Raman Scattering by Magnetoplasma Oscillations in Many-Valley Semiconductors

A thesis submitted in accordance with the requirements for the degree of Doctor of Philosophy

John Sanders

Department of Physics

ABSTRACT

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RAMAN SCATTERING IN SEMICONDUCTORS SANDERS

Raman Scattering by Magnetoplasma Oscillations in Many-Valley Semiconductors

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A thesis submitted to the Faculty of Graduate Studies and Research in partial fulfilment of requirements for the degree of Doctor of Philosophy.

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PREFACE

The results of the calculations in this thesis are an original contribution to knowledge. Both the Raman scattering process and the excitations considered are well-known; however, the combination of the two is original. In the calculation many standard techniques are employed and published results of others are used freely; all these contributions to the thesis are acknowledged in the bibliography.

ABSTRACT

The Raman scattering cross sections are calculated for the longitudinal collective modes in n-type PbTe in a static magnetic field oriented symmetrically with respect to the four ellipsoidal energy surfaces, and varying in strength from 10 Kgauss to 200 Kgauss. Only modes propagating parallel to this field are considered. Because of the anisotropy of the energy surfaces, a low-frequency charge density oscillation can exist in the plasma. It is shown that the presence of this mode can be detected most easily through its interaction with the longitudinal optical phonons or the usual plasmons. A one-band model is used to describe the carriers, and the electron-electron interaction is treated within the random phase approximation. The results can be adapted easily to Ge by elimination of the phonons.

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CHAPTER I

INTRODUCTION

The availability of lasers has stimulated much interest in the problem of light scattering by solid-state plasmas[1]. In this thesis we deal with the solid state plasmas of lightly-doped many-valley semiconductors, consisting of carriers with anisotropic energy surfaces. In a DC magnetic field these plasmas, under suitable conditions, support a low-frequency charge density oscillation[2]. Such a mode must not be confused with the sound mode of two-carrier plasmas[3]. The mode we discuss exists only in a magnetic field, and results from the coupling of motion along the field to motion transverse to the field (which is quantized in Landau levels) through the anisotropic effective-mass tensor.

The purpose of this thesis is to calculate the inelastic light-scattering cross section by this mode. The scattering process will be treated to lowest order in perturbation theory in the photon field. The carriers of the plasma will be treated in the effective mass approximation[4]. All other crystal structure effects will be neglected, except for screening through virtual interband transition which will be accounted for by an optical dielectric constant ε_∞ (we assume ε_∞ to be independent of frequency for the frequencies with which we work). The interaction between carriers will be calculated in a random phase

approximation (RPA)[†]. In a polar semiconductor the coulomb interaction will be augmented in an important way by an interaction due to the exchange of longitudinal optical (LO) phonons; the two can be conveniently combined as shown in reference (1).

We will work in particular with n-type PbTe which is a polar substance. Our results will then be easily adaptable to Ge by elimination of the phonons. Both crystals have a bcc inverse lattice structure with four ellipsoidal energy surfaces in the [111] and equivalent directions. We will treat each ellipsoid separately, ignoring intervalley effects.

Finally, we restrict ourselves to a static magnetic field in the [001] direction, and consider only propagation of the mode parallel to the field.

The one-band model we use is valid only if the incident photon frequency is far from the frequency corresponding to the band gap.For PbTe the gap is 0.19 ev [5], so that a convenient wavelength is probably 10.6 μ such as provided by the CO_2 laser.

[†]The bare electron propagators used in the irreducible polarization part will be Landau state propagators rather than free-particle ones.

CHAPTER II

THE MODEL

A. The Hamiltonian

Figure 1 shows the ellipsoids in k-space occupied by the carriers in n-type PbTe or Ge. The coordinate system we denote by $\mathcal{C}$. To find the effective one-band hamiltonian for the crystal we assume parabolic bands of the form*

$$\mathcal{E}(k) = \frac{1}{2m}\,\alpha_{ij}\,k_i\,k_j \qquad (2.1)$$

for each of the ellipsoids, where k is measured from the Brillouin zone boundary. The shape of each ellipsoid is characterized by constants α_T and α_L so that in the proper coordinate systems we have the energy relationship

$$\mathcal{E}(k) = \frac{1}{2m}\left[\alpha_T\left(k_{\bar{1}}^2 + k_{\bar{2}}^2\right) + \alpha_L\, k_{\bar{3}}^2\right] \qquad (2.2)$$

where $k_{\bar{i}}$ is expressed with respect to a coordinate system $\bar{\mathcal{C}}$. Within the effective mass approximation, the effective hamiltonian, for one surface "ℓ", in a DC magnetic field is

$$\mathcal{H}_{cr}^{(\ell)} = \frac{1}{2m}\,\underset{\sim}{\Pi}\cdot\underset{\approx}{\alpha}^{(\ell)}\cdot\underset{\sim}{\Pi} - e\varphi + \frac{1}{2}\,g^{*(\ell)}\mu_B\,\underset{\sim}{B}\cdot\underset{\sim}{\sigma} \qquad (2.3)$$

where $\underset{\sim}{\Pi} = \underset{\sim}{p} + e\underset{\sim}{A}^{DC}$ (the charge of the electron is -e), p is the canonical momentum, $g^{*(\ell)}$ is the effective g-factor, $B = \nabla \times A^{DC}$, and φ is a potential due to other electrons in the plasma. Later, when we calculate the interaction of the plasma with incident photons, we will replace $\underset{\sim}{\Pi}$ by $\underset{\sim}{\Pi} + e\underset{\sim}{A}$.

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* In the formalism we use natural units $\hbar = 1 = c$. In numerical calculations cgs units will be used.

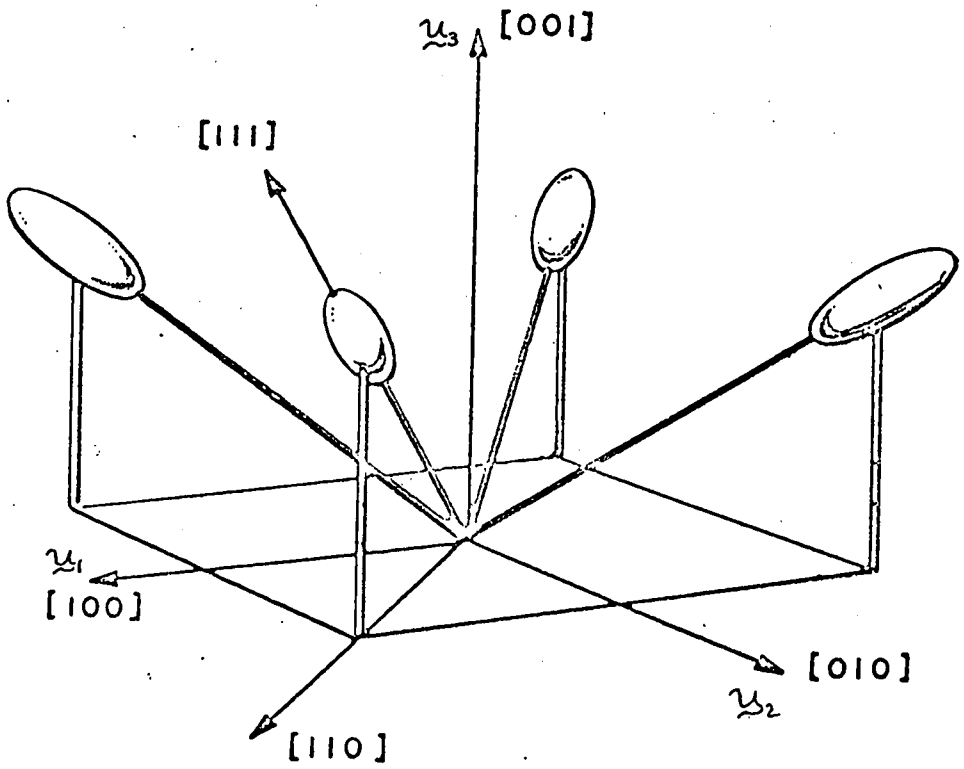

Figure 1. The four prolate spheroids of carriers in k-space are shown for n-type PbTe and Ge. The spheroids are centred on the Brillouin zone faces.

B. The Single-Particle States

We consider only the case of B pointing in the $\underset{\sim}{u}_3$ direction. Working with one surface at a time we look for eigenstates of the hamiltonian

$$\mathcal{H}_{cr}^{o} = \frac{1}{2m}\underline{\Pi}\cdot\underline{\underline{\alpha}}\cdot\underline{\Pi} + \frac{1}{2}g^{*}\mu_B\underline{B}\cdot\underline{\sigma} \tag{2.4}$$

Since the two terms of this hamiltonian commute, we treat them separately. As indicated in equation (2.2) we perform a rotation of the coordinate system from $\mathcal{C}$ to $\overline{\mathcal{C}}$ so that

$$k_{\bar{i}} = R_{ij}\,k_j \tag{2.5}$$

and

$$\mathcal{H}_{cr}^{o} = \frac{1}{2m}\left[\alpha_T\left(\Pi_{\bar{1}}^2 + \Pi_{\bar{2}}^2\right) + \alpha_L\,\Pi_{\bar{3}}^2\right] \tag{2.6}$$

By rescaling length according to

$$K_{\bar{i}} = \sqrt{\alpha_i}\,k_{\bar{i}} \qquad X_{\bar{i}} = \frac{x_{\bar{i}}}{\sqrt{\alpha_i}}$$

$$\overline{A}_{\bar{i}} = \sqrt{\alpha_i}\,A_{\bar{i}} \qquad \overline{B}_{\bar{i}} = \sqrt{\alpha_j\alpha_k}\,B_{\bar{i}} \quad \text{(i,j,k cyclic)} \tag{2.7}$$

with $\alpha_1 = \alpha_2 = \alpha_T$ and $\alpha_3 = \alpha_L$, and with no summation over repeated indices, we can rewrite the hamiltonian

$$\mathcal{H}_{cr}^{o} = \frac{1}{2m}\left(\frac{\overline{\nabla}}{i} + e\underline{\overline{A}}^{DC}\right)^2 \tag{2.8}$$

We now perform a second rotation to $\overline{\overline{\mathcal{C}}}$ where

$$K_{\bar{i}} = S_{ij} K_J \tag{2.9}$$

so that the rescaled field $\underline{\bar{B}}$ has components $\bar{B}_{\bar{i}} = \bar{B}\delta_{i,3}$, and we will have the usual Landau wave functions as solutions. In the coordinate system $\bar{\bar{\mathcal{C}}}$ we choose the gauge

$$\underline{\bar{A}}^{DC} = (0, X_{\bar{1}}\bar{B}, 0) \tag{2.10}$$

and the Schrödinger equation becomes

$$-\frac{1}{2m}\left[\frac{\partial^2}{\partial X_{\bar{1}}^2} + \left(\frac{\partial}{\partial X_{\bar{2}}} + ie\bar{B}X_{\bar{1}}\right)^2 + \frac{\partial^2}{\partial X_{\bar{3}}^2}\right] \Psi(\underline{X}) = E\,\Psi(\underline{X}) \tag{2.11}$$

whose solutions are

$$\Psi_{nQK}(\underline{X}) = \frac{1}{2\pi(\alpha_T^2\alpha_L)^{1/4}}\, e^{iQX_{\bar{2}} + iKX_{\bar{3}}}\, u_n\left(X_{\bar{1}} + \frac{Q}{m\omega_c}\right) \tag{2.12}$$

where

$$\omega_c = \frac{e\bar{B}}{m}$$

$$E_{nK} = \left(n + \tfrac{1}{2}\right)\omega_c + \frac{K^2}{2m} \tag{2.13}$$

$$u_n(X_{\bar{1}}) = \left(\frac{m\omega_c}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}\, e^{-\frac{1}{2}m\omega_c X_{\bar{1}}^2}\, H_n\left(\sqrt{m\omega_c}\, X_{\bar{1}}\right)$$

and H_n are the Hermite polynomials.

The coordinates in system $\bar{\bar{\mathcal{C}}}$ are related to those in $\mathcal{C}$ as follows

$$x_i = X_{\bar{k}} M_{ki} \tag{2.14}$$

with

$$M_{ki} = S_{kj} \sqrt{\alpha_j} R_{ji} \tag{2.15}$$

Note that the matrices M will differ for the four ellipsoids.

From the properties of Hermite polynomials it is easy to verify that the $u_n(\xi)$ satisfy the relationships

$$\begin{aligned} u_n(\xi) &= (-)^n u_n(-\xi) \\ \xi u_n(\xi) &= \frac{1}{\sqrt{2m\omega_c}}\left[\sqrt{n}\, u_{n-1}(\xi) + \sqrt{n+1}\, u_{n+1}(\xi)\right] \\ \frac{d}{d\xi} u_n(\xi) &= \sqrt{\frac{m\omega_c}{2}}\left[\sqrt{n}\, u_{n-1}(\xi) - \sqrt{n+1}\, u_{n+1}(\xi)\right] \end{aligned} \tag{2.16}$$

Going back to the unscaled coordinates in $\mathcal{C}$ we define our wave functions

$$\Phi_{nQK}(\underline{x}) = \Psi_{nQK}(\underline{X}) \tag{2.17}$$

for each surface, with $x_i = X_{\bar{k}} M_{ki}$. The normalizations

have been chosen so that

$$\int \Phi^{*}_{nQK}(\underline{x})\,\Phi_{n'Q'K'}(\underline{x})\,d^{3}x = \delta_{nn'}\,\delta(K-K')\,\delta(Q-Q')$$

$$\int u_{n}(\xi)\,u_{n'}(\xi)\,d\xi = \delta_{nn'} \qquad (2.18)$$

If we now include the spin part of our hamiltonian (2.4), we get solutions

$$\Phi_{nQK\sigma}(\underline{x}) = \Psi_{nQK}(\underline{X})\,\chi_{\sigma} \qquad (2.19)$$

with energies

$$E_{nK\sigma} = \left(n+\tfrac{1}{2}\right)\omega_{c} + \frac{K^{2}}{2m} + \frac{1}{4}\,g^{*}\omega_{0}\sigma \qquad (2.20)$$

where $\sigma = 1(-1)$ for spin parallel (antiparallel) to the magnetic field $\underline{B}$. χ_{σ} is a two-component eigenspinor of σ_{z}.

For purposes of second quantization we will use electron operators

$$\psi^{(\ell)}_{\sigma}(\underline{x}) = \sum_{n}\int dQ\,dK\; c^{(\ell)}_{n\sigma}(Q,K)\,\Phi^{(\ell)}_{nQK\sigma}(\underline{x}) \qquad (2.21)$$

with the c's satisfying the anticommutation relations

$$\left\{c^{(\ell)}_{n}(Q,K),\,c^{(\ell')}_{n'}(Q',K')\right\} = \delta_{\ell\ell'}\,\delta_{nn'}\,\delta(Q-Q')\,\delta(K-K') \qquad (2.22)$$

C. The Matrices M

We calculate the matrix M for the [111] ellipsoid. The two coordinate systems $\mathcal{C}$ and $\overline{\mathcal{C}}$ are shown in figure 2. Expressing all vectors with respect to $\mathcal{C}$, we write $\overline{\underset{\sim}{u}}_2=(a,b,c)$ and choose it orthogonal to $\underset{\sim}{B}$ as well as to $\overline{\underset{\sim}{u}}_3=\frac{1}{\sqrt{3}}(1,1,1)$. We find

$$\overline{\underset{\sim}{u}}_2=\frac{1}{\sqrt{2}}(-1,1,0)$$

Then $\overline{\underset{\sim}{u}}_1=\overline{\underset{\sim}{u}}_2\times\overline{\underset{\sim}{u}}_3=\frac{1}{\sqrt{6}}(1,1,-2)$. Characterizing the rotation by R_{ij} (equation 2.5), and expressing an arbitrary vector $\underset{\sim}{V}$ with respect to both coordinate systems $\mathcal{C}$ and $\overline{\mathcal{C}}$, we find

$$V_i\,\underset{\sim}{u}_i=R_{ij}V_j\,\overline{\underset{\sim}{u}}_i$$

Accordingly

$$R_{ij}=\overline{\underset{\sim}{u}}_i\cdot\underset{\sim}{u}_j$$

or

$$R^{(111)}=\begin{pmatrix}\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}}\\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}\end{pmatrix} \qquad (2.23)$$

Applying the rescaling prescription to $\underset{\sim}{B}$ we find

$$\begin{aligned}\overline{B}_1&=-\frac{2}{\sqrt{6}}\sqrt{\alpha_L\alpha_T}\,B\\ \overline{B}_2&=0 \qquad (2.24)\\ \overline{B}_3&=\frac{\alpha_T}{\sqrt{3}}B\end{aligned}$$

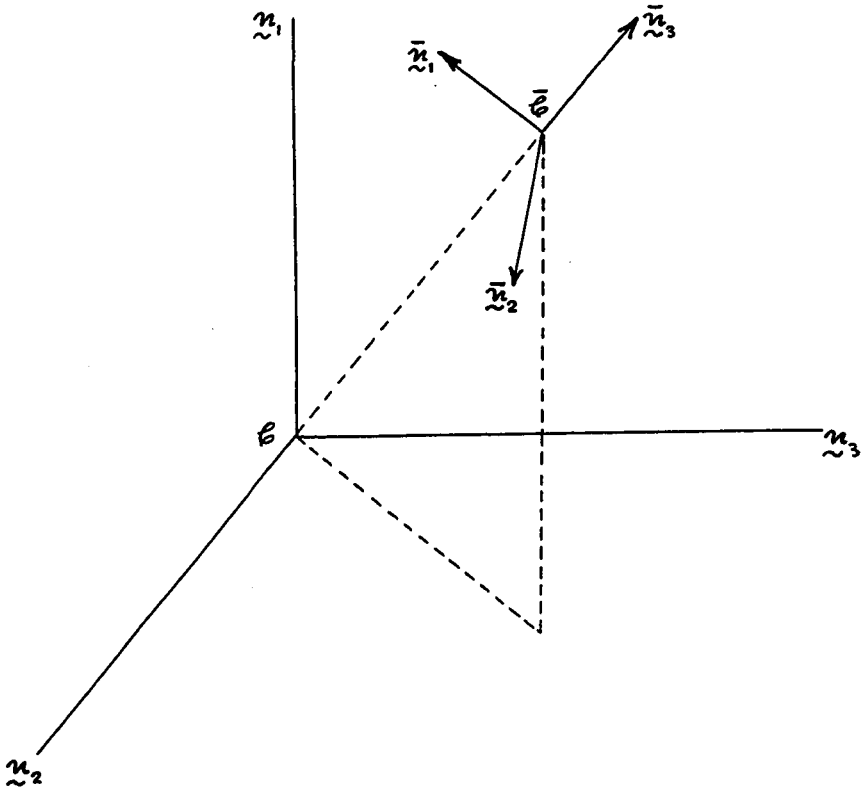

Figure 2. The two coordinate systems $\mathcal{C}$ and $\bar{\mathcal{C}}$.

We perform one more rotation to get $\underline{\overline{B}}$ into the form $(0,0,\overline{B})$. With the same procedure as for our first rotation we find

$$S^{(III)}=\begin{pmatrix} \sqrt{\frac{\alpha_T}{\alpha_T+2\alpha_L}} & 0 & \sqrt{\frac{2\alpha_L}{\alpha_T+2\alpha_L}} \\ 0 & 1 & 0 \\ -\sqrt{\frac{2\alpha_L}{\alpha_T+2\alpha_L}} & 0 & \sqrt{\frac{\alpha_T}{\alpha_T+2\alpha_L}} \end{pmatrix} \qquad (2.25)$$

From (2.15) we now find

$$M^{(III)}=\begin{pmatrix} \sqrt{\frac{\alpha_T+2\alpha_L}{6}} & \sqrt{\frac{\alpha_T+2\alpha_L}{6}} & \sqrt{\frac{2}{3}}\frac{\alpha_L-\alpha_T}{\sqrt{\alpha_T+2\alpha_L}} \\ -\sqrt{\frac{\alpha_T}{2}} & \sqrt{\frac{\alpha_T}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3\alpha_L\alpha_T}{\alpha_T+2\alpha_L}} \end{pmatrix} \qquad (2.26)$$

The same treatment of the other ellipsoids yields

$$M^{(III)}=\begin{pmatrix} -\sqrt{\frac{\alpha_T+2\alpha_L}{6}} & \sqrt{\frac{\alpha_T+2\alpha_L}{6}} & \sqrt{\frac{2}{3}}\frac{\alpha_L-\alpha_T}{\sqrt{\alpha_T+2\alpha_L}} \\ -\sqrt{\frac{\alpha_T}{2}} & -\sqrt{\frac{\alpha_T}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3\alpha_L\alpha_T}{\alpha_T+2\alpha_L}} \end{pmatrix}$$

$$M^{(1-11)} = \begin{pmatrix} \sqrt{\frac{\alpha_T+2\alpha_L}{6}} & -\sqrt{\frac{\alpha_T+2\alpha_L}{6}} & \sqrt{\frac{2}{3}}\frac{\alpha_L-\alpha_T}{\sqrt{\alpha_T+2\alpha_L}} \\ \sqrt{\frac{\alpha_T}{2}} & \sqrt{\frac{\alpha_T}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3\alpha_L\alpha_T}{\alpha_T+2\alpha_L}} \end{pmatrix} \tag{2.27}$$

$$M^{(-1-11)} = \begin{pmatrix} -\sqrt{\frac{\alpha_T+2\alpha_L}{6}} & -\sqrt{\frac{\alpha_T+2\alpha_L}{6}} & \sqrt{\frac{2}{3}}\frac{\alpha_L-\alpha_T}{\sqrt{\alpha_T+2\alpha_L}} \\ \sqrt{\frac{\alpha_T}{2}} & -\sqrt{\frac{\alpha_T}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3\alpha_L\alpha_T}{\alpha_T+2\alpha_L}} \end{pmatrix}$$

Detailed calculation shows that ω_c is the same for each ellipsoid (as one would expect from symmetry)

$$\omega_c = \omega_o\sqrt{\frac{\alpha_T(\alpha_T+2\alpha_L)}{3}} \tag{2.28}$$

where $\omega_o = \frac{eB}{m}$ is the usual cyclotron frequency for a free electron.

D. Electron-Electron Interactions

To complete the description of our crystal model we specify the electron-electron interactions. In a polar crystal there are two. The first is the coulomb interaction screened

by virtual interband transitions

$$V(\underset{\sim}{x}_1-\underset{\sim}{x}_2)=\frac{e^2}{\epsilon_\infty}\frac{1}{|\underset{\sim}{x}_1-\underset{\sim}{x}_2|} \tag{2.29}$$

The second is the interaction due to the exchange of virtual LO phonons, for which we need to consider the phonon field.

At long wavelengths we can start off with a macroscopic lagrangian density

$$\mathcal{L}=\frac{\gamma}{2}\dot{P}^2+\frac{\alpha}{2}\left(\partial_i P_j\right)^2+\frac{\beta}{2}P^2+\underset{\sim}{P}\cdot\underset{\sim}{D} \tag{2.30}$$

where $\underset{\sim}{P}(\underset{\sim}{x})$ is the polarization at the point $\underset{\sim}{x}$ due to the LO phonons, and $\underset{\sim}{D}(\underset{\sim}{x})$ is the electric displacement. Note that other simple derivative terms need not be included because of the condition $\nabla \times \underset{\sim}{P}=0$. The last term is the Fröhlich interaction[6] of a macroscopic field due to the conduction electrons with the phonon polarization. $\underset{\sim}{D}$ satisfies the Maxwell equation

$$\nabla\cdot\underset{\sim}{D}=4\pi\rho \tag{2.31}$$

where ρ is the conduction charge density. To determine the phenomenological constants in this lagrangian we need Fröhlich's original argument that a conduction electron in a crystal causes a total polarization $\underset{\sim}{P}_t$ made up of that due to the phonons, $\underset{\sim}{P}$, and that due to virtual interband transitions, $\underset{\sim}{P}_\infty$:

$$\underset{\sim}{P}_t(\underset{\sim}{x})=\underset{\sim}{P}(\underset{\sim}{x})+\underset{\sim}{P}_\infty(\underset{\sim}{x}) \tag{2.32}$$

The latter is approximately independent of frequency for frequencies much less than the band gap. Thus, from the high-frequency response we find

$$\underset{\sim}{D} = \epsilon_\infty \underset{\sim}{E}$$

and

$$\underset{\sim}{P}_\infty(x) = \frac{1}{4\pi}(\underset{\sim}{D} - \underset{\sim}{E}) = \frac{1}{4\pi}\underset{\sim}{D}\left(1 - \frac{1}{\epsilon_\infty}\right) \tag{2.33}$$

At zero frequency we have

$$\underset{\sim}{D} = \epsilon_o \underset{\sim}{E}$$

and

$$\underset{\sim}{P}_t = \frac{1}{4\pi}(\underset{\sim}{D} - \underset{\sim}{E}) = \frac{1}{4\pi}\underset{\sim}{D}\left(1 - \frac{1}{\epsilon_o}\right) \tag{2.34}$$

where ϵ_o is the static dielectric constant. Hence, for the static case

$$\underset{\sim}{P} = \frac{\underset{\sim}{D}}{4\pi}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_o}\right) \tag{2.35}$$

since $\underset{\sim}{P}_\infty$ is independent of frequency. With the additional fact that the undoped crystal will vibrate at a frequency ω_L, we find that

$$\beta = -4\pi\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_o}\right)^{-1}$$

$$\gamma = \frac{4\pi}{\omega_L^2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_o}\right)^{-1} \tag{2.36}$$

in order that (2.28) will give us the correct equations of motion. The constant α will come into the dispersion relation of the phonon. However, since we deal with wave numbers

much smaller than an inverse lattice vector, we will neglect dispersion.

The usual normal coordinate-creation, destruction operator formalism gives the following results:

$$H_{ph}^{o} = \int d^3q \; \omega_L(\underset{\sim}{q})\, b^{\dagger}(\underset{\sim}{q})\, b(\underset{\sim}{q}) \tag{2.37}$$

with

$$\left[b(\underset{\sim}{q}), b^{\dagger}(\underset{\sim}{q}')\right] = \delta^3(\underset{\sim}{q}-\underset{\sim}{q}') \tag{2.38}$$

and

$$P_i(\underset{\sim}{x}) = \frac{1}{(2\pi)^{3/2}} \frac{\partial}{\partial x_i} \int \frac{d^3q}{|\underset{\sim}{q}|} \frac{1}{\sqrt{2\gamma\omega_L}}\, e^{-i\underset{\sim}{q}\cdot\underset{\sim}{x}} \left[b(-\underset{\sim}{q}) + b^{\dagger}(\underset{\sim}{q})\right] \tag{2.39}$$

The Fröhlich interaction becomes

$$H_I^F = -\int \underset{\sim}{P}\cdot\underset{\sim}{D}\; d^3x \tag{2.40}$$

$$= q\sqrt{\frac{4\pi e^2}{\epsilon_\infty}} \sum_{l\sigma} \int d^3x\, \psi_\sigma^{(l)\dagger}(\underset{\sim}{x})\psi_\sigma^{(l)}(\underset{\sim}{x}) \int \frac{d^3q}{|\underset{\sim}{q}|}\, e^{-i\underset{\sim}{q}\cdot\underset{\sim}{x}} \left[b(-\underset{\sim}{q}) + b^{\dagger}(\underset{\sim}{q})\right]$$

with

$$q = -\frac{1}{2\pi}\sqrt{\frac{\omega_L}{4\pi}\left(1-\frac{\omega_T^2}{\omega_L^2}\right)} \tag{2.41}$$

We have used the Lyddane, Sachs, Teller relation

$$\frac{\omega_T^2}{\omega_L^2} = \frac{\epsilon_\infty}{\epsilon_o} \tag{2.42}$$

CHAPTER III

THE SCATTERING CROSS SECTION

A. The Photon Field

The free-field lagrangian density in vacuum is

$$\mathcal{L} = -\frac{1}{16\pi}\left(\partial_\mu A_\nu - \partial_\nu A_\mu\right)^2 \tag{3.1}$$

in unrationalized units. The Greek subscripts run from 1 to 4, and the Latin ones from 1 to 3. The equations of motion are

$$\partial^2 A_i = 0 \tag{3.2}$$

in the radiation gauge $\partial_i A_i = 0$. An easy way to adapt this lagrangian to a medium characterized by a dielectric constant ε_∞ is to reinterpret $\frac{\partial}{\partial x_4}$ as follows

$$\frac{\partial}{\partial x_4} = -i\eta\frac{\partial}{\partial t} \tag{3.3}$$

where η is the optical index of refraction, $\eta = \sqrt{\varepsilon_\infty}$. The equation of motion becomes

$$\nabla^2 A_i - \eta^2\frac{\partial^2 A_i}{\partial t^2} = 0 \tag{3.4}$$

which is equivalent to the macroscopic Maxwell equations. The canonical momentum is†

$$\pi_i = \frac{i\eta}{4\pi}A_{i,4} = \frac{\eta^2}{4\pi}\dot{A}_i \tag{3.5}$$

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† This $\underset{\sim}{\pi}$ must not be confused with the $\underset{\sim}{\Pi}$ we used in Chapter II. We will not use this form of $\underset{\sim}{\Pi}$ again after this section.

and the hamiltonian density,

$$\mathcal{H} = \frac{1}{8\pi}\left[\eta^2 E^2 + B^2\right] \tag{3.6}$$

This verifies that the choice of normalization of (3.1) is correct. Introduction of creation and destruction operators, via normal coordinates, leads to the following results

$$H = \sum_{\lambda,\underset{\sim}{k}} \omega(\underset{\sim}{k})\, a^{\dagger}_{\lambda}(\underset{\sim}{k})\, a_{\lambda}(\underset{\sim}{k}) \tag{3.7}$$

with the dispersion relation

$$\omega(\underset{\sim}{k}) = \frac{|\underset{\sim}{k}|}{\eta} \tag{3.8}$$

and with λ denoting the two kinds of polarization, and

$$A_i(\underset{\sim}{x}) = \frac{1}{\eta}\sqrt{\frac{2\pi}{V}} \sum_{\underset{\sim}{k}} \sqrt{\frac{1}{\omega(k)}}\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}} \left[a_i(-\underset{\sim}{k}) + a^{\dagger}_i(\underset{\sim}{k})\right] \tag{3.9}$$

with

$$\begin{aligned} a_i(\underset{\sim}{k}) &= \sum_{\lambda} e^{(\lambda)}_i(\underset{\sim}{k})\, a_{\lambda}(\underset{\sim}{k}) \\ \left[a_{\lambda}(\underset{\sim}{k}), a^{\dagger}_{\lambda'}(\underset{\sim}{k}')\right] &= \delta_{\underset{\sim}{k}\underset{\sim}{k}'}\, \delta_{\lambda\lambda'} \\ \sum_{\lambda=1}^{2} e^{(\lambda)}_i(\underset{\sim}{k})\, e^{(\lambda)*}_j(\underset{\sim}{k}) &= \delta_{ij} - \frac{k_i k_j}{\underset{\sim}{k}^2} \end{aligned} \tag{3.10}$$

V is the quantization volume which drops out at the end of the calculation.

In finding the cross section we will need the density of photons and the density of final states in k-space. The former is calculated from

$$\langle \underset{\sim}{k}\lambda | \underset{\sim}{k}\lambda \rangle = 1 \tag{3.11}$$

which shows a density of photons of $\frac{1}{V}$. The latter is given by

$$1 = \sum_{\underset{\sim}{k}\lambda} |\underset{\sim}{k}\lambda\rangle\langle\underset{\sim}{k}\lambda| = \sum_{\lambda} \frac{V}{(2\pi)^3} \int |\underset{\sim}{k}\lambda\rangle\langle\underset{\sim}{k}\lambda| \, d^3k$$

which shows a density of states in k-space of $\frac{V}{(2\pi)^3}$.

B. The Cross Section- Formalism

In the absence of perturbing photons, the hamiltonian for our system is

$$H_{cr} = \sum_{l\sigma} \int \psi_{\sigma}^{(l)\dagger}(\underset{\sim}{x}) \left[\frac{\underset{\sim}{\Pi}\cdot\underset{\sim}{\alpha}^{(l)}\cdot\underset{\sim}{\Pi}}{2m} + \frac{1}{2} g^* \mu_B \underset{\sim}{B}\cdot\underset{\sim}{\sigma} \right] \psi_{\sigma}^{(l)}(\underset{\sim}{x}) \, d^3x + \tag{3.12}$$

$$+ \int d^3q \, \omega_L(\underset{\sim}{q}) b^{\dagger}(\underset{\sim}{q}) b(\underset{\sim}{q}) + H_I^C + H_I^F$$

where H_I^F is given by (2.40) and

$$H_I^C = \frac{e^2}{2\epsilon_\infty} \sum_{\substack{l_1 l_2 \\ \sigma_1 \sigma_2}} \int \psi_{\sigma_1}^{(l_1)\dagger}(\underset{\sim}{x}_1) \psi_{\sigma_2}^{(l_2)\dagger}(\underset{\sim}{x}_2) \frac{1}{|\underset{\sim}{x}_1 - \underset{\sim}{x}_2|} \psi_{\sigma_2}^{(l_2)}(\underset{\sim}{x}_2) \psi_{\sigma_1}^{(l_1)}(\underset{\sim}{x}_1) d^3x_1 d^3x_2 \tag{3.13}$$

We have neglected intervalley effects, and have assumed g^* to be the same for each ellipsoid. Since the $\Phi(\underset{\sim}{x})$ are solutions of $\mathcal{H}_{cr}^{o}$ we can rewrite (3.11)

$$H_{cr} = H_o + H_I^C + H_I^F \tag{3.14}$$

with

$$H_o = \sum_{\substack{n\sigma \\ l}} \int dQ\,dK\, E_{nK\sigma}^{(l)} C_{n\sigma}^{(l)\dagger}(Q,K) C_{n\sigma}^{(l)}(Q,K) + \int d^3q\, \omega_L(\underset{\sim}{q})\, b^{\dagger}(\underset{\sim}{q})\, b(\underset{\sim}{q}) \tag{3.15}$$

We find the hamiltonian in the presence of the photons by replacing $\underset{\sim}{\pi}$ by $\underset{\sim}{\pi} + e\underset{\sim}{A}$ in (3.12) and adding the free photon hamiltonian (3.7):

$$H = H_{cr} + H_{em} + H_I^{em} \tag{3.16}$$

with

$$H_I^{em} = \frac{1}{2m} \sum_{l\sigma} \int \psi_{\sigma}^{(l)\dagger}(\underset{\sim}{x}) \left[e\alpha_{ij}^{(l)} (A_i \pi_j + \pi_i A_j) + e^2 \alpha_{ij}^{(l)} A_i A_j \right] \psi_{\sigma}^{(l)}(\underset{\sim}{x})\, d^3x \tag{3.17}$$

In calculating the cross section we treat the crystal exactly (at least in principle) and treat the field $\underset{\sim}{A}$ to second order in perturbation theory. It is well-known that, as long as the effective mass approximation holds,

$$H_{II}^{em} = \frac{e}{2m} \sum_{l\sigma} \int \psi_{\sigma}^{(l)\dagger}(\underset{\sim}{x})\, \alpha_{ij}^{(l)} (A_i \pi_j + \pi_i A_j)\, \psi_{\sigma}^{(l)}(\underset{\sim}{x})\, d^3x \tag{3.18}$$

contributes a negligible amount to the cross section compared with

$$H_{I2}^{em} = \frac{e^2}{2m} \sum_{l\sigma} \int \psi_\sigma^{(l)\dagger}(\underset{\sim}{x}) \psi_\sigma^{(l)}(\underset{\sim}{x}) \alpha_{ij}^{(l)} A_i(\underset{\sim}{x}) A_j(\underset{\sim}{x}) \, d^3x \qquad (3.19)$$

Therefore we will neglect H_{I1}^{em} [7,8].

We now consider the scattering process in which a photon $|\underset{\sim}{k}_1 \lambda_1\rangle$ scatters off the crystal in the state $|i\rangle$ into the state $|\underset{\sim}{k}_2 \lambda_2\rangle$, leaving the crystal in the state $|f\rangle$. In the end we shall be left with matrix elements of the type $\langle i|.....|i\rangle$ by which we mean an average over the grand canonical ensemble, and which we shall write simply as $\langle .....\rangle$. Using only H_{I2}^{em}, and to lowest order in $\underset{\sim}{A}$, we get for the transition amplitude

$$T_{12}^{if} = \langle f | a_{\lambda_2}(\underset{\sim}{k}_2)(-i)\int H_{I2}^{em}(t)\,dt\, a_{\lambda_1}^\dagger(\underset{\sim}{k}_1) | i\rangle \qquad (3.20)$$

The time dependence of the interaction hamiltonian is of the form

$$H_{I2}^{em}(t) = e^{i(H_{em}+H_{cr})t} H_{I2}^{em} e^{-i(H_{em}+H_{cr})t} \qquad (3.21)$$

Using (3.19), (3.10), (3.9) and (3.7) in (3.20) we find[†]

[†]The density is not a spinor as we have taken the product $\chi_\sigma^\dagger \chi_\sigma = 1$.

$$T_{12}^{if} = -\frac{i2\pi e^2}{mV\eta^2\sqrt{\omega_1\omega_2}} \sum_{l\sigma} \int d^4x\, e^{i\underset{\sim}{q}\cdot\underset{\sim}{x} - i\omega t}\, e_i^{(\lambda_2)*}(\underset{\sim}{k}_2)\alpha_{ij}^{(l)} e_j^{(\lambda_1)}(\underset{\sim}{k}_1) \langle f | \rho_\sigma^{(l)}(\underset{\sim}{x}) | i \rangle \qquad (3.22)$$

where

$$\begin{aligned} &\underset{\sim}{k}_1 - \underset{\sim}{k}_2 = \underset{\sim}{q} \\ &\omega_1 - \omega_2 = \omega(\underset{\sim}{k}_1) - \omega(\underset{\sim}{k}_2) = \omega \\ &\rho_\sigma^{(l)}(\underset{\sim}{x}) = \psi_\sigma^{(l)\dagger}(\underset{\sim}{x})\psi_\sigma^{(l)}(\underset{\sim}{x}) \end{aligned} \qquad (3.23)$$

The transition probability is just the modulus squared of this transition amplitude. We include all possible excitations of the crystal by summing this probability over all final states[3]. The generalized transition probability W_{12} is then

$$W_{12} = \sum_f \left| T_{12}^{if} \right|^2 = \frac{4\pi^2 e^4}{m^2\eta^4 V^2 \omega_1\omega_2} \sum_{ll'\sigma\sigma'} \int dt\, dt'\, e^{-i\omega(t-t')} \times \qquad (3.24)$$

$$\times \langle \rho_{\sigma'}^{(l')}(\underset{\sim}{q}, t') \rho_\sigma^{(l)}(-\underset{\sim}{q}, t) \rangle\, \lambda_{21}^{(l)}\, \lambda_{21}^{(l')*}$$

We have defined

$$\begin{aligned} &\rho_\sigma^{(l)}(\underset{\sim}{q}, t) = \int d^3x\, \rho_\sigma^{(l)}(\underset{\sim}{x}, t)\, e^{-i\underset{\sim}{q}\cdot\underset{\sim}{x}} \\ &\lambda_{21}^{(l)} = \underset{\sim}{e}^{(\lambda_2)*}(\underset{\sim}{k}_2) \cdot \underset{\approx}{\alpha}^{(l)} \cdot \underset{\sim}{e}^{(\lambda_1)}(\underset{\sim}{k}_1) \end{aligned} \qquad (3.25)$$

Since the integrand is a function of (t-t') we can do one time integration to get

$$W_{12} = \frac{4\pi^2 r_o^2 T}{V^2 \omega_1 \omega_2 \eta^4} \sum_{\substack{\ell\ell' \\ \sigma\sigma'}} \int dt\, e^{i\omega t} \left\langle \rho_{\sigma'}^{(\ell')}(\underset{\sim}{q}, t)\, \rho_{\sigma}^{(\ell)}(-\underset{\sim}{q}, 0) \right\rangle \lambda_{21}^{(\ell)} \lambda_{21}^{(\ell')*} \qquad (3.26)$$

where T is the total time and r_o , the classical electron radius.

The cross section is the transition probability per unit time per unit incoming flux, times the density of final states

$$d\sigma = \frac{W_{12}}{T} \frac{1}{v} \frac{V}{(2\pi)^3} k_2^2\, dk_2\, d\Omega \qquad (3.27)$$

where v is the velocity of light in the crystal. We find

$$\frac{d\sigma}{d\Omega\, d\omega} = \frac{r_o^2}{2\pi\eta^3} \frac{\omega_2}{\omega_1} \sum_{\substack{\ell\ell' \\ \sigma\sigma'}} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \left\langle \rho_{\sigma'}^{(\ell')}(\underset{\sim}{q}, t)\, \rho_{\sigma}^{(\ell)}(-\underset{\sim}{q}, 0) \right\rangle \lambda_{21}^{(\ell)} \lambda_{21}^{(\ell')*} \qquad (3.28)$$

Because retarded commutators are simply related to temperature Green's functions, we write the correlation function as a commutator[3]

$$\int_{-\infty}^{\infty} dt\, e^{i\omega t} \left\langle \rho_{\sigma'}^{(\ell')}(\underset{\sim}{q}, t)\, \rho_{\sigma}^{(\ell)}(-\underset{\sim}{q}, 0) \right\rangle = \frac{1}{1 - e^{-\beta\omega}} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \left\langle \left[\rho_{\sigma'}^{(\ell')}(\underset{\sim}{q}, t), \rho_{\sigma}^{(\ell)}(-\underset{\sim}{q}, 0) \right] \right\rangle \qquad (3.29)$$

The cross section becomes

$$\frac{d\sigma}{d\Omega\, d\omega} = \frac{r_0^2}{\pi\eta^3}\frac{\omega_2}{\omega_1}\frac{1}{1-e^{-\beta\omega}}\,\mathrm{Re}\sum_{\substack{ll'\\ \sigma\sigma'}}\int_0^\infty dt\, e^{i\omega t}\left\langle\left[\rho_{\sigma'}^{(l')}(\underset{\sim}{q},t),\rho_{\sigma}^{(l)}(-\underset{\sim}{q},0)\right]\right\rangle\lambda_{21}^{(l)}\lambda_{21}^{(l')*} \qquad (3.30)$$

Because we deal often with the Fourier transform of this retarded commutator, we give it a symbol

$$F_{\sigma\sigma'}^{ll'}(\underset{\sim}{q},\omega) = \int_0^\infty e^{i\omega t}\, dt\left\langle\left[\rho_{\sigma}^{(l)}(\underset{\sim}{q},t),\rho_{\sigma'}^{(l')}(-\underset{\sim}{q},0)\right]\right\rangle \qquad (3.31)$$

and the cross section is

$$\frac{d\sigma}{d\Omega\, d\omega} = \frac{r_0^2}{\pi\eta^3}\frac{\omega_2}{\omega_1}\frac{1}{1-e^{-\beta\omega}}\,\mathrm{Re}\sum_{\substack{ll'\\ \sigma\sigma'}}F_{\sigma\sigma'}^{ll'}(\underset{\sim}{q},\omega)\lambda_{21}^{(l)*}\lambda_{21}^{(l')} \qquad (3.32)$$

CHAPTER IV

THE RETARDED COMMUTATOR $F(\underline{q},\omega)$

A. The Thermodynamic Correlation Function

At finite temperatures the commutator (3.31) is not a convenient quantity to calculate directly. Rather one defines and calculates the temperature correlation function

$$\mathcal{F}^{ll'}_{\sigma\sigma'}(\underline{q},\tau,\tau') = \langle T\, \rho^{(l)}_{\sigma}(\underline{q},\tau)\, \overline{\rho}^{(l')}_{\sigma'}(\underline{q},\tau')\rangle \qquad (4.1)$$

where $\langle\ldots\ldots\rangle$ again denotes an average over the grand canonical ensemble. τ and τ' are restricted to the region $(-\beta\ ,\ \beta)$ and the τ-dependence of the operators is given by[9]

$$\rho(\underline{q},\tau) = e^{(H-\mu N)\tau}\ \rho(\underline{q},0)\ e^{-(H-\mu N)\tau}$$

$$\overline{\rho}(\underline{q},\tau) = e^{(H-\mu N)\tau}\ \rho^{\dagger}(\underline{q},0)\ e^{-(H-\mu N)\tau} \qquad (4.2)$$

It is easy to show that

$$\mathcal{F}(\underline{q},\tau-\beta) = \mathcal{F}(\underline{q},\tau) \qquad (4.3)$$

for $\tau\ \varepsilon(0,\beta)$. Defining $\mathcal{F}(\underline{q},\tau)$ outside the region $(-\beta\ ,\ \beta)$ by requiring periodicity, we can expand it in the usual Fourier

series

$$\mathcal{F}(\underset{\sim}{q},\tau)=\frac{1}{\beta}\sum_{\omega_n}\mathcal{F}(\underset{\sim}{q},\omega_n)\,e^{-i\omega_n\tau} \tag{4.4}$$

with

$$\omega_n=\frac{2n\pi}{\beta}\qquad n=0,\pm1,\ldots.$$

and

$$\mathcal{F}(\underset{\sim}{q},\omega_n)=\int_0^\beta \mathcal{F}(\underset{\sim}{q},\tau)\,e^{i\omega_n\tau}\,d\tau \tag{4.5}$$

The two functions F and $\mathcal{F}$ are related to each other through their analytic properties in the ω-plane. They have the following spectral representations

$$F^{ll'}_{\sigma\sigma'}(\underset{\sim}{q},\omega)=\sum_{mn} i\,e^{\beta(\Omega+\mu N_n-E_n)}\left\{\frac{\langle n|\rho^{(l)}_{\sigma}(\underset{\sim}{q})|m\rangle\langle m|\rho^{(l')}_{\sigma'}(-\underset{\sim}{q})|n\rangle}{\omega+E_n-E_m+i\delta}+\right.$$
$$\left.-\frac{\langle n|\rho^{(l')}_{\sigma'}(-\underset{\sim}{q})|m\rangle\langle m|\rho^{(l)}_{\sigma}(\underset{\sim}{q})|n\rangle}{\omega+E_m-E_n+i\delta}\right\} \tag{4.6}$$

$$\mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{q},\omega_s)=-\sum e^{\beta(\Omega+\mu N_n-E_n)}\left\{\frac{\langle n|\rho^{(l)}_{\sigma}(\underset{\sim}{q})|m\rangle\langle m|\rho^{(l')}_{\sigma'}(-\underset{\sim}{q})|n\rangle}{E_n-E_m+i\omega_s}+\right.$$
$$\left.-\frac{\langle n|\rho^{(l')}_{\sigma'}(-\underset{\sim}{q})|m\rangle\langle m|\rho^{(l)}_{\sigma}(\underset{\sim}{q})|n\rangle}{E_m-E_n+i\omega_s}\right\} \tag{4.7}$$

where $e^{-\beta\Omega} = \mathrm{Tr}\, e^{\beta(\mu N - H)}$. We can analytically continue F in the ω-plane to obtain the equality

$$F^{ll'}_{\sigma\sigma'}(\underset{\sim}{q}, i\omega_s) = -i\, \mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{q}, \omega_s) \tag{4.8}$$

for $\omega_s > 0$. Conversely we can analytically continue $\mathcal{F}$ uniquely[10] and obtain

$$F^{ll'}_{\sigma\sigma'}(\underset{\sim}{q}, \omega) = -i\, \mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{q}, -i\omega) \tag{4.9}$$

for ω in the upper half-plane.

B. Perturbation Theory

The most important part of the problem still remains; namely, to calculate the quantity $\mathcal{F}(\underset{\sim}{q}, \tau)$. Of course, we are unable to do so exactly, but will use the RPA (which is equivalent to the self-consistent field approximation, and which can be argued to be a good approximation in the high density limit of the electron gas that we encounter in PbTe[11]). Before making this approximation, however, we will continue with some well-known thermodynamic Green's function formalism[9], partly for the sake of continuity, and partly to establish our conventions.

Following Abrikosov et al. we write

$$e^{-(H-\mu N)\tau} = e^{-(H_0-\mu N)\tau}\, \mathcal{S}(\tau) \tag{4.10}$$

where we have assumed that H can be written as $H_o + H_I$. This defines $\mathcal{S}(\tau)$

$$\mathcal{S}(\tau) = e^{(H_o - \mu N)\tau}\, e^{-(H-\mu N)\tau} \tag{4.11}$$

which can also be written as

$$\mathcal{S}(\tau) = T\, exp\left[-\int_0^\tau H_I(\tau')\, d\tau'\right] \tag{4.12}$$

with $H_I(\tau)$ in the interaction representation

$$H_I(\tau) = e^{(H_o - \mu N)\tau}\, H_I\, e^{-(H_o-\mu N)\tau} \tag{4.13}$$

We can now write (4.1), in which the operators are in the Matsubara representation, in the interaction representation*

$$\mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{q},\tau,\tau') = \langle T\, \rho^{(l)}_{\sigma}(\underset{\sim}{q},\tau)\, \rho^{(l')}_{\sigma'}(\underset{\sim}{q},\tau')\, \mathcal{S}(\beta)\rangle^{conn}_{o} \tag{4.14}$$

Here $\langle \ldots\ldots \rangle^{conn}_{o}$ means $Tr\{e^{\beta(\Omega_o + \mu N - H_o)} \ldots\ldots\}$ where only connected diagrams are allowed, and $e^{-\beta\Omega_o} = Tr\, e^{\beta(\mu N - H_o)}$.

Via (3.25) we can rewrite (4.14)

$$\mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{q},\tau) = \int d^3x\, d^3x'\, e^{-i\underset{\sim}{q}\cdot(\underset{\sim}{x}-\underset{\sim}{x}')} \times$$
$$\times \langle T\, \psi^{(l)}_{\sigma}(\underset{\sim}{x},\tau)\, \overline{\psi}^{(l)}_{\sigma}(\underset{\sim}{x},\tau^+)\, \psi^{(l')}_{\sigma'}(\underset{\sim}{x}',0)\, \psi^{(l')}_{\sigma'}(\underset{\sim}{x}',0^+)\, \mathcal{S}(\beta)\rangle^{conn}_{o} \tag{4.15}$$

---

*From this point on all operators will be written in the interaction representation.

We call the matrix element of the integrand the polarization part

$$\mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0)=\langle T\psi^{(l)}_{\sigma}(\underset{\sim}{x},\tau)\bar{\psi}^{(l)}_{\sigma}(\underset{\sim}{x},\tau^{+})\psi^{(l')}_{\sigma'}(\underset{\sim}{x}',0)\bar{\psi}^{(l')}_{\sigma'}(\underset{\sim}{x}',0^{+})\mathcal{S}(\beta)\rangle^{conn}_{0} \qquad (4.16)$$

and represent it by the diagram in figure 3. The solid lines represent bare particle propagators, and the shaded portion includes all possible processes. This polarization part can be expanded in terms of the proper polarization part[12] (proper with respect to both the coulomb interaction ------ and the phonon interaction ∧∧∧∧) as shown in figure 4. The proper polarization part is represented by the shaded bubble. If we denote the total interaction by ∼∼∼∼ = ----- + ∧∧∧∧ we may redraw figure 4 as shown in figure 5, where the braided line denotes the screened interaction between electrons and whose expansion is shown in figure 6.

Figures 4,5 and 6 all represent integral equations which we write down in section D.

Thus far we have not yet made any approximations (at least not for $\mathcal{F}$). The approximation is the subject of the next section.

C. The Random Phase Approximation

We now approximate the proper polarization part by the simple bubble diagram as shown in figure 7.

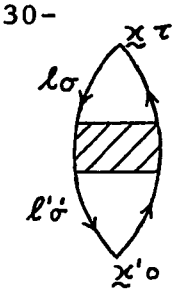

Figure 3. Diagrammatic representation of the polarization part $\mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0)$. The solid lines denote bare particle propagators, and the shaded portion includes all possible processes.

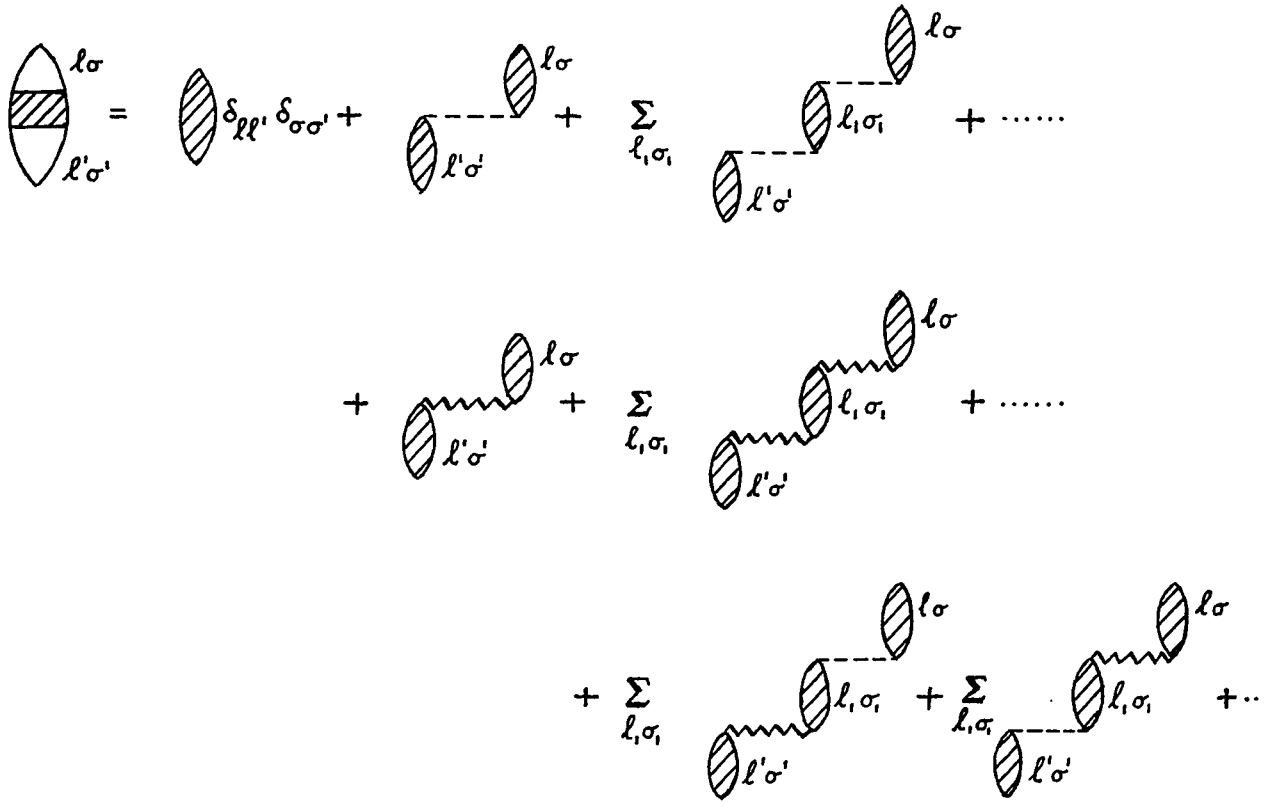

Figure 4. Expansion of the polarization part in terms of the proper polarization part.

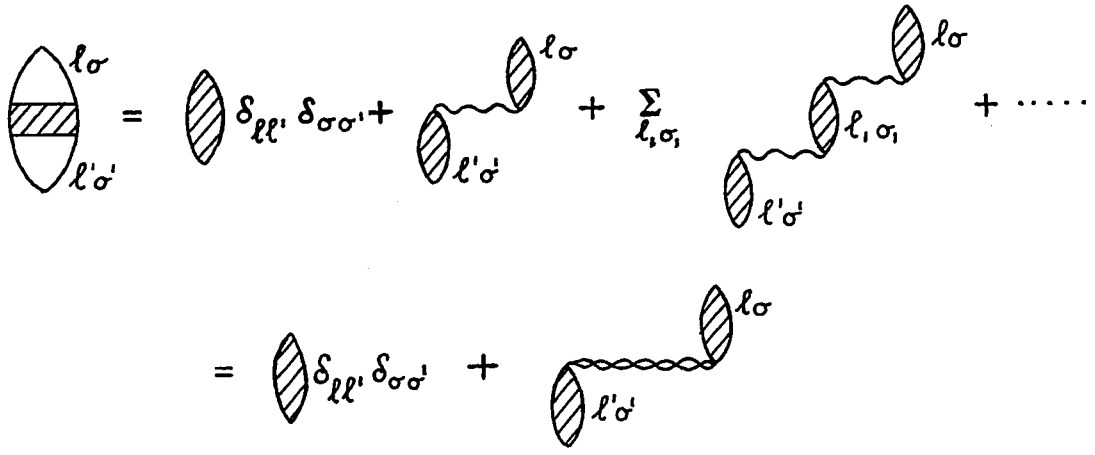

Figure 5. Expansion of the polarization part in terms of the proper polarization part using the screened electron-electron interaction.

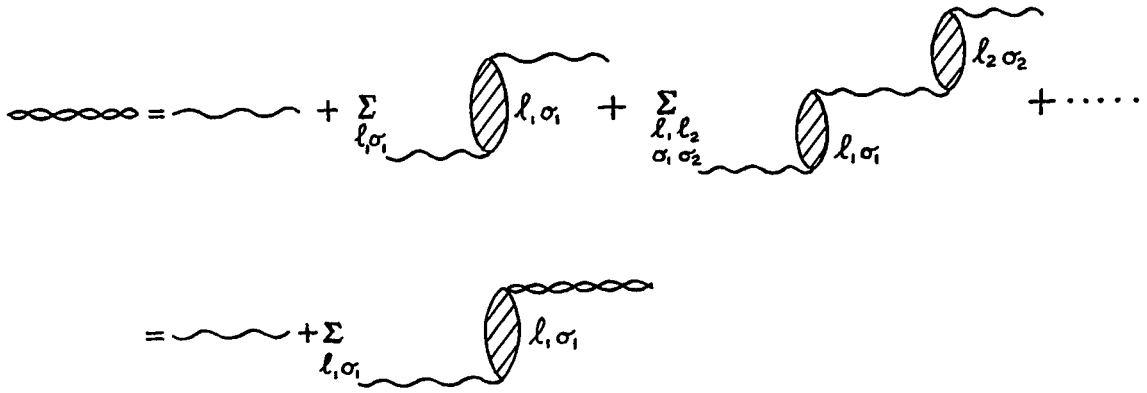

Figure 6. Expansion of the screened electron-electron interaction in terms of the proper polarization part.

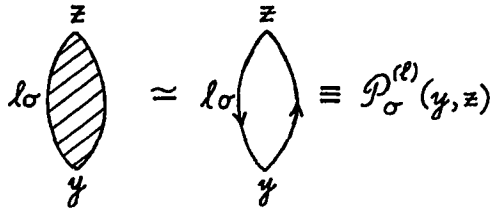

Figure 7. Diagrammatic representation of the RPA.

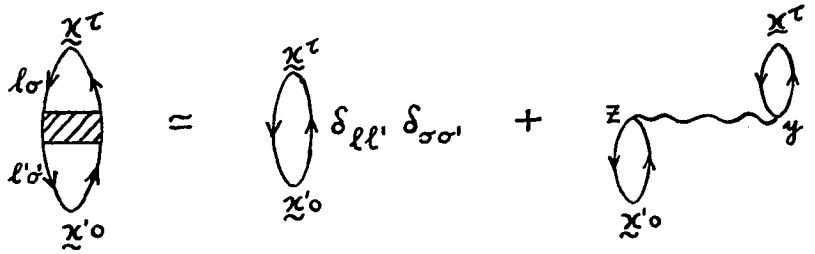

Figure 8. A first order approximation for the polarization part $\mathcal{F}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0)$ in the RPA.

We will show that $\mathcal{P}(y,z)$ depends only on the difference of its coordinates $y-z$. As a result we will be able to change the integral equations represented by figures 5 and 6 into algebraic ones. This dependence of $\mathcal{P}$ on $y-z$ can be understood if we note that in (2.3) a translation is equivalent to a gauge transformation of A^{DC}. And physical quantities such as the dielectric constant to which $\mathcal{P}(y,z)$ is closely related must not depend on gauge.

We define the bare particle Green's function[†]

$$\mathcal{G}_\sigma^{(\ell)}(y,z) = \langle T\psi_\sigma^{(\ell)}(y)\bar{\psi}_\sigma^{(\ell)}(z)\rangle_0$$

The function $\mathcal{P}$ is

$$\mathcal{P}_\sigma^{(\ell)}(y,z) = \mathcal{G}_\sigma^{(\ell)}(y,z)\mathcal{G}_\sigma^{(\ell)}(z,y)$$

For $\tau_y > \tau_z$ we have, using (2.21)

$$\mathcal{G}_{\sigma>}^{(\ell)}(y,z) = \sum_{nn'}\int dQ\,dQ'\,dK\,dK'\,\Phi_{nQK}^{(\ell)}(y)\Phi_{n'Q'K'}^{(\ell)*}(z)\langle C_{n\sigma}^{(\ell)}(Q,K,\tau_y)\bar{C}_{n'\sigma}^{(\ell)}(Q',K',\tau_z)\rangle_0$$

$$= \sum_n \int dQ\,dK\,\Phi_{nQK}^{(\ell)}(y)\Phi_{nQK}^{(\ell)*}(z)\, e^{(E_{nK\sigma}^{(\ell)}-\mu^{(\ell)})(\tau_z-\tau_y)}\left(1-f_{nK\sigma}^{(\ell)}\right)$$

[†] We omit the spinor part of the wave function as $\mathcal{G}$ is diagonal in spin.

Similarly, for $\tau_y < \tau_z$

$$\mathcal{G}^{(\ell)}_{\sigma<}(y,z) = \sum_n \int dQ\,dK\, \Phi^{(\ell)}_{nQK}(y)\, \Phi^{(\ell)*}_{nQK}(z)\, e^{(E^{(\ell)}_{nK\sigma} - \mu^{(\ell)})(\tau_z - \tau_y)}\, f^{(\ell)}_{nK\sigma}$$

The function $f_{nK\sigma}$ is the usual fermi function

$$f^{(\ell)}_{nK\sigma} = \left[e^{\beta(E^{(\ell)}_{nK\sigma} - \mu^{(\ell)})} + 1 \right]^{-1} \tag{4.17}$$

and $\mu^{(\ell)}$ is the fermi level for carriers of ellipsoid ℓ.

An easy way to find the time Fourier transform of $\mathcal{P}$ is to notice that it has the same periodicity in τ as $\mathcal{F}$. Calling $\tau = \tau_y - \tau_z$ we see that

$$\mathcal{P}(y,z,\tau) = \mathcal{G}(y,z,\tau)\,\mathcal{G}(z,y,-\tau) \tag{4.18}$$

for $\tau \in (0,\beta)$. Using the fact that[9]

$$\mathcal{G}(\tau) = -\mathcal{G}(\tau - \beta) \tag{4.19}$$

for τ in this same interval, we have

$$\mathcal{P}(y,z,\tau) = \mathcal{P}(y,z,\tau-\beta) \tag{4.20}$$

Therefore

$$\mathcal{P}(y,z,\omega_m) = \int_0^\beta \mathcal{P}(y,z,\tau)\, e^{i\omega_m \tau}\, d\tau \tag{4.21}$$

with $\omega_m = \frac{2m\pi}{\beta}$. We find

$$\mathcal{P}(\underset{\sim}{y},\underset{\sim}{z},\omega_m) = -\sum_{nn'}\int dK dK' dQ dQ' \Phi_{nQK}(\underset{\sim}{y})\Phi^*_{nQK}(\underset{\sim}{z})$$
$$\Phi_{n'Q'K'}(\underset{\sim}{z})\Phi^*_{n'Q'K'}(\underset{\sim}{y})\frac{f_{nK\sigma}-f_{n'K'\sigma}}{E_{n'K'\sigma}-E_{nK\sigma}+i\omega_m} \tag{4.22}$$

We suppress the superscript ℓ until it becomes relevant.

Next we take the Fourier transforms with respect to $\underset{\sim}{y}$ and $\underset{\sim}{z}$.

$$\mathcal{P}(\underset{\sim}{q},\underset{\sim}{q}',\omega_m) = \int \mathcal{P}(\underset{\sim}{y},\underset{\sim}{z},\omega_m)\, e^{-i\underset{\sim}{q}\cdot\underset{\sim}{y}+i\underset{\sim}{q}'\cdot\underset{\sim}{z}}\, d^3y\, d^3z$$
$$= -\sum_{nn'}\int dK dK' I_1 \frac{f_{nK\sigma}-f_{n'K'\sigma}}{E_{n'K'\sigma}-E_{nK\sigma}+i\omega_m} \tag{4.23}$$

where

$$I_1 = \int dQ dQ' d^3y\, d^3z\, e^{-i\underset{\sim}{q}\cdot\underset{\sim}{y}+i\underset{\sim}{q}'\cdot\underset{\sim}{z}}\, \Phi_{nQK}(\underset{\sim}{y})\Phi^*_{nQK}(\underset{\sim}{z})\Phi_{n'Q'K'}(\underset{\sim}{z})\Phi^*_{n'Q'K'}(\underset{\sim}{y}) \tag{4.24}$$

Substituting in the functions Φ from (2.17) and (2.12) we find

$$I_1 = \delta\left(M_{2i}(q_i-q_i')\right)\delta\left(M_{3i}(q_i-q_i')\right)\delta\left(K'-K+M_{3i}q_i\right)\int dQ\, dZ_{\mp}\, dY_{\mp}\, e^{\frac{iQ}{m\omega_c}M_{1i}(q_i-q_i')}$$
$$e^{-iM_{1i}q_iY_{\mp}}\, e^{iM_{1i}q_i'Z_{\mp}}\, u_n(Y_{\mp})u_{n'}\left(Y_{\mp}-\frac{M_{2i}q_i}{m\omega_c}\right)u_n(Z_{\mp})u_{n'}\left(Z_{\mp}-\frac{M_{2i}q_i}{m\omega_c}\right) \tag{4.25}$$

The integral over the degenerate quantum number Q gives us the desired result

$$I_1 = \frac{2\pi m\omega_c}{\sqrt{\alpha_T^2\alpha_L}}\,\delta^3(\underset{\sim}{q}-\underset{\sim}{q}')\,\delta(K'-K+M_{3i}q_i)\left|\gamma_{nn'}(M_{1i}q_i,-M_{2j}q_j)\right|^2 \tag{4.26}$$

where the matrix elements $\gamma_{nn'}$ are defined

$$\gamma_{nn'}(q_1,q_2) = \int dx\, e^{-iq_1x}\,u_n(x)\,u_{n'}\left(x+\frac{q_2}{m\omega_c}\right) \tag{4.27}$$

Putting (4.26) back into (4.23) and integrating over K' we obtain

$$\mathcal{P}_\sigma(\underset{\sim}{q},\underset{\sim}{q}',\omega_m) = -\frac{2\pi m\omega_c}{\sqrt{\alpha_T^2\alpha_L}}\,\delta^3(\underset{\sim}{q}-\underset{\sim}{q}')\sum_{nn'}\left|\gamma_{nn'}(M_{1i}q_i,-M_{2j}q_j)\right|^2 \times \int dK\,\frac{f_{nK\sigma}-f_{n'K'\sigma}}{E_{n'K'\sigma}-E_{nK\sigma}+i\omega_m} \tag{4.28}$$

where we understand that $K' = K - M_{3i}q_i$.

We have shown explicitly that $\mathcal{P}$ is a function of the difference of its coordinates only. We define a new space Fourier transform

$$\mathcal{P}_\sigma(\underset{\sim}{q},\underset{\sim}{q}',\omega_m) = (2\pi)^3\,\delta^3(\underset{\sim}{q}-\underset{\sim}{q}')\,\mathcal{P}_\sigma(\underset{\sim}{q},\omega_m) \tag{4.29}$$

We use the properties of $f_{nK\sigma}$ and $\gamma_{nn'}$ to write

$$\mathcal{P}_\sigma(q,\omega_m) = -\frac{m\omega_c}{2\pi^2\sqrt{\alpha_T^2\alpha_L}} \sum_{nn'} \left| \gamma_{nn'}(M_{1i}q_i, -M_{2j}q_j) \right|^2 \int dK \, f_{n\kappa\sigma} \frac{E_{n'\kappa'\sigma} - E_{n\kappa\sigma}}{(E_{n'\kappa'\sigma} - E_{n\kappa\sigma})^2 + \omega_m^2} \quad (4.30)$$

The matrix elements $\gamma_{nn'}$ can be evaluated in closed form. We do so in section E.

D. Evaluation of the Polarization Part and the Dielectric Constant

We shall write down and solve the integral equations which correspond to the diagrams in figures 5 and 6 (within the RPA).

To establish the Feynman rules which conform to our conventions, we do a first order calculation of the polarization part $\mathcal{F}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0)$. The diagrams are shown in figure 8. Using the appropriate expansion of (4.12) with the hamiltonian $H_I = H_I^F + H_I^C$, we find

$$\begin{aligned} \mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0) \equiv \langle T\psi^{(l)}_\sigma(\underset{\sim}{x},\tau)\bar{\psi}^{(l)}_\sigma(\underset{\sim}{x},\tau^+)\psi^{(l)}_\sigma(\underset{\sim}{x}',0)\bar{\psi}^{(l)}_\sigma(\underset{\sim}{x}',0^+)\rangle_0^{conn} \delta_{ll'}\delta_{\sigma\sigma'} + \\ -\int_0^\beta d\tau_1 \langle T\psi^{(l)}_\sigma(\underset{\sim}{x},\tau)\bar{\psi}^{(l)}_\sigma(\underset{\sim}{x},\tau^+)\psi^{(l')}_{\sigma'}(\underset{\sim}{x}',0)\bar{\psi}^{(l')}_{\sigma'}(\underset{\sim}{x}',0^+)H_I^c(\tau_1)\rangle_0^{conn} + \quad (4.31) \\ +\tfrac{1}{2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T\psi^{(l)}_\sigma(\underset{\sim}{x},\tau)\bar{\psi}^{(l)}_\sigma(\underset{\sim}{x},\tau^+)\psi^{(l')}_{\sigma'}(\underset{\sim}{x}',0)\psi^{(l')}_{\sigma'}(\underset{\sim}{x}',0^+)H_I^F(\tau_1)H_I^F(\tau_2)\rangle_0^{conn} \end{aligned}$$

where we have yet to choose the proper contractions. For convenience we write

$$H_I^c(\tau_y)=\frac{1}{2}\sum_{\substack{l_1 l_2\\ \sigma_1\sigma_2}}\int \psi_{\sigma_1}^{(l_1)}(y)\psi_{\sigma_2}^{(l_2)}(z)\,U(y-z)\,\psi_{\sigma_2}^{(l_2)}(z)\psi_{\sigma_1}^{(l_1)}(y)\,d^4z\,d^3y \tag{4.32}$$

with

$$U(y-z)=\frac{e^2}{\epsilon_\infty}\frac{\delta(\tau_y-\tau_z)}{|\underset{\sim}{y}-\underset{\sim}{z}|} \tag{4.33}$$

Using Wick's theorem we obtain

$$\mathcal{F}_{\sigma\sigma'}^{ll'}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0)=\delta_{ll'}\delta_{\sigma\sigma'}\mathcal{P}_\sigma^{(l)}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0)-\int d^4y\,d^4z\,\mathcal{P}_\sigma^{(l)}(\underset{\sim}{x},\tau;y)\,U(y-z)\,\mathcal{P}_{\sigma'}^{(l')}(z;\underset{\sim}{x}',0)+$$
$$+\int d^4y\,d^4z\,\mathcal{P}_\sigma^{(l)}(\underset{\sim}{x},\tau;y)\,W(y-z)\,\mathcal{P}_{\sigma'}^{(l')}(z;\underset{\sim}{x}',0) \tag{4.34}$$

with the effective potential due to the phonon exchange

$$W(y-z)=\frac{4\pi e^2}{\epsilon_\infty}q^2\int\frac{d^3q}{q^2}\,e^{i\underset{\sim}{q}\cdot(\underset{\sim}{y}-\underset{\sim}{z})}\left\{\langle T\,b(\underset{\sim}{q},\tau_y)\bar{b}(\underset{\sim}{q},\tau_z)\rangle_0+\right.$$
$$\left.+\langle T\,b(-\underset{\sim}{q},\tau_z)\bar{b}(-\underset{\sim}{q},\tau_y)\rangle_0\right\} \tag{4.35}$$

We define the bare phonon propagator

$$\mathcal{D}(\underset{\sim}{q},\tau_1,\tau_2)=\langle T\,b(\underset{\sim}{q},\tau_1)\bar{b}(\underset{\sim}{q},\tau_2)\rangle_0 \tag{4.36}$$

Its Fourier transform is†

$$\mathcal{D}(\underset{\sim}{q},\omega_s) = \frac{1}{\omega_L - i\omega_s} \tag{4.37}$$

with $\omega_s = \frac{2\pi s}{\beta}$. The Fourier transform of the potential (4.35) is then

$$w(\underset{\sim}{q},\omega_s) = \frac{4\pi e^2}{\epsilon_\infty q^2} \frac{\omega_L^2 - \omega_T^2}{\omega_L^2 + \omega_s^2} \tag{4.38}$$

The rules are now evident. Remembering to associate a negative sign with each closed fermion loop, we can make the following identifications

$-v(y-z)$ $\quad y$ - - - - - z

$w(y-z)$ $\quad y$ ∿∿∿∿ z

The negative sign associated with $v(y-z)$ automatically takes care of the $(-)^n$ associated with any n-th order perturbation diagram. The phonon interaction only appears in even orders.

The RPA result for the polarization part is

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†As mentioned earlier, we neglect the dependence of ω_L on wave number (section II D).

$$\mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0) = -\delta_{ll'}\delta_{\sigma\sigma'}\mathcal{P}^{(l)}_{\sigma}(\underset{\sim}{x},\tau;\underset{\sim}{x}',0) + \\ -\int d^4y\, d^4z\, \mathcal{P}^{(l)}_{\sigma}(\underset{\sim}{x},\tau;y)\,\mathcal{U}(y-z)\,\mathcal{P}^{(l')}_{\sigma'}(z;\underset{\sim}{x}',0) \tag{4.39}$$

We have chosen the sign of $\mathcal{U}$ so that in the absence of phonons it reduces to the screened coulomb potential. The equation for $\mathcal{U}$ is

$$-\mathcal{U}(y-z) = \left[-V(y-z)+W(y-z)\right] + \\ +\sum_{l\sigma}\int\left[-V(y-z_1)+W(y-z_1)\right]\mathcal{P}^{(l)}_{\sigma}(z_1,z_2)\,\mathcal{U}(z_2-z)\,d^4z_1\,d^4z_2 \tag{4.40}$$

Because $\mathcal{P}$ depends only on the difference of its coordinates, we can Fourier transform equations (4.39) and (4.40)

$$\mathcal{F}^{ll'}_{\sigma\sigma'}(\underset{\sim}{q},\omega_m) = -V\left[\delta_{ll'}\delta_{\sigma\sigma'}\mathcal{P}^{(l)}_{\sigma}(\underset{\sim}{q},\omega_m) + \mathcal{P}^{(l)}_{\sigma}(\underset{\sim}{q},\omega_m)\,\mathcal{U}(\underset{\sim}{q},\omega_m)\,\mathcal{P}^{(l')}_{\sigma'}(\underset{\sim}{q},\omega_m)\right] \tag{4.41}$$

where V is the volume of the crystal, and

$$\mathcal{U}(\underset{\sim}{q},\omega_m) = V(\underset{\sim}{q},\omega_m) - W(\underset{\sim}{q},\omega_m) + \\ +\left[V(\underset{\sim}{q},\omega_m)-W(\underset{\sim}{q},\omega_m)\right]\sum_{l\sigma}\mathcal{P}^{(l)}_{\sigma}(\underset{\sim}{q},\omega_m)\,\mathcal{U}(\underset{\sim}{q},\omega_m) \tag{4.42}$$

The last equation has the solution

$$U(\underset{\sim}{q},\omega_m)=\frac{V(\underset{\sim}{q},\omega_m)-W(\underset{\sim}{q},\omega_m)}{1-[V(\underset{\sim}{q},\omega_m)-W(\underset{\sim}{q},\omega_m)]\sum_{l\sigma}\mathcal{P}_\sigma^{(l)}(\underset{\sim}{q},\omega_m)} \tag{4.43}$$

The sum of the bare interactions can be conveniently written

$$V(\underset{\sim}{q},\omega_m)-W(\underset{\sim}{q},\omega_m)=\frac{4\pi e^2}{\epsilon_\infty q^2}\,\frac{\omega_T^2+\omega_m^2}{\omega_L^2+\omega_m^2} \tag{4.44}$$

so that (4.43) becomes

$$U(\underset{\sim}{q},\omega_m)=\frac{\frac{4\pi e^2}{\epsilon_\infty q^2}\,\frac{\omega_T^2+\omega_m^2}{\omega_L^2+\omega_m^2}}{1-\frac{4\pi e^2}{\epsilon_\infty q^2}\,\frac{\omega_T^2+\omega_m^2}{\omega_L^2+\omega_m^2}\sum_{l\sigma}\mathcal{P}_\sigma^{(l)}(\underset{\sim}{q},\omega_m)} \tag{4.45}$$

At this stage it is appropriate to go back to physically-meaningful quantities by the analytic continuation of equation (4.9). Defining

$$\begin{aligned} P_\sigma^{(l)}(\underset{\sim}{q},\omega)&=\mathcal{P}_\sigma^{(l)}(\underset{\sim}{q},-i\omega)\\ U(\underset{\sim}{q},\omega)&=U(\underset{\sim}{q},-i\omega)\end{aligned} \tag{4.46}$$

we get from (4.41) and (4.45)

$$F^{ll'}_{\sigma\sigma'}(\underset{\sim}{q},\omega)=iV\left[\delta_{ll'}\delta_{\sigma\sigma'}P^{(l)}_{\sigma}(\underset{\sim}{q},\omega)+U(\underset{\sim}{q},\omega)\,P^{(l)}_{\sigma}(\underset{\sim}{q},\omega)\,P^{(l')}_{\sigma'}(\underset{\sim}{q},\omega)\right] \tag{4.47}$$

$$U(\underset{\sim}{q},\omega)=\frac{\frac{4\pi e^2}{\epsilon_\infty q^2}\,\frac{\omega_L^2-\omega^2}{\omega_L^2-\omega^2}}{1-\frac{4\pi e^2}{\epsilon_\infty q^2}\,\frac{\omega_T^2-\omega^2}{\omega_L^2-\omega^2}\sum_{l\sigma}P^{(l)}_{\sigma}(\underset{\sim}{q},\omega)} \tag{4.48}$$

and from (4.30)

$$P^{(l)}_{\sigma}(\underset{\sim}{q},\omega)=-\frac{m\omega_c}{2\pi^2\sqrt{\alpha_T^2\alpha_L}}\sum_{nn'}\left|\gamma_{nn'}\left(M^{(l)}_{1i}q_{i\tau}-M^{(l)}_{2j}q_{j\tau}\right)\right|^2\int dK\int^{(l)}_{nK\sigma}\frac{E^{(l)}_{n'K'\sigma}-E^{(l)}_{nK\sigma}}{\left(E^{(l)}_{n'K'\sigma}-E^{(l)}_{nK\sigma}\right)^2-\omega^2} \tag{4.49}$$

In all these expressions ω is assumed to have a small positive imaginary part. $U(\underset{\sim}{q},\omega)$ is the effective interaction between the conduction electrons in the crystal. It is conventional to lump all the screening factors into a dielectric constant

$$U(\underset{\sim}{q},\omega)=\frac{4\pi e^2}{\epsilon(\underset{\sim}{q},\omega)\,q^2} \tag{4.50}$$

with the dielectric constant defined

$$\epsilon(\underset{\sim}{q},\omega)=\epsilon_\infty\frac{\omega^2-\omega_L^2}{\omega^2-\omega_T^2}-\frac{4\pi e^2}{q^2}\sum_{l\sigma}P_\sigma^{(l)}(\underset{\sim}{q},\omega) \tag{4.51}$$

The first term is the lattice contribution and the second term is due to the conduction electrons. We see that the polarizabilities are additive, and in this respect we have found nothing new[13].

In terms of the dielectric constant, the function $F(\underset{\sim}{q},\omega)$ becomes

$$F_{\sigma\sigma'}^{ll'}(\underset{\sim}{q},\omega)=iV\left[\delta_{ll'}\delta_{\sigma\sigma'}P_\sigma^{(l)}(\underset{\sim}{q},\omega)+\frac{4\pi e^2}{q^2}\frac{P_\sigma^{(l)}(\underset{\sim}{q},\omega)P_{\sigma'}^{(l')}(\underset{\sim}{q},\omega)}{\epsilon(\underset{\sim}{q},\omega)}\right] \tag{4.52}$$

E. The Matrix Elements $\gamma_{nn'}$

The only quantities that remain to be calculated are given by (4.27)

$$\gamma_{nn'}(q_1,q_2)=\int dx\, e^{-iq_1x}\,u_n(x)\,u_{n'}\left(x+\frac{q_2}{m\omega_c}\right)$$

$$=\sqrt{\frac{m\omega_c}{\pi}}\frac{1}{\sqrt{2^{n+n'}n!n'!}}\int dx\, e^{-iq_1x}\,e^{-\frac{1}{2}m\omega_c x^2}H_n\left(\sqrt{m\omega_c}\,x\right)\times \quad (4.27)$$

$$\times\, e^{-\frac{1}{2}m\omega_c\left(x+\frac{q_2}{m\omega_c}\right)^2}H_{n'}\left(\sqrt{m\omega_c}\left(x+\frac{q_2}{m\omega_c}\right)\right)$$

Through a change of variable we get

$$\gamma_{nn'}(q_1,q_2)=\frac{e^{\frac{iq_1q_2}{2m\omega_c}}\,e^{-\frac{q_1^2+q_2^2}{4m\omega_c}}}{\sqrt{\pi\,2^{n+n'}n!n'!}}\int d\xi\, e^{-(\xi+b)^2}H_n(\xi)H_{n'}\left(\xi+\frac{q_2}{\sqrt{m\omega_c}}\right)$$

with

$$b=\frac{q_2+iq_1}{2\sqrt{m\omega_c}} \quad (4.53)$$

Calling the integral I_2, we have

$$I_2=\int d\xi\, e^{-\xi^2}H_n(\xi-b)H_{n'}(\xi+b^*)$$

These Hermite polynomials can be expanded about the point ξ [14].

$$H_n(\xi-a)=\sum_{m=0}^{n}\frac{(-2a)^{n-m}n!}{m!(n-m)!}\,H_m(\xi) \quad (4.54)$$

Substituting, and using the orthogonality relation of the Hermite polynomials

$$\int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = 2^n n! \sqrt{\pi}\, \delta_{mn} \tag{4.55}$$

we find

$$I_2 = \sum_{m=0} \sqrt{\pi}\, (-)^{n-m} 2^{n+n'-m} \frac{b^{n-m} b^{*n'-m} n! n'!}{(n-m)!\,(n'-m)!\, m!}$$

where the largest value of m is determined by the factorials. We have the result

$$\gamma_{nn'}(q_1, q_2) = e^{\frac{i q_1 q_2}{2 m \omega_c}} e^{-\frac{q_1^2 + q_2^2}{4 m \omega_c}} \sum_{m=0} (-)^{n-m} \frac{2^{\frac{n+n'}{2} - m} \sqrt{n! n'!}\, b^{n-m} b^{*n'-m}}{m!\,(n-m)!\,(n'-m)!} \tag{4.56}$$

A case of special importance is $q_2 = 0$. Then

$$\left| \gamma_{nn'}(q_1, 0) \right|^2 = e^{-\frac{q_1^2}{2 m \omega_c}} \sum_{m, m'=0} \frac{(-)^{m+m'} n! n' ! \left(\frac{q_1^2}{2 m \omega_c} \right)^{n+n'-m-m'}}{m! m'! (n-m)! (n-m')! (n'-m)! (n'-m')!} \tag{4.57}$$

a result which will prove useful later.

CHAPTER V

THE SPECIAL CASE $\underset{\sim}{q} = (0,0,q)$

A. The Cross Section

We restrict ourselves to modes traveling in the direction of the static magnetic field. The function $P(\underset{\sim}{q},\omega)$ simplifies to

$$P_\sigma^{(\ell)}(\underset{\sim}{q},\omega) = -\frac{m\omega_c}{2\pi^2\sqrt{\alpha_T^2\alpha_L}} \sum_{nn'} \left|\gamma_{nn'}\left(M_{13}^{(\ell)} q, 0\right)\right|^2 \int dK \oint_{nK\sigma}^{(\ell)} \frac{E^{(\ell)}_{n'K'\sigma} - E^{(\ell)}_{nK\sigma}}{\left(E^{(\ell)}_{n'K'\sigma} - E^{(\ell)}_{nK\sigma}\right)^2 - \omega^2 - i\delta} \qquad (5.1)$$

for positive frequencies, and with $K' = K - M_{33}^{(\ell)} q$. Expressions (2.26) and (2.27) show that M_{13} and M_{33} are the same for each ellipsoid. Hence $P(\underset{\sim}{q},\omega)$ no longer depends on ℓ , and we shall often suppress the superscript. The real part of the retarded commutator $F(\underset{\sim}{q},\omega)$, which we need for the cross section (3.33), becomes

$$\mathrm{Re}\, F^{\ell\ell'}_{\sigma\sigma'}(\underset{\sim}{q},\omega) = -V\left[\delta_{\ell\ell'}\delta_{\sigma\sigma'}\, \mathrm{Im}\, P_\sigma(\underset{\sim}{q},\omega) + \frac{4\pi e^2}{q^2}\, \mathrm{Im}\, \frac{P_\sigma(\underset{\sim}{q},\omega) P_{\sigma'}(\underset{\sim}{q},\omega)}{\epsilon(\underset{\sim}{q},\omega)}\right] \qquad (5.2)$$

Since we are interested in the collective modes given by the zeros of $\epsilon(\underset{\sim}{q},\omega)$, the first term in (5.2) does not contribute.

Substituting the second term into the cross section we have

$$\frac{d\sigma}{d\Omega d\omega} = -\frac{r_o^2}{\pi \eta^3} \frac{\omega_2}{\omega_1} \frac{V}{1-e^{-\beta\omega}} \frac{4\pi e^2}{q^2} \operatorname{Im} \frac{\left(\sum_\sigma P_\sigma(\underset{\sim}{q},\omega)\right)^2}{\epsilon(\underset{\sim}{q},\omega)} \left| \sum_\ell \lambda_{21}^{(\ell)} \right|^2 \qquad (5.3)$$

In the absence of damping (i.e. $\operatorname{Im} P(\underset{\sim}{q},\omega) = \operatorname{Im} \epsilon(\underset{\sim}{q},\omega) = 0$) we obtain

$$\left.\frac{d\sigma}{d\Omega d\omega}\right|_{\tilde{\omega}} = \frac{r_o^2 V}{\eta^3(1-e^{-\beta\tilde{\omega}})} \frac{\omega_2}{\omega_1} \frac{4\pi e^2}{q^2} \left(\sum_\sigma P_\sigma(\underset{\sim}{q},\omega)\right)^2 \left| \sum_\ell \lambda_{21}^{(\ell)} \right|^2 \frac{\delta(\omega-\tilde{\omega})}{\epsilon'(\underset{\sim}{q},\tilde{\omega})} \qquad (5.4)$$

where $\epsilon'(\underset{\sim}{q},\tilde{\omega})$ is the derivative of $\epsilon(\underset{\sim}{q},\omega)$ with respect to ω , evaluated at the resonance $\tilde{\omega}$ given by $\epsilon(\underset{\sim}{q},\tilde{\omega}) = 0$.

B. <u>The Photon Polarization</u>

The polarization factor is

$$\left| \sum_\ell \lambda_{21}^{(\ell)} \right|^2 = \left| \sum_\ell \underset{\sim}{e}_2^* \cdot \underset{\approx}{\alpha}^{(\ell)} \cdot \underset{\sim}{e}_1 \right|^2 \qquad (5.5)$$

(for convenience we have written $\underset{\sim}{e}^{(\lambda_i)}(\underset{\sim}{k}_i)$ as $\underset{\sim}{e}_i$)
To evaluate it, we need to express $\underset{\approx}{\alpha}^{(\ell)}$ with respect to the coordinate system $\mathcal{C}$. In $\overline{\mathcal{C}}$, $\underset{\approx}{\alpha}$ is diagonal, and the energy surface is

$$\varepsilon(\underset{\sim}{k}) = \frac{1}{2m}\left(\alpha_1 k_1^2 + \alpha_2 k_2^2 + \alpha_3 k_3^2\right)$$

With equation (2.5) this becomes in $\mathcal{C}$

$$\varepsilon(\underset{\sim}{k}) = \frac{1}{2m}\left(R^{-1}\bar{\alpha}R\right)_{ij} k_i k_j$$

where $\bar{\alpha}$ means the matrix expressed with respect to $\bar{\mathcal{C}}$. Therefore

$$\alpha_{ij} = \left(R^{-1}\bar{\alpha}R\right)_{ij} \tag{5.6}$$

Calling $\alpha_T - \alpha_L = \Delta$, we find

$$\alpha^{(111)} = \begin{pmatrix} \frac{2\alpha_T+\alpha_L}{3} & -\frac{\Delta}{3} & -\frac{\Delta}{3} \\ -\frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} & -\frac{\Delta}{3} \\ -\frac{\Delta}{3} & -\frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} \end{pmatrix}$$

$$\alpha^{(-111)} = \begin{pmatrix} \frac{2\alpha_T+\alpha_L}{3} & \frac{\Delta}{3} & \frac{\Delta}{3} \\ \frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} & -\frac{\Delta}{3} \\ \frac{\Delta}{3} & -\frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} \end{pmatrix}$$

$$\alpha^{(1-11)} = \begin{pmatrix} \frac{2\alpha_T+\alpha_L}{3} & \frac{\Delta}{3} & -\frac{\Delta}{3} \\ \frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} & \frac{\Delta}{3} \\ -\frac{\Delta}{3} & \frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} \end{pmatrix}$$

$$\alpha^{(-1-11)} = \begin{pmatrix} \frac{2\alpha_T+\alpha_L}{3} & -\frac{\Delta}{3} & \frac{\Delta}{3} \\ -\frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} & \frac{\Delta}{3} \\ \frac{\Delta}{3} & \frac{\Delta}{3} & \frac{2\alpha_T+\alpha_L}{3} \end{pmatrix} \qquad (5.7)$$

Thus $\sum_l \alpha_{ij}^{(l)} = \frac{4}{3}(2\alpha_T+\alpha_L)\,\delta_{ij}$ and (5.5) becomes

$$\left|\sum_l \lambda_{21}^{(l)}\right|^2 = \frac{16}{9}(2\alpha_T+\alpha_L)^2 \left|\underset{\sim}{e}_2^* \cdot \underset{\sim}{e}_1\right|^2 \qquad (5.8)$$

The largest cross section will be obtained for light polarized in a plane perpendicular to the scattering plane.

C. The Long-Wavelength Limit

For values of $q \leq 10^4$ cm^{-1} and magnetic fields $B \geq 10$ Kgauss it is usually sufficient to work to lowest order in q (see Appendix). We obtain this limit by expanding both the integrand and $\left|\gamma_{nn'}\right|^2$ in expression (5.1) to order q^2:

$$P_\sigma(\underset{\sim}{q},\omega) = -\frac{m\omega_c}{2\pi^2\sqrt{\alpha_T^2\alpha_L}} \sum_n \int dK \int_{n\kappa\sigma} \frac{q_\beta^2}{2m} \left\{\frac{M_{13}^2}{\omega_c^2-\omega^2} - \frac{M_{33}^2}{\omega^2}\right\} + O(q^4) \qquad (5.9)$$

The sum and integral over n and K is related to the total number of electrons

$$N_\sigma^{(\ell)} V = \sum_n \int dQ\, dK \int_{n K \sigma}^{(\ell)} \frac{\bar{L}_\perp \bar{L}_z}{(2\pi)^2}$$

$$= \frac{m\omega_c \bar{V}}{(2\pi)^2} \sum_n \int dK \int_{n K \sigma}^{(\ell)}$$

where $\bar{V}$ is the rescaled volume. We find

$$\sum_n \int dK \int_{n K \sigma}^{(\ell)} = \frac{4\pi^2 \sqrt{\alpha_T^2 \alpha_L}}{m\omega_c} N_\sigma^{(\ell)} \tag{5.10}$$

where $N_\sigma^{(\ell)}$ is the electron density of spin σ due to ellipsoid ℓ. The function $P(\underset{\sim}{q},\omega)$ becomes

$$P_\sigma^{(\ell)}(\underset{\sim}{q},\omega) = \frac{N_\sigma^{(\ell)} q^2}{m} \left\{ \frac{M_{33}^2}{\omega^2} - \frac{M_{13}^2}{\omega_c^2 - \omega^2} \right\} \tag{5.11}$$

and the dielectric constant,

$$\epsilon(0,\omega) = \epsilon_\infty \left[\frac{\omega^2 - \omega_L^2}{\omega^2 - \omega_T^2} - \frac{\omega_p^2}{\omega^2} \frac{\omega^2 - 5\omega_c^2}{\omega^2 - \omega_c^2} \right] \tag{5.12}$$

with

$$\zeta^2 = \frac{M_{33}^2}{M_{13}^2 + M_{33}^2}$$

$$\omega_p^2 = \frac{4\pi N e^2}{m \epsilon_\infty} \left(M_{13}^2 + M_{33}^2 \right) \qquad (5.13)$$

These results are identical with those of reference (11). Figure 9 shows the general structure of $\varepsilon(0,\omega)$ for $\omega_c > \omega_T$. It is not valid to extend the graph to frequencies that approach the band gap frequency, as then ε_∞ becomes frequency dependent.

The derivative of $\varepsilon(0,\omega)$ is

$$\frac{d}{d\omega} \epsilon(0,\omega) = \epsilon_\infty \left[2\omega \frac{\omega_L^2 - \omega_T^2}{(\omega^2 - \omega_T^2)^2} + 2 \frac{\omega_p^2}{\omega^3} \frac{\omega^4 + \zeta^2 \omega_c^2 (\omega_c^2 - 2\omega^2)}{(\omega^2 - \omega_c^2)^2} \right] \qquad (5.14)$$

Numerical results for the modes and their cross sections were obtained for PbTe with the following parameters[5,15,16]

$\alpha_T = 42$ $\quad \alpha_L = 4.2$

$\omega_L = 1.8 \times 10^{13} \text{sec}^{-1}$ $\quad \omega_T = 4.9 \times 10^{12} \text{sec}^{-1}$ $\quad \varepsilon_\infty = 30$

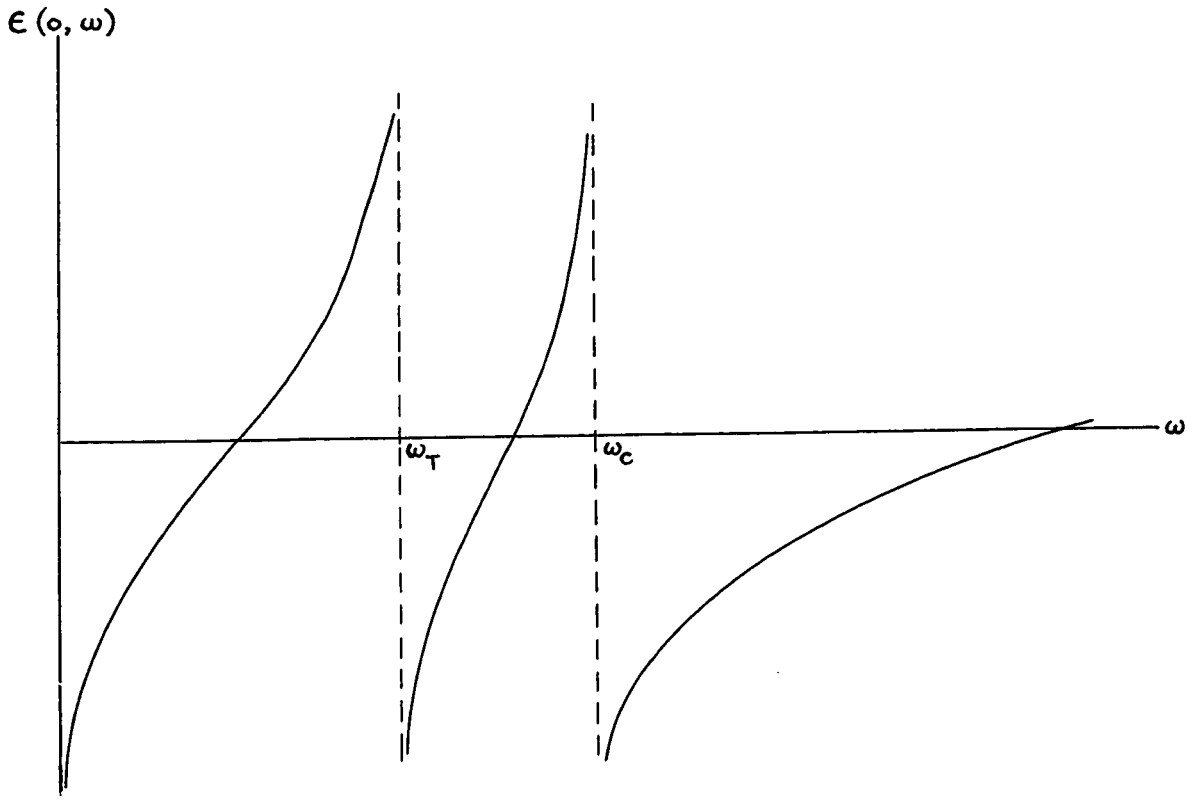

Figure 9. The general structure of the long-wavelength dielectric constant as a function of frequency, for $\omega_c > \omega_T$.

g^* [001] = 29

$N = 10^{18}$ cm^{-3} and $V = 10^{-3}$ cm.

The modes were calculated by Newton's method. Although the equation $\varepsilon(0,\omega) = 0$ is a cubic equation whose roots can be found analytically, Newton's method was found more convenient. The results are shown in Table 1 for various magnetic field strengths. The quantity $\Lambda(\omega)$ is given by

$$\Lambda(\omega) = \frac{64\pi e^2 V}{9\eta^3 q_0^4}(2\alpha_T + \alpha_L)^2 \frac{(\Sigma_\sigma P_\sigma(q,\omega))^2}{|\epsilon'(0,\omega)|} \qquad (5.15)$$

where the long-wavelength limit of $P(\underset{\sim}{q},\omega)$ is used. In terms of $\Lambda(\omega)$, the cross section is

$$\frac{d\sigma}{d\Omega\, d\omega} = \Lambda(\tilde{\omega})\, r_0^2 q_0^2 \frac{\omega_2}{\omega_1} \left|\underset{\sim}{e}_2^* \cdot \underset{\sim}{e}_1\right|^2 \delta(\omega - \tilde{\omega}) \qquad (5.16)$$

for the mode at $\tilde{\omega}$.

At 10.5 Kgauss $\omega_c = \omega_T$, and only two modes exist in the plasma. Physically what happens is that as ω_c approaches ω_T, the zero of ε between ω_c and ω_T is forced into the damping region near ω_c (the long-wavelength limit of ε is no longer valid; see section D); the mode becomes damped, and eventually the resonance becomes so wide that it is no longer well-defined. If one sets $\omega_c = \omega_T$ in (5.12), the equation $\varepsilon(0,\omega) = 0$ reduces to a quadratic.

Table 1

The collective modes and their relative cross sections $\Lambda(\omega)$ are shown for various magnetic fields.

Magnetic Field (Kgauss)	Cyclotron Frequency (10^{13} sec^{-1})	Mode Frequency (10^{13} sec^{-1})	$\frac{\varepsilon'(0,\omega)}{\varepsilon_\infty}$ (10^{-13} sec)	$\Lambda(\omega)$ (cgs units)
10	.47	5.86	.343	1390
		.49	4.03×10^5	1650
		.27	1720	118
10.5	.49	5.86	.343	1390
		.28	1510	144
12	.56	5.86	.343	1390
		.50	31000	1400
		.31	1090	249
15	.70	5.87	.344	1390
		.54	2040	1040
		.36	764	616

Table 1 (continued)

Magnetic Field (Kgauss)	Cyclotron Frequency (10^{13} sec^{-1})	Mode Frequency (10^{13} sec^{-1})	$\frac{\varepsilon'(0,\omega)}{\varepsilon_\infty}$ (10^{-13} sec)	$\Lambda(\omega)$ (cgs units)
20	.93	5.89	.345	1390
		.64	339	455
		.40	779	1170
50	2.33	6.13	.361	1350
		1.44	15.1	15
		.43	1150	1570
100	4.67	7.06	.441	1150
		2.50	2.26	63
		.43	1220	1600
200	9.34	10.50	.820	657
		3.35	.781	388
		.43	1240	1600

The frequencies of the three modes are plotted versus magnetic field in Figure 10. The graph shows the usual repulsion of interacting modes. For fields less than 50 Kgauss the low-frequency (LF) plasmon and phonon modes mix strongly. For larger fields it is the LF and high frequency (HF) plasmons that mix. Table 1 suggests that the LF plasmon is most easily detected at fields of 10 - 15 Kgauss, although at higher fields it can be detected through the magnetic field dependence of the HF plasmon.

Numerical calculations show that if the phonons are eliminated (but the other parameters remain unchanged), the LF plasmon has a very small cross section compared with the HF plasmon for fields less than 100 Kgauss. The results are tabulated in Table 2. Comparison with Table 1 shows that it is the phonons that enable one to detect the LF plasmon at low magnetic fields. Furthermore, direct evidence of the LF plasmon may be easier to obtain in a nonpolar substance, provided one goes to high enough magnetic fields.

D. Damping

We wish to consider two types of damping. The first is damping as predicted by our theory; the second is collision damping which we introduce in an ad hoc manner with a phenomenological relaxation time.

For the first type of damping we return to (5.1), perform the integration, and substitute the result into (4.51).

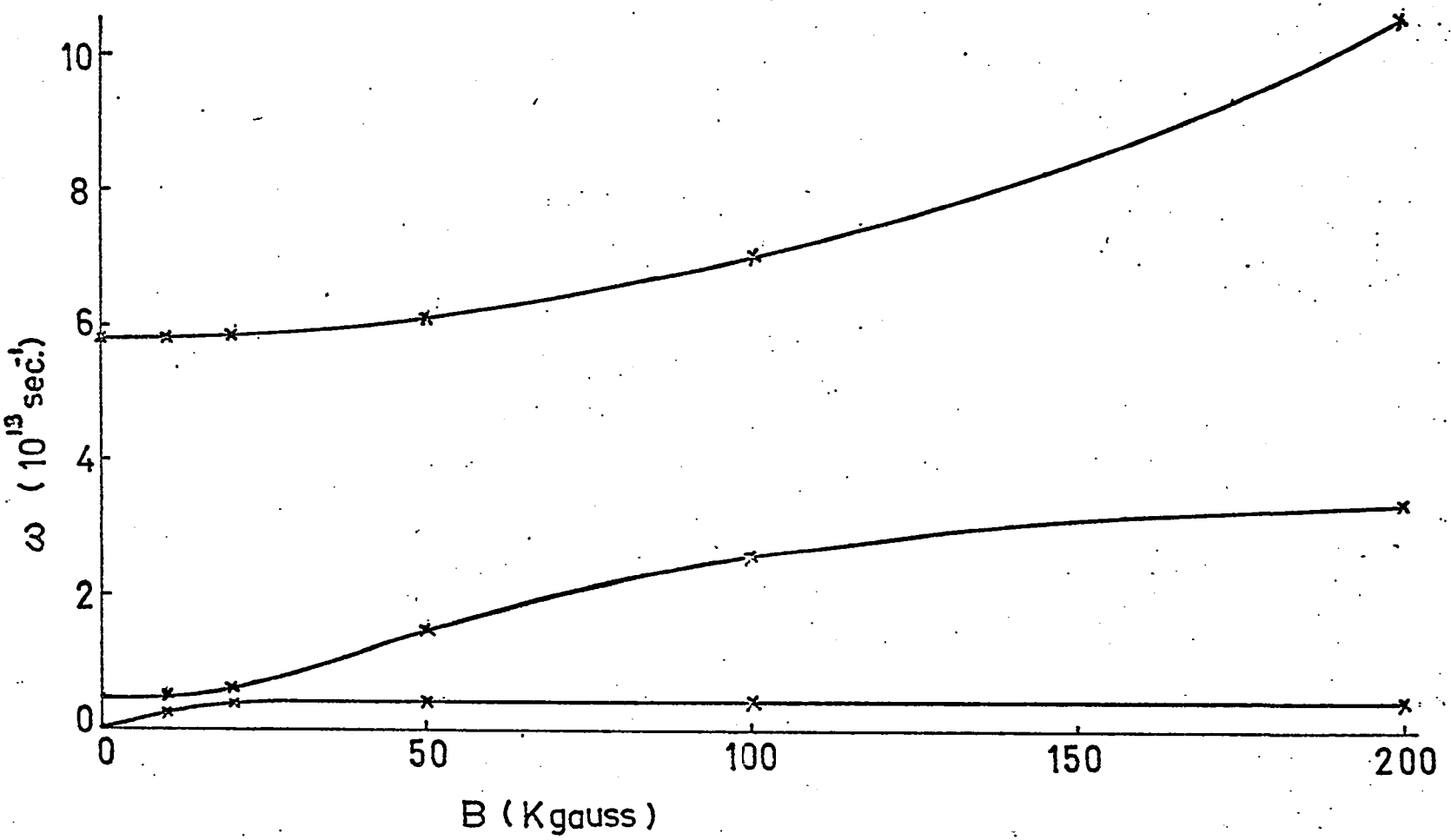

Figure 10. The three collective mode frequencies are plotted against magnetic field.

Table 2

Collective modes and their relative cross sections for various magnetic fields for a model substance which is nonpolar, but has the same parameters α_T, α_L, and ε_∞ as PbTe.

Magnetic Field (Kgauss)	Mode Frequency 10^{13} sec^{-1}	$\Lambda(\omega)$ (cgs units)
10	5.59	1600
	.28	.4
15	5.59	1580
	.42	1.2
50	5.91	1510
	1.32	40
100	6.92	1220
	2.25	250
200	10.4	620
	3.0	680

We find the real part of the dielectric constant, at zero temperature,

$$\mathrm{Re}\,\epsilon(\underset{\sim}{q},\omega) = \epsilon_\infty \frac{\omega^2-\omega_L^2}{\omega^2-\omega_T^2} - \frac{4e^2m^2\omega_c}{\pi\sqrt{\alpha_T^2\alpha_L}} \frac{1}{M_{33}q^3} \sum_{\substack{nn'\\ \sigma}} \left|\gamma_{nn'}(M_{13}q,0)\right|^2 \times$$
$$\times \ln\left|\frac{\left[(n'-n)\omega_c - \frac{M_{33}qK_{n\sigma}}{m} + \frac{M_{33}^2q^2}{2m}\right]^2 - \omega^2}{\left[(n'-n)\omega_c + \frac{M_{33}qK_{n\sigma}}{m} + \frac{M_{33}^2q^2}{2m}\right]^2 - \omega^2}\right| \qquad (5.17)$$

$K_{n\sigma}$ is the maximum value of K for the level (n, σ). The imaginary part of the dielectric constant, at any temperature, is

$$\mathrm{Im}\,\epsilon(\underset{\sim}{q},\omega) = \frac{4e^2m^2\omega_c}{\sqrt{\alpha_T^2\alpha_L}} \frac{1}{M_{33}q^3} \sum_{\substack{nn'\\ i\sigma}} \left|\gamma_{nn'}(M_{13}q,0)\right|^2 f_{nK_i\sigma}\,\mathrm{sign}\left(E_{n'K_i-M_{33}q} - E_{nK_i}\right) \qquad (5.18)$$

for $\omega > 0$, and with K_i the solutions of

$$\left|(n'-n)\omega_c - \frac{M_{33}qK}{m} + \frac{M_{33}^2q^2}{2m}\right| = \omega \qquad (5.19)$$

Although (5.17) is a complicated function, careful examination shows that it has the general form indicated in Figure 11, at least in the regions $\omega\ \epsilon(\omega_2,\omega_3)$ and $\omega_4 < \omega < 2\omega_c$. The asymptotes are given by

$$\omega_1 = \frac{M_{33}qK_{o\downarrow}}{m} - \frac{M_{33}^2q^2}{2m}$$

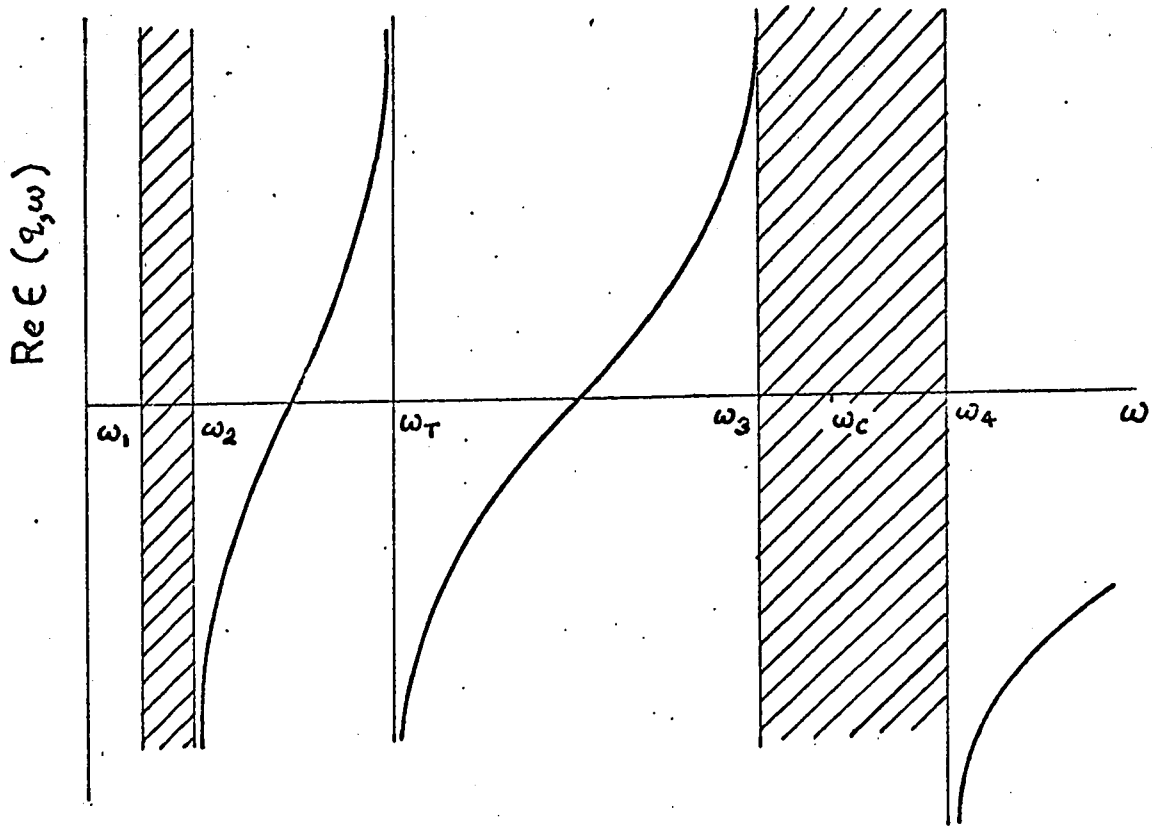

Figure 11. The general structure of Re $\varepsilon(\underset{\sim}{q},\omega)$ shown only in the regions $\omega\ \varepsilon(\omega_2,\omega_3)$ and $\omega>\omega_4$. The shaded regions are those for which Im $\varepsilon(\underset{\sim}{q},\omega)$ is nonzero (for $T = o$) .

$$\omega_2 = \frac{M_{33} q K_{o\downarrow}}{m} + \frac{M_{33}^2 q^2}{2m}$$

$$\omega_3 = \omega_c - \frac{M_{33} q K_{o\downarrow}}{m} + \frac{M_{33}^2 q^2}{2m} \qquad (5.20)$$

$$\omega_4 = \omega_c + \frac{M_{33} q K_{o\downarrow}}{m} + \frac{M_{33}^2 q^2}{2m}$$

To determine the location of these asymptotes, we estimate $K_{o\downarrow}$ by calculating the fermi momentum while ignoring the Landau level structure. We write

$$2\frac{\bar{V}}{(2\pi)^3}\,\frac{4}{3}\pi K_F^3 = NV$$

where $\bar{V}$ denotes the rescaled volume, so that

$$K_F^3 = 3\pi^2 \sqrt{\alpha_T^2 \alpha_L}\, N$$

or

$$K_F = 1.4 \times 10^7 \text{ cm}^{-1} \qquad (5.21)$$

Assuming that $K_{o\downarrow}$ is of this order, we find for $q = 10^4$,

$$\omega_1 \simeq \omega_2 \simeq 5 \times 10^{11} \text{ sec}^{-1}$$

$$\omega_3 \simeq \omega_c - 5 \times 10^{11} \qquad (5.22)$$

$$\omega_4 \simeq \omega_c + 5 \times 10^{11}$$

Of course there are more asymptotes (and hence modes) than

those shown in Figure 11; there are asymptotes near each of the frequencies $2\omega_c$, $3\omega_c$ and so on. However, contributions to the dielectric constant due to terms with $|n - n'| \geq 2$ are negligible at frequencies of interest because of the factor $\left|\gamma_{nn'}(M_{13}q, 0)\right|^2$ in the expression (5.17). In the long-wavelength limit these contributions reduce to zero.

At $T = 0$ the imaginary part of $\varepsilon(\underline{q},\omega)$ is non-zero in the shaded regions of Figure 11. Since the modes are given by the zeros of $\varepsilon(\underline{q},\omega)$, they are undamped as long as $\omega_3 > \omega_2$, and ω_T falls outside the damping regions. In view of the values given in (5.22), temperature effects on damping may be neglected for the low temperatures in which we are interested ($4.2^{\circ}K$).

We introduce collision damping through the replacement of ω by $\omega + i/\tau$ in the conductivity $\sigma(\underline{q},\omega)$, where τ is a relaxation time determined by experiment. If we have no damping due to the vanishing of the denominators in (5.1) (i.e., expression (5.18) is zero), the whole function $\varepsilon(\underline{q},\omega)$ is given by its real part. In regions of frequency in which the long-wavelength limit is valid we then have

$$\epsilon^{\tau}(0,\omega) = \epsilon_{\infty}\left[\frac{\omega^2-\omega_L^2}{\omega^2-\omega_T^2} - \frac{\omega_p^2}{\omega(\omega+i/\tau)}\,\frac{(\omega+i/\tau)^2 - \zeta^2\omega_c^2}{(\omega+i/\tau)^2-\omega_c^2}\right]$$

If $\omega\tau \gg 1$ we calculate the imaginary part of the dielectric constant to be

$$\mathrm{Im}\,\epsilon^{\tau}(0,\omega) = \frac{\epsilon_\infty \omega_p^2}{\omega^3\tau(\omega^2-\omega_c^2)^2}\left[\omega^4+\omega^2\omega_c^2+\beta^2\omega_c^2(\omega_c^2-3\omega^2)\right]$$

while its real part is unchanged from (5.12).

To translate this result into a scattering linewidth, we return to (5.3) and reconsider the factor

$$\mathrm{Im}\,\frac{(P^{\tau}(q,\omega))^2}{\epsilon^{\tau}(0,\omega)}$$

where $P^{\tau}(\underline{q},\omega) = \sum_{\sigma} P^{\tau}_{\sigma}(\underline{q},\omega)$ and the superscript indicates, as in $\varepsilon^{\tau}(0,\omega)$ that collision damping has been included. Assuming that $\mathrm{Im}\,\varepsilon^{\tau}(0,\omega)$ is constant over the width of the line we find

$$\mathrm{Im}\,\frac{(P^{\tau}(q,\omega))^2}{\epsilon^{\tau}(0,\omega)} = -\frac{\epsilon_I^{\tau}}{\epsilon_R^2(0,\omega)+(\epsilon_I^{\tau})^2}P_R^2(\underline{q},\omega)$$

The subscripts denote real and imaginary parts. Near the mode $\tilde{\omega}$ we get for this expression

$$-\frac{\epsilon_I^{\tau}}{\left[\epsilon_R'(0,\tilde{\omega})(\omega-\tilde{\omega})\right]^2+(\epsilon_I^{\tau})^2}$$

which gives a Lorentzian line shape of width

$$\Delta\omega = \frac{\epsilon_I^\tau}{|\epsilon_R'(0,\omega)|}$$

We can find a relaxation time τ from the data of Bobayashi et al.[17]. For PbTe at 4.2°K they give a mobility

$$\mu = 1.5 \times 10^6 \text{ cm}^2/\text{Vsec}$$

Using the transport effective mass which appears in ω_p^2, we find a relaxation time

$$\tau = 2.9 \times 10^{-11} \text{ sec}$$

For example, the mode $\omega = .54 \times 10^{13} \text{ sec}^{-1}$ at 15 Kgauss has a calculated linewidth

$$\Delta\omega = 1.3 \times 10^{10} \text{ sec}^{-1}$$

CHAPTER VI

SOME EXPERIMENTAL CONSIDERATIONS

Because of the high optical dielectric constant of PbTe, $\eta = 5.48$, large reflection and refraction will take place at the surfaces of the crystal in any optical experiment. Reflection coefficients for oblique incidence are readily available[18]. To investigate the restrictions imposed by refraction, we consider a slab of crystal shown in Figure 12. Using the equations

$$\begin{aligned} \sin\theta_1 &= \eta \sin\theta_2 \\ \eta \sin\theta_3 &= \sin\theta_4 \\ \underset{\sim}{k}_1 &= \underset{\sim}{k}_2 + \underset{\sim}{q} \end{aligned} \tag{6.1}$$

with $\underset{\sim}{k}_1$ and $\underset{\sim}{k}_2$ the photon momenta in the crystal, we find the following relationship between θ_1 and θ_4

$$\sin^2\theta_4 = \frac{\sin^2\theta_1}{1 + \frac{q^2}{k_1^2} - 2\frac{q}{k_1}\sqrt{1 - \frac{\sin^2\theta_1}{\eta^2}}}$$

which simplifies to

$$\sin^2\theta_4 = \frac{\sin^2\theta_1}{\left(1 - \frac{q}{k_1}\right)^2 + \frac{q}{\eta^2 k_1}\sin^2\theta_1} \tag{6.2}$$

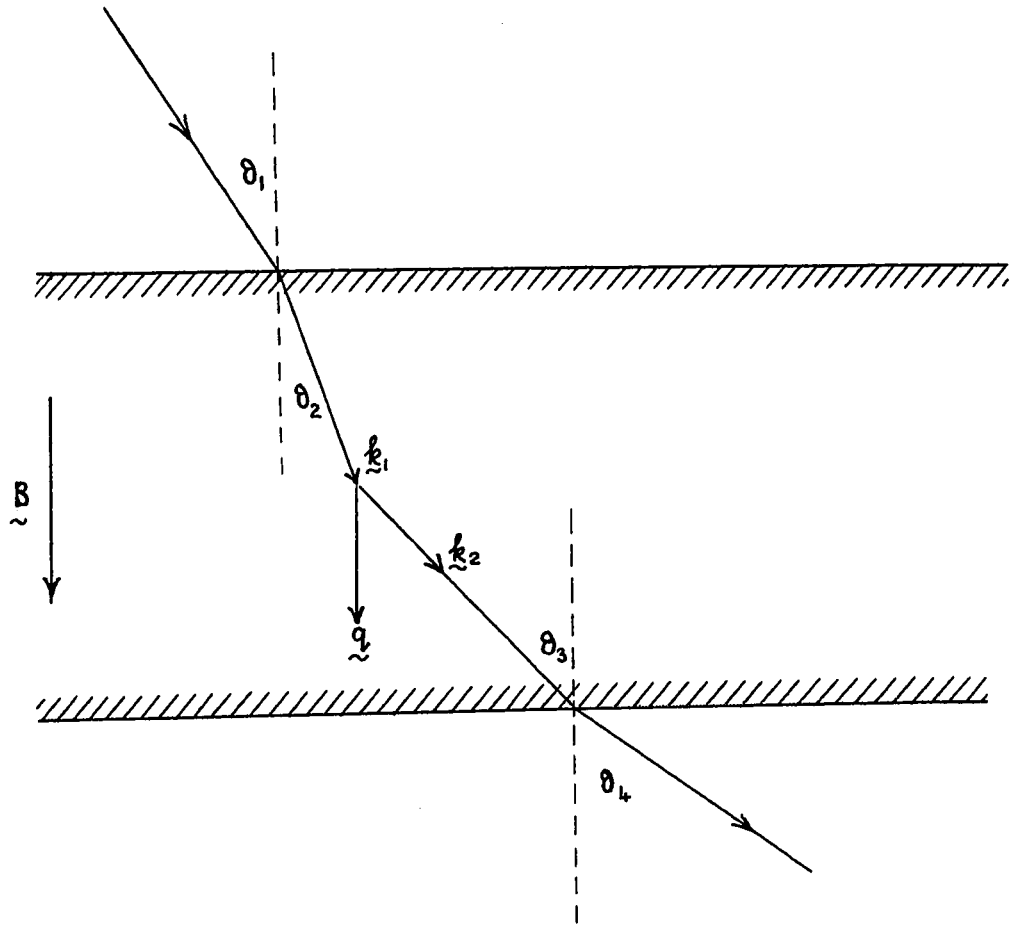

Figure 12. Refraction at the surfaces of the crystal.

when we use the fact that $\sin^2\theta_1 \ll \eta^2$. Since $q \sim 10^4$, $k_1 \sim 3 \times 10^4$, we have approximately

$$\sin\theta_4 = \frac{\sin\theta_1}{1 - \frac{q}{k_1}} \tag{6.3}$$

The maximum value of θ_1 is then about 42° before total internal reflection takes place at the second interface.

CHAPTER VII

CONCLUSIONS

The existence of a LF magnetoplasma mode should be observable in PbTe in a Raman scattering experiment. Both the HF plasmon and the LO phonon modes have appreciable cross sections; at low fields ($B < 50$ Kgauss) the LF plasmon mixes with the LO phonon, and at higher fields, with the HF plasmon. In nonpolar crystals evidence of its existence through a Raman experiment can be obtained only at high magnetic fields.

APPENDIX

We derive the long-wavelength limit of $\varepsilon(\underset{\sim}{q},\omega)$. If we are outside the damping regions, the dielectric constant is given by (5.17)

$$\epsilon(\underset{\sim}{q},\omega)=\epsilon_\infty\frac{\omega^2-\omega_L^2}{\omega^2-\omega_T^2}-\frac{4e^2m^2\omega_c}{\pi\hbar\alpha_T^2\alpha_L}\frac{1}{M_{33}q^3}\sum_{nn'\sigma}\left|\gamma_{nn'}(M_{13}q,0)\right|^2\times$$
$$\times\ln\left|\frac{\left[(n'-n)\omega_c-\frac{M_{33}qK_{n\sigma}}{m}+\frac{M_{33}^2q^2}{2m}\right]^2-\omega^2}{\left[(n'-n)\omega_c+\frac{M_{33}qK_{n\sigma}}{m}+\frac{M_{33}^2q^2}{2m}\right]-\omega^2}\right| \qquad (A.1)$$

We expand the matrix element $|\gamma|^2$ to order q^2 (equation 4.57)

$$\left|\gamma_{nn'}(M_{13}q,0)\right|^2=\delta_{nn'}\left[1-(2n+1)\frac{M_{13}^2q^2}{2m\omega_c}\right]+$$
$$+\delta_{n'n+1}(n+1)\frac{M_{13}^2q^2}{2m\omega_c}+\delta_{n'n-1}n\frac{M_{13}^2q^2}{2m\omega_c} \qquad (A.2)$$

For the term n' = n the logarithm is (in cgs units)

$$\ln\frac{\omega^2-\left(\frac{M_{33}qK_{n\sigma}\hbar}{m}-\frac{M_{33}^2q^2\hbar}{2m}\right)^2}{\omega^2-\left(\frac{M_{33}qK_{n\sigma}\hbar}{m}+\frac{M_{33}^2q^2\hbar}{2m}\right)^2}$$

If we put in some numbers, $M_{33} = 3.24$, $q = 10^4$, $K_{n\sigma} = 10^7$ we find

$$\frac{M_{33} q K_{n\sigma} \hbar}{m} \sim 3.8 \times 10^{11} \text{ sec}^{-1}$$
$$\frac{M_{33}^2 q^2 \hbar}{2m} \sim 6.1 \times 10^{8} \text{ sec}^{-1} \qquad \text{(A.3)}$$

Any modes in which we are interested lie in the range 10^{12} to 10^{13} sec^{-1}. Therefore for these modes we can expand the logarithm

$$\ln \frac{\omega^2 - \left(\frac{M_{33} q K_{n\sigma}}{m} - \frac{M_{33}^2 q^2}{2m}\right)^2}{\omega^2 - \left(\frac{M_{33} q K_{n\sigma}}{m} + \frac{M_{33}^2 q^2}{2m}\right)^2} \simeq \frac{2 M_{33}^3 q^3 K_{n\sigma}}{m^2 \omega^2 - M_{33}^2 q^2 K_{n\sigma}^2} \qquad \text{(A.4)}$$

For the term $n' = n + 1$ the logarithm is

$$\ln \left| \frac{\left(\omega_c + \frac{M_{33}^2 q^2}{2m}\right)^2 + \frac{M_{33}^2 q^2 K_{n\sigma}^2}{m^2} - \omega^2 - \frac{2 M_{33} q K_{n\sigma}}{m}\left(\omega_c + \frac{M_{33}^2 q^2}{2m}\right)}{\left(\omega_c + \frac{M_{33}^2 q^2}{2m}\right)^2 + \frac{M_{33}^2 q^2 K_{n\sigma}^2}{m^2} - \omega^2 + \frac{2 M_{33} q K_{n\sigma}}{m}\left(\omega_c + \frac{M_{33}^2 q^2}{2m}\right)} \right|$$

For fields of 10 Kgauss or greater ω_c exceeds 4×10^{12} sec^{-1}. Because of (A.3) we therefore simplify this factor to

$$\ln \left| \frac{\omega_c^2 - \omega^2 - \frac{2 M_{33} q_\parallel K_{n\sigma} \omega_c}{m}}{\omega_c^2 - \omega^2 + \frac{2 M_{33} q_\parallel K_{n\sigma} \omega_c}{m}} \right|$$

For frequencies not near ω_c we expand this logarithm and obtain

$$- \frac{4 M_{33} q_\parallel K_{n\sigma} \omega_c}{m(\omega_c^2 - \omega^2)}$$

Note that this expansion is not valid for the mode between ω_T and ω_c if ω_c approaches ω_T. Finally the term for which $n' = n - 1$ becomes

$$\frac{4 M_{33} q_\parallel K_{n\sigma} \omega_c}{m(\omega_c^2 - \omega^2)}$$

If we combine these approximations, and work to order q^3 we find

$$\epsilon(\underset{\sim}{q}, \omega) \simeq \epsilon_\infty \frac{\omega^2 - \omega_L^2}{\omega^2 - \omega_T^2} - \frac{8 e^2 \omega_c}{\pi \sqrt{\alpha_T^2 \alpha_L}} \left[\frac{M_{33}^2}{\omega^2} - \frac{M_{13}^2}{\omega_c^2 - \omega^2} \right] \sum_{n\sigma} K_{n\sigma}$$

By counting states one can show that (equation 5.10)

$$\sum_{n\sigma} K_{n\sigma} = \frac{\pi^2 \sqrt{\alpha_T^2 \alpha_L} N}{2 m \omega_c}$$

and (5.12) follows.

BIBLIOGRAPHY

1. Platzman P.M. and Tzoar N., Phys. Rev. 182, 510 (1969).
2. Wallace P.R., Can. J. Phys. 43, 2162 (1965).
3. Platzman P.M., Phys. Rev. 139, A379 (1965).
4. Luttinger J.M. and Kohn W., Phys. Rev. 97, 869 (1955).
5. Cuff K.F., Eliett M.R., Kuglin C.D., and Williams L.R., In Physics of Semiconductors Proceedings, Paris Conference (1964).
6. Fröhlich H., Adv. in Phys. 3, 325 (1954).
7. Platzman P.M. and Tzoar N., Phys. Rev. 136, A11 (1964).
8. Platzman P.M., Wolff P.A., and Tzoar N., Phys. Rev. 174, 489 (1968).
9. Abrikosov A.A., Gorkov L.P., and Dzyaloshinski I.E., "Methods of Quantum Field Theory in Statistical Physics", Prentice-Hall (1963).
10. Ambegaokar V., "Astrophysics and the Many-Body Problem", Brandeis Summer Institute 1962, Benjamin (1963).
11. Wallace P.R., In "Physics of Solids in Intense Magnetic Fields" (Edited by E.D. Haidemenakis), Plenum Press (1969).
12. Schultz T.D., "Quantum Field Theory and the Many-Body Problem", Gordon and Breach (1962).
13. Varga B.B., Phys. Rev. 137, A1896 (1965).
14. Morse P.M. and Feshbach H., "Methods of Theoretical Physics", McGraw-Hill (1953).

BIBLIOGRAPHY (continued)

15. Wallace P.R., Chandler K.K., and Harnad J., Can. J. Phys. 46, 243 (1968).

16. Butler J.F. and Calawa A.R., In Physics of Quantum Electronics Conference Proceedings, Puerto Rico (1965).

17. Bobayashi A., Sato Y., and Fujimoto M., In Physics of Semiconductors Proceedings, Paris Conference (1964).

18. Jackson J.D., "Classical Electrodynamics", John Wiley and Sons (1962).