TEMPERATURE DEPENDENCE OF THE HIGH-FREQUENCY ELECTRONIC DIELECTRIC FUNCTION

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Abstract: The temperature dependence of the high-frequency polarizability in a degenerate electron gas is investigated. The calculation is performed by extending the RPA to the diagonal exchange terms. Contrary to the imaginary part of the polarizability which is expressed through a general formula valid in the whole temperature region, the real part is calculated retaining only quadratic terms in the temperature. The correction terms are of interest in semimetals and semiconductors with small carrier concentration.

1. Introduction

The behaviour of the polarizability of an electron gas has been extensively investigated both in the classical and in the quantum limit[1]. Whereas in low-density systems, such as gas discharge plasmas, the electron polarizability can be evaluated by assuming that particles are distributed in the momentum space according to the Maxwell-Boltzmann law, for high-density gases the quantum treatment must be applied. Quantum effects play a predominant role if the temperature is lowered below the degeneracy temperature T_F. This situation is realized in a gas of metallic electrons, where its degeneracy temperature is about hundred times higher than room temperature. Thus the collective motion of conduction electrons can be determined by the zero temperature approximation for all temperatures of interest.

The aim of the present paper is to calculate the high-frequency electronic polarizability in the intermediate region of weakly degenerate systems. We

consider the case when an electron gas is heated to the temperature T, which is lower but not negligible in comparison with T_F. In order to make the calculation simpler, only the lowest order terms in the ratio T/T_F will be retained. Although for normal metals temperature effects are of no importance, this calculation is not of pure academic interest. The picture of a free electron gas, developed for metals, can also be applied to semimetals and semiconductors having a substantially lower electron concentration. By adding the impurities to semiconductors it is possible to change the electronic density in the conduction band and hence continuously vary the degeneracy temperature.

The properties of a high-density electron gas can be calculated on the basis of the random phase approximation[1, 2]. The inclusion of higher-order effects can be achieved along the lines proposed by Suhl and Werthamer[3]. The first corrections to the RPA expressions are represented by the diagonal exchange terms. This approximation is applied in the present paper. We assume the validity of the RPA and estimate the influence of the non-RPA processes by taking into account the electron exchange.

2. Constitutive equations

We study the dielectric properties of electrons in a neutral electron-ion system. For the sake of simplicity we shall suppose that ions form a uniform sea of positive charge. The system Hamiltonian up to constant terms is

$$H_0 = \sum_{sp} E_p N_{sp} + \frac{1}{2} \sum_k V_k \rho_k^* \rho_k . \tag{1}$$

In (1) s refers to the spin and p to the electron wave number, E_p is the free particle energy

$$E_p = \frac{\hbar^2 p^2}{2m} ;$$

N_{sp} is the occupation number operator

$$N_{sp} = c_{sp}^* c_{sp} ;$$

V_k is the Fourier transform of the Coulomb potential

$$V_k = \frac{4\pi e^2}{k^2} ;$$

ρ_k is the k-th density fluctuation

$$\rho_k = \sum_{sp} c^*_{sp} c_{sp+k} ;$$

while c^*_{sp} and c_{sp} are the electron creation and annihilation operators, respectively.

Now suppose that our system is in interaction with test charges, whose time behaviour is described by $e^{-i\omega t}$. Denoting the corresponding density fluctuation by R_k, for the effective Coulomb energy of the probe on $\vec{r}$ we have

$$U(\vec{r}) = \sum_k V_k (R_k + \rho_k) e^{i\vec{k}\vec{r}} = \sum_k V_k R_k e^{i\vec{k}\vec{r}} (1 + \frac{\rho_k}{R_k}) . \qquad (2)$$

From (2) we define the frequency and wave number dependent electronic dielectric function[1,4]

$$\frac{1}{\varepsilon(k,\omega)} = 1 + \frac{\rho_k}{R_k} . \qquad (3)$$

The ratio ρ_k/R_k will be determined by considering the equation of motion for the electron-hole pair $\rho_{spk} = c^*_{sp} c_{sp+k}$. Starting from the Hamiltonian $H = H_0 + H_{int}$, where H_{int} describes the interaction of the probe with the electron gas

$$H_{int} = \sum_k V_k R_k \rho^*_k ,$$

one can calculate the time derivative of ρ_{spk}

$$\frac{d}{dt} \rho_{spk} = \frac{i}{\hbar} [H, \rho_{spk}].$$

On the other hand

$$\frac{d}{dt} \rho_{spk} = -i\omega \rho_{spk} ,$$

giving

$$\hbar\omega \rho_{spk} + [H, \rho_{spk}] = 0 . \qquad (4)$$

Applying the anticommutation rules for the creation and annihilation ope·rators, it follows

$$[H, \rho_{spk}] = \rho_{spk} (E_p - E_{p+k}) + \frac{1}{2} \sum_{k'} V_{k'} \{(\rho_{k'} + 2 R_{k'}) (c^*_{sp+k'} c_{sp+k} -$$

$$- c^*_{sp} c_{sp+k-k'}) + (c_{sp+k'} c_{sp+k} - c^*_{sp} c_{sp+k-k'}) \rho_{k'}\}. \tag{5}$$

The sum over k' contains the terms of the form $c_1^* c_2 c_3^* c_4$, representing two-pair electron-hole excitations. Writing the equation of motion for these excitations and proceeding in the same way, we arrive at an infinite chain of equations. This approach is known as the generalized RPA[3]. Confining ourselves to the first step, we linearize equation (5), obtaining

$$\rho_{spk} (\hbar\omega + E_p - E_{p+k}) + V_k (\rho_k + R_k) (N_{sp+k} - N_{sp}) - \tag{6}$$

$$- \sum_{p'} V_{p-p'} \{(N_{sp+k} - N_{sp}) \rho_{sp'k} - (N_{sp'+k} - N_{sp'}) \rho_{spk}\} = 0.$$

Now we introduce the function F_p satisfying the integral equation

$$F_p = \frac{1}{\hbar\omega - \Delta E_p} \{1 - \sum_{p'} V_{p-p'} \Delta N_{p'} (F_p - F_{p'})\}, \tag{7}$$

where

$$\Delta N_p = N_{sp+k} - N_{sp} \qquad \Delta E_p = E_{p+k} - E_p.$$

Then by multiplying (6) by F_p and summing it over all electron states, one obtains

$$\rho_k + (\rho_k + R_k) V_k \sum_{sp} \Delta N_p F_p = 0. \tag{8}$$

The first term on the right-hand side of (7) represents the RPA contribution, while the second one gives the exchange correction. To include correlation effects into the latter, we shall restrict the sum over $\vec{p'}$ in (7) only to terms for which $|\vec{p'} - \vec{p}| > k_c$. This restriction may be understood on the basis of the work by Bohm and Pines[2], who have shown that the long-range part of the Coulomb interaction is described by plasmons. Hence electrons effectively interact via short range forces expressed by the term

$$H_{\text{eff}} = \frac{1}{2} \sum_{k > k_c} V_\lambda \, \rho_k^* \, \rho_k.$$

Here k_c is the wave number above which it is meaningless to introduce variables representing the collective behaviour of electrons. The same procedure was also applied by Bailyn[5], Hone[6] and Bross and Holz[7] in their study of the electron-phonon matrix element.

Combining (3) and (8), for the dielectric constant it follows

$$\varepsilon(k, \omega) = 1 + 4\pi\alpha(k, \omega) \tag{9}$$

where $\alpha(k, \omega)$ is the electronic polarizability

$$4\pi\alpha(k, \omega) = V_k \sum_{sp} F_p \Delta N_p. \tag{10}$$

3. Calculation

We shall perform the calculation under the following assumptions:

— the wave number k is much less than the Fermi momentum k_F,

— the frequency ω is much higher than the individual frequency kv_F, where v_F is the Fermi velocity, and

— the temperature T is low in comparison with the degeneracy temperature

$$T_F = \frac{\hbar^2 k_F^2}{2mK},$$

where K is Boltzmann's constant.

For small k we have

$$\Delta E_p = \frac{\hbar^2 \vec{k} \vec{p}}{m}, \quad \Delta N_p = \frac{\vec{k} \vec{p}}{p} \frac{d N_p}{dp},$$

N_p being the Fermi-Dirac distribution function. The influence of exchange and correlation will be taken into account by iterating equation (7). As the zero-order approximation we take the RPA value

$$F_{po} = \frac{1}{\hbar\omega - \Delta E_p}$$

Then the polarizability calculated to the first-order becomes

$$4 \pi \alpha (k, \omega) = V_k \left\{ \sum_{sp} F_{po} \Delta N_p - \right.$$

$$\left. - \sum_{spp'} V_{p-p'} \Delta N_p \Delta N_{p'} F_{po} (F_{po} - F_{p'o}) \right\} , \tag{11}$$

where the prime in the second sum denotes that $|\vec{p'} - \vec{p}| > k_c$. It can be easily seen that for small k the second term on the right-hand side of (11) is of the order k^2 compared with the first term. This is a general rule. Every new iteration of equation (7) leads to a contribution which is smaller by a factor $(k/k_F)^2$ than the preceding one. In other words, in the long-wavelength limit the high-frequency electronic polarizability is given by the first-order approximation.

By adopting the adiabatic boundary condition, we add a small positive imaginary part to the frequency

$$\omega \rightarrow \omega + i \eta.$$

Then with the help of the relations

$$\lim_{\eta \to 0} \frac{1}{x + i \eta} = P \frac{1}{x} - i \pi \delta (x),$$

$$\lim_{\eta \to 0} \frac{1}{(x + i \eta)^2} = P \frac{1}{x} + i \pi \frac{d\delta (x)}{dx},$$

where the symbol P denotes that the principal value has to be taken, for the real and the imaginary part of (11) it follows

$$\mathrm{Re} \; 4 \pi \alpha (k, \omega) = V_k \left\{ P \sum_{sp} \frac{\Delta N_p}{\hbar \omega - \Delta E_p} - \right. \tag{12}$$

$$\left. - P \sum_{spp'} V_{p-p'} \Delta N_p \Delta N_{p'} \frac{\Delta E_p - \Delta E_{p'}}{(\hbar \omega - \Delta E_p)^2 (\hbar \omega - \Delta E_{p'})} \right\}$$

and

$$\text{Im } 4\,\pi\alpha\,(k,\omega) = -\pi V_k \left\{ \sum_{sp} \Delta N_p\, \delta\,(\hbar\omega - \Delta E_p) + \right. \tag{13}$$

$$\left. + P \sum_{spp'} V_{p-p'}\, \Delta N_p\, \Delta N_{p'}\,(-\frac{d}{d\Delta E_p} + \frac{2}{\hbar\omega - \Delta E_{p'}})\,\delta\,(\hbar\omega - \Delta E_p) \right\}.$$

Expanding (12) in powers of k and retaining only terms up to k^2, one obtains

$$\text{Re } 4\,\pi\alpha\,(k,\omega) = -\frac{2\,V_k}{\hbar^2\omega^2} \sum_{sp} N_p\, \Delta E_p \left[1 + (\frac{\Delta E_p}{\hbar\omega})^2 \right] -$$

$$-\frac{V_k}{2\,m^2\omega^2} \sum_{spp'}' V_{p-p'}\, \frac{\vec{k}\,\vec{p}}{p}\, \frac{\vec{k}\,\vec{p'}}{p'}\, \frac{dN_p}{dp}\, \frac{dN_{p'}}{dp'}\,(\vec{k}\,\vec{p} - \vec{k}\,\vec{p'})^2.$$

Transforming the sum over the wave vector to the integral over energy, after applying Sommerfeld's formula[8]

$$-\int_0^\infty G\,(E)\frac{dN}{dE}\,dE = G\,(\mu) + \frac{(\pi KT)^2}{6}\, \frac{d^2G}{d\mu^2} + \ldots \quad T \ll T_F, \tag{14}$$

— μ being the chemical potential — the integration gives (see Appendix)

$$\text{Re } 4\,\pi\alpha\,(k,\omega) = -(\frac{\omega_r}{\omega})^2 - \frac{3\,k^2\,v_F^2\,\omega_p^2}{5\,\omega^4} \left\{ 1 - 0.0553\,r_s\,(1 + \frac{\beta^2}{4} - \frac{\beta^4}{8}) + \right.$$

$$\left. + \frac{5\pi^2}{12}(\frac{T}{T_F})^2 \left[1 + 0.0166\,r_s\,(1 + \frac{\beta^2}{6} + \frac{4}{3}\ln\frac{2}{\beta}) \right] \right\}. \tag{15}$$

In (15) ω_p is the classical plasma frequency

$$\omega_p^2 = \frac{4\,\pi\,Ne^2}{m}, \tag{16}$$

N being the electron concentration, β is the cut-off wave number expressed in units of k_F

$$\beta = \frac{k_c}{k_F}, \tag{17}$$

and r_s is the radius of the unit sphere expressed in Bohr radii

$$\frac{4\pi}{3}(r_s a_0)^3 N = 1. \tag{18}$$

Writing (14), we have supposed that $T \ll T_F$, and consequently we have kept only terms of the lowest order in T/T_F. If the temperature is close to T_F, then higher-order terms must also be taken into account.

The RPA contribution to the imaginary part is

$$\text{Im } 4\pi\alpha_0(k,\omega) = \pi V_t \frac{2}{(2\pi)^3} \frac{h^2}{mKT} \int \vec{k}\vec{p}\, \delta\left(\hbar\omega - \frac{\hbar^2 \vec{k}\vec{p}}{m}\right) \frac{e^{\frac{E_p - \mu}{KT}}}{\left(e^{\frac{E_p - \mu}{KT}} + 1\right)^2} d^3p.$$

Taking $\vec{k}$ in the direction of the z-axis, after applying the δ-function, we obtain

$$p^2 = p_x^2 + p_y^2 + \left(\frac{m\omega}{\hbar k}\right)^2 \geq \left(\frac{m\omega}{\hbar k}\right)^2 \tag{19}$$

leading to the inequality $E_p \gg KT$. Hence it approximately follows

$$\text{Im } 4\pi\alpha_0(k,\omega) = \frac{2}{(2\pi)^3} \frac{\pi V_k}{KT} \iiint\limits_{-\infty}^{\infty} p_z\, \delta\left(p_z - \frac{m\omega}{\hbar k}\right) e^{\frac{\mu - E_p}{KT}}\, dp_x\, dp_y\, dp_z =$$

$$= \frac{V_k m^2 \omega}{2\pi k \hbar^3} e^{\frac{1}{KT}\left(\mu - \frac{m\omega^2}{2k^2}\right)}.$$

In the limit of small momentum transfers the exchange effect does not influence the imaginary part of the polarizability. This becomes obvious on noticing that in the exchange contribution there appears the factor $V_{p-p'}$, which is small because according to (19) p is large for the long wavelength limit. Thus, expressing the phase velocity by $v = \omega/k$ and the most probable thermal velocity by $c = \sqrt{2KT/m}$, we may write

$$\text{Im } 4\pi\alpha(k,\omega) = \frac{2 e^2 m^2 v}{k^2 \hbar^3} e^{\frac{\mu}{KT} - \left(\frac{v}{c}\right)^2}. \tag{20}$$

The imaginary part of the high-frequency polarizability is due to the Maxwellian tail in the non-zero Fermi-Dirac distribution function.

4. Discusion

In our model the imaginary part of the polarizability is given by the Landau term (20). We wish to point out that expression (20) is also valid for high--temperature systems. If electrons behave like classical particles, then the normalizing condition yields

$$e^{\frac{\mu}{KT}} = 4 N \hbar^3 (\frac{\pi}{2 m K T})^{3/2},$$

which inserted in (20) gives the well known expression

$$\text{Im } 4 \pi \alpha (k, \omega) = \frac{2 \sqrt{\pi} \omega_p^2 v}{k^2 c^3} e^{-(\frac{v}{c})^2}, \quad T \gg T_F. \tag{21}$$

On the contrary, if the temperature is low enough, then with the help of $N = k_F^3/3 \pi^2$ we obtain

$$\text{Im } 4 \pi \alpha (k, \omega) = \frac{3 \pi \omega_p^2 v}{2 k^2 v_F^3} e^{\frac{T_F}{T} - (\frac{v}{c})^2}, \quad T \ll T_F. \tag{22}$$

By virtue of the inequality $(v/c)^2 \gg T_F/T$, which follows from the smallness of the wave number, expression (22) goes to zero for $T = 0$. At zero temperature electronic energies are too small, real processes do not occur, the imaginary part of the polarizability vanishes and oscillations are undamped.

Let us consider the change in the real part of the polarizability caused by varying the temperature of the electron gas. Generally, we may write

$$\text{Re } 4 \pi \alpha (k, \omega) = -\frac{\omega^2}{\omega_p^2} (1 + \frac{k^2}{\omega^2} A), \quad \omega \gg k v_F. \tag{23}$$

Now, choosing β to be given by[1]

$$\beta = 0.470 \sqrt{r_s}$$

at the zero temperature one finds

$$A = \frac{3}{5} v_F^2 [1 - 0.0553 r_s (1 + 0.0553 r_s - 0.00306 r_s^2)], \quad T = 0. \tag{24}$$

If the system is heated, then in the region of low temperatures the additional contribution increases quadratically with T

$$A = \frac{3}{5} v_F^2 \{1 - 0.0553 \, r_s \, (1 + 0.0553 \, r_s - 0.00306 \, r_s^2) +$$

<div align="right">(25'</div>

$$+ \frac{5 \pi^2}{12} (\frac{T}{T_F})^2 [1 + 0.0166 \, r_s \, (2.930 + 0.0369 \, r_s - \frac{2}{3} \ln r_s)]\}, \quad T \ll T_F.$$

For higher temperatures this increase is not so fast and, finally, high above the degeneracy temperature the term corresponding to the expression in the curly bracket of (25) behaves like T/T_F, giving

$$A = \frac{3 \, KT}{m}, \quad T \gg T_F.$$

In applying the results derived to semimetals and semiconductors, the effects of crystal periodicity and polarization must be taken into account. If we consider, for instance, III—IV semiconductor compounds, then expression (18) for the mean interelectronic spacing has to be replaced by

$$r_s = \frac{m^* c^2}{\hbar^2 \varepsilon_0} \sqrt[3]{\frac{3}{4 \pi N}},$$

where the typical values for the effective electronic mass and the static dielectric constant are $m^* = 0.05$ and $\varepsilon_0 = 15$, respectively. Hence by lowering the concentration from $10^{18} \, cm^{-3}$ to $10^{16} \, cm^{-3}$, T_F decreases from 840 K to 40 K, while r_s increases from 0.4 to 1.8. Of course, in the latter case the non-RPA contributions to the polarizability are not negligible. It must be emphasized that in these materials the dispersion relation for an electron plasma is not given by $\varepsilon (k, \omega) = 0$. Under the above conditions plasmons are strongly coupled to phonons, and the assumption that ions are motionless particles becomes inadequate. Thus the dispersion relation can be derived by calculating the total electron-phonon dielectric function and equating it to zero[9, 10].

Appendix

With the help of (14), the RPA term Re $4 \pi \alpha (k, \omega)$ can be calculated in a straightforward manner

$$\text{Re } 4 \pi \alpha_{RPA} (k, \omega) = - (\frac{\omega_p}{\omega})^2 \{1 + \frac{3 \, k^2 \, v_F^2}{5 \, \omega^2} [1 + \frac{5 \pi^2}{12} (\frac{T}{T_F})^2]\}. \tag{A1}$$

where we have taken into account that

$$\mu = K T_F [1 - \frac{\pi^2}{12} (\frac{T}{T_F})^2]. \tag{A2}$$

The corresponding exchange contribution is

$$\text{Re } 4\pi\alpha_{ex}(k,\omega) = -\frac{V_k}{2m^2\omega^3}\sum_{spp'}{}' V_{p-p'}\frac{\overrightarrow{kp}}{p}\frac{\overrightarrow{kp'}}{p'}\frac{dN_p}{dp}\frac{dN_{p'}'}{dp'}(\overrightarrow{kp}-\overrightarrow{kp'})^2.$$

With

$$\frac{\overrightarrow{kp}}{kp} = \cos\theta = t, \qquad \frac{\overrightarrow{pp'}}{pp'} = \cos\theta' = t',$$

we have

$$\frac{\overrightarrow{kp'}}{kp'} = \sin\theta\sin\theta'\cos(\varphi-\varphi') + \cos\theta\cos\theta' = \tau.$$

Hence

$$\text{Re } 4\pi\alpha_{ex}(k,\omega) = -\frac{V_k}{m^2\omega^4}\frac{2}{(2\pi)^6}\int\frac{4\pi e^2 k^4 t\tau}{F^2+p'^2-2pp't'}\frac{dN_p}{dp}\frac{dN_{p'}'}{dp'}\cdot$$

$$\cdot(p^2 t^2 - pp' t\tau)\,p^2 p'^2\,dp\,dp'\,dt\,dt'\,d\varphi\,d\varphi'.$$

(A3)

Here it must be born in mind that by virtue of the restriction $|\overrightarrow{p'}-\overrightarrow{p}| > k_c$, the maximal value for t' is not unity but

$$t'_{max} = \frac{p'^2+p^2-k_c^2}{2pp'}.$$

Thus, after performing the angular integration we arrive at

$$\text{Re } 4\pi\alpha_{ex}(k,\omega) = -\frac{2V_k e^2 k^4}{15\pi^3 h^4\omega^3}\int\!\!\int_0^\infty\Bigg[\frac{E_c^2-4E_pE_{p'}'-2E_pE_c-4E_p\sqrt{E_pE_{p'}'}}{4} +$$

$$+ E_p(E_p-E_{p'}')\ln\frac{\sqrt{E_p}+\sqrt{E_{p'}'}}{\sqrt{E_c}}\Bigg]\frac{dN_p}{dE_p}\frac{dN_{p'}'}{dE_{p'}'}-dE_p\,dE_{p'}',$$

where $E_c = h^2 k_c^2/2m$. Then, applying expression (14) up to quadratic terms in the temperature it follows

$$4\pi\alpha_{ex}(k,\omega) = \frac{4V_k e^2\mu^2 k^4}{15\pi^3 h^4\omega^3}\Bigg[1+\frac{E_c}{4\mu}-\frac{E_c^2}{8\mu^2}+\frac{\pi^2}{24}\Big(\frac{KT}{\mu}\Big)^2\Big(1-$$

(A4)

$$-4\ln 2\sqrt{\frac{\mu}{E_c}}\Big)\Bigg].$$

With the help of (A2), this transforms into

$$4\,\pi\alpha_{ex}\,(k,\omega) = \frac{3}{20}(\frac{k}{k_f})^2\,(\frac{\omega_p}{\omega})^4\left[1 + \frac{\beta^2}{4} - \frac{\beta^4}{8} - \frac{\pi^2}{8}(\frac{T}{T_F})^2\,(1 + \frac{\beta^2}{6} + \frac{4}{3}\ln\frac{2}{\beta})\right],$$

(A5)

which together with (A1) yields (15).

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TEMPERATURNA OVISNOST VISOKOFREKVENTNE ELEKTRONSKE DIELEKTRIČNE FUNKCIJE

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Sadržaj

Izračunata je temperaturna zavisnost polarizabilnosti degenerirane elektronske plazme u području visokih frekvencija i malih valnih vektora za sisteme s niskom temperaturom. Račun je proveden za plazmu dovoljno visoke koncentracije, za koju korekcije aproksimacii slučajnih faza ne igraju značajniju ulogu.

Pretpostavljajući da je omjer temperature i temperature degeneracije malen, realni dio polarizabilnosti izračunat je do uključivo kvadratičnih članova u temperaturi.