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Damping of Phonons in an Electron-Ion Gas

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Abstract

Relaxation time and phonon mean free path have been obtained for an electron-ion gas (a quantum plasma) from the expression for the angle of dielectric loss. The familiar formula for the dielectric constant given by Nozières and Pines¹⁾ has been extended so as to include the life time effect of electronic levels. In this way a quantum mechanical version of Pippard's semi-classical theory²⁾ for the phonon mean free path has been shown in a simple but convincing manner. The result can be applied to liquid metals and classical plasmas. The problem at finite temperatures is also considered. As another application the polarizability in the presence of a static magnetic field is obtained.

§ 1 Introduction

The theory of an electron-ion gas serves as a realistic model of metals and plasmas as far as the long range phenomena are concerned. This theory affords us useful fundamental information about the elementary excitations and the relaxation processes. One of the most important quantities is the phonon mean free path which determines the rate of approach to thermal equilibrium, the absorption rate of ultra-sonic wave and the thermoelectricity in metals.

According to Pippard the phonon mean free path Λ_p increases by a factor $(\nu_p \tau)^{-1}$ for long wave lengths compared with shorter wave lengths such as $\lambda < \Lambda_e$, where ν_p , λ , τ and Λ_e are the phonon frequency, the phonon wave length, the electron relaxation time and the electron mean free path, respectively. His derivation of the result depends upon a classical reasoning and involves some intuitive assumptions. In this paper it will be shown that the corresponding result can be derived from the recent theory of the dielectric constant for electron gases developed by Nozières, Pines, Schrieffer and others,³⁾ by taking account of the life time of the single particle excitation near the Fermi surface. The origins of the level broadening may be perturbations due to collisions of electrons with ion cores, impurities and others besides those by the screened potential. The electrostatic effect such as the screening effect is already involved in the dielectric formulation.

The elementary excitations are given as poles of the inverse dielectric constant. If the imaginary part of the dielectric constant is negligible at the phonon frequency, the phonon would become a pure elementary excitation. Usually the imaginary part is not negligible, the phonon level is broadened and the life time effect appears, even if the electron levels are sharp and their level breadths are negligible. As pointed out by Wentzel⁴⁾ and the author⁵⁾, the phonon behaves as if it were an unstable particle met in the field theory. In the classical theory of plasma the frequency of

the plasma oscillation may be imaginary. This fact is known as the Landau damping.⁶⁾ From the classical point of view the phonon damping is considered as a reflection of the Landau damping to the ionic oscillation.

In § 1 the half level width of the phonon spectrum will be given in terms of the angle of dielectric loss. In § 2 the life time of electronic levels near the Fermi surface will be introduced and the Pippard formula will be examined. In § 3 the magnitude of the life time will be estimated for liquid metals. The mean free path and the relaxation time of the phonon will be obtained. In § 4 the result will be extended to the problem at finite temperatures. In § 5 the problem of a static magnetic field will be considered.

§ 1 . Half level widths of phonons

The relaxation time or the level breadth of the phonon excitation is obtained from the expression for the dielectric constant of the electron-ion system which becomes

$$\epsilon(k, \nu) = \epsilon_e(k, \nu) - \frac{\omega_i^2}{\nu^2} \quad , \quad (1.1)$$

where ϵ_e is the electronic dielectric constant and ω_i is the ionic plasma frequency. Usually the expression depends on the wave number k and the frequency ν and is given by the fourier transform of the retarded longitudinal dielectric constant. If the imaginary part of the dielectric constant ϵ_2 is negligible, the inverse dielectric constant would have a pole at the phonon frequency. Near the phonon frequency we expand the real part of the dielectric constant ϵ_1 and put

$$\epsilon_1(k, \nu) = \epsilon_1'(k, \nu) (\nu - \nu_p) \quad . \quad (1.2)$$

Near the phonon frequency ν_p the inverse dielectric constant is expressed by

$$\frac{1}{\epsilon(k, \nu)} = \frac{\epsilon(k, \nu_p)}{\epsilon_1'(k, \nu_p)^2 (\nu - \nu_p)^2 + \epsilon_2(k, \nu_p)^2} \quad (1.3)$$

This expression has a peak at the phonon frequency and the half width $\Gamma/2$ is given by the derivative of ϵ_1 and ϵ_2 ; $\Gamma/2 = \epsilon_2(k, \nu_p) / \epsilon_1'(k, \nu_p)$. The relaxation time is defined as the inverse of the half level width. As a solution of the dispersion equation; $\epsilon(k, \nu) = 0$, the phonon frequency with the imaginary part is written as⁵⁾

$$\nu_p = \omega_p + i\Gamma/2 \quad (1.4)$$

For small wave numbers, the real part ω_p approaches to the well-known value $(zm/3M)^{1/2} v_f k$, where z , M and v_f are the ionic charge, the ionic mass and the Fermi velocity of electron, respectively. The derivative $\epsilon_1'(k, \nu_p)$ can be expressed in terms of the real part of the electronic dielectric constant $\epsilon_1^e(k, \nu_p)$ from (1.1); $\epsilon_1'(k, \nu_p) = \nu_p / 2 \epsilon_1^e(k, \nu)$. The imaginary part is also replaced by the electronic value $\epsilon_2^e(k, \nu)$, the value in the absence of the ionic oscillation. The explicit form of these quantities will be given in the next section. Introducing the angle of dielectric loss; $\varphi(k, \nu) = \arctan(\epsilon_2^e / \epsilon_1^e)$, the level breadth may be written as

$$\Gamma = \nu_p \tan \varphi(k, \nu) \quad (1.5)$$

§ 2. Electronic dielectric constant.

The free-electron polarizability $4\pi\alpha(k, \nu)$ is given by⁷⁾

$$4\pi\alpha(k, \nu) = \frac{4\pi e^2}{k^2} \sum_K \frac{f(K+\frac{k}{2}) - f(K-\frac{k}{2})}{\hbar(\nu - \nu_{K,k}) + i\delta} \quad (2.1)$$

Here δ is an infinitesimal positive quantity and $f(K)$ is the distribution function of an electron in state K , energy $E(K) = \hbar^2 K^2 / 2m$; at thermal equilibrium one has the familiar Fermi-Dirac result

$$f(K) = 1 / [\exp((E(K) - \mu) / \kappa T) + 1] \quad (2.2)$$

where μ is the chemical potential and κ is the Boltzmann constant. We have also introduced one-electron excitation frequency $\nu_{K,k} = E(K + \frac{k}{2}) - E(K - \frac{k}{2})$. The electronic dielectric constant becomes

$$\epsilon_e(k, \nu) = \epsilon_1^e(k, \nu) + i\epsilon_2^e(k, \nu) = 1 + 4\pi\alpha(k, \nu) \quad (2.3)$$

We assume that the electronic states near the Fermi surface have a common constant breadth denoted by γ , and consider that the energy of an electron (outside the Fermi sphere) has a positive imaginary part and the energy of a hole has a negative imaginary part. In this case the electron polarizability can be written as

$$4\pi\alpha(k, \nu) = \frac{4\pi e^2}{k^2} \left\{ \begin{array}{l} \sum_{E(K+\frac{k}{2}) < \mu} \frac{1}{\nu + \nu_{K,k} + i\gamma} \\ \sum_{E(K-\frac{k}{2}) > \mu} \frac{1}{\nu - \nu_{K,k} + i\gamma} \end{array} \right. \quad (2.4)$$

in the low temperature limit. After a simple calculation we obtain the following result

$$\epsilon_1^e(k, \nu) = 1 + \frac{4\pi e^2}{k^2} \left\{ 2N(0) + \frac{\nu}{2\nu_0} N(0) \ln \frac{(\nu - \nu_0)^2 + \gamma^2}{(\nu + \nu_0)^2 + \gamma^2} - \frac{\gamma}{\nu_0} N(0) \left(\arctan(\nu_0 - \nu/\gamma) + \arctan(\nu_0 + \nu/\gamma) \right) \right\} \quad (2.5)$$

$$\epsilon_2^e(k, \nu) = \frac{\gamma}{2\nu_0} \ln \frac{(\nu_0 - \nu)^2 + \gamma^2}{(\nu_0 + \nu)^2 + \gamma^2} + \frac{\nu}{\nu_0} \left\{ \arctan\left(\frac{\nu_0 - \nu}{\gamma}\right) + \arctan\left(\frac{\nu_0 + \nu}{\gamma}\right) \right\} \quad (2.6)$$

where $N(0)$ is the usual level density and ν_0 is the maximum excitation frequency $\nu_f k$. Hereafter we are only interested in the low frequency region since the phonon frequency is much smaller than ν_0 .

If the level breadth is infinitesimal we are led to the previous result. In this case, in the small wave number limit, we get

$$\epsilon_1^e = 1 + \frac{8\pi e^2}{k^2} N(0), \quad \epsilon_2^e = \frac{4\pi^2 e^2}{k^2} N(0) (\nu/\nu_0),$$

$$\varnothing = \arctan(\pi\nu/2\nu_0), \quad \Gamma = \pi\nu^2/2\nu_0. \quad (2.7)$$

If the breadth of the electronic states is much larger than the maximum excitation energy $\ll \nu_0$; $\gamma > \nu_0$, or in other words the wave number is smaller than the inverse electron mean free path; $\lambda_e^{-1} > k$ we find

$$\epsilon_1^e = \frac{8\pi e^2}{3k^2} N(0) (\nu_0^2/\gamma^2), \quad \epsilon_2^e = \frac{16\pi e^2}{3k^2} N(0) (\nu_0^2/\gamma^3) \nu$$

$$\varnothing = \arctan(2\nu/\gamma), \quad \Gamma = 2\nu^2/\gamma, \quad (2.8)$$

Using the electron relaxation time $\tau = 2/\gamma$, the phonon level breadth becomes as simply as $\nu^2 \tau$, which is smaller than the value given in (2.7)

by a factor $2\nu_0\tau/\pi$. When we define the phonon mean free path by s/Γ , using the sound velocity s , we find the mean free path increases by a factor $\pi/2\nu_0\tau$ and

$$\frac{1}{\Lambda_p} = (\nu_p \tau) k \quad (2.9)$$

at the phonon frequency $\nu_p = sk$. This result is slightly larger than Pippard's classical value by a factor $5/4$. Froelich's theory of dielectrics gives also the same result as (2.9) in this limit.

§ 3. Life time due to collisions with ion cores.

As pointed out by Ziman and others,⁸⁾ the scattering of electrons due to ion cores is important in describing the relaxation phenomena in liquid metals, especially in polyvalent metals. Here we would simplify the problem so that the electrons are scattered by an average potential of ion cores which is obtained from the resistivity of a metal at its melting point. The scattering due to the screened potential is important for monovalent metals, especially for Na and Li. The scattering by this potential exhausts almost the whole transition probability. It can be shown that the matrix element of this scattering is exactly the same as that for the electron-phonon scattering. The relaxation time of phonons due to this scattering becomes twice the inverses of Γ given in (2.7). By this fact, it is implied that this type of scattering process is an electrostatic one and is already included in our formulation. For polyvalent metals, on the other hand, this effect plays the minor role and usually negligible. According to Ziman, the contribution from this scattering is 7% for Zn, 1% for Hg, 3% for Ga, 4% for In, 2% for Sn and 1% for Pb.

The transition probability W_k for the momentum transfer $\hbar k$ is given by the ion-core potential U_k and the x-ray distribution function a_k

$$W_k = \frac{2\pi}{\hbar} U_k^2 a_k N(0)/N, \quad (3.1)$$

where N is the total number of ions and $2N(0)/N = 3z/2\epsilon_f$; $\epsilon_f = mv_f^2/2 = \mu$. Ziman obtained the resistivity using this expression and estimated the magnitude of the average potential from the experimental values obtained for liquid metals. We subtract the contribution from the screened potential and find the value for the average ion-core potential. The values for W_k which may be identified to the level breadth are listed in Table. 1

	Zn	Hg	Ga	In	Sn	Pb	Bi
z	2	2	3	3	4	4	5
$W_k \times 10^{-15}$	4.3	5.6	3.9	2.6	5.1	9.1	1.6

Table. 1

These values are as large as about hundred times of the values for Na and Ce.

Considering these large level width we are allowed to apply the expressions given in (2.8). Using Froelich's theory of dielectrics we can derive formally the same expression for the level breadth, if we could identify the relaxation time appearing in Froelich's theory to the inverse of the half width of the electron state. Such an identification, however, opens to many questions so that it seems not to be fully justified at present. In this respect our formulation is more reasonable and pertinent to our problem to present a quantum mechanical reformulation of Pippard's theory.

§ 4. A plasma with high electron temperature.

As a limiting case, we consider a high temperature plasma.

At finite temperatures, the sound waves are well defined only when the effective positive charge temperature T^+ is small compared to that for electrons T ; $T \gg T^+$. This is not the case of complete thermal equilibrium. In this case we can obtain $\epsilon_2(k, \nu)$ from (2.1) using the Boltzmann distribution function for $f(k)$. For over all range of frequency ν , we find

$$\epsilon_2^e(k, \nu) = \frac{4\pi e^2}{k^3} n(m/\hbar) \sinh(\hbar\nu\beta) , \quad (4.1)$$

where we have put $f(K) = n \exp(-\beta E(K))$ and n is the number density of electrons. With the aide of the Cauchy relation, the real part is found by

$$\begin{aligned} \epsilon_1^e(k, \nu) &= \int \frac{2\nu' \epsilon_2^e(k, \nu')}{\nu'^2 - \nu^2} d\nu' \\ &= \frac{4\pi e^2}{k^2} n\beta (\beta \rightarrow 0) . \end{aligned} \quad (4.2)$$

In this limit the phonon level breadth approaches to

$$\Gamma = 2 (\pi m z / 8 M)^{1/2} \nu_p , \quad \nu_p = (z \kappa T / M)^{1/2} k , \quad (4.3)$$

which is tantamount to the classical result derived from the Vlasov equation and compared to the expression for the Landau damping :

$$\Gamma = \frac{\pi}{n} \frac{\nu_e^2}{k^2} \frac{df(\nu_p/k)}{dv} \nu_p , \quad (4.4)$$

where ν_e is the electron plasma frequency ; $(4\pi n e^2 / m)^{1/2}$ and v is the electron velocity ; $v = \hbar K / m$. The phonon half level width may be regarded as the rate of growing up of sound waves in a plasma. Such excitations of sound waves or ionic oscillations are considered as a . origin of instabilities occuring in a hot plasma which is known as the two-stream instability. The growing up of sound waves in the presence of a static magnetic field is an interesting problem and will be discussed briefly in the next section.

§ 5. External constant magnetic field

It can be shown that the polarizability for a constant magnetic field B_0 parallel to the z -axis is given by

$$4\pi\alpha = \frac{4\pi e^2}{k^2} \sum_{\substack{m, n \\ p, Q}} \left[\frac{1}{\hbar\nu + E_{m, Q-q} - E_{n, Q} - i\delta} - \frac{1}{\hbar\nu + E_{n, Q} - E_{m, Q+q} - i\delta} \right] P_{mn}(\epsilon) f_n(Q). \quad (5.1)$$

Here $f_n(Q) = f(E_{n, Q})$, $E_{n, Q} = (n + 1/2)\hbar\nu_B + \hbar^2 Q^2 / 2m$ and ν_B is the Lamor frequency ; eB_0/m (magnetic unit). $P_{mn}(\epsilon)$ means the square of the matrix element of the phase factor ; $\exp(ik \cdot r)$ between the Landau states specified by the quantum numbers n, P, Q and $m, P-1, Q-q$ where l and q are the y - and z - component of the wave vector k , respectively and $\epsilon = \hbar(l^2 + q^2) / 2m\nu_B$. The analytical expression for $P_{mn}(\epsilon)$ will be given in the Appendix. Here we restrict ourselves to the propagation along the magnetic field, the z axis. The real and imaginary part of the polarizability turn out to be

$$4\pi\alpha_1 = \frac{4\pi e^2}{q^2} \frac{m\nu_B}{(2\pi\hbar)^2} \sum_n I_n(q), \quad (5.2)$$

$$4\pi\alpha_2 = \frac{4\pi e^2}{q^2} \frac{m^2\nu_B}{4\pi\hbar^3} \frac{\Lambda}{q}, \quad (5.3)$$

$$I_n(q) = \int_{-K_n}^{K_n} \left(\frac{1}{\nu - \frac{\hbar Q}{m} q + \frac{\hbar q^2}{2m}} - \frac{1}{\nu - \frac{\hbar Q}{m} q - \frac{\hbar q^2}{2m}} \right) f_n(Q) dQ \quad (5.4)$$

where Λ is the difference of Λ_+ and Λ_- which are defined by

$$\Lambda_{\pm} = \sum_n f_n(Q_{\pm}), \quad Q_{\pm} = \frac{m}{mq} \left(\nu \pm \frac{\hbar q^2}{2m} \right), \quad (5.5)$$

and $K_n = (2m/\hbar^2)^{\frac{1}{2}} [\mu - (n + \frac{1}{2}) \hbar \nu_B]^{\frac{1}{2}}$. The quantities $\Lambda_{+,-}$ become integers which are not larger than $[\frac{\mu}{\hbar \nu_0} - \frac{1}{2} \frac{m\nu^2}{2q^2 \hbar \nu_B} (1 \pm \frac{\hbar q^2}{2\nu m})^2]$ in low temperature limit. In terms of these quantities the level breadth of the phonon spectrum becomes

$$\Gamma = \nu_p \frac{\alpha_2}{\alpha_1} = \frac{\pi}{\hbar q} \frac{\nu_p}{g(q)} \quad (5.6)$$

In low temperature limit the quantity $g(q) = \sum I_n(q)$ is a periodic function with respect to the inverse of the frequency ν_B as shown by Quinn and Rodriguez⁹⁾.

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Appendix

The quantity appeared in (5.1) ; $P_{mn}(\epsilon)$ is expressed by the Charlier polynomials :

$$P_{mn}(\epsilon) = e^{-\epsilon} C(m, n, \epsilon)^2 \epsilon^{m+n} / m!n! \quad . \quad (A.1)$$

The Charlier polynomials are related to the associated Laguerres polynomials by

$$C(m, n, \epsilon) = C(n, m, \epsilon) = (-\epsilon)^{-m} m! L_m^{n-m}(-\epsilon) \quad .$$

It is readily seen that

$$\sum_m P_{mn}(\epsilon) = 1, \quad \sum_m m P_{mn}(\epsilon) = n + \epsilon, \quad (A.2)$$

which confirms the sum rule for the dielectric constant and we obtain the classical plasma frequency in small wave number limit. From the equation (5.1), in the high frequency limit, we get

$$1 + 4\pi\alpha = \frac{4\pi e^2}{k^2} \sum_{n, m} \sum_{P, Q} \frac{-2(m-n)\hbar\nu_B - \frac{\hbar^2 q^2}{m}}{\hbar^2 \nu^2} P_{mn}(\epsilon) f_n(Q) + 1 = 0 \quad (A.3)$$

Using (A.2) and the definition of ϵ we are led to the exact classical plasma frequency :

$$1 - \frac{4\pi n e^2}{m \nu^2} = 0 \quad . \quad (A.4)$$