Scattering of Electromagnetic Waves by an Electron-Phonon System*

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A theory is developed which described the scattering of electromagnetic waves by the electron density fluctuation of an electron-phonon system. The frequency spectrum of the scattered radiation is calculated by the temperature-dependent Green's function method and is alternatively derived by an elementary treatment in terms of dressed electrons and phonons. The theory may find its application in the study of incoherent scattering of electromagnetic waves in the vacuum ultraviolet region by thin metals. The resulting frequency spectrum of the scattered radiation shows resonances corresponding to the collective response of the electrons to the lattice vibrations, and to the collective excitation of plasma oscillations.

I. INTRODUCTION

THE present work is concerned with the derivation of an expression for the cross section of incoherent scattering of electromagnetic waves from a normal metal. We consider a simplified model for the metal, composed of electrons and phonons, and study the power scattered from the system when it is exposed to incident electromagnetic waves with frequencies above the penetration frequency. The radiation scattered is the sum of the Thomson scattering from each of the electrons in the system (the ions contribution is clearly negligible because of their large mass), and thus depends on the density fluctuations of the electrons. While in the usual Thomson scattering problem one deals with randomly distributed fixed electrons, the present theory is concerned with the effect of the motion of the electrons due to the thermal fluctuation of the system.

The problem of the scattering of x rays and light from solids was thoroughly investigated in the last decades,[1,2] and theoretically satisfactory explanations of the experiments have been given. Less attention was paid to the incoherent scattering of electromagnetic waves in the vacuum uv region from metals. In this region the wavelength is much *larger* then the lattice spacing and, if the frequency is above the penetration frequency and the system is optically *thin*, the scattering is predominantly due to the *conduction* electrons so that the cross section shows some features of these electrons. The purpose of our work is to give a *microscopic* treatment of the scattering mechanism, taking into account both the Coulomb interaction between electrons and the electron-phonon interaction.

The scattered radiation is determined by the spectrum of electron density fluctuations and this, in turn, depends on the coupled motion of electrons and ions in the metal as well as the individual and collective aspects of the motion of the electrons. The tendency of the electrons to screen out the ions and each other influences significantly the spectrum of density fluctuations. This is reflected especially in the fact that there are large density fluctuations, for a given wavelength, at both the frequencies of the lattice vibrations and the frequency of the collective plasma oscillations of the conduction electrons. Hence, it is expected that the spectral shape of the scattered waves will show resonances at these frequencies. While the effect of lattice vibrations is similar to that studied at other frequency regions of electromagnetic waves, the resonance at the vicinity of the plasma frequency of the conduction electrons is peculiar to the region to be discussed here. To some extent our treatment is similar to the one employed in classical plasmas.[3]

We start with the expression of the scattering cross section given in terms of the autocorrelation function of the electron-density operators.[3] The system is assumed to be represented by the Bardeen-Pines[4] Hamiltonian, and thus both electron-phonon and electron-electron interactions are explicitly introduced. The autocorrelation function is investigated by the *temperature-dependent Green's function* method[5,6] employing a diagram technique to obtain the leading asymptotic contribution for the scattering cross section when the number of electrons in the Bohr radius is large, and the wavelength of the field is larger than the Bohr radius. We also assume that the waves are not attenuated appreciably, i.e., the system is optically thin, but still there are many particles present across it. An alternative method employing a *self-consistent test particle* is also applied to facilitate an elementary derivation of the results and to obtain a simple physical interpretation for them. We conclude the paper with a brief discussion of the results, pointing out the possibility of utilizing

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the scattering of electromagnetic waves from thin metals to study some properties of the electron-phonon system.

II. THE GENERAL FORMALISM

Following Rosenbluth and Rostoker[3] we consider a plane wave with frequency ω_0 and wave vector $\mathbf{K}_0=\omega_0/c$ incident on the system, which occupies the volume V. In the first Born approximation, the differential cross section for the scattered waves per unit frequency per unit solid angle in the direction of $\mathbf{K}$ per unit incident power is given by[3]

$$\sigma(\omega)=Nr_0^2[1-\sin^2\alpha\cos^2(\phi-\phi_0)]S(\mathbf{K}_0-\mathbf{K},\omega_0-\omega), \quad (1)$$

where $N=nV$ is the total number of electrons, $r_0=e^2/mc^2$ is the classical electron radius, α is the angle between $\mathbf{K}$ and $\mathbf{K}_0$, and ϕ and ϕ_0 are the azimuthal angles that locate $\mathbf{K}$ and the incident electric field. Relativistic effects are neglected and the system is assumed to be in thermal equilibrium. The spectrum of electron density fluctuations $S(\mathbf{k},\omega)$ is defined by

$$S(\mathbf{k},\omega)=2\,\mathrm{Re}S^\dagger(\mathbf{k},\omega), \quad (2)$$

where

$$S^\dagger(\mathbf{k},\omega)=\frac{1}{2Vn}\int_0^\infty d\tau\epsilon^{i\omega\tau}\cdot \times\langle n(\mathbf{k},\tau)n(-\mathbf{k},0)+n(-\mathbf{k},0)n(\mathbf{k},\tau)\rangle \quad (3)$$

and Re stands for the real value. In Eq. (3)

$$n(\mathbf{k},t)=\epsilon^{iHt}n(\mathbf{k},0)\epsilon^{-iHt} \quad (4)$$

is the spatial Fourier transform of the electron density operator in the Heisenberg representation, H is the total Hamiltonian of the system, and the average of an operator A is given by

$$\langle A\rangle=\mathrm{Tr}\{e^{\beta(\Omega+\mu N-H)}A\}, \quad (5)$$

where β is the inverse temperature in energy units, μ and N are, respectively, the chemical potential and the total number operator of the electrons and

$$e^{-\beta\Omega}=\mathrm{Tr}\{e^{\beta(\mu N-H)}\}. \quad (6)$$

We also set $\hbar=1$. The remainder of the report is devoted to the calculation of the function $S(\mathbf{k},\omega)$.

In order to facilitate the temperature-dependent Green's function method[5,6] we define a real function

$$\Phi(\mathbf{k},\omega)=\frac{1}{V}\sum_{m,s}\exp[\beta(\Omega+\mu N_m-E_m)] \times\langle m|n(\mathbf{k},0)|s\rangle\langle s|n(-\mathbf{k},0)|m\rangle\delta(E_s-E_m-\omega), \quad (7)$$

thus,

$$S^\dagger(\mathbf{k},\omega)=-i\frac{1}{2n}\int\frac{d\omega'}{\omega'-\omega-i\epsilon}(1+\epsilon^{-\beta\omega'})\Phi(\mathbf{k},\omega'), \quad (8)$$

and Eq. (2) reads

$$S(\mathbf{k},\omega)=\pi\frac{1+\epsilon^{-\beta\omega}}{n}\Phi(\mathbf{k},\omega). \quad (9)$$

In Eq. (7) m and s represent eigenstates of the Hamiltonian and the total number operator, with

$$H|m\rangle=E_m|m\rangle, \quad N|m\rangle=N_m|m\rangle, \quad (10)$$

and $N_m=N_s$ in Eq. (7), due to the fact that $n(\mathbf{k},t)$ commutes with N.

We now define a Green's function

$$G(\mathbf{k},u)=\frac{1}{V}\langle T\{n(\mathbf{k},u)n(-\mathbf{k},0)\}\rangle \quad (11)$$

in the real domain $-\beta<u<\beta$. In Eq. (11), T is the Dyson ordering operator and

$$n(\mathbf{k},u)=\epsilon^{uH}n(\mathbf{k},0)\epsilon^{-uH}. \quad (12)$$

By expressing $G(\mathbf{k},u)$ in terms of the sum over states, as in Eq. (7), one easily convinces himself that

$$G(\mathbf{k},u+\beta)=G(\mathbf{k},u); \quad (13)$$

hence, its "Fourier transform" with respect to u

$$G_n(\mathbf{k})=\int_0^\beta du\,e^{i2\pi nu/\beta}G(\mathbf{k},u) \quad n=0,\pm1,\pm2,\cdots, \quad (14)$$

enjoys the property

$$G_n(\mathbf{k})=\int\frac{d\omega'}{\omega'-i2\pi n/\beta}(1-e^{-\beta\omega'})\Phi(\mathbf{k},\omega'). \quad (15)$$

If we now introduce a function

$$F(\mathbf{k},z)=\int\frac{d\omega'}{\omega'-z}(1-e^{-\beta\omega'})\Phi(\mathbf{k},\omega'), \quad (16)$$

which is analytic in the entire z plane, except for a cut on the real axis, we find that $F(\mathbf{k},z)$ is the analytical continuation of $G_n(\mathbf{k})$ from the infinite set of points $i2\pi n/\beta(n\neq0)$ on the imaginary axis of z to the entire plane, except for the real axis. Furthermore, if for any function $f(z)$ in the complex z plane, we denote by

$$f^\pm(\omega)=\lim_{z\to\omega\pm i\epsilon}f(z), \quad \epsilon\to+0, \quad (17)$$

we obtain from Eq. (16)

$$\Phi(\mathbf{k},\omega)=-i\frac{F^+(\mathbf{k},\omega)-F^-(\mathbf{k},\omega)}{2\pi(1-\epsilon^{-\beta\omega})}, \quad (18)$$

and finally

$$S(\mathbf{k},\omega)=-\frac{1}{n}\coth(\tfrac{1}{2}\beta\omega)\frac{F^+(\mathbf{k},\omega)-F^-(\mathbf{k},\omega)}{2i}. \quad (19)$$

Equation (19) provides us with the required relation

between the spectrum fluctuation of the density and the analytical continuation of the "Fourier transforms" of the temperature-dependent Green's function $G(\mathbf{k},u)$. The problem is thus reduced to the calculation of $G_n(\mathbf{k})$.

III. THE SPECTRUM OF THE ELECTRON-DENSITY FLUCTUATIONS

A. The Electron-Phonon Hamiltonian

Before we turn to the calculation of $S(\mathbf{k},\omega)$ we discuss briefly the electron-phonon Hamiltonian to be used here. We follow Bardeen and Pines[4] assuming a monatomic crystal of n ions and electrons per unit volume. We introduce phonon coordinates to represent the ion motion, and second quantization representation for the electrons. The phonons are assumed to be either longitudinal or transversal, and only the longitudinal phonons interact with the electrons (long-wavelength region). We define creation and annihilation operators, $a_p^\dagger$ and a_p, obeying the usual anticommutation relations, to represent the Bloch states ψ_p. The Bloch equation is

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial \mathbf{r}^2}+V(\mathbf{r})\right]\psi_p(\mathbf{r})=E(\mathbf{p})\psi_p(\mathbf{r}), \tag{20}$$

where $V(\mathbf{r})$ stands for the effective potential due to the equilibrium position of the ions, compensated by a uniform negative charge. An extended zone scheme is to be used. The Hamiltonian for the electrons is

$$H_e=\sum_p E(\mathbf{p})a_p^\dagger a_p + \frac{1}{2V}\sum_k{}' \phi(k)\sum_{p,p'} a_{p+k}^\dagger a_p a_{p'+k}^\dagger a_{p'} \tag{21}$$

with

$$\phi(k)=\int d\mathbf{r}d\mathbf{r}'\,\psi_{p+k}^\dagger(\mathbf{r})\psi_{p'}^\dagger(r')\frac{e^2}{(\mathbf{r}-\mathbf{r}')}\psi_{p'+k}(\mathbf{r}')\psi_p(\mathbf{r}), \tag{22}$$

where we assume, in the spirit of Bloch's theory, that $\phi(k)$ depends on the absolute value of $\mathbf{k}$ [for free electrons $\phi(k)=4\pi e^2/k^2$].

The longitudinal phonons are represented by the Hamiltonian

$$H=\sum_{\mathbf{k}\,(\text{zone})}\Omega_k b_\mathbf{k}^\dagger b_\mathbf{k}, \tag{23}$$

where $b_\mathbf{k}^\dagger$ and $b_\mathbf{k}$ are the creation and annihilation operators of phonons in the $\mathbf{k}$ state obeying the usual commutation relations, and Ω_k is determined solely by the ion-ion interaction (in the negative background). The summation is restricted to the first Brillioun zone for the phonons.

The interaction between the electrons and the phonons is represented by the Hamiltonian

$$H_{ep}=\sum_\mathbf{k} V_\mathbf{k}Q_\mathbf{k}\sum_p a_{p-k}^\dagger a_p, \tag{24}$$

where

$$V_\mathbf{k}=(-nM)^{-1/2}\int d\mathbf{r} \times\psi_{p+k}^*(\mathbf{r})\left[\sum_j \boldsymbol{\varepsilon}_k\cdot\frac{\partial}{\partial\mathbf{r}}U(\mathbf{r}-\mathbf{R}_j)e^{i\mathbf{k}\cdot\mathbf{R}_j}\right]\psi_p(\mathbf{r}). \tag{25}$$

The matrix element of the interaction depends only on the wave vector difference between the initial and the final states of the electrons. We have also $V_\mathbf{k}^*=V_{-\mathbf{k}}$. The sum over $\mathbf{k}$ in Eq. (24) extends over all values, while

$$Q_\mathbf{k}=(2\Omega_k)^{-1/2}[b_\mathbf{k}+b_{-\mathbf{k}}^\dagger] \tag{26}$$

refers to the reduced vector in the first zone. This amounts to the inclusion of Peierls-umklapp processes.[7] In Eq. (25), M is the ion mass, $\boldsymbol{\varepsilon}_\mathbf{k}$ is a unit vector in the $\mathbf{k}$ direction, and $U(\mathbf{r}-\mathbf{R}_j)$ is the effective potential of interaction between an electron in position $\mathbf{r}$ and an ion in equilibrium position $\mathbf{R}_j$. The total Hamiltonian is now

$$H=H_e+H_p+H_{ep}, \tag{27}$$

with the irrelevant parts (e.g., the transverse phonons) left out.

B. Green Function Technique

We rewrite Eq. (11) in the interaction representation

$$G(\mathbf{k},u)=\frac{1}{V}\sum_{p,p'}\langle U(\beta)\rangle_0^{-1} \times\langle T\{a_{p+k}^\dagger(u)a_p(u)a_{p'-k}^\dagger(0)a_{p'}(0)U(\beta)\}\rangle_0, \tag{28}$$

where use has been made of the second-quantization representation of the density operator

$$n(\mathbf{k})=\sum_p a_{p+k}^\dagger a_p. \tag{29}$$

The symbol $\langle\ \rangle_0$ corresponds to the average defined in Eq. (5), but for noninteracting particles ($H_0=\sum_p E(\mathbf{k})a_p^\dagger a_p+\sum_\mathbf{k}\Omega_k b_\mathbf{k}^\dagger b_\mathbf{k}$),

$$U(\beta)=\exp\left\{-\int_0^\beta du H_I(u)\right\}, \tag{30}$$

where

$$H_I=\frac{1}{2V}\sum_k\phi(k)\sum_{p,p'}a_{p+k}^\dagger a_{p'}^\dagger a_{p'-k}a_p + \sum_\mathbf{k}V_\mathbf{k}Q_\mathbf{k}\sum_p a_{p-k}^\dagger a_p \tag{31}$$

and

$$H_I(u)=e^{uH_0}H_I e^{-uH_0}, \tag{32}$$

with the same convention for $a_p(u)$.

The basic rules for the perturbation expansion of

[7] The umklapp processes are not explicitly treated in this paper but they may be included without major changes of the theory.

$G_n(\mathbf{k})$, the Fourier transform of Eq. (28), are given by Luttinger and Ward[5] with a slightly modified procedure to include the ions' motion. We employ a diagram technique, indicating by a solid line the free-electron propagator

$$g_{\mathbf{p}}(u)=\langle T\{a_{\mathbf{p}}^{\dagger}(u)a_{\mathbf{p}}(0)\}\rangle_0, \tag{33}$$

which has the form

$$g_{\mathbf{p}}(\zeta_l)=[\zeta_l-E(\mathbf{p})]^{-1}, \tag{34}$$

in the "Fourier transform" representation, with

$$\zeta_l=i\pi(2l+1)\frac{1}{\beta}+\mu, \quad l=0,\pm1,\pm2,\cdots. \tag{35}$$

By a wavy line we indicate the free phonon propagator

$$D_{\mathbf{k}}^{0}(u)=\langle T\{Q_{\mathbf{k}}(u)Q_{\mathbf{k}}(0)\}\rangle_0, \tag{36}$$

or

$$D_{\mathbf{k}}^{0}(\alpha_m)=\frac{-1}{\Omega_k^2-\alpha_m^2}, \tag{37}$$

$$\alpha_m=i2\pi m/\beta, \quad m=0\pm1,\pm2,\cdots, \tag{38}$$

and by a dashed line the Coulomb interaction $\phi(k)$ of Eq. (22). After Migdal[8] we assign to each electron-phonon vertex the quantity $V_{\mathbf{k}}$ (or $V_{\mathbf{k}}^{*}$) and neglect all vertex corrections. Thus to each phonon line corresponds the factor $|V_{\mathbf{k}}|^2$.

C. The Approximation Method

We consider the leading asymptotic contribution to the electron-density fluctuation spectrum in the long-wavelength region, in the limit where many electrons are in the Bohr sphere, and the electron-ion mass ratio m/M is small. The class of diagrams contributing to $S(\mathbf{k},\omega)$ in this case are given in Fig. 1. The saw-toothed line represents the effective interaction shown in Fig. 2 and it it is given by[9]

$$U_{\mathbf{k}}(\alpha_m)=\phi(k)+|v_{\mathbf{k}}|^2D_{\mathbf{k}}^{0}(\alpha_m)+[\phi(k)+|v_{\mathbf{k}}|^2D^{0}{}_{\mathbf{k}}(\alpha_m)]$$
$$\times\frac{1}{V}\sum_{\mathbf{p}}\frac{1}{\beta}\sum_{l}g_{\mathbf{p}+\mathbf{k}/2}(\zeta_l+\alpha_m)g_{\mathbf{p}-\mathbf{k}/2}(\zeta_l)U_{\mathbf{k}}(\alpha_m), \tag{39}$$

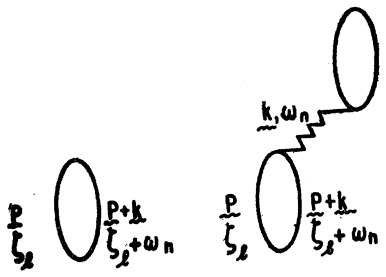

FIG. 1. The class of diagrams which contribute to the spectrum of electron density fluctuations in the present approximation.

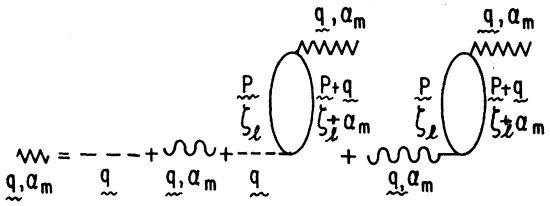

FIG. 2. The diagrammatic representation of the integral equation for the effective electron-electron interaction.

where α_m is given by Eq. (38). Equation (39) is now solved for $U_k(\alpha_m)$, and yields

$$U_{\mathbf{k}}(\alpha_m)=\frac{\phi(k)+|V_{\mathbf{k}}|^2D_{\mathbf{k}}^{0}(\alpha_m)}{1-Q_{\mathbf{k}}(\alpha_m)[\phi(k)+|V_{\mathbf{k}}|^2D_{\mathbf{k}}^{0}(\alpha_m)]}, \tag{40}$$

where

$$Q_{\mathbf{k}}(\alpha_m)=+\frac{1}{V}\sum_{\mathbf{p}}\frac{1}{\beta}\sum_{l}g_{\mathbf{p}+\mathbf{k}/2}(\zeta_l+\alpha_m)g_{\mathbf{p}-\mathbf{k}/2}(\zeta_l)$$
$$=\frac{1}{(2\pi)^3}\int d\mathbf{p}\frac{f_{\mathbf{p}+\mathbf{k}/2}-f_{\mathbf{p}-\mathbf{k}/2}}{E(\mathbf{p}+\mathbf{k}/2)-E(\mathbf{p}-\mathbf{k}/2)-\alpha_m} \tag{41}$$

and

$$f_{\mathbf{k}}=[e^{\beta[E(p)-\mu]}+1]^{-1} \tag{42}$$

is the Fermi distribution for the electrons.

It is convenient to cast Eq. (40) into another form showing explicitly the Coulomb and phonon parts of it. Defining the electron dielectric function (in its Fourier representation)

$$\epsilon(\mathbf{k},\alpha_m)=1-\phi(k)Q_{\mathbf{k}}(\alpha_m), \tag{43}$$

and the "dressed" phonon propagator

$$D_{\mathbf{k}}(\alpha_m)=D_{\mathbf{k}}^{0}(\alpha_m)\left[1-\frac{|V_{\mathbf{k}}|^2Q_{\mathbf{k}}(\alpha_m)}{\epsilon(\mathbf{k},\alpha_m)}D_{\mathbf{k}}^{0}(\alpha_m)\right]^{-1}, \tag{44}$$

we are able to write

$$D_{\mathbf{k}}^{0}(\alpha_m)=D_{\mathbf{k}}(\alpha_m)\left[1+\frac{|V_{\mathbf{k}}|^2Q_{\mathbf{k}}(\alpha_m)}{\epsilon(\mathbf{k},\alpha_m)}D_{\mathbf{k}}(\alpha_m)\right]^{-1} \tag{45}$$

and thus

$$U_{\mathbf{k}}(\alpha_m)=\frac{\phi(k)}{\epsilon(\mathbf{k},\alpha_m)}+\frac{|V_{\mathbf{k}}|^2D_{\mathbf{k}}(\alpha_m)}{[\epsilon(\mathbf{k},\alpha_m)]^2}. \tag{46}$$

The physical interpretation of the right-hand side of Eq. (46) is simple. The first term represents the usual dynamically screened Coulomb potential due to the collective motion of the electrons, and the second term corresponds to a "dressed" phonon $D_{\mathbf{k}}(\alpha_m)$ interacting with the electrons through a dynamically screened electron-phonon interaction $V_{\mathbf{k}}/\epsilon(\mathbf{k},\alpha_m)$.

Using the prescription of Luttinger and Ward[5] generalized to include the phonon effects, we calculate

[8] A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **34**, 1438 (1958) [translation: Soviet Phys.—JETP **6**, 966 (1958)].
[9] D. Pines, in *Introduction to The Many Body Problem* (W. A. Benjamin, Inc., New York, 1961).

the contribution of the diagrams of Fig. 1, and obtain

$$G_n(\mathbf{k})=Q_{\mathbf{k}}(\omega_n)[1+U_{\mathbf{k}}(\omega_n)Q_{\mathbf{k}}(\omega_n)], \quad (47)$$

with $\omega_n=2\pi in/\beta$, $n=0, \pm1, \pm2, \cdots$. The analytical continuation of $G_n(\mathbf{k})$ causes no difficulties and yields [see Eq. (16)]

$$F(\mathbf{k},z)=Q_{\mathbf{k}}(z)[1+U_{\mathbf{k}}(z)Q_{\mathbf{k}}(z)], \quad (48)$$

where by Eq. (41)

$$Q_{\mathbf{k}}(z)=\frac{1}{(2\pi)^3}\int d\mathbf{p}\frac{f_{\mathbf{p}+\mathbf{k}/2}-f_{\mathbf{p}-\mathbf{k}/2}}{E(\mathbf{p}+\mathbf{k}/2)-E(\mathbf{p}-\mathbf{k}/2)-z}, \quad (49)$$

and similar definitions for $U_{\mathbf{k}}(z)$, $D_{\mathbf{k}}(z)$, and $\epsilon(\mathbf{k},z)$.

The spectrum of density fluctuation is now given by substituting Eq. (48) into Eq. (19) [with Eq. (17)]

$$S(\mathbf{k},\omega)=\frac{1}{n}\coth(\tfrac{1}{2}\beta\omega)\frac{Q_{\mathbf{k}}^{+}(\omega)[1+U_{\mathbf{k}}^{+}(\omega)Q_{\mathbf{k}}^{+}(\omega)]-Q_{\mathbf{k}}^{-}(\omega)[1+U_{\mathbf{k}}^{-}(\omega)Q_{\mathbf{k}}^{-}(\omega)]}{2i} \quad (50)$$

or, by using Eq. (46), we obtain our final general result

$$S(\mathbf{k},\omega)=\frac{1}{n}\coth(\tfrac{1}{2}\beta\omega)\frac{1}{2i}\left\{\frac{Q_{\mathbf{k}}^{+}(\omega)-Q_{\mathbf{k}}^{-}(\omega)}{|\epsilon(\mathbf{k},\omega)|^2}+|V_{\mathbf{k}}|^2\left[\left(\frac{Q_{\mathbf{k}}^{+}(\omega)}{\epsilon^{+}(\mathbf{k},\omega)}\right)^2 D_{\mathbf{k}}^{+}(\omega)-\left(\frac{Q_{\mathbf{k}}^{-}(\omega)}{\epsilon^{-}(\mathbf{k},\omega)}\right)^2 D_{\mathbf{k}}^{-}(\omega)\right]\right\} \quad (51)$$

The first part of S on the right-hand side of Eq. (51) is clearly due to the electron density fluctuation *without* taking into account the presence of the phonons in the system. This would be the result one obtains dealing with an electron gas. The second part has the effect of the *presence* of phonons with the electrons dynamically shielding them.

For a given wave-vector $\mathbf{k}$, that is, a given incident wave and detector location, the ω dependence of the scattering cross section is essentially the following:

(i) The first part of s, the "electron" part, can be written explicitly as

$$S_{\mathrm{el}}(k,\omega)=\frac{\pi}{n}\coth(\tfrac{1}{2}\beta\omega)\frac{1}{|\epsilon(k,\omega)|^2}\frac{1}{(2\pi)^3}\times\int d\mathbf{p}\,(f_{\mathbf{p}+\mathbf{k}/2}-f_{\mathbf{p}-\mathbf{k}/2})\times\delta[E(\mathbf{p}+\mathbf{k}/2)-E(\mathbf{p}-\mathbf{k}/2)-\omega], \quad (52)$$

with

$$\epsilon(k,\omega)=1-\phi(k)\frac{1}{(2\pi)^3}\times\int d\mathbf{p}\frac{f_{\mathbf{p}+k/2}-f_{\mathbf{p}-\mathbf{k}/2}}{E(\mathbf{p}+k/2)-E(\mathbf{p}-\mathbf{k}/2)-\omega-i\delta}, \quad \delta\to+0. \quad (53)$$

The main body of S_{el} corresponds to a Doppler broadening, due to the *individual* motion of the electrons, and is characterized by a weak *continuum*, as shown schematically in Fig. 3. Besides this continuum there is a *sharp* resonance, corresponding to the *collective* effect of the density fluctuation, located at the vicinity of the point where both the integral and $\epsilon(k,\omega)$ of Eq. (52) decrease simultaneously (see Fig. 3). Rewriting Eq. (52) as

$$S_{\mathrm{el}}(k,\omega)=\frac{\pi}{n}\coth(\tfrac{1}{2}\beta\omega)\frac{1}{\phi(k)}\frac{\mathrm{Im}\epsilon(k,\omega)}{|\epsilon(k,\omega)|^2}, \quad (54)$$

we notice that the resonance occurs at the point where the real part of the electron dielectric function vanishes, $\mathrm{Re}\epsilon(k,\omega)=0$, namely near the frequency, ω_p, of the electron plasma oscillation of the system. The height and the width of this peak are determined by $\mathrm{Im}\epsilon(k,\omega)$ at the vicinity of ω_p.

(ii) The "phonon" part of the cross section contributes mostly at low frequencies, i.e., frequencies of the order of the phonon spectrum, and dies away at higher frequencies. Thus, we can rewrite the second part of Eq. (51) approximately as

$$S_{\mathrm{ph}}(\mathbf{k},\omega)=\frac{1}{n}\coth(\tfrac{1}{2}\omega\beta)\frac{1}{2i}\frac{|V_{\mathbf{k}}|^2}{[\phi(k)]^2}\left|\frac{1-\epsilon(k,\omega)}{\epsilon(k,\omega)}\right|^2\times[D_{\mathbf{k}}^{+}(\omega)-D_{\mathbf{k}}^{-}(\omega)], \quad (55)$$

where use has been made of Eqs. (43) and (53). Further, if we use Eqs. (44) and (37) and define

$$D(k,\omega)\equiv D_{\mathbf{k}}^{+}(\omega)=D_{\mathbf{k}}^{0+}(\omega)\left(1-\frac{|V_{\mathbf{k}}|^2}{\phi(k)}\frac{1-\epsilon^{+}(\mathbf{k},\omega)}{\epsilon^{+}(\mathbf{k},\omega)}D_{\mathbf{k}}^{0+}(\omega)\right)^{-1}, \quad (56)$$

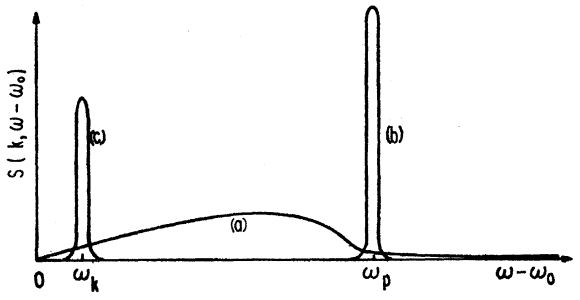

FIG. 3. Schematic sketch (not to scale) of the spectrum of the electron density fluctuations. (a) The *individual* electron continuum. (b) The *collective* electron-electron resonance due to excitation of plasma oscillations. (c) The *collective* electron-phonon resonance, due to the cloud of electrons participating in the lattice vibrations.

or with Eq. (53)

$$D(k,\omega)=1\Big/\left((\omega+i\delta)^2-\Omega_k^2-\frac{|V_{\mathbf{k}}|^2}{\phi(k)}\frac{1-\epsilon(k,\omega)}{\epsilon(k,\omega)}\right)^{-1},$$

$$\times\delta\to+0 \quad (57)$$

we find

$$\frac{1}{2i}D_{\mathbf{k}}^{+}(\omega)-D_{\mathbf{k}}^{-}(\omega)=\mathrm{Im}D(k,\omega), \quad (58)$$

and finally

$$S_{\mathrm{ph}}(k,\omega)=\frac{1}{n}\coth(\tfrac{1}{2}\beta\omega)\left|\frac{V_{\mathbf{k}}}{\phi(k)}\right|^2\times\left(\frac{1-\epsilon(k,\omega)}{\epsilon(k,\omega)}\right)^2\mathrm{Im}D(k,\omega). \quad (59)$$

The function S_{ph} shows a resonance shape centered around the "real" frequencies of the phonons, corresponding to the given wavelength $\mathbf{k}$. The resonance frequencies are determined by the dispersion relation

$$F(\omega)=\omega^2-\Omega_k^2-\frac{|V_{\mathbf{k}}|^2}{\phi(k)}\frac{1-\epsilon(k,\omega)}{\epsilon(k,\omega)}=0. \quad (60$$

Under the assumption that the damping of the lattice waves is very small, the dressed phonons frequency obeys

$$\omega_k^2=\Omega_k^2+\frac{|V_{\mathbf{k}}|^2}{\phi(k)}\mathrm{Re}\left[\frac{1-\epsilon(k,\omega_k)}{\epsilon(k,\omega_k)}\right] \quad (61)$$

and the damping is given by

$$\gamma_k=-\frac{|V_k|^2}{2\omega_k\phi(k)}\frac{\mathrm{Im}\epsilon(k,\omega_k)}{|\epsilon(k,\omega_k)|^2}, \quad |\gamma_k|\ll\omega_k. \quad (62)$$

A further simplification is apparent if we notice that $\omega_k\ll E_F$ (the Fermi energy) and we may write

$$\omega_k^2\approx\Omega_k^2+\frac{V_k^2}{\phi(k)}\frac{1-\epsilon(k,0)}{\epsilon(k,0)}, \quad (63)$$

which leads to the well-known result

$$\omega_k=\pm ck$$

for long wavelengths, with $c=(m/3M)^{1/2}U_F$—the sound velocity, and U_F the Fermi velocity.

To conclude we notice that for positive frequencies (the negative frequencies may be treated in the same manner)

$$\mathrm{Im}D(k,\omega)=\frac{1}{2\omega_k}\frac{|\gamma_k|}{(\omega-\omega_k)^2+\gamma_k^2}, \quad (64)$$

and due to the resonance behavior around ω_k

$$S_{\mathrm{ph}}(k,\omega)=\frac{1}{n}\coth(\tfrac{1}{2}\beta\omega_k)\left|\frac{V_k}{\phi(k)}\right|^2\times\left|\frac{1-\epsilon(k,\omega_k)}{\epsilon(k,\omega_k)}\right|^2\frac{1}{2\omega_k}\frac{|\gamma_p|}{(\omega-\omega_k)^2+\gamma_n^2}. \quad (65)$$

S_{ph} is the contribution to the scattering cross section due to the coupled motion of the electrons and the phonons. Equation (65) shows a Lorentzian shape around the phonon frequencies ω_k; the width and the height are determined by γ_k and $1/\gamma_k$, respectively.

IV. SELF-CONSISTENT TEST-PARTICLE APPROACH

In the present section we rederive the results of the previous section by employing a method, well known in classical problems, of the self-consistent test particle.[3] This method facilitates an elementary derivation and, moreover, leads to a very simple physical interpretation of the results. The response of the system to a *"test particle"* with an assigned motion and dynamics is calculated and then an *ensemble* average with respect to the test particle taken in a *self-consistent* manner. The concept of a *"dressed particle"* is thus introduced naturally.

A. Dressed Electrons

Consider a test particle, with the same properties as the electrons, embedded into the system of interacting electrons. The Hamiltonian of the system is given by Eq. (21) and by the interaction term

$$H_I=\sum_{\mathbf{q}}{}'\,\phi(q)\sum_{\mathbf{p}}a_{\mathbf{p}+\mathbf{q}}{}^{\dagger}\alpha_{\mathbf{p}_0-\mathbf{q}}{}^{\dagger}\alpha_{\mathbf{p}_0}a_{\mathbf{p}}, \quad (66)$$

where $\mathbf{p}_0$ is the assigned momentum of the test particle and $\alpha_{\mathbf{p}}{}^{\dagger}$, $\alpha_{\mathbf{p}}$ are its Fermion creation and annihilation operators. The equation of motion of the (field) electron annihilation operator is given by

$$i\frac{\partial}{\partial t}a_{\mathbf{p}}=E(\mathbf{p})a_{\mathbf{p}}+\sum_{\mathbf{k}}\phi(k)\sum_{\mathbf{p}'}a_{\mathbf{p}}{}^{\dagger}a_{\mathbf{p}'+\mathbf{k}}a_{\mathbf{p}-\mathbf{k}}+\sum_{\mathbf{q}}\phi(q)\alpha_{\mathbf{p}_0-\mathbf{q}}{}^{\dagger}\alpha_{\mathbf{p}_0}a_{\mathbf{p}-\mathbf{q}} \quad (67)$$

and a similar one for $a_{\mathbf{p}}{}^{\dagger}$. If we define a "distribution function" $\langle\mathbf{p}+\mathbf{k}|\rho|\mathbf{p}\rangle$ by the equation (in the Heisenberg representation)

$$\langle\mathbf{p}+\mathbf{k}|\rho(t)|\mathbf{p}\rangle=\mathrm{Tr}\{Da_{\mathbf{p}}{}^{\dagger}(t)a_{p+\mathbf{k}}(t)\}, \quad (68)$$

where D is the density matrix of the system, we obtain

$$\left[i\frac{\partial}{\partial t}+E(\mathbf{p})-E(\mathbf{p}+\mathbf{k})\right]\langle\mathbf{p}+\mathbf{k}|\rho|\mathbf{p}\rangle=\sum_{\mathbf{k}'}\phi(\mathbf{k}')[n(\mathbf{k}',t)+\alpha_{\mathbf{p}_0-\mathbf{k}'}{}^{\dagger(t)}\alpha_{\mathbf{p}_0}{}^{(t)}]\times[\langle\mathbf{p}+\mathbf{k}-\mathbf{k}'|\rho|\mathbf{p}\rangle-\langle\mathbf{p}+\mathbf{k}|\rho|\mathbf{p}+\mathbf{k}'\rangle], \quad (69)$$

where, to first approximation, correlations and exchange terms were neglected.[10] Here,

$$n(\mathbf{k},t)=\sum_{\mathbf{p}}\langle\mathbf{p}+\mathbf{k}|\rho|\mathbf{p}\rangle$$

is the density of the field electrons.

The response of the field electrons to the test particle is now obtained by assuming the right-hand side of Eq. (69) to be a small perturbation on the thermal equilibrium solution

$$\langle\mathbf{p}+\mathbf{k}|\rho|\mathbf{p}\rangle=\delta_{\mathbf{k},0}f_p, \tag{71}$$

where $f_\mathbf{p}$ is the Fermi distribution function given by Eq. (42). Thus, the perturbed part of $\langle\mathbf{p}+\mathbf{k}|\rho|\mathbf{p}\rangle$ obeys the equation

$$\left\{i\frac{\partial}{\partial t}+E(\mathbf{p})-E(\mathbf{p}+\mathbf{k})+\phi(k)(f_{\mathbf{p}+\mathbf{k}}-f_\mathbf{p})\sum_{\mathbf{p}}\right\}\times\langle\mathbf{p}+\mathbf{k}|\rho^{(1)}(t)|\mathbf{p}\rangle$$
$$=\phi(k)[f_\mathbf{p}-f_{\mathbf{p}+\mathbf{k}}]\alpha_{\mathbf{p}_0-\mathbf{k}}{}^\dagger\alpha_{\mathbf{p}_0}e^{-i[E(\mathbf{p}_0)-E(\mathbf{p}_0-\mathbf{k})]t}, \tag{72}$$

where use has been made of

$$\alpha_\mathbf{p}(t)=\alpha_\mathbf{p}\epsilon^{-iE(\mathbf{p})t}, \tag{73}$$

and a similar expression for $\alpha_p{}^\dagger(t)$. Solving Eq. (72) for the density response we obtain

$$n^{(1)}(\mathbf{k},t)=\frac{\phi(k)}{\epsilon[k,E(\mathbf{p}_0)-E(\mathbf{p}_0-\mathbf{k})]}\times\sum_{\mathbf{p}}\frac{f_{\mathbf{p}+\mathbf{k}}-f_\mathbf{p}}{E(\mathbf{p}+\mathbf{k})-E(\mathbf{p})-E(\mathbf{p}_0)+E(\mathbf{p}_0-\mathbf{k})-i\delta}\times\alpha_{\mathbf{p}_0-\mathbf{k}}{}^\dagger\alpha_{\mathbf{p}_0}\epsilon^{-i[E(\mathbf{p}_0)-E(\mathbf{p}_0-\mathbf{k})]t},\quad\delta\to+0 \tag{74}$$

where $\epsilon(k,\omega)$ is given by Eq. (53).

We now consider the test particle with its associated cloud [Eq. (74)] as a dressed electron with an assigned momentum $\mathbf{p}_0$; hence, the corresponding density operator reads

$$\hat{n}(k,t)=a_{\mathbf{p}_0-\mathbf{k}}{}^\dagger(t)a_{\mathbf{p}_0}(t)+n^{(1)}(\mathbf{k},t)=\frac{1}{\epsilon[\mathbf{k},E(\mathbf{p}_0)-E(\mathbf{p}_0-\mathbf{k})]}\times e^{-i[E(\mathbf{p}_0)-E(\mathbf{p}_0-\mathbf{k})]t}a_{\mathbf{p}_0-\mathbf{k}}{}^\dagger a_{\mathbf{p}_0}, \tag{75}$$

where the α's were replaced by the usual a's. Substituting Eq. (75) into Eq. (3) yields

$$S^\dagger(\mathbf{k},\omega)=\frac{1}{2nV}\int d\tau\,\epsilon^{i\omega\tau}\sum_{\mathbf{p}_0}\langle a_{\mathbf{p}_0-\mathbf{k}/2}{}^\dagger a_{\mathbf{p}_0+\mathbf{k}/2}a_{\mathbf{p}_0+\mathbf{k}/2}{}^\dagger a_{\mathbf{p}_0-\mathbf{k}/2}+a_{\mathbf{p}_0+\mathbf{k}/2}{}^\dagger a_{\mathbf{p}_0-\mathbf{k}/2}a_{\mathbf{p}_0-\mathbf{k}/2}{}^\dagger a_{\mathbf{p}_0+\mathbf{k}/2}\rangle\times\frac{1}{|\epsilon[k,E(\mathbf{p}_0-\mathbf{k}/2)-E(\mathbf{p}_0+\mathbf{k}/2)]|^2}\times e^{-i[E(\mathbf{p}_0-\mathbf{k}/2)-E(\mathbf{p}_0+\mathbf{k}/2)]\tau}, \tag{76}$$

where the average is to be taken over a "free" Hamiltonian of the dressed electrons. The spectrum density is now, by Eq. (2) and $\mathbf{p}_0\to-\mathbf{p}$

$$S(k,\omega)=\frac{\pi}{n}\frac{1}{V}\sum_{\mathbf{p}}\frac{1}{|\epsilon(k,\omega)|^2}\times[f_{\mathbf{p}+\mathbf{k}/2}(1-f_{\mathbf{p}-\mathbf{k}/2})+f_{\mathbf{p}-\mathbf{k}/2}(1-f_{\mathbf{p}+\mathbf{k}/2})]\times\delta[E(\mathbf{p}+\mathbf{k}/2)-E(\mathbf{p}-\mathbf{k}/2)-\omega], \tag{77}$$

and, after some algebraic manipulation and replacing $(1/V)\sum_\mathbf{p}$ by $[1/(2\pi)^3]\int d\mathbf{p}$, we recover Eq. (52), which is the required result.

By this approach we are led to a simple picture of the physics behind the mechanism of the scattering. The scattering comes from a system of particles dressed by a cloud around them. Both the core and the cloud contributes to the cross section, the first leads to a one-particle continuum and the latter to a sharp resonance due to the collective excitations.

B. Dressed Phonons

In a similar way we can treat the formation of the cloud around a test-phonon. We consider a test phonon in the $\mathbf{k}$ state immersed in the system of interacting electrons. The Hamiltonian is given by Eqs. (21), (23), and (24) without the summation over $\mathbf{k}$ in the last two equations. The equation of motion for $a_\mathbf{p}$ is the same as in Eq. (67) with the last term on the right replaced by

$$V_\mathbf{k}Q_\mathbf{k}a_{\mathbf{p}-\mathbf{k}}. \tag{78}$$

Making the same approximations as before, we end with the equation

$$\left\{i\frac{\partial}{\partial t}+E(\mathbf{p})-E(\mathbf{p}+k)+\phi(\mathbf{k})(f_{\mathbf{p}+\mathbf{k}}-f_\mathbf{p})\sum_{\mathbf{p}}\right\}\times\langle\mathbf{p}+\mathbf{k}|\rho^{(1)}(t)|\mathbf{p}\rangle=V_\mathbf{k}[f_\mathbf{p}-f_{\mathbf{p}+\mathbf{k}}]Q_\mathbf{k}(t), \tag{79}$$

for the response of the electrons to the test phonon [compare with Eq. (72) and Ref. 11], while the

[10] H. Ehrenreich and M. H. Cohen, Phys. Rev. **115**, 786 (1959).

[11] A. Ron, Phys. Rev. **131**, 2040 (1963).

dynamics of the phonon are given by

$$\left(\frac{\partial^2}{\partial t^2}+\Omega_k^2\right)Q_{\mathbf{k}}(t)=-V_{\mathbf{k}}^*\sum_{\mathbf{p}}\langle\mathbf{p}+\mathbf{k}|\rho^{(1)}(t)|\mathbf{p}\rangle. \quad (80)$$

We now Fourier transform Eqs. (79) and (80) in time and use Eq. (53) to obtain

$$n^{(1)}(\mathbf{k},\omega)=\frac{V_{\mathbf{k}}}{\phi(k)}\frac{1-\epsilon(k,\omega)}{\epsilon(k,\omega)}Q_{\mathbf{k}}(\omega), \quad (81)$$

and thus $Q_k(\omega)$ obeys

$$\left[-\omega^2+\Omega_k^2+\frac{|V_{\mathbf{k}}|^2}{\phi(k)}\frac{1-\epsilon(k,\omega)}{\epsilon(k,\omega)}\right]Q_{\mathbf{k}}(\omega)=0. \quad (82)$$

The "true" frequencies of the dressed phonon are thus given by

$$\omega^2-\Omega_k^2-\frac{|V_{\mathbf{k}}|^2}{\phi(k)}\frac{1-\epsilon(k,\omega)}{\epsilon(k,\omega)}=0, \quad (83)$$

which is the same dispersion relation displayed by Eq. (60). For very small damping factor γ_k we can write

$$Q_{\mathbf{k}}(t)=(2\omega_k)^{-1/2}[b_{\mathbf{k}}\epsilon^{-i(\omega_k+i\gamma_k)t}+b_{-\mathbf{k}}^{\dagger}\epsilon^{i(\omega_k-i\gamma_k)t}], \quad (84)$$

where $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^{\dagger}$ are the annihilation and creation operators for the phonons. Finally, going back to Eq. (81), we find for the electron cloud

$$n(\mathbf{k},t)=\frac{V_{\mathbf{k}}}{\phi(k)}\frac{1}{(2\omega_k)^{1/2}}\left\{\frac{1-\epsilon(k,\omega_k+i\gamma_k)}{\epsilon(k,\omega_k+i\gamma_k)}b_{\mathbf{k}}\epsilon^{-i(\omega_k+i\gamma_k)t}+\frac{1-\epsilon(k,\omega_k-i\gamma_k)}{\epsilon(k,\omega_k-i\gamma_k)}b_{-\mathbf{k}}^{\dagger}\epsilon^{i(\omega_k-i\gamma_k)t}\right\}. \quad (85)$$

We now substitute Eq. (83) into Eq. (3) and read

$$S^{\dagger}(\mathbf{k},\omega)=\frac{1}{2nV}\frac{|V_{\mathbf{k}}|^2}{2\omega_k}\frac{1}{[\phi(k)]^2}\left|\frac{1-\epsilon(k,\omega_k)}{\epsilon(k,\omega_k)}\right|^2\times\int_0^{\infty}d\tau\,\epsilon^{i\omega\tau}\{\langle b_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}^{\dagger}b^{\dagger}\rangle\epsilon^{-i(\omega_k+i\gamma_k)\tau}+\langle b_{-\mathbf{k}}^{\dagger}b_{-\mathbf{k}}+b_{-\mathbf{k}}b_{-\mathbf{k}}^{\dagger}\rangle\epsilon^{+i(\omega_k-i\gamma_k)\tau}\}. \quad (86)$$

Performing the time integration and noticing that

$$\langle b_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\rangle=\coth(\tfrac{1}{2}\beta\omega_k), \quad (87)$$

where the average is with respect to the "free" dressed phonons, we finally obtain, for positive frequencies

$$S(k,\omega)=\frac{1}{n}\frac{|V_{\mathbf{k}}|^2}{2\omega_k[\phi(k)]^2}\left|\frac{1-\epsilon(k,\omega_k)}{\epsilon(k,\omega_k)}\right|^2\times\coth(\tfrac{1}{2}\beta\omega_k)\frac{|\gamma_k|}{(\omega-\omega_k)^2+\gamma_k^2}, \quad (88)$$

which recovers Eq. (65).

The interpretation of this result is now simple. The scattering comes from electrons associated with the dressed phonons, i.e., from electrons participating in the lattice vibrations by following the ions of the lattice in their motion. The ions of the lattice are shielded by the electrons and while oscillating they carry with them their electron clouds, which gives rise to the resonance in the scattering cross section.

V. DISCUSSION

The coupled motion of electrons and ions in a metal is reflected in the spectrum of the density fluctuations of the electrons, and this, in turn, can be observed by detecting the incoherent scattering of electromagnetic waves from thin films of metal. Although a simplified model for the metal was the basis of the theoretical investigation in the present paper, it is conceivable that the theory would yield a fairly good agreement with the real situation, when applied to metals like Na. Thus, the incoherent scattering experiment can, in principle, provide a tool for studying the elementary collective excitations in the electron-phonon system, i.e., lattice vibrations, with the electrons participating collectively in the motion of the lattice, and the electron plasma oscillations.

To conclude we wish to make the following comments:

(i) The amount of radiation scattered from the system is extremely small (the cross section is proportional to $r_0^2\approx10^{-25}$ cm^2) and very sensitive detectors must be used. Moreover, we were concerned only with an incident radiation with highly peaked frequency spectrum, while in reality care should be taken to correct for the width of the spectrum.

(ii) The frequencies of the incident waves are much higher then the lattice vibrations frequencies; hence, the shifts due to the phonon resonances are very small, and can be detected only by very sensitive equipment. Furthermore, the influence of the transverse phonons was not considered here and should be taken into account for practical problems.

(iii) The widths and heights of the resonances are also influenced by other processes (e.g., electron-phonon collisions contribute to the very small width of the plasma oscillation resonance) and should be considered for practical problems.

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