=(\hbar/2\omega)^{1/2}(a_{\mathbf{K}}-a_{-\mathbf{K}}^{+}),$$

$$p_{\mathbf{K}}=i(\hbar\omega/2)^{1/2}(a_{\mathbf{K}}^{+}+a_{-\mathbf{K}}). \tag{18}$$

The plasma frequency ω has to be determined according to the condition that, up to the first power of α, there should be no electron-plasmon coupling either in the Hamiltonian or in the subsidiary conditions, in the new representation performed by the second canonical transformation. The dispersion equation which results from here eliminates also the plasmon-plasmon coupling to the same degree of accuracy.

The second Bohm-Pines canonical transformation is performed from the old set of operators $(\mathbf{r}_{mi}, \mathbf{p}_{mi}, a_{\mathbf{K}}, a_{\mathbf{K}}^+)$ to the new set of operators $(\mathbf{R}_{mi}, \mathbf{P}_{mi}, A_{\mathbf{K}}, A_{\mathbf{K}}^+)$, according to the relations

$$\mathbf{r}_{mi} = \exp(-i\,S/\hbar)\,\mathbf{R}_{mi}\exp(i\,S/\hbar) \tag{19}$$

and so on, the generator S being given by

$$S = -i(e/M)\sum_{\substack{mi,\,\kappa\mathbf{k}\\ k<k_c}}(2\pi\hbar/\omega)^{1/2}\frac{\dfrac{\mathbf{k}}{K}\left(\mathbf{P}_{mi}-\dfrac{\hbar\,\mathbf{k}}{2}\right)A_{\mathbf{K}}}{\omega-\mathbf{k}\,\mathbf{P}_{mi}/M+\hbar\,k^2/2M}$$

$$\cdot\exp(i\,\kappa\,m\,a)\exp(i\,\mathbf{k}\,\mathbf{R}_{mi})+\text{h.c.} \tag{20}$$

The new Hamiltonian H_{new} can be calculated from

$$H_{\text{new}} = \exp(-i\,S/\hbar)\,\mathscr{H}\exp(i\,S/\hbar) = \sum_{l=0}^{\infty}\frac{(-i/\hbar)^l}{l!}[S,\mathscr{H}]_{(l)}, \tag{21}$$

where $\mathscr{H}$ is the same function of the new variables as H is of the old variables. This new Hamiltonian will be calculated up to the first power of α. This is achieved by keeping only the terms up to the first order commutators, at most. With this degree of accuracy and applying the in-plane RPA, the electron-plasmon coupling in the new operator of the subsidiary conditions, $(\Omega_{\mathbf{K}})_{\text{new}}$, is eliminated providing the following dispersion equation be satisfied:

$$\omega(\kappa,k)(2\pi L^{-1})\sum_{\kappa'}\omega(\kappa',k)\,g_n(\kappa-\kappa')\,A_{\kappa'\mathbf{k}}$$

$$=\mathscr{B}^{-1}(\omega,\mathbf{k})\,A_{\kappa\mathbf{k}}, \tag{22}$$

where $k<k_c$ and

$$\mathscr{B}(\omega,\mathbf{k}) = N^{-1}\sum_i[(\omega-\mathbf{k}\mathbf{P}_{mi}/M)^2-(\hbar\,k^2/2M)^2]^{-1}. \tag{23}$$

Assuming an isotropic Fermi distribution of electrons in each plane this quantity does not depend on m and may be expanded as

$$\mathscr{B}(\omega,\mathbf{k}) \cong \omega^{-2}[1+\tfrac{1}{4}(3+\beta^2)\,\alpha], \tag{24}$$

with $\beta = k/k_F$. The operator $(\Omega_{\mathbf{K}})_{\text{new}}$ is

$$(\Omega_{\mathbf{K}})_{\text{new}} = \sum_{mi}\omega^2[\omega^2-(\mathbf{k}\,\mathbf{P}_{mi}/M-\hbar\,k^2/2M)^2]^{-1}$$

$$\cdot\exp(i\,\kappa\,m\,a)\exp(i\,\mathbf{k}\,\mathbf{R}_{mi}) \tag{25}$$

and contains only the individual electron coordinates. The new subsidiary conditions inhibit the long range fluctuations of electron density and favour the correlated plasma oscillations. The above operator provides us with the collective component of the electron density operator which oscillates harmonically with the frequency ω. It will be used in Section 4 in the equation-of-motion method.

There is a convenient grouping of terms in $\mathscr{H}$ which considerably simplifies the calculation of H_{new} in Eq. (21). Let us consider

$$\mathscr{H}_a = \sum_{mi}\mathbf{P}_{mi}^2/2M + \sum_{\substack{\kappa\mathbf{k}\\ k<k_c}}\frac{\hbar\,\omega}{2}(A_{\kappa\mathbf{k}}^+A_{\kappa\mathbf{k}}+A_{\kappa\mathbf{k}}A_{\kappa\mathbf{k}}^+), \tag{26}$$

the last term arising from

$$\mathscr{H}_{\text{field}} = \sum_{\substack{\kappa\mathbf{k}\\ k<k_c}}\frac{\hbar\,\omega}{2}(A_{\kappa\mathbf{k}}^+A\quad+A_{\kappa\mathbf{k}}A_{\kappa\mathbf{k}}^+)+\mathscr{H}_{\text{pl-pl}}, \tag{27}$$

where

$$\mathscr{H}_{\text{pl-pl}} = \sum_{\substack{\kappa\kappa'\mathbf{k}\\ k<k_c}}\frac{\hbar}{4\omega}[\omega^2\delta_{\kappa\kappa'}$$

$$-(2\pi L^{-1})\,\omega(\kappa,k)\,\omega(\kappa',k)\,g_n(\kappa-\kappa')]$$

$$\cdot[(A_{\kappa\mathbf{k}}A_{-(\kappa'\mathbf{k})}+A_{-(\kappa\mathbf{k})}^+A_{\kappa'\mathbf{k}}^+)-(A_{\kappa\mathbf{k}}A_{\kappa'\mathbf{k}}^++A_{\kappa'\mathbf{k}}^+A_{\kappa\mathbf{k}})]. \tag{28}$$

It is easy to verify that

$$\frac{i}{\hbar}[S,\mathscr{H}_a] = \mathscr{H}_{\text{int}}, \tag{29}$$

so that in Eq. (21) only the commutators

$$-\frac{i}{2\hbar}[S,\mathscr{H}_{\text{int}}]-\frac{i}{\hbar}[S,\mathscr{H}_{\text{pl-pl}}] \tag{30}$$

remain to be calculated. If the eigenvalue dispersion equation (22) is satisfied, $\mathscr{H}_{\text{pl-pl}}$ (which arises in Eq. (21) from $[S,\mathscr{H}]_{(0)}=\mathscr{H}$) cancels that part of the commutator $-(i/2\hbar)[S,\mathscr{H}_{\text{int}}]$ which contains only the plasmon variables. With the same dispersion equation the plasmon-plasmon term (28) of the Hamiltonian is proved to be proportional to α, so that its commutator with S in Eq. (30) will give contributions of order greater than α and, therefore, they will be neglected. In this way both the electron-plasmon and plasmon-plasmon decoupling is accomplished to the desired degree of approximation (first power of α).

The new Hamiltonian is

$$H_{\text{new}} = H_{\text{electron}}+H_{\text{plasmon}}+H_{\text{res part}}, \tag{31}$$

where

$$H_{\text{electron}}=\sum_{mi}\mathbf{P}_{mi}^2/2M-2\pi e^2 M^{-2} L^{-1}\sum_{\substack{mi,\kappa\mathbf{k}\\k<k_c}}(\mathbf{k}\mathbf{P}_{mi}/K)^2$$
$$\cdot\left[(\omega-\hbar k^2/2M)^2-(\mathbf{k}\,\mathbf{P}_{mi}/M)^2\right]^{-1}$$
$$-2\pi e^2 nNL^{-1}\sum_{\substack{\kappa\mathbf{k}\\k<k_c}}K^{-2}+\mathscr{H}_{sr},$$

$$H_{\text{plasmon}}=\sum_{\substack{\kappa\mathbf{k}\\k<k_c}}\frac{\hbar\omega}{2}(A^+_{\kappa\mathbf{k}}A_{\kappa\mathbf{k}}+A_{\kappa\mathbf{k}}A^+_{\kappa\mathbf{k}}),$$

$$H_{\text{res part}}=-\pi e^2 M^{-2}L^{-1}$$
$$\cdot\sum_{\substack{mi,m'i',\kappa\mathbf{k}\\m\neq m',i\neq i',k<k_c}}\frac{\left[(\mathbf{k}/K)\left(\mathbf{P}_{mi}-\frac{\hbar\mathbf{k}}{2}\right)\right]\left[(\mathbf{k}/K)\left(\mathbf{P}_{m'i'}+\frac{\hbar\mathbf{k}}{2}\right)\right]}{\omega(\omega-\mathbf{k}\mathbf{P}_{m'i'}/M-\hbar k^2/2M)}$$
$$\cdot\exp[i\kappa(m-m')a]\exp[i\mathbf{k}(\mathbf{R}_{mi}-\mathbf{R}_{m'i'})]+\text{h.c.}\qquad(32)$$

The second term in H_{electron} acts to increase the electron mass as a consequence of the inertial effect of the associated cloud of collective oscillations. The residual part $H_{\text{res part}}$ describes an extremely weak attractive velocity dependent electron-electron interaction which may be neglected in a first approximation, if a calculation of the ground state energy is in mind. H_{plasmon} represents a set of independent harmonic oscillators whose frequency ω will be determined in the next section.

3. Plasma Frequency

Letting $L\to\infty$ the eigenvalue dispersion equation (22) is converted into an integral equation

$$\omega(\kappa,k)\int_{-\infty}^{+\infty}d\kappa'\,\omega(\kappa',k)\,g_n(\kappa-\kappa')A_{\kappa'\mathbf{k}}=\mathscr{B}^{-1}(\omega,\mathbf{k})A_{\kappa\mathbf{k}}\qquad(33)$$

which is easy to solve in the thermodynamic limit. As is well known, $g_n(\kappa-\kappa')$ tends to $\delta(\kappa-\kappa'+G)$ for $n\to\infty$, where $G=(2\pi/a)p$, p running over all integers, are vectors in the reciprocal lattice of our layered structure. Therefore, the equation

$$\omega(\kappa,k)\sum_G\omega(\kappa+G,k)A_{\kappa+G\mathbf{k}}=\mathscr{B}^{-1}(\omega,\mathbf{k})A_{\kappa\mathbf{k}}\qquad(34)$$

is obtained, whose solution is

$$\mathscr{B}^{-1}(\omega,\mathbf{k})=\sum_G\omega^2(\kappa+G,k).\qquad(35)$$

The summation in Eq. (35) is easy to perform. By taking into account Eq. (14) we get [6]

$$\mathscr{B}^{-1}(\omega,\mathbf{k})=\omega_p^2\frac{ak}{2}\frac{\sinh ak}{\cosh ak-\cos a\kappa},\qquad(36)$$

or, with the expansion (24),

$$\omega^2=\omega_p^2\frac{ak}{2}\left[\frac{\sinh ak}{\cosh ak-\cos a\kappa}+\frac{1}{4}(3+\beta^2)k\right].\qquad(37)$$

This frequency is periodic in κ, with period $2\pi/a$, so that κ may be restricted to the first Brillouin zone, $-\pi/a\leqq\kappa<\pi/a$. The expansion parameter α is given by

$$\alpha=k\frac{\cosh ak-\cos a\kappa}{\sinh ak}\qquad(38)$$

and the cut-off momentum k_c must be restricted to those values of k for which $\alpha<1$. This condition is satisfied for sufficiently small values of $(\kappa,\mathbf{k})$ (κ restricted to the first Brillouin zone), but finite; these values represent the wave vectors of the plasmons.
The plasma frequency (37) corresponds to the free-ends system. If the cyclic condition $L=na$ is imposed, the summation in (15) yields

$$g_n^{\text{cyc}}(\kappa-\kappa')=na(2\pi)^{-1}\delta_{\kappa+G,\kappa'}\qquad(39)$$

and the solution of Eq. (22) has the form (37). In the thermodynamic limit $L=na\to\infty$, κ becomes a continuous variable and the two bands of plasma frequency (free-ends and cyclic condition) coincide.
If the electron-plasmon coupling H_{int} in Eq. (8) is neglected, the remaining plasmon-plasmon interaction in H_{field} (13) can be easily diagonalized by requiring $(L\to\infty)$

$$\omega(\kappa,k)\int_{-\infty}^{+\infty}d\kappa'\,\omega(\kappa',k)\,g_n(\kappa-\kappa')\,q_{-(\kappa'\mathbf{k})}=\omega^2 q_{-(\kappa\mathbf{k})}.\qquad(40)$$

This dispersion equation may be derived from Eq. (33) by taking $\alpha=0$ in the expansion (24) of the factor $\mathscr{B}(\omega,\mathbf{k})$. The frequency obtained in this way reduces to the first term in Eq. (37) (which contains κ-dependence). Thus, terms which contain even powers of k arise from the electron-plasmon coupling H_{int}, while the κ-band of frequencies is due to the interaction between plasmons in different layers. If one considers only a layer by taking $\alpha\to\infty$, Eq. (37) becomes

$$\omega^2=(2\pi e^2N/M)k\left[1+\tfrac{1}{4}(3+\beta^2)k\right],\qquad(41)$$

a dispersion relation which depends only on the wave vector $\mathbf{k}$.
The band of frequencies (37) is essentially the same as that given by Fetter in Eq. (1). There is only a difference in replacing s^2 from (1) by $\frac{3}{4}v_F^2$ and, in addition, a new k^4-term is contained in (37). The value of the adiabatic speed of sound at zero temperature, s, is also given by Fetter in terms of the thermodynamics of the two-dimensional Fermi gas being $s^2=\frac{1}{2}v_F^2$. This value differs from that obtained here in the framework of a

consistent microscopic theory ($\frac{3}{4}v_F^2$). The additional k^4-term is of the form $(\hbar k^2/2M)^2$. It does not appear in the classical limit $\hbar \to 0$, and, therefore, is a quantum mechanical effect of the electron-plasmon interaction. In consequence of the above discussion, it may be said that the plasma dispersion relation (1) represents the classical limit of that given in Eq. (37) by means of a quantum mechanical method. The asymptotic behaviour of (37) in the limit of long-wavelengths, $\kappa \to 0$, $k \to 0$, is the same as in Eq. (14) given in [2].

4. The Equation-of-Motion Method

The physical content of the subsidiary conditions (9) written in the new variables ($(\Omega_{\mathbf{K}})_{\text{new}}$ being given by (25)) results from the following identity which holds when the subsidiary conditions are satisfied:

$$\sum_{mi} \exp(i\kappa m a) \exp(i\mathbf{k}\mathbf{R}_{mi})\,\psi$$
$$= \sum_{mi} \frac{(\mathbf{k}\mathbf{P}_{mi}/M - \hbar k^2/2M)^2}{\omega^2 - (\mathbf{k}\mathbf{P}_{mi}/M - \hbar k^2/2M)^2}$$
$$\cdot \exp(i\kappa m a) \exp(i\mathbf{k}\mathbf{R}_{mi})\,\psi. \tag{42}$$

Hence it can be seen that the density fluctuations of long wavelength ($(\mathbf{k}\mathbf{P}_{mi}/M\omega) < \alpha < 1$) are reduced due to the fact that these density fluctuations are taken in the collective oscillations. The operator associated with these collective oscillations is furnished by the operator $(\Omega_{\mathbf{K}})_{\text{new}}$ as being

$$\rho^{\text{coll}}_{-(\kappa\mathbf{k})} = \sum_{mi} [\omega^2 - (\mathbf{k}\mathbf{p}_{mi}/M + \hbar k^2/2M)^2]^{-1}$$
$$\cdot \exp(i\kappa m a) \exp(i\mathbf{k}\mathbf{r}_{mi}). \tag{43}$$

This operator oscillates harmonically in the old representation ($\mathbf{r}_{mi}, \mathbf{p}_{mi}$) and its effect on the wave function is zero in the new representation ($\mathbf{R}_{mi}, \mathbf{P}_{mi}$) (as it is shown by the subsidiary conditions) because these new variables describe electron motion in the absence of any collective oscillation (there is no electron-plasmon coupling in H_{new}). The equation-of-motion method will be applied with this operator in the second quantization formalism.

The single-particle wave functions of the unperturbed eigenstates of electrons are given by

$$\varphi_{m\mathbf{k}}(x, \mathbf{r}) = \chi(x - ma) \exp(i\mathbf{k}\mathbf{r}). \tag{44}$$

The spin is disregarded for simplicity. The function $\chi(x - ma)$ is arbitrarily highly localized on the m-th plane and it is effectively the square root of a $\delta(x - ma)$ function [1]. The functions (44) are normalized to unity $(\varphi_{m\mathbf{k}}, \varphi_{m'\mathbf{k}'}) = \delta_{mm'}\delta_{\mathbf{k}\mathbf{k}'}$. The Hamiltonian of the system may be written as

$$H = \sum_{m\mathbf{k}} \varepsilon_k a^+_{m\mathbf{k}} a_{m\mathbf{k}} + Ma(2LN)^{-1}$$
$$\cdot \sum_{\substack{m_1 m_2 \\ \kappa\mathbf{k}\mathbf{k}_1\mathbf{k}_2}} k^{-2}\omega^2(\kappa, k) \exp[i\kappa(m_1 - m_2)a]$$
$$\cdot a^+_{m_1\mathbf{k}_1+\mathbf{k}} a^+_{m_2\mathbf{k}_2-\mathbf{k}} a_{m_2\mathbf{k}_2} a_{m_1\mathbf{k}_1}, \tag{45}$$

where $\varepsilon_k = \hbar^2 k^2/2M$, $\omega^2(\kappa, k)$ is given by Eq. (14) and $a_{m\mathbf{k}}(a^+_{m\mathbf{k}})$ is the annihilation (creation) operator of an electron localized on the plane m with the wave vector $\mathbf{k}$ ($\mathbf{k}=0$ is excluded). The electron density operator $\sum_{mi} \exp(i\kappa m a) \exp(i\mathbf{k}\mathbf{r}_{mi})$ is given in this representation by

$$\rho_{-(\kappa\mathbf{k})} = \sum_{m\mathbf{k}_1} \exp(i\kappa m a)\, a^+_{m\mathbf{k}_1+\mathbf{k}} a_{m\mathbf{k}_1}, \tag{46}$$

and the collective oscillation operator $\rho^{\text{coll}}_{-(\kappa\mathbf{k})}$ becomes

$$\rho^{\text{coll}}_{-(\kappa\mathbf{k})} = \sum_{m\mathbf{k}_1} [\omega^2 - (\hbar\mathbf{k}\mathbf{k}_1/M + \hbar k^2/2M)^2]^{-1}$$
$$\cdot \exp(i\kappa m a)\, a^+_{m\mathbf{k}_1+\mathbf{k}} a_{m\mathbf{k}_1}. \tag{47}$$

It is convenient to introduce (as in [4])

$$\xi_{-(\kappa\mathbf{k})}(\omega) = \sum_{m\mathbf{k}_1} [\omega - (\hbar\mathbf{k}\mathbf{k}_1/M + \hbar k^2/2M)]^{-1}$$
$$\cdot \exp(i\kappa m a)\, a^+_{m\mathbf{k}_1+\mathbf{k}} a_{m\mathbf{k}_1} \tag{48}$$

which is related to $\rho^{\text{coll}}_{-(\kappa\mathbf{k})}$ by

$$\rho^{\text{coll}}_{(\kappa\mathbf{k})} = \frac{1}{2\omega} [\xi_{-(\kappa\mathbf{k})}(\omega) - \xi_{-(\kappa\mathbf{k})}(-\omega)]. \tag{49}$$

If the $\xi_{-(\kappa\mathbf{k})}(\omega)$ satisfy

$$\dot{\xi}_{-(\kappa\mathbf{k})}(\omega) - i\omega\,\xi_{-(\kappa\mathbf{k})}(\omega) = 0, \tag{50}$$

then

$$\ddot{\rho}^{\text{coll}}_{-(\kappa\mathbf{k})} + \omega^2 \rho^{\text{coll}}_{-(\kappa\mathbf{k})} = 0. \tag{51}$$

By using the Heisenberg equation

$$\dot{\xi}_{-(\kappa\mathbf{k})}(\omega) = (i\hbar)^{-1} [\xi_{-(\kappa\mathbf{k})}(\omega), H],$$

it immediately follows

$$i\dot{\xi}_{-(\kappa\mathbf{k})}(\omega) + \omega\,\xi_{-(\kappa\mathbf{k})}(\omega) = \rho_{-(\kappa\mathbf{k})}$$
$$+ Ma(2\hbar LN)^{-1} \sum_{m\kappa'\mathbf{k}'\mathbf{k}_1} k'^{-2}\omega^2(\kappa', k') \exp[i(\kappa - \kappa')ma]$$
$$\cdot \{(\omega - \hbar\mathbf{k}\mathbf{k}_1/M + \hbar k^2/2M)^{-1}$$
$$- [\omega - \hbar\mathbf{k}(\mathbf{k}_1 + \mathbf{k}')/M + \hbar k^2/2M]^{-1}\}$$
$$\cdot [a^+_{m\mathbf{k}_1} a_{m\mathbf{k}_1-\mathbf{k}+\mathbf{k}'} \rho_{-(\kappa'\mathbf{k}')} + \rho_{-(\kappa'\mathbf{k}')} a^+_{m\mathbf{k}_1} a_{m\mathbf{k}_1-\mathbf{k}+\mathbf{k}'}]. \tag{52}$$

If the RPA ($\mathbf{k}' = \mathbf{k}$) is applied and the usual approximation

$$a^+_{m\mathbf{k}_1} a_{m\mathbf{k}_1} \to \langle a^+_{m\mathbf{k}_1} a_{m\mathbf{k}_1} \rangle = 1 \quad \text{for } k_1 \leq k_F$$

and

$$\langle a^+_{m\mathbf{k}_1} a_{m\mathbf{k}_1} \rangle = 0 \quad \text{for } k_1 > k_F$$

(Fermi distribution at zero temperature) is performed then Eq. (50) is satisfied by taking

$$\rho_{-(\kappa\mathbf{k})}\, 1 - 2\pi L^{-1} \sum_{\kappa'} \omega^2(\kappa', k)\mathscr{B}(\omega, \mathbf{k}) \cdot g_n(\kappa-\kappa')\rho_{-(\kappa'\mathbf{k})} = 0, \tag{53}$$

a dispersion equation which formally differs from Eq. (22) but which has the same solution (37).

It is possible to apply the equation-of-motion method with the electron density operator $\rho_{-(\kappa\mathbf{k})}$. The dispersion equation is, in this case,

$$\rho_{-(\kappa\mathbf{k})}\, 1 - 2\pi L^{-1} \sum_{\kappa'} k^{-2}\omega^2(\kappa', k)\mathscr{D}(\omega, \mathbf{k}) \cdot g_n(\kappa-\kappa')\rho_{-(\kappa'\mathbf{k})} = 0, \tag{54}$$

where

$$\mathscr{D}(\omega, \mathbf{k}) = MN^{-1} \sum_{\mathbf{k}_1} \frac{n_{\mathbf{k}_1} - n_{\mathbf{k}_1+\mathbf{k}}}{\hbar\omega + \varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}_1+\mathbf{k}}}, \tag{55}$$

$n_{\mathbf{k}}$ being the Fermi distribution at zero temperature. By a straightforward manipulation we get $\mathscr{D}(\omega, \mathbf{k}) = k^2\mathscr{B}(\omega, \mathbf{k})$, so that Eqs. (53) and (54) coincide.

For small values of k the leading term in (55) is k^2/ω^2, so that the plasma frequency is the first term (κ-dependent) in (37). Even powers of k could be added to this first term by expanding Eq. (55) further and so that the electron-plasmon interaction can be considered. In so doing, no estimate exists of the extent to which this interaction is taken into account. By using the operator $\rho^{\text{coll}}_{-(\kappa\mathbf{k})}$ the electron-plasmon coupling can be handled under control (up to the first power of α).

5. Conclusions

The Bohm-Pines theory was proved to be useful in calculating the plasma frequency in the layered electron gas of Visscher and Falicov in many respects. In the framework of this many body theory it is possible to take into account in a definite manner (up to the first power of α) both the electron-plasmon and the plasmon-plasmon coupling. The theory permits the dispersion equation (22) of the plasma frequency for a finite sample of n planes to be found and, thus, permits the part played by the boundary conditions to be investigated. The oscillatory component of the electron density operator is furnished by this theory; the equation-of-motion method can be applied with this operator.

The band of plasma frequency given by Eq. (37) represents a quantum mechanical extension of the classical result (1) obtained by Fetter [3]. The asymptotic behaviour of (37) for $\kappa \to 0$, $k \to 0$ is the same as that given by Grecu [2].

It was shown that the mathematical device of the cyclic condition leads, in the thermodynamic limit, to the plasma frequency of the physical free-ends system.

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M. Apostol
Laboratory of theoretical physics
Institute of Atomic Physics
P.O. Box 5206
Bucharest-Magurele
Romania