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Optical Properties of an Electron Gas in the Generalized Hartree-Fock Approximation

ALMA A. *G.* ***de*** **BASSI**

Instituto de Física Gleb Wataghin, UNICAMP, Campinas

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The dielectric constant and absorption coefficient of an electron gas whose ground state displays a static charge density wave with exchange interaction via a §-potential, is studied and applied to an alkali metal, sodium. An additional contribution to the absorption coefficient was found which manifests itself in the form of a band that precedes and overlaps with the initial part of the interband contribution. Furthermore, this contribution is several orders of magnitudes smaller than the interband contribution so that it can only be detected using very high resolution instruments.

A constante dielétrica e o coeficiente de absorção de um gás de eletrons cujo estado fundamental apresenta uma densidade estática de carga com interação de troca via um potencial § são estudados e aplicados a um metal alcalino, o sódio Uma contribuição adicional ao coeficiente de absorção foi encontrada, manifestando-se na forma de uma banda que precede e se superpõe à parte inicial da contribuição interbanda. Além disso, esta contribuição é menor, por várias ordens de grandeza, que a contribuição interbanda, de modo que só pode ser detetada pelo de instrumentos de alta resolução.

1. INTRODUCTION

Many optical experiments are capable of furnishing information concerning solid state properties. In general, solids are classified as metals and insulators with intermediate cases being called semiconductors[1]. Although this classification is based primarily on electrical conductivity, the charge carriers also influence optical propertiessuch that insulators tend to be transparent and metals opaque in the visible part of the spectrum. Semiconductors tend to be opaque in the visible region and transparent in thc infrared.

Generally optical properties are studied by measurements ofthe reflectivity at normal incidence, followed by a Kraners - Kronig analysis relating the real and imaginary parts of $\varepsilon(\omega)$. Thus two parts of the dielectric constant, eãch dependent on frequency, $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, or the optical constants, $\eta(\omega)$ and $\kappa(\omega)$, are obtained^2.

In the usual experiments, the optical properties of metais are associated with their high reflectivities and low transmission. Ina more quantitative way, these optical properties are given in terms of two material constants, the index of refraction η and the coefficient of extinction κ, which allow one to relate the complex dielectric constant to observables such as the reflectivity. In metals, because of their high optical absorption at low frequencies, the effects caused by free charge carriers arealmost always studied by application of reflectivity techniques. The conductivity of these free charge carriers appears to be well explained by Drude's theory. On the other hand the manifestations caused by free charge carriers in semiconductors are usually more conveniently studied using absorption techniques.

In solid state studies we must also consider the contributions of various electronic processes of energy bands on the optical properties. Among these contributions, the intraband process, which corresponds to electronic conduction by free charge carriers, is important in conductors such as metals and degenerate semiconductors.

The interaction between itinerant electrons in the interior of the metal can be studied by means of the response of the metal toa charge which varies with time and space. The function which describes this type of interaction is the dielectric constant, which is dependent on the wave vector, q, and the frequency, ω. With the object ofstudying the dielectric constant and the absorption coefficient of an electron gas, as well as its applications to alkali metals, we investigate here the dielectric constant of an electron gas whose ground state corresponds to the state of a static charge density wave in the form proposed by Overhauser[3]. We will discuss the modifications which the dielectric constant and absorption coefficient suffer in relation to their respective values in normal metals (NHF).

2. THE GENERALIZED HARTREE-FOCK APPROXIMATION (GHF): THE STATIC CHARGE DENSITY WAVE STATE

The normal Hartree-Fock approximation (NHF) describes the wave function by means of a single Slater determinant formed using electron functions of the type $\phi_{K\sigma}(\xi)$. We propose to modify the Slater determinant by using one-particle wave functions of the type

$$u_K\phi_K(r)\,|\sigma> + v_K\phi_{K+Q}(r)\,|\sigma'> ,$$

where the $\phi_K(r)$ are NHF solutions with u_K and v_K normalized such that $u_K^2 + v_K^2 = 1$. These last two quantities are variational parameters specified by the minimization of the total energy. The many-particle wavefunctions will be given by

$$\psi_{GHF} = \det\|\,u_K\phi_K(r)\,|\sigma> + v_K\phi_{K+Q}(r)\,|\sigma'>\| = \det\|\,\phi(r,\xi)\,\| \qquad (1)$$

The second quantization formalism will be used because it permits considerable simplification of the mathematical treatment and is more adequate for our present work. The basic Hamiltonian of the system consisting of an electron gas of point particles immersed in a neutralizing, continuous distribution of positive charge, is

$$H = \sum_{K,\sigma} \varepsilon_K^0\, C^+_{K\sigma} C_{K\sigma} + \frac{1}{2} \sum_{\substack{K,K',q\\ \sigma,\sigma'}} <K+q, K'-q|V|K',K> \, C^+_{K+q\sigma}\, C^+_{K'-q\sigma'} C_{K\sigma'} C_{K\sigma} , \qquad (2)$$

where the first term of the RHS of Eq. (2) is the Bloch-band hamiltonian and the second represents the interaction between the electrons. The equation of motion for $C^+_{K\sigma}$ is

$$[H, C^{+}_{K\sigma}] = \varepsilon^{0}_{K} C^{+}_{K\sigma} + \sum_{\substack{K',q\\ \sigma,\sigma'}} \langle K+q, K'-q | V | K', K \rangle \, C^{+}_{K+q\sigma} \, C^{+}_{K'-q\sigma'} \, C_{K'\sigma'} \tag{3}$$

The linearization of the generalized Hartree-Fock approximation, using wave function (1) gives

$$\langle C^{+}_{K\sigma} \, C_{K'\sigma'} \rangle = n_{K\sigma} \, \delta_{KK'} \, \delta_{\sigma\sigma} \, ,$$

and

$$\langle C^{+}_{K\sigma} \, C_{K'\sigma'} \rangle = b_{K\sigma} \, \delta_{KK'-Q} \, \delta_{\sigma\sigma'} \quad ,$$

where Q is a wave vector to be specified. Taking the interaction term of Eq.(3) and all the possible combinations of the operator pairs we obtain

$$[H, C^{+}_{K\sigma}] = \varepsilon^{0}_{K} C^{+}_{K\sigma} + \sum_{K',\sigma'} \langle K, K' | V | K', K \rangle \, n_{K'\sigma'} C^{+}_{K\sigma}$$

$$- \sum_{K'} \langle K', K | V | K', K \rangle \, n_{K'\sigma} C^{+}_{K\sigma} + \sum_{K',\sigma'} \langle K+Q \; K'-Q | V | K', K \rangle$$

$$b_{K'\sigma'} C^{+}_{K+Q\sigma} - \sum_{K'} \langle K', K+Q | V | K'+Q, K \rangle b_{K'\sigma} C^{+}_{K+Q\sigma'}$$

where we can immediately identify one part of this equation as the normal Hartree-Fock energy given by

$$\varepsilon^{0}_{K} + i_{K',\sigma'} \langle K, K' | V | K', K \rangle n K'\sigma' - \sum_{K'} \langle K', K | V | K', K \rangle n_{K'\sigma} = \varepsilon^{NHF}_{K} \; .$$

The other term we call

$$\Delta_{K} = \sum_{K',\sigma'} \langle K+Q, K'-Q | V | K', K \rangle b_{K'\sigma'} - \sum_{K'} \langle K', K+Q | V | K'+Q, K \rangle b_{K'\sigma}$$

Then

$$[H, C^+_{K\sigma}] = i\hbar C^+_{K\sigma} = \omega C^+_{K\sigma} = \varepsilon^{NHF}_{K} C^+_{K\sigma} - \Delta_K C^+_{K+Q\sigma} \tag{4}$$

This equation of motion, as compared with Eq. (3) contains one more term involving the operator $C^+_{K+Q\sigma}$, whose equation of motion is

$$[H, C^+_{K+Q\sigma}] = \varepsilon^0_{K+Q} C^+_{K+Q\sigma} + \sum_{K',\sigma',q} \langle K+Q+q, K'-q|V|K', K+Q\rangle$$

$$C^+_{K+Q+q\sigma} \quad C^+_{K'+q\sigma'} \quad C_{K'\sigma'}$$

The generalization of the Hartree-Fock approximation then produces

$$[H, C^+_{K+Q\sigma}] = i\hbar C_{K+Q\sigma} = \omega C^+_{K+Q\sigma} = \varepsilon^{NHF}_{K+Q} C^+_{K+Q\sigma} - \Delta^*_K C^+_{K\sigma} \tag{5}$$

Letting $\varepsilon^{NHF}_K = \tilde{\varepsilon}_K$ Eqs. (4) and (5) can be rewritten as

$$(\omega - \tilde{\varepsilon}_K) C^+_{K\sigma} + \Delta_K C^+_{K+Q\sigma} = 0$$

$$\Delta^*_K C^+_{K\sigma} + (\omega - \tilde{\varepsilon}_{K+Q}) C^+_{K+Q\sigma} = 0$$

whose secular determinant is

$$\begin{vmatrix} (\omega - \tilde{\varepsilon}_K) & \Delta_K \\ \Delta^*_K & (\omega - \tilde{\varepsilon}_{K+Q}) \end{vmatrix} = 0 \tag{6}$$

Solving this equation we obtain the new energy spectra of the quasi-particles,

$$\omega^{\pm} = \frac{1}{2} (\tilde{\varepsilon}_{K+Q} - \tilde{\varepsilon}_K) \pm \sqrt{\frac{1}{4} (\tilde{\varepsilon}_{K+Q} - \tilde{\varepsilon}_K)^2 \; |\Delta_K|^2}$$

To calculate the total system energy in its ground state we fix the wave number Q as half a reciprocal lattice vector and set $|\sigma\rangle = |\sigma'\rangle$ for the wave functions of the quasi-particles. In this way the self consistent potential has a periodicity of twice that of the lattice potential with the first Brillouin zone reduced to one **half.** The ground state energy can then be written as

$$E_0 = \sum_{K,\sigma}^{(1)} \left[\tilde{\varepsilon}_K \cos^2\theta_K + \tilde{\varepsilon}_{K+Q} \sin^2\theta_K - \Delta_K \sin^2\theta_K\right]$$

where $\Sigma_{K\sigma}^{(1)}$ is a sum over the new reduced Brillouin zone.

The wave function of the ground state has been selected to be

$$|\psi_0> = \prod_{K,\sigma}^{(1)} \left[\cos\theta_K C^{+}_{K\sigma} + \sin\theta_K C^{+}_{K+Q\sigma}\right]|0>$$

which indicates that the first N states of a quasi-particle of lowest energy $\bar{\omega}_K$ are occupied. Minimizing this energy with respect to 0_K one has

$$\mathrm{tg}2\theta_K = \frac{2\Delta_K}{\tilde{\varepsilon}_{K+Q} - \tilde{\varepsilon}_K} ,$$

where

$$\Delta_K = \sum_{K'}^{(1)} \left[V(Q) - V(K-K')\right] \sin\theta_{K'}\cos\theta_{K'} =$$

$$= \sum_{K'}^{(1)} \frac{\Delta_{K'}\left[V(Q) - V(K-K')\right]}{\sqrt{(\tilde{\varepsilon}_{K'\,Q} - \tilde{\varepsilon}_{K'})^2 + 4\Delta^2_{K'}}} \qquad (7)$$

which is the self consistent equation. Here $V(Q) = <K+Q, K'-Q|V|K;K>$ and $V(K-K') = <K',K+Q|V|K'+Q,K>$.

Utilizing the wave function selected by GHF, the charge density becomes

$$\rho(r) = \sum_{K}^{(1)} |\cos^2\theta_K|\phi_K(r)|^2 + \sin^2\theta_K|\phi_{K+Q}(r)|^2 + \sin\theta_K\cos\theta_K$$
$$\left[\phi^{*}_K(r)\,\phi_{K+Q}(r) + \phi^{*}_{K+Q}(r)\quad \phi_K(r)\right]$$

Approximating the function ϕ by plane waves this equation becomes

$$\rho(r) = 1 + \frac{1}{N}\sum_K^{(1)} \sin 2\theta_K \cos(Q.r) = 1 + A\cos(Q.r), \qquad (8)$$

where

$$A = \frac{1}{N}\sum_K^{(1)} \sin 2\theta_K = \frac{1}{N}\sum_K^{(1)} \frac{2\Delta_K}{\sqrt{(\varepsilon_{K+Q}-\varepsilon_K)^2 + 4\Delta_K^2}} .$$

Since $\sin 2\theta_K$ is proportional to Δ_K it goes to zero as Δ_K goes to zero and therefore $\rho(r)=1$ which is the normal state charge density with plane waves, as it should be. Eq. (8) clearly shows that the ground state of the system described by the wave function, $|\psi_0>$, develops a static charge density wave with periodicity $\lambda = 2\pi/|Q|$. It is easy to verify that the magnetic density is zero and therefore magnetic order is not present. We will denote states described in this way as "non-normal" metallic states.

3. DIELECTRIC CONSTANT

We introduce a test charge in the system defined by Eq.(2) and consider that this charge varies spacially and temporally following the expression

$$er_0\, e^{i(q.r - \omega t)} - C.C.$$

This density of external charge introduced in the gas at a point **r** is relevant vector $D(r,t)$ by means of Poisson's equation[4],

$$\text{div } D(r,t) = 4\pi e r_0 (e^{i(q.r - \omega t)} + C.C) \qquad (9)$$

The external field acts to polarize the system of electrons. The fluctuations of induced charge can be considered as responsible for the field E_p. According to the laws of electrostatics the electric field within the system is

$$E(r,t) = D(r,t) + E_p(r,t) , \qquad (10)$$

where $E_p(r,t)$ can be related to the polarization charge density by the equation

$$\mathrm{div}\, E_p(r,t) = 4\pi e \;\langle\rho(r,t)\rangle \tag{11}$$

Taking the divergence of (10) and substituting into it the values given by (9) and (11) we obtain

$$\mathrm{div}\, E(r,t) = 4\pi e(r_0 + \langle\rho(r,t)\rangle) \tag{12}$$

which is the equation that relates the electric field to the fluctuations of externa1 and induced charge. Taking the Fourier transforms of (9) and (12) we have

$$\mathrm{iq}\; D(q,\omega) = 4\pi e r_0 \tag{13a}$$

and

$$\mathrm{iq}\; E(q,\omega) = 4\pi e(r_0 + \langle\rho(q,\omega)\rangle) \tag{13b}$$

For a macroscopic field these equations express the usual laws of electrostatics for a dielectric material. Extending them to the microscopic level and considering them applicable to all the wave vectors q and frequencies ω, they correspond to fields that vary in an arbitrary (and rapid) way in space and time. Besides this, in analogy with the electrostatic laws[4], we write in the linear approximation

$$E(q,\omega) = \frac{D(q,\omega)}{\varepsilon(q,\omega)} \tag{14}$$

Here $\varepsilon(q,\omega)$ is the dielectric constant dependent on the frequency w and wave vector q. In other words it is the generalization (to fields that vary in space and time) of the homogeneous dielectric constant of the electrostatic.

Taking the value of $D(q,\omega)$ in Eq.(14) and substituting it into (13a), inverting the order of Eqs. (13) and dividing them member by member we have

$$\frac{1}{\varepsilon(q,\omega)} - 1 = \frac{\langle\rho(q,\omega)\rangle}{r_0} = 4\pi\chi(q,\omega) \;, \tag{15}$$

where $\chi(q,\omega)$ is the electric susceptibility of the system. At this point we use the Green's function technique described in the classic article by Zubarev[5]. We can express

$$\chi(q,\omega) = -2 \, \frac{\langle\langle \rho(q) | V(0) ; \omega \rangle\rangle}{r_0} , \qquad (16)$$

where <<.....>> is abreviated notation for the corresponding Green function.

The interaction energy with a test charge is given by

$$V(t) = \frac{4\pi e^2}{q^2} \left[r_0 \rho^+(q,t) \, e^{-i\omega t} + C.C. \right] ,$$

where

$$\rho(q) = \sum_{K\sigma} C^+_{K+q\sigma} \, C_{K\sigma}$$

and $C^+_{K+q\sigma}$ and $C_{K\sigma}$ are respectively creation operator of a electron spin in plane wave states, $|K + q\rangle$, and anihilation operator of o electron spin in the state $|K\rangle$. Applying these values to Eq.(16) we have

$$\chi(q,\omega) = \frac{8\pi^2 e^2}{q^2} \sum_{\substack{K,\sigma \\ K',\sigma'}} \langle\langle C^+_{K+q\sigma} \, C_{K\sigma} | C^+_{K'\sigma'} C_{K'+q\sigma'} \; ; \; \omega + is \rangle\rangle \qquad (17)$$

It remains to resolve the equations of motion for Green's functions for pairs of operators $C^+_{K+q\sigma} C_{K\sigma}$ and $C_{K+Q+q\sigma} C_{K+Q\sigma}$. Instead of invoking the NHF approximation we use the generalized Hartree-Fock form discussed in Section 2.

Performing the required analysis we obtain in the following results:

$$\left[C^+_{K+q\sigma} \, C_{K\sigma}, H \right] = (\varepsilon^{HF}_K - \varepsilon^{HF}_{k+q}) \, C^+_{K+q\sigma} C_{K\sigma} - (n_{K\sigma} - n_{K+q\sigma}) \, V(q)$$

$$\sum_{K'\sigma'} C^+_{K'+q\sigma'} \, C_{K'\sigma'} + b_{K\sigma} \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} C^+_{K'+q\sigma'} C_{K'+Q\sigma'} - b_{K+q\sigma}$$

$$\sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} C^+_{K'+Q+q\sigma'} C_{K'\sigma'} - \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} C^+_{K+q\sigma} C_{K+Q\sigma}$$

$$+ \sum_{K'\sigma'} b_{K'+q\sigma'} W_{\sigma\sigma'} C^+_{K+Q+q\sigma} C_{K\sigma} \qquad (18)$$

$$
\begin{aligned}
\left[C^{+}_{K+Q+q\sigma}\, C_{K+Q\sigma}, H\right] = {} & (\varepsilon^{HF}_{K+Q} - \varepsilon^{HF}_{K+Q+q})\, C^{+}_{K+Q+q\sigma} C_{K+Q\sigma} \\
& -(n_{K+Q\sigma} - n_{K+Q+q\sigma}) V(q) \sum_{K'\sigma'} C^{+}_{K'+q\sigma'} C_{K'\sigma'} + b_{K\sigma} \sum_{\sigma'} \\
& W_{\sigma\sigma'} \sum_{K'} C^{+}_{K'+Q+q\sigma'} C_{k'\sigma'} - b_{K+q\sigma} \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} C^{+}_{K'+q\sigma'} \\
& C_{K'+Q\sigma'} - \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} C_{K+Q+q\sigma}\, C_{K\sigma} + \sum_{K'\sigma'} b_{K'+q\sigma'} \\
& W_{\sigma\sigma'}\, C^{+}_{K+q\sigma}\, C_{K+Q\sigma} \quad ,
\end{aligned}
\tag{19}
$$

where

$$
n_{K\sigma} = < C^{+}_{K\sigma}\; C_{K\sigma} >
$$

$$
b_{K\sigma} = < C^{+}_{K\sigma}\; C_{K+Q\sigma} >
$$

and $\sum_{\sigma'} W_{\sigma\sigma'} = \sum_{\sigma'} \left[U\delta_{\sigma\sigma'} - V(Q)\right]$ is the interaction energy. This energy is the difference between the exchange interaction (which we approximated by a contect-type interaction of strenght U) and the direct coulombic contribution associated with a component Q of electronic charge density. As we can see Eqs. (18) and (19) are coupled to the pairs of operators $C^{+}_{K+Q+q\sigma} C_{K\sigma}$ and $C^{+}_{K+q\sigma} C_{K+Q\sigma}$. We have then the calculated equations of motions for Green's functions of these pair of operators

$$
\begin{aligned}
\left[C_{K+Q+q\sigma} C_{K\sigma}, H\right] = {} & (\varepsilon^{HF}_{K} - \varepsilon^{HF}_{K+Q+q})\; C^{+}_{K+Q+q\sigma}\; C_{K\sigma} \\
& + (n_{K\sigma} - n_{K+Q+q\sigma}) \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} C^{+}_{K'+Q+q\sigma'} C_{K'\sigma'} \\
& - b_{K\sigma}\; V(q) {}_{K'\sigma'}\; C^{+}_{K'+Q+q\sigma'} C_{K'+Q\sigma'}\; b_{K+q\sigma}\; V(q)
\end{aligned}
\tag{20}
$$

$$\sum_{K'\sigma'} C^+_{K'+q\sigma'} C_{K'\sigma'} - \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} C^+_{K+Q+q\sigma}$$

$$C_{K+Q\sigma} + \sum_{K'\sigma'} b_{K'+q\sigma'} W_{\sigma\sigma'} C^+_{K+q\sigma} C_{K\sigma}$$

and

$$\begin{aligned}
[C^+_{K+q\sigma} C_{K+Q\sigma}, H] &= (\varepsilon^{\mathrm{HF}}_{K+Q} - \varepsilon^{\mathrm{HF}}_{K+q}) C^+_{K+q\sigma} C_{K+Q\sigma} \\
&-(n_{K+q\sigma} - n_{K+Q\sigma}) \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} C^+_{K'+q\sigma'} C_{K'+Q\sigma'} \\
&-b_{K\sigma} V(q) \sum_{K'\sigma'} C^+_{K'+q\sigma'} C_{K'\sigma'} + b_{K+q\sigma} V(q) \sum_{K'\sigma'} \\
&C^+_{K'+Q+q\sigma'} C_{K'+Q\sigma'} - \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} C^+_{K+q\sigma} C_{K\sigma} \\
&+ \sum_{K'\sigma'} b_{K'+q\sigma'} W_{\sigma\sigma'} C^+_{K+Q+q\sigma} C_{K+Q\sigma} \ .
\end{aligned} \tag{21}$$

Adding to these four equations their respective independent terms and summing over Ku we obtain the system of equations

$$\begin{aligned}
\sum_{K\sigma} \langle\langle C^+_{K+q\sigma} C_{K\sigma} | \overset{+}{\rho}(q) ; \omega + is \rangle\rangle &= - \frac{1}{2\pi} \sum_{K\sigma} \frac{n_{K\sigma} - n_{K+q\sigma}}{\Omega_K} \\
&\sum_{K\sigma} \frac{n_{K\sigma} - n_{K+q\sigma}}{\Omega_K} V(q) \sum_{K'\sigma'} \langle\langle C^+_{K'+q\sigma'} C_{K'\sigma'} | \rho^+(q) ; \omega + is \rangle\rangle \\
&+ \sum_{K\sigma} \frac{b_{K\sigma} - b_{K+q\sigma}}{\Omega_K} \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} \langle\langle C^+_{K'+Q+q\sigma'} C_{K'\sigma} | \rho^+(q) ; \omega + is \rangle\rangle \\
&- \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{\langle\langle C^+_{K+q\sigma} C_{K+Q\sigma} | \rho^+(q) ; \ \omega + is \rangle\rangle}{\Omega_K} \\
&+ \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{\langle\langle C^+_{K+Q+q\sigma} C_{K\sigma} | \rho^+(q) ; \ \omega + is \rangle\rangle}{\Omega_K}
\end{aligned} \tag{22}$$

$$\sum_{K\sigma} << C^{+}_{K+Q+q\sigma}\ C_{K+Q\sigma} | \rho^{+}(q)\ ;\ \omega + is >> = -\frac{1}{2\pi} \sum_{K\sigma} \frac{n_{K+Q\sigma} - n_{K+Q+q\sigma}}{\Omega_{K+Q}}$$

$$- \sum_{K\sigma} \frac{n_{K+Q\sigma} - n_{K+Q+q\sigma}}{\Omega_{K+Q}} V(q) \sum_{K'\sigma'} << C^{+}_{K'+Q+q\sigma'} , C_{K'+Q\sigma'} | \rho^{+}(q)\ ; \omega + is >>$$

$$+ \sum_{K\sigma} \frac{b_{K\sigma} - b_{K+q\sigma}}{\Omega_{K+Q}} \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} << C^{+}_{K'+q\sigma'} , C_{K'+Q\sigma'} | \rho^{+}(q)\ ;\ \omega + is >>$$

$$- \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{<< C^{+}_{K+Q+q\sigma}\ C_{K\sigma} | \rho^{+}(q)\ ; \omega + is >>}{\Omega_{K+Q}}$$

$$+ \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{<< C^{+}_{K+q\sigma}\ C_{K+Q\sigma} | P^{+}(q)\ ;\ \omega + is >>}{R_{K+Q}}$$

$$\sum_{K\sigma} << C^{+}_{K+Q+q\sigma}\ C_{K\sigma} | \rho^{+}(q)\ ;\ \omega + is >> = - \frac{1}{2\pi} \sum_{K\sigma} \frac{b_{K\sigma} - b_{K+q\sigma}}{\Omega'_{K}}$$

(23)

$$+ \sum_{K\sigma} \frac{n_{K\sigma} - n_{K+Q+q\sigma}}{\Omega'_{K}} \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} << C^{+}_{K'+Q+q\sigma'} , C_{K'\sigma'} | \rho^{+}(q)\ ; \omega + is >>$$

$$- \sum_{K\sigma} \frac{b_{K\sigma} - b_{K+q\sigma}}{\Omega'_{K}} V(q) \sum_{K'\sigma'} << C^{+}_{K'+Q+q\sigma'}\ C_{K'+Q\sigma'} | \rho^{+}(q)\ ;\ \omega + is >>$$

$$- \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{<< C^{+}_{K+Q+q\sigma} C_{K+Q\sigma} | \rho^{+}(q)\ ;\ \omega + is >>}{\Omega'_{K}}$$

$$+ \sum_{K'\sigma'} b_{K'+q\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{<< C^{+}_{K+q\sigma}\ C_{K\sigma} | \rho^{+}(q)\ ;\ \omega + is >>}{\Omega'_{K}} \tag{24}$$

and

$$\sum_{K\sigma} \langle\langle C^{+}_{K+q\sigma} C_{K+Q\sigma} | \rho^{+}(q) ; \omega + is \rangle\rangle = - \frac{1}{2\pi} \sum_{K\sigma} \frac{b_{K\sigma} - b_{K+q\sigma}}{\Omega'_{K+Q}}$$

$$+ \sum_{K\sigma} \frac{n_{K+Q\sigma} - n_{K+q\sigma}}{\Omega'_{K+Q}} \sum_{\sigma'} W_{\sigma\sigma'} \sum_{K'} \langle\langle C^{+}_{K'+q\sigma'} C_{K'+Q\sigma'} | \rho^{+}(q) ; \omega + is \rangle\rangle$$

$$- \sum_{K\sigma} \frac{b_{K\sigma} - b_{K+q\sigma}}{\Omega'_{K+Q}} V(q) \sum_{K'\sigma'} \langle\langle C^{+}_{K'+q\sigma'} C_{K'\sigma'} | \rho^{+}(q) ; \omega + is \rangle\rangle$$

$$- \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{\langle\langle C^{+}_{K+q\sigma} C_{K\sigma} | \rho^{+}(q) ; \omega + is \rangle\rangle}{\Omega'_{K+Q}}$$

$$+ \sum_{K'\sigma'} b_{K'\sigma'} W_{\sigma\sigma'} \sum_{K\sigma} \frac{\langle\langle C_{K+Q+q\sigma} C_{K+Q\sigma} | \rho^{+}(q) ; \omega + is \rangle\rangle}{\Omega'_{K+Q}} \qquad (25)$$

where

$$\begin{aligned} \Omega_{K} &= \omega - \varepsilon_{K} + \varepsilon_{K+q} \\ \Omega_{K+Q} &= \omega - \varepsilon_{K+Q} + \varepsilon_{K+Q+q} \\ \Omega'_{K} &= \omega - \varepsilon_{K} + \varepsilon_{K+Q+q} \end{aligned} \qquad (26)$$

and

$$\Omega'_{K+Q} = \omega - \varepsilon_{K+Q} + \varepsilon_{K+q}$$

Omitting the extensive and tedious intermediary calculational steps, the final result is given by

$$\varepsilon(q,\omega) = 1 + V(q)\, F'(q,\omega) +$$

$$+ \frac{V(q) \sum_{\sigma'} W_{\sigma\sigma'} \left([F'(q,\omega)]^{2} - [F''(q,\omega)]^{2} \right) \left(1 - L'(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'} \right)}{\left(1 - L'(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'} \right)^{2} + \left(L''(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'} \right)^{2}}$$

$$- \frac{2V(q) \sum_{\sigma'} W_{\sigma\sigma'} P'(q,\omega)P''(q,\omega)L''(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'}}{(1-L'(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'})^2 + (L''(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'})^2}$$

$$- i \{ \; V(q)F''(q,\omega) + \qquad (27)$$

$$+ \frac{V(q) \sum_{\sigma'} W_{\sigma\sigma'}([P'(q,\omega)]^2 - [P''(q,\omega)]^2)L''(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'}}{(1-L'(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'})^2 + (L''(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'})^2}$$

$$+ \frac{2V(q) \sum_{\sigma'} W_{\sigma\sigma'} P'(q,\omega)P''(q,\omega) \; [1-L'(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'}]}{(1-L'(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'})^2 + (L''(q,\omega) \sum_{\sigma'} W_{\sigma\sigma'})^2} \}$$

where

$$F'(q,\omega) = \text{p.v.} \sum_{K\sigma} \frac{n_{K\sigma} - n_{K+q\sigma}}{\omega - \varepsilon_K + \varepsilon_{K+q}} \; ,$$

$$F''(q,\omega) = \pi \sum_{K\sigma} (n_{K\sigma} - n_{K+q\sigma}) \, \delta(\omega - \varepsilon_K + \varepsilon_{K+q}) \; ,$$

$$L'(q,\omega) = \text{p.v.} \sum_{K\sigma} \frac{n_{K\sigma} - n_{K+Q+q\sigma}}{\omega - \varepsilon_K + \varepsilon_{K+Q+q}} \; ,$$

$$L''(q,\omega) = \pi \sum_{K\sigma} (n_{K\sigma} - n_{K+Q+q\sigma}) \, \delta(\omega - \varepsilon_K + \varepsilon_{K+Q+q}) \; ,$$

$$P'(q,\omega) = \text{p.v.} \sum_{K\sigma} \frac{b_{K\sigma} - b_{K+q\sigma}}{\omega - \varepsilon_K + \varepsilon_{K+Q+q}} \; ,$$

and

$$P''(q,\omega) = \pi \sum_{K\sigma} (b_{K\sigma} - b_{K+q\sigma}) \, \delta(\omega - \varepsilon_K + \varepsilon_{K+Q+q}) \; .$$

Eq. (27) furnishes the dieletric constant of the electron gas in the GHF approximation. Letting

$$\text{Im}\ \varepsilon_N(q,\omega) = -\ V(q)F''(q,\omega)$$

and

$$\text{Im}\ \varepsilon_G(q,\omega) = -\frac{V(q)\sum_{\sigma'} W_{\sigma\sigma'}([P'(q,\omega)]^2 - [P''(q,\omega)]^2)L''(q,\omega)\sum_{\sigma'} W_{\sigma\sigma'}}{(1-L'(q,\omega)\sum_{\sigma'} W_{\sigma\sigma'})^2 + (L''(q,\omega)\sum_{\sigma'} W_{\sigma\sigma'})^2}$$

$$\frac{2V(q)\sum_{\sigma'} W_{\sigma\sigma'}P'(q,\omega)P''(q,\omega)(1-L'(q,\omega)\sum_{\sigma'} W_{\sigma\sigma'})}{(1-L'(q,\omega)\sum_{\sigma'} W_{\sigma\sigma'})^2+(L''(q,\omega)\sum_{\sigma'} W_{\sigma\sigma'})^2}$$

we can write

$$\text{Im}\ \varepsilon(q,\omega) = \text{Im}\ \varepsilon_N(q,\omega) + \text{Im}\ \varepsilon_G(q,\omega)\ . \qquad (28)$$

As we can see the imaginary term is separated into two parts, the imaginary part of the normal intraband dielectric constant of the electron gas, (Im $\varepsilon_N(q,\omega)$)[6], and the part due to the presence of the static charge density wave, (Im $\varepsilon_G(q,\omega)$), which is represented in Fig.1 using numerical data ispppropriate to sodium metal. The coefficient of absorption is given by

$$\alpha(\omega) = -\ \omega\ \text{Im}\ \varepsilon(\omega) = -\omega\ \text{Im}\ \varepsilon_N(\omega) - \omega\ \text{Im}\ \varepsilon_G(\omega) = \alpha_N(\omega) + \alpha_G(\omega)\ . \qquad (29)$$

Clearly, $a_G(\omega)$ is the contribution due to the presence of the static charge density wave shown in Fig.2. It can be proved thàt in the limit $A \to 0$, i.e. when the amplitude of the static wave of charge tends toward zero, the term $\alpha_G(\omega)$ is zero, as must be the case. Finally, with the aid of the Butcher's formula[7] we estimate the interband contribution to the absorption coefficient using the appropriate values for sodium metal[3].1n Fig.3 we show this contribution ($\alpha_0(\omega)$) and in Fig.4 we show it together with the coritribution associated with the presence of the static wave of charge. Note: that the contribution of the latter to the total absorption coefficient is much smaller than the interband contribution,

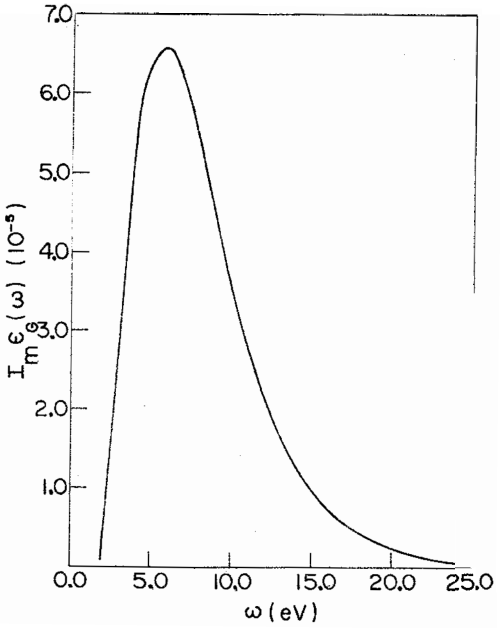

Fig.1 - The imaginary part of the dielectric constant due to the presence of the static charge density wave.

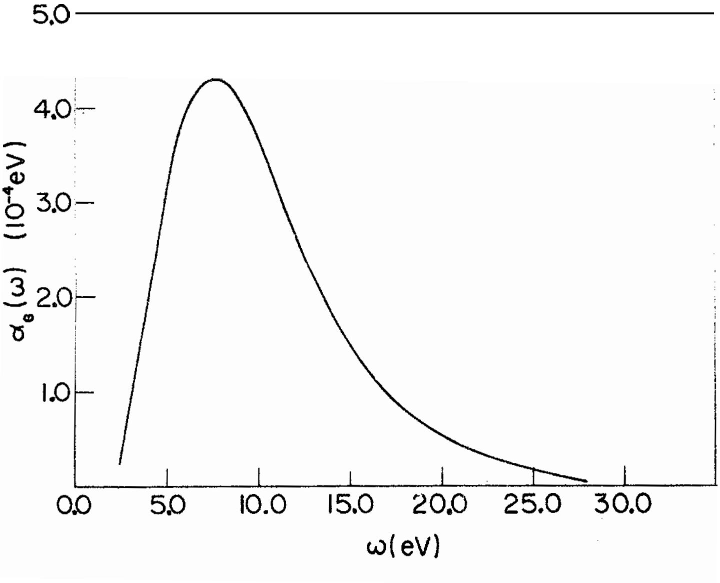

Fig.2 - Contribution to the absorption coefficient due to the presence of the static charge density wave.

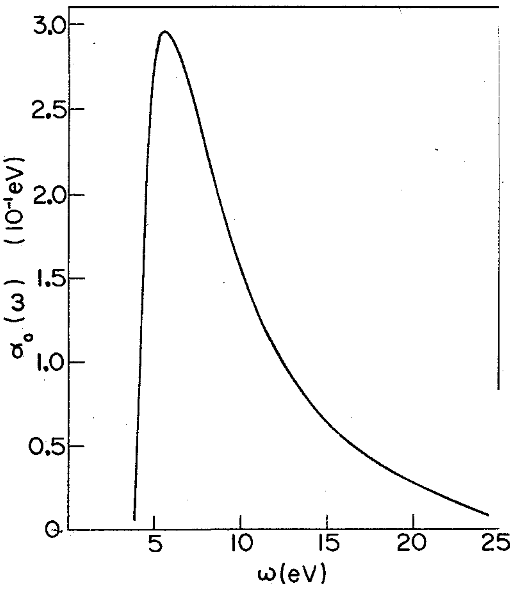

Fig.3 - The interband contribution to the absorption coefficient using the appropriate values for sodium metal[3].

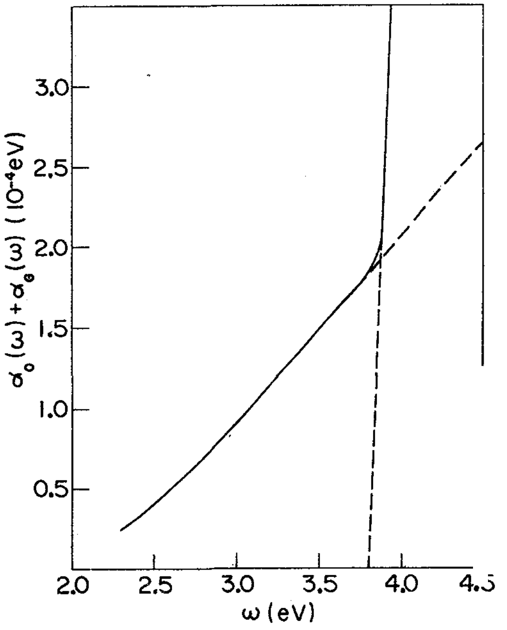

Fig.4 - The interband contribution together with the contribution associated with the presence of the static charge density wave to the absorption coefficient.

Nevertheles, it can be seen that it produces a contributionto the absorption in the material at frequencies below the intraband absorption edge. Since this contribution is always three orders of magnitude smaller than that of the interband contribution, its experimental detection is extremely difficult in the case of metals. However charge density waves have been evidenced recently by means of some types of measurements, such as electron diffraction[8], neutron scattering[9] and others[10,11].

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