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SOUND PROPAGATION IN α Sn (*)

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Résumé. — La propagation d'ondes sonores dans l'étain α, semiconducteur à gap nul, est étudiée dans les deux régimes adiabatique et non adiabatique, dans l'approximation de la phase aléatoire. On montre que la vitesse des ondes est la même dans les deux régimes et que le domaine non adiabatique est caractérisé par une absorption en $q^{\frac{3}{2}}$. L'influence des interactions à N électrons sur ces résultats est ensuite brièvement discutée.

Abstract. — The sound propagation in the gapless semiconductor α Sn is studied in both adiabatic and non-adiabatic regimes within the R.P.A. scheme. It is shown that the sound velocity is the same in both regimes, while the latter is characterized by a $q^{\frac{3}{2}}$ sound absorption. The validity of these results when the many-body interactions are taken into account is briefly discussed.

1. **Introduction.** — This paper is devoted to a theoretical study of the sound propagation in a second-type gapless semiconductor [1], namely α Sn. The problem is of basic interest because this is one of the few situations where the adiabatic approximation for the force constants is bound to be invalid. Indeed, let $C_{ss'}^{\alpha\beta}(\mathbf{R}_l - \mathbf{R}_{l'}, \mathbf{t} - \mathbf{t}')$ be the coupling coefficient between the displacement at time t, and in the direction α, of the atom s which is in the cell centered at R_l, and the force exerted at time $t' > t$, in the direction β, on the atom $(s', R_{l'})$. Its time Fourier transform $C_{ss'}^{\alpha\beta}(\mathbf{R}_l - \mathbf{R}_{l'}, \omega)$ is, in practice, independent of ω in the two following cases [2] :

— Metals : $\omega \ll \omega_{pl}$, where ω_{pl} is the plasmon frequency ;

— Insulators : $\omega < \omega_p$ where $\hbar\omega_p$ is the energy of the electronic gap.

None of these conditions are satisfied in infinitely pure α Sn at 0 K where the valence and the conduction bands belong to the same irreducible representation Γ_8^+ at the center of the Brillouin zone ; this substance is the prototype of a gapless semiconductor of the second type, i.e. one in which the one-electron energy is quadratic in $\| \mathbf{k} \|$ around Γ.

The study of this sound propagation can be performed following methods first introduced by Keating [3], Pick *et al.* [2] and Sham [4] who have shown how to relate the force constant $C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega)$ to the irreducible part of the susceptibility function $\chi(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ ([1]).

Such a study was in fact undertaken by Sherrington [5] who was able to show that, within the limit of the random phase approximation (R.P.A.) of the susceptibility, a sound wave should always propagate in α Sn. Nevertheless two different regimes exist for $q \gg q_c$ and $q \ll q_c$ where $q_c \sim 10^4\ \mathrm{cm}^{-1}$: for $q \gg q_c$ the adiabatic approximation is valid while it is not in the latter case. Sherrington then concluded that there were two different sound velocities for the two regimes, and the original goal of this study was to look for the evaluation of the difference between those two values. It rapidly turned out that a certain number of points were overlooked in [5] so that a more complete study had to be undertaken.

In order to make this paper a rather self contained one, section 2 summarizes the results and methods of [6] which are necessary for a complete study of the sound propagation. Section 3 is devoted to the study of the susceptibility function within the same R.P.A. framework as used in [5] ; the analytic dependence of the real and imaginary parts of this quantity, as functions of $\| \mathbf{q} \|$, $\mathbf{G}$ and $\mathbf{G}'$ are studied for the three various cases ($\mathbf{G}$ and $\mathbf{G}' = 0$; $\mathbf{G}$ or $\mathbf{G}' = 0$; $\mathbf{G}$ and $\mathbf{G}' \neq 0$), once ω has been set equal to vq (where v,

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([1]) There and throughout this paper $\mathbf{q}$ is a vector of the first Brillouin zone and $\mathbf{G}$, $\mathbf{G}'$ are vectors of the reciprocal lattice.

the sound velocity, is kept as a free parameter). Section 4 analyses the various terms of the dynamical matrix of the acoustical phonons and concludes that only the non-electric terms will contribute to it, with coefficients the hermitian part of which is identical in both adiabatic and non-adiabatic regimes. Finally in section 5, the form of the hermitian and non-hermitian part of the dynamical matrix is discussed. It is shown that the non-adiabatic regime can only be characterized by a $q^{\frac{3}{2}}$ sound absorption. The modifications due to the non validity of the random-phase approximation in the non-adiabatic regime are also briefly discussed and it is suggested that while no changes are expected from the sound velocity, the expression for the sound absorption may be invalid.

2. **A phonon theory summary.** — 2.1 INTRODUCTION. — Let us briefly summarize here the elements of the phonon theory which are necessary for the rest of this paper ; we shall use the notations of [6] where most of the developments can be found and shall simply quote the microscopic expressions of the force constants and the technique one must use in the long wave-length limit in order to study the acoustical phonons.

2.2 MICROSCOPIC EXPRESSIONS OF THE FORCE CONSTANTS. — The microscopic theory of phonons allows one to express the Fourier transforms of the harmonic force constants $C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega)$ through the irreducible part of the polarisation function of all the electrons $\chi(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ and the charge Z_s of the nuclei. For this, it is convenient to consider, for fixed ω and $\mathbf{q}$, this function as an infinite square matrix, $\mathbf{G}$ and $\mathbf{G}'$ being respectively the row and column and furthermore, to introduce the following two additional matrices

$$S(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) = \delta_{\mathbf{G},\mathbf{G}'} - \frac{4\pi}{|\mathbf{q} + \mathbf{G}|} \chi(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) \frac{1}{|\mathbf{q} + \mathbf{G}'|} \tag{2.1}$$

$$^{r}S(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) = (1 - \delta_{\mathbf{G},\mathbf{0}})(1 - \delta_{\mathbf{G}',\mathbf{0}}) S(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) . \tag{2.2}$$

The force constants are then expressed as the sum of two terms, the behaviour of which may be different in the $\omega \to 0$, $\mathbf{q} \to 0$ limit.

$$C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) = C_{1ss'}^{\alpha\beta}(\mathbf{q}, \omega) + G_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) . \tag{2.3}$$

The first term (which is always analytic) is

$$C_{1ss'}^{\alpha\beta}(\mathbf{q}, \omega) = Z_s \sum_{\mathbf{G},\mathbf{G}'}{}' e^{i\mathbf{G}.\mathbf{R}_s} (\widehat{\mathbf{q} + \mathbf{G}})_\alpha ({}^{r}S)^{-1} (\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) (\widehat{\mathbf{q} + \mathbf{G}'})_\beta e^{-i\mathbf{G}'.\mathbf{R}'_s} Z_{s'} - \delta_{ss'} K_{ss'}^{\alpha\beta} \tag{2.4}$$

where $(\widehat{\mathbf{q} + \mathbf{G}})_\alpha$ is the α projection of the unit vector

$$\widehat{\mathbf{q} + \mathbf{G}} = \frac{\mathbf{q} + \mathbf{G}}{\| \mathbf{q} + \mathbf{G} \|}$$

and $K_{ss'}^{\alpha\beta}$ is a constant (which value is given in [6]) which ensures the translational invariance of the total energy of the crystal.

The second term, usually referred to as the electrical term is

$$G_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) = Z_s^{\alpha}(\mathbf{q}, \omega) \frac{1}{L(\mathbf{q}, \mathbf{q}, \omega)} Z_{s'}^{\beta}(\mathbf{q}, \omega) \tag{2.5}$$

where

$$Z_{s'}^{\beta}(\mathbf{q}, \omega) = Z_{s'} \left\{ \hat{q}_\beta - \sum_{\mathbf{G},\mathbf{G}'}{}' (\widehat{\mathbf{q} + \mathbf{G}})_\beta e^{-i\mathbf{G}.\mathbf{R}_{s'}} ({}^{r}S)^{-1} (\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) S(\mathbf{q} + \mathbf{G}', \mathbf{q}, \omega) \right\} \tag{2.6}$$

and

$$L(\mathbf{q}, \mathbf{q}, \omega) = S(\mathbf{q}, \mathbf{q}, \omega) - \sum_{\mathbf{G},\mathbf{G}'}{}' S(\mathbf{q}, \mathbf{q} + \mathbf{G}, \omega) ({}^{r}S)^{-1} (\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) S(\mathbf{q} + \mathbf{G}', \mathbf{q}, \omega) . \tag{2.7}$$

In insulators, both $Z_s^{\alpha}(q, \omega)$ and $L(\mathbf{q}, \mathbf{q}, \omega)$ have a $\hat{q}$ dependent limit, and, as we shall see in section 4, similar problems arise in α Sn.

2.3 THE ELASTIC LIMIT OF THE PHONON DYNAMICAL MATRIX. — In order to discuss the existence of acoustical phonons, it is convenient [6] to write the phonon dynamical matrix in the following form

$$O = \left\| \begin{matrix} \sum_{ss'} C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) - \sum_{s} M_s \delta_{\alpha\beta} \omega^2 & \sum_{s} C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) - M_{s'} \delta_{\alpha\beta} \omega^2 \\ \sum_{s'} C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) - M_s \delta_{\alpha\beta} \omega^2 & C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) - \delta_{ss'} \delta_{\alpha\beta} M_s \omega^2 \end{matrix} \right\| \tag{2.8}$$

where the new determinant has been built by summing some rows and columns of the usual dynamical matrix of a crystal (M_s is the mass of the atoms, and here runs from 1 to 2 with $M_1 = M_2 = M$).

In a crystal where only the non electric term of the force constants exists (metal, as well as diamond, silicon and germanium) one shows that

$$\lim_{\omega \to 0,\, \mathbf{q} \to 0} \sum_{ss'} C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) = q^2 \sum_{\gamma,\delta} \hat{q}_\gamma V^{\alpha\gamma,\beta\delta} \hat{q}_\delta \tag{2.9}$$

$$\lim_{\omega \to 0,\, \mathbf{q} \to 0} \sum C_{ss'}^{\alpha\beta}(\mathbf{q}, \omega) = q \sum_{\gamma} \hat{q}_\gamma J_{s'}^{\alpha\gamma,\beta} . \tag{2.10}$$

The splitting of (2.9) in submatrices respectively proportional to q^2, q and unity implies the existence of eigenvalues ω proportional to q, and, more precisely, if $\omega = v \parallel \mathbf{q} \parallel$, v is the solution of

$$O = \left\| \sum_{\gamma,\delta} \hat{q}_\gamma [V^{\alpha\gamma,\delta\beta} - J_s^{\alpha\gamma,\eta} [C_{ss'}^{\eta\varepsilon}(0, 0)]^{-1} J_{s'}^{\varepsilon,\delta\beta}] \hat{q}_\delta - \sum_s M_s \,\delta\alpha\beta v^2 \right\| \tag{2.11}$$

where the second term of the parenthesis comes from the relaxation of the lattice under an acoustical wave.

In insulators, as well as in semiconductors, the same treatment must be applied to the electric term, and it generally leads to a more complicated form of (2.11). The situation we shall encounter in α Sn will be different : an electrical term does exist, and it has a complicated behaviour; nevertheless, when forming the determinant (2.8) each electrical term will give rise to a contribution of higher order in q than the corresponding non-electrical term : as a consequence they will be neglected and the sound velocity will be a solution of (2.11).

3. **The R.P.A. susceptibility functions.** — 3.1 GENERALITIES. — As we restrict ourselves to the R.P.A. (see section 5 for a more general discussion) we can closely follow [5] in the calculation of the susceptibility function, (a quantity also studied under various limits in e.g. [8, 9, 10]) and discuss only some special aspects of this calculation. The method used in this former paper may be summarized as follows.

First, one writes $\omega = v \parallel \mathbf{q} \parallel$ where v must, in principle, be self consistently determined.

Second, one notices that the R.P.A. susceptibility function may be split into two parts, one, $\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ in which the matrix elements entering into its numerator contains zero (type A) or only one (type B) wave function connected with the Γ_8^+ point, the second, $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ in which both waves functions are connected with the Γ_8^+ point (matrix elements of type C). In the $\mathbf{q} \to 0$ limit, the analytic form of $\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ is that of an ordinary insulator and is given in table I.

TABLE I

$$4\pi\chi^r(\mathbf{q}, \mathbf{q}) = q^2 \sum_{\alpha,\beta} B^{\alpha\beta} \hat{q}_\alpha \hat{q}_\beta + O(q^4)$$

$$4\pi\chi^r(\mathbf{q}, \mathbf{q} + \mathbf{G}) = -q \sum_\alpha A^\alpha(\mathbf{G}) \hat{q}_\alpha + O(q^2) \qquad G \neq 0$$

$$4\pi\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}') = 4\pi\chi^A(\mathbf{G}, \mathbf{G}') + O(q) \qquad \mathbf{G} \text{ and } \mathbf{G}' \neq 0 .$$

Analytic behaviour of $\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}')$ in the vicinity of $\mathbf{q} = 0$.

This table takes into account the fact that a center of inversion of the crystal has been taken as the origin of coordinate in the real space, so that the two following relations are satisfied :

$$\chi(-\mathbf{q} - \mathbf{G}, -\mathbf{q} - \mathbf{G}', \omega) = \chi(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) \tag{3.1}$$

$$\mathrm{Jm}\, \chi(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', 0) = 0 . \tag{3.2}$$

Finally $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ is given by

$$\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{M}{E_v(\mathbf{k}) - E_c(\mathbf{k} + \mathbf{q}) - \omega - i\delta} + \frac{M^*}{E_v(\mathbf{k}) - E_c(\mathbf{k} + \mathbf{q}) + \omega + i\delta} \tag{3.3}$$

with

$$M = \sum_{v_v, v'_c} \langle \mathbf{k} + \mathbf{q}, v'_c \mid e^{i(\mathbf{q}+\mathbf{G}).\mathbf{r}} \mid v_v, \mathbf{k} \rangle \langle \mathbf{k}, v_v \mid e^{-i(\mathbf{q}+\mathbf{G}').\mathbf{r}} \mid v'_c, \mathbf{k} + \mathbf{q} \rangle \tag{3.4}$$

where v_c (resp. v_v) labels the two conduction (resp. valence) bands connected to Γ_8^+, and $\mid v, \mathbf{k} \rangle$ is the electronic wave function associated with the eigenvalue $E_v(\mathbf{k})$, and following [8], those have the expressions :

$$\mid v, \mathbf{k} \rangle = \left[\sum_{\alpha=1}^{3} A_v^\alpha \mid \theta_\mathbf{k}, \psi_\mathbf{k} \rangle \varepsilon^\alpha_{(\mathbf{r})} \right] e^{i\mathbf{k}.\mathbf{r}} \tag{3.5a}$$

$$E_v(\mathbf{k}) = \frac{1}{2} \frac{k^2}{mv} . \tag{3.5b}$$

In this expression, $A_v^\alpha(\theta_\mathbf{k}, \psi_\mathbf{k})$ depends only on the two angular spherical coordinates of $\hat{k}$ with respect to the crystalline axes, $\varepsilon^\alpha(\mathbf{r})$ being one of the three eigen values of the $\Gamma_{25'}$ level which gives rise to the Γ_8^+ level by the spin orbit splitting. Furthermore, the effective masses are identical for the two valence (or conduction) bands.

Let us note that, as the three $\varepsilon^\alpha(\mathbf{r})$ functions transform as xy, yz and zx under the operations of the O_h group, it is convenient to label them respectively with the indices z, x and y, or (using the usual elasticity convention) with 3, 1 and 2. In the rest of this section we shall use this last convention and use $1 \leqslant \alpha \leqslant 3$ both as an ordinary index and as one labeling a specified cartesian coordinate.

The complex behaviour of (3.3), whatever are $\mathbf{G}$ and $\mathbf{G}'$, in the vicinity of $\omega = 0$, $\mathbf{q} = 0$ has two different origins.

One is related to the vanishing of its denominator, and Sherrington showed that, if q_c is such that

$$\frac{q_c^2}{2\,\mu^*} = v q_c \qquad \left(\frac{1}{\mu^*} = \frac{1}{m_c} + \frac{1}{m_v}\right) \tag{3.6}$$

— for $q \gg q_c$ one could write directly $\omega = 0$ in the denominator (adiabatic regime),

— for $q \ll q_c$ the exact form of the denominator had to be taken into account (non-adiabatic regime) and led to different results (as well as to an imaginary part that we shall compute in order to discuss the sound attenuation problem),

— for $q \simeq q_c$ no predictions can be made, as $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ is no longer analytic in ω and q.

The second origin for a complicated behaviour of $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ is related to the non-analytic form of the Liu and Brust wave functions (eq. (3.4)) and needs some discussion. This will be done in the next paragraph, while the final results for $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ will be summarized in paragraph 3.3.

3.2 Influence of the wave functions and related problems. — 3.2.1 *The wave function problem.* — The role of the numerator (3.4) is best understood when a change of axes is done so that $\hat{q}$ is taken as the new polar axis for the spherical coordinates, k, $\Theta_{\mathbf{k}}$, $\psi_{\mathbf{k}}$ being the new variables. Clearly the denominator of (3.3) does not depend on $\psi_{\mathbf{k}}$, and its numerator can be integrated over $\psi_{\mathbf{k}}$.

One then finds (7) that :

$$\int_0^{2\pi} M_{\mathbf{G},\mathbf{G}',\mathbf{q}}(k, \Theta_{\mathbf{k}}, \psi_{\mathbf{k}})\, \mathrm{d}\psi_k = = N^1 \frac{k^2}{|\,\mathbf{k} + \mathbf{q}\,|^2} + N^2 \frac{kq}{|\,\mathbf{k} + \mathbf{q}\,|^2} + N^3 \frac{q^2}{|\,\mathbf{k} + \mathbf{q}\,|^2} \tag{3.7}$$

where each function N depends on $\mathbf{G}$, $\mathbf{G}'$, $\Theta_{\mathbf{k}}$ and $\hat{q}$ where, furthermore, N^1 is equal to zero for $\mathbf{G}$ or $\mathbf{G}' = 0$ while N^2 is equal to zero under the stronger condition $\mathbf{G}$ and $\mathbf{G}' = 0$.

The form of (3.7) is easy to understand.

On the one hand, the wave functions (3.5*a*) are mutually orthogonal for all values of $\mathbf{k}$; a matrix element entering the numerator M is then proportional to $\|\,\mathbf{q}\,\|$ if $\mathbf{G}$ or $\mathbf{G}' = 0$. The zero values of N^1 and N^2 is simply a reassertion of this remark.

On the other hand, these wave functions depend only on $\hat{k}$ (except for a phase factor) and, more precisely, on products of $\sin \Theta_{\mathbf{k}}$ and $\cos \Theta_{\mathbf{k}}$; $q/\|\,\mathbf{k} + \mathbf{q}\,\|$ factors appear when one expresses e.g. $\cos \Theta_{\mathbf{k}+\mathbf{q}}$ as a function of $\cos \Theta_{\mathbf{k}}$, and $\sin \Theta_{\mathbf{k}}$, and the very existence of such factors simply reflects the non-analyticity of the waves functions around the Γ_8^+ point. Such a non-analyticity will be carried over by integration as will be apparent in table II.

3.2.2 *The cut-off problem.* — The Liu and Brust wave functions (3.5) are valid for wave vectors $\mathbf{k}$ which are small with respect to a reciprocal lattice vector i.e. for $\|\,\mathbf{k}\,\| \lesssim k_c \simeq 10^6\ \mathrm{cm}^{-1}$, a value much larger than $q_c \simeq 10^4\ \mathrm{cm}^{-1}$. k_c is thus a natural cut-off for such an integration and the contribution of the rest of the bands is a normal one which must be included in $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$. In fact, as it should, the actual value of k_c is irrelevant.

Indeed the denominator of (3.3) is proportional to k^2 for large k. As a result the $k^2\,\mathrm{d}k$ integration of the N^3 term is absolutely convergent and it is easily seen that it converges much below k_c.

The N^2 term is not absolutely convergent (the integrand is proportional to $\mathrm{d}k/k$) but this leading term is cancelled by the integration over $\Theta_{\mathbf{k}}$ (a point which was overlooked in [5]) and the next term has the same behaviour as the N^3 term. As a consequence, $\chi^t(\mathbf{q}, \mathbf{q}, vq)$ and $\chi^t(\mathbf{q}, \mathbf{q} + \mathbf{G}, vq)$ will have the same analytic behaviour in q.

Finally, the integral over the N^1 term depends on k_c, because the integrand is proportional to $\mathrm{d}k$ for large k, but it is easily seen that the result is identical in both regimes, and that the lowest order term is q independent. As N^1 gives the leading contribution to :

Table II

	$\frac{q}{q_c} \ll 1$ (non-adiab.)	$\frac{q}{q_c} \gg 1$ (adiab.)
$4\,\pi\chi^r(\mathbf{q}, \mathbf{q}, vq)$	$-(1 + i)\sqrt{\frac{2\,\mu^*}{v}}\, q^{\frac{3}{2}}$	$-3\,qC_0$
$4\,\pi\chi^r(\mathbf{q}, \mathbf{q} + \mathbf{G}, vq)$	$-(1 + i)\sqrt{\frac{2\,\mu^*\, q^{\frac{3}{2}}}{v}} \sum_{\alpha,\beta} D^{\alpha\beta}(\mathbf{G})\, \hat{q}_\alpha\, \hat{q}_\beta$	$-D_0\, q \sum_{\alpha,\beta} D'^{\alpha\beta}(\mathbf{G})\, \hat{q}_\alpha\, \hat{q}_\beta$
$4\,\pi\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$	$\sum_{p,p'=1}^{6} m_p(\mathbf{G})\, T_{pp'}\, m_{p'}(\mathbf{G}')\,(1 + i\lambda q^{\frac{1}{2}})$	$\sum_{p,p'=1}^{6} m_p(\mathbf{G})\, T_{pp'}\, m_{p'}(\mathbf{G}')$

Analytic behaviour of $\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$ in the vicinity of $\mathbf{q} = 0$.

$\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$, the role of the cut-off is seen to cancel out when both $\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$ and $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$ are added.

3.2.3 *The q development problem.* — All the results which will be quoted in the next paragraph correspond to the leading q term. It turns out that such a term is the only one which needs to be considered for a sound velocity problem, because any higher order term would give a negligible contribution.

3.3 Results and remarks on $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$. — The actual calculations of $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$ are described in [7], and are summarized in table II.

In this table λ, C_0 and D_0 are simple smoothly varying functions of the effective masses m_c and m_v, the exact expression of which are given in [7];

$$m_p(\mathbf{G}) \equiv m_{\alpha\beta}(\mathbf{G}) = \langle \varepsilon_\alpha(\mathbf{r}) \mid e^{i\mathbf{G}.\mathbf{r}} \mid \varepsilon_\beta(\mathbf{r}) \rangle \quad (3.8)$$

where $1 \leqslant p \leqslant 6$, p being the usual contracted index used in elasticity theory (e.g. $p \equiv 5 \Leftrightarrow \alpha = 1, \beta = 2$ or $\alpha = 2, \beta = 1$);

$$D^{\alpha\beta}(\mathbf{G}) = \frac{2\pi}{5}[6\, a m_{\alpha\beta}(\mathbf{G}) - \delta_{\alpha\beta}[(10 + a)\,\mathrm{Trace}\, m_{\alpha\beta}(\mathbf{G}) + \tfrac{3}{2}(3\,a - 1)\, m_{\alpha\alpha}(\mathbf{G})]]\,; \quad (3.9)$$

$$D'^{\alpha\beta}(\mathbf{G}) = \frac{2\pi}{3}[m_{\alpha\beta}(\mathbf{G}) + \tfrac{1}{2}\,\delta_{\alpha\beta}[\mathrm{Trace}\, m_{\alpha\beta}(\mathbf{G}) - m_{\alpha\alpha}(\mathbf{G})]]\,; \quad (3.10)$$

$$a = \frac{m_c - m_v}{m_c + m_v}\,; \quad (3.11)$$

$$T_{ij} = A_{ij}\,\mu^*\,\frac{kc}{45\,\pi} \quad \text{with} \quad A_{ij} = \begin{cases} -\ 64\,;\ i = j = 1, 2, 3 \\ -\ 192\,;\ i = j = 4, 5, 6 \\ \quad 32\,;\ i \neq j \neq 4, 5, 6. \end{cases} \quad (3.12)$$

Let us finally remark that:

— as $\varepsilon^\alpha(\mathbf{r})$ is even under the inversion with respect to the origin in the real space, so is $m_{\alpha\beta}(\mathbf{G})$ under the same inversion in the reciprocal space, and, furthermore $\mathrm{Im}\,(m_{\alpha\beta}(\mathbf{G})) = 0$. As a result, each term of tables I and II fulfils the relation (3.2*a*) though, $\chi^r(\mathbf{q}, \mathbf{q} + \mathbf{G}, vq)$ and $\chi^t(\mathbf{q}, \mathbf{q} + \mathbf{G}, vq)$ have an opposite parity with respect to $\mathbf{G}$:

— in both regimes, $\chi^t(\mathbf{q}, \mathbf{q} + \mathbf{G}, vq)$ has the same q dependence as $\chi^t(\mathbf{q}, \mathbf{q}, vq)$. The underlying reason has been given in 3.2.2, but this result may be an artefact of the R.P.A. method in the non-adiabatic regime.

4. **The elements of the dynamical matrix.** — 4.1 Introduction. — This fourth part is devoted to the study of the analytical behaviour of the elements of the dynamical matrix (2.8). It will be shown here that, even in the very severe limit of 0 K and no impurity, the elements of this matrix are practically identical to those of e.g. silicon. More precisely, its hermitian part has exactly the same form in both the adiabatic and the non-adiabatic regimes, this form being identical to that of the above mentioned typical semiconductor. The only difference comes from the existence of a non-hermitian part which exists only in the non-adiabatic regime and will eventually lead to a sound absorption.

A brief look at table II shows that such results are possible only if the sole contribution of the bands in contact comes from $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$ with $\mathbf{G}$ and $\mathbf{G}' = 0$. This is indeed the purpose of this section which will be divided in three paragraphs. Analytical expressions of the constituants of the dynamical matrix will be given in the first one. The second one will analyse the properties of the non-electric part of (2.8): it will be shown that their hermitian part fulfils the relations (2.9, 2.10) while the non-hermitian ones have a similar form but are smaller by a $q\,\frac{1}{2}$ factor. Finally, the third paragraph will be devoted to the same problem for the electric part which will be shown to be of higher order in q that their non-electric counterpart, and thus not contributing to (2.8).

4.2 The constituting elements of the force constants. — Formulae (2.4, 5, 6, 7) allow us to express the non-electric and the electric part of the dynamical force constants in terms of the three quantities $1/L(\mathbf{q}, \mathbf{q}, vq)$, $S(\mathbf{q} + \mathbf{G}, \mathbf{q}, vq)$ and $({}^rS)^{-1}\,(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$, each of them being a function of the electronic susceptibilities. In order to clarify the foregoing discussion, it is useful to summarize in table III the analytic behaviour of each of these quantities in both regimes, as it results from tables I and II and eq. (2.1, 2.2) and (2.7). It reads table III.

All quantities entering this table have been defined in (3.8, 3.12) and in table I, and furthermore

$$R(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq) = (1 - \delta_{\mathbf{G},\mathbf{o}})(1 - \delta_{\mathbf{G}',\mathbf{o}}) \times \times \left(\delta_{\mathbf{G},\mathbf{G}'} - \frac{4\pi}{|\mathbf{q}+\mathbf{G}|}\,\chi^r(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}')\,\frac{1}{|\mathbf{q}+\mathbf{G}'|}\right). \quad (4.1)$$

Let us simply recall that, due to the existence of a center of inversion in the crystal (see (3.2)) $A^\alpha(\mathbf{G})$ is odd in $\mathbf{G}$, while $D^{\alpha\beta}(\mathbf{G})$, $D'^{\alpha\beta}(\mathbf{G})$ and $m_p(\mathbf{G})$ are even in $\mathbf{G}$, and $R^{-1}(\mathbf{G}, \mathbf{G}')$ is even in $\mathbf{G}$, $\mathbf{G}'$ and a real quantity.

TABLE III

	$\frac{q}{q_c} \ll 1$ (non-adiab.)	$\frac{q}{q_c} \gg 1$ (adiab.)
$\frac{1}{L(\mathbf{q}, \mathbf{q}, vq)}$	$\frac{1}{1+i\sqrt{\frac{v}{2\mu^*}}q^{\frac{1}{2}}} + O(q^2)$	$\frac{1}{3C_0}q + O(q^2)$
$S(\mathbf{q}, \mathbf{q}+\mathbf{G}, vq)$	$\frac{1}{\lvert\mathbf{q}+\mathbf{G}\rvert}\left\{\sum_\alpha A^\alpha(\mathbf{G})\hat{q}_\alpha + q\frac{1}{2}(1+i)\sqrt{\frac{2\mu^*}{v}}\sum_{\alpha\beta} D^{\alpha\beta}(\mathbf{G})\hat{q}_\alpha\hat{q}_\beta\right\}$	$\frac{1}{\lvert\mathbf{q}+\mathbf{G}\rvert}\left\{\sum_\alpha A^\alpha(\mathbf{G})\hat{q}_\alpha + D_0\sum_{\alpha\beta} D'^{\alpha\beta}(\mathbf{G})\hat{q}_\alpha\hat{q}_\beta\right\}$
$({}^rS)^{-1}(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}', vq)$	$R^{-1}(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}') - \sum_{pp'}\left[\sum_{G_1}' R^{-1}(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}_1)\frac{1}{\lvert\mathbf{q}+\mathbf{G}_1\rvert}m_p(\mathbf{G}_1)\right] \times \left[\frac{1}{T_{pp'}(1+i\lambda q^{\frac{1}{2}})} + \sum_{G_3G_4}' \frac{m_p(\mathbf{G}_3)}{\lvert\mathbf{q}+\mathbf{G}_3\rvert}R^{-1}(\mathbf{q}+\mathbf{G}_3, \mathbf{q}+\mathbf{G}_4)\frac{m'_p(\mathbf{G}_4)}{\lvert\mathbf{q}+\mathbf{G}_4\rvert}\right]^{-1} \times \left[\sum_{G_2} m_{p'}(\mathbf{G}_2)\frac{1}{\lvert\mathbf{q}+\mathbf{G}_2\rvert}R^{-1}(\mathbf{q}+\mathbf{G}_2, \mathbf{q}+\mathbf{G})\right]$ $\lambda \neq 0$	$\lambda = 0$

Analytic behaviour of the functions entering into the force constants in the vicinity of $\mathbf{q} = 0$.

One may also notice that :

— the behaviour of $1/L(\mathbf{q}, \mathbf{q}, vq)$ is in fact governed by that of $\chi^t(\mathbf{q}, \mathbf{q}, vq)$; this explains why its analytical form is quite simple ;

— conversely, $\chi^r(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}', vq)$ and $\chi^t(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}', vq)$ have the same analytical behaviour ; the cumbersome form of $({}^rS)^{-1}$ $(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}', vq)$ comes only from the special form of the second term ;

— finally, the real part of this quantity has the same expression in both regimes, while its imaginary part only exists in the non-adiabatic one.

4.3 THE NON-ELECTRIC ELEMENTS OF THE DYNAMICAL MATRIX. — Let us study here the non-electric contribution to the elements of the dynamical matrix (2.8). We shall first show that their hermitian part does fulfil the usual relations (2.9, 2.10) which are a pre-requisite for the existence of acoustical waves. We shall prove afterwards that their non-hermitian part is such that its ratio to the corresponding hermitian part is always of order $q^{\frac{1}{2}}$. The important point which has to be noticed is that the proofs which will be given only involve symmetry considerations on the one hand, and the translational properties of the total crystal on the other hand.

4.3.1 *The hermitian part.* — Following (2.4) and table III, one has

$$C^{\alpha\beta}_{1ss'}(\mathbf{q}) = \sum_{\mathbf{G},\mathbf{G}'}' Z_s[\cos(\mathbf{G}.\mathbf{R}_s) + i\sin(\mathbf{G}.\mathbf{R}_s)]\,(\widehat{\mathbf{q}+\mathbf{G}})_\alpha \times$$
$$\times\,({}^rS)^{-1}(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}', 0)\,(\widehat{\mathbf{q}+\mathbf{G}'})_\beta$$
$$\times\,[\cos(\mathbf{G}'.\mathbf{R}_{s'}) - i\sin(\mathbf{G}'.\mathbf{R}_{s'})]\,Z_{s'} - K^{\alpha\beta}_s\,\delta_{ss'}\,; \quad (4.2)$$

in which the adiabatic approximation has been made, in accordance with the remarks made in the preceeding paragraph.

Clearly $C^{\alpha\beta}_{1ss'}(0)$ is a real constant, the imaginary terms giving a zero contribution due to parity considerations.

Let us prove that (2.9) is verified i.e.

$$\left(\lim_{\mathbf{q}\to 0}\ \sum_s C^{\alpha\beta}_{1ss'}(\mathbf{q}) = O(q)\right) \quad (4.3)$$

In order to do it, we shall momentally admit (see paragraph 4.4) that the electric term $G^{\alpha\beta}_{ss'}(\mathbf{q})$ is equal to zero for $\mathbf{q} \to 0$. The translational invariance of the crystal then implies the usual adiabatic result that the left hand side of (4.3) must be zero for $\mathbf{q} = 0$. Furthermore, the inversion symmetry property of the crystal implies that, in the same limit, the first derivative of $\widehat{\mathbf{q}+\mathbf{G}}$ or $({}^rS)^{-1}$ $(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}')$ has a parity opposite to that of the related function : as a consequence,

— the left hand side of (4.3) is of order q, each non zero by symmetry term being proportional to q ;

— in fact, this symmetry consideration shows that the $\cos(\mathbf{G}.\mathbf{R}_s)\sin(\mathbf{G}.\mathbf{R}_{s'})$ term is the only one which can contribute.

The summation over s' then immediately yields

$$\sum_{ss'} C^{\alpha\beta}_{1ss'}(\mathbf{q}) = O(q^2) \quad (4.4)$$

the term of order q giving a zero contribution in the summation over s'.

4.3.2 *The non-hermitian part.* — Table III shows that, in the non-adiabatic regime, the non-electric terms contain a non-hermitian contribution which comes from a term which is readily seen to be

$$\mathrm{Im}\,\{ ({}^{r}S)^{-1} (\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq) \} = - \lambda q \tfrac{1}{2} \times \times \sum_{p,p'=1}^{6} f_p(\mathbf{q}, \mathbf{G}) \frac{1}{T_{pp'}} f_{p'}(\mathbf{q}, \mathbf{G}') \quad (4.5)$$

where $T_{pp'}$ is defined in (3.12) and

$$f_p(\mathbf{q}, \mathbf{G}) = \sum_{p_1} \left[\sum_{\mathbf{G}_1} R^{-1}(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}_1) \times \times \frac{1}{|\mathbf{q} + \mathbf{G}_1|} mp_1(\mathbf{G}_1) \right] \left[\frac{1}{T_{p_1 p}} + \sum_{\mathbf{G}_3, \mathbf{G}_4} \frac{mp_1(\mathbf{G}_3)}{\| \mathbf{q} + \mathbf{G}_3 \|} R^{-1}(\mathbf{q} + \mathbf{G}_3, \mathbf{q} + \mathbf{G}_4) \frac{m_p(\mathbf{G}_4)}{\| \mathbf{q} + \mathbf{G}_4 \|} \right]^{-1} . \quad (4.6)$$

$f_p(\mathbf{O}, \mathbf{G})$ being even in $\mathbf{G}$, one can use the same reasoning as above to study this non-hermitian part. It is easily seen that :

— the only contribution to Im $C^{\alpha\beta}_{1ss'}(0)$ comes from a sin $(\mathbf{G}.\mathbf{R}_s) \times$ sin $(\mathbf{G}.\mathbf{R}_{s'})$ term, the summation over $\mathbf{G}$ and $\mathbf{G}'$ being decoupled (see (2.4) and (4.5)); this contribution is proportional to $q\,\tfrac{1}{2}$;

— furthermore, this contribution is odd in $\mathbf{R}_s$. The lowest order corresponding term in $\sum_s C^{\alpha\beta}_{1ss'}(\mathbf{q})$ is thus proportional to $q\,\tfrac{3}{2}$, and comes from a cos $(\mathbf{G}.\mathbf{R}_s)$ sin $(\mathbf{G}.\mathbf{R}_{s'})$ factor;

— the latter is still odd in $\mathbf{R}_{s'}$ so that the non-hermitian part of $\sum_{ss'} C^{\alpha\beta}_{1ss'}(\mathbf{q})$ is proportional to $q\,\tfrac{5}{2}$.

4.3.3 *Summary and remarks.* — This paragraph may be summarized by the following table (Table IV).

TABLE IV

$$\lim_{\mathbf{q}\to 0} C^{\alpha\beta}_{122}(\mathbf{q}, vq) = C^{\alpha\beta}_{22} + iq\,\tfrac{1}{2}\, C'^{\alpha\beta}_{22}$$

$$\lim_{\mathbf{q}\to 0} \sum_s C^{\alpha\beta}_{1s2}(\mathbf{q}, vq) = iq \sum_\gamma [J^{\alpha\gamma,\beta}_2 + iq\,\tfrac{1}{2}\, J'^{\alpha\gamma,\beta}_2]\, \hat{q}_\gamma$$

$$\lim_{\mathbf{q}\to 0} \sum_{s'} C^{\alpha\beta}_{12s'}(\mathbf{q}, vq) = - iq \sum_\gamma [J^{\alpha,\beta\gamma}_2 + iq\,\tfrac{1}{2}\, J'^{\alpha,\beta\gamma}_2]\, \hat{q}_\gamma$$

$$\lim_{\mathbf{q}\to 0} \sum_{ss'} C^{\alpha\beta}_{1ss'}(\mathbf{q}, vq) = q^2 \sum_{\gamma,\delta} [V^{\alpha\gamma,\beta\delta} + iq\,\tfrac{1}{2}\, V'^{\alpha\gamma,\beta\delta}]\, \hat{q}_\gamma\, \hat{q}_\delta$$

Analytic behaviour of the non-electric elements of the acoustical phonon matrix in the vicinity of $\mathbf{q} = 0$.

These results take into account the fact that α Sn has an inversion symmetry center, but it does not have the other symmetry properties of the group $\mathrm{O_h}$. When those are used, one obtains the same results as in e.g. Silicon, i.e.

$$C^{\alpha\beta}_{122} = \delta_{\alpha\beta}\, C \quad (4.7a)$$

$$J^{\alpha\gamma,\beta}_2 = (1 - \delta_{\alpha\beta})\,(1 - \delta_{\alpha\gamma})\,(1 - \delta_{\beta\gamma})\, J \quad (4.7b)$$

$$V^{\alpha\gamma,\beta\delta} = \delta_{\alpha\gamma}\, \delta_{\beta\delta}[V_{11}\, \delta_{\alpha\beta} + (1 - \delta_{\alpha\beta})\, V_{12}] + + \delta_{\alpha\beta}\, \delta_{\gamma\delta}(1 - \delta_{\alpha\beta})\, V_{44} \quad (4.7c)$$

and the same relations for the primed quantity.

4.4 THE ELECTRIC ELEMENTS OF THE DYNAMICAL MATRIX. — In this last paragraph, we shall very briefly show that the electric terms of the dynamical matrix (2.8) never contribute to it because they are of higher order in q that the non-electric ones.

4.4.1 *The hermitian part.* — It results from the preceeding paragraph that the electric term will not contribute to the dynamical matrix provided that

$$\lim_{\mathbf{q}\to 0} Z^{x_\alpha}_s(\mathbf{q}, vq) \frac{1}{L(\mathbf{q}, \mathbf{q}, vq)} Z^\beta_{s'}(\mathbf{q}, vq) = O(q^m) \quad (4.8a)$$

$$\lim_{\mathbf{q}\to 0} \left(\sum_s Z^{x_\alpha}_s(\mathbf{q}, vq) \right) \frac{1}{L(\mathbf{q}, \mathbf{q}, vq)} Z^\beta_{s'}(\mathbf{q}, vq) = O(q^{m+1}) \quad (4.8b)$$

$$\lim_{\mathbf{q}\to 0} \left(\sum_s Z^{x_\alpha}_s(\mathbf{q}, vq) \right) \frac{1}{L(\mathbf{q}, \mathbf{q}, vq)} \left(\sum_{s'} Z^\beta_{s'}(\mathbf{q}, vq) \right) = = O(q^{m+2}) \quad (4.8c)$$

with $m > 0$, $Z^\beta_{s'}(\mathbf{q}, vq)$ being defined by (2.6).

The study of those quantities was partly undertaken in [5]. We need to repeat it for three specific reasons :

— only (4.8*a*) was considered in Sherrington's paper ;

— the aim of that paper was to prove the existence of sound waves in both regimes. One could then satisfied oneself with $m = 0$, which is a weaker constraint than the one we need here ;

— the proof given was only partly correct, and needs to be re-examined.

Those various points are shortly discussed in the appendix (and with more details in [7]) where it is indeed shown that these relations are always verified with m at least equal to $\tfrac{1}{2}$ in the non-adiabatic regime, and to 1 in the adiabatic one.

4.4.2 *The non-hermitian part and conclusion.* — The discussion of this part is lengthy but otherwise straight-forward as it involves only parity considerations. One then finds [7] that the three relations (4.8) are satisfied with $m > \tfrac{1}{2}$. As, for the non-electric part, they are satisfied with $m = \tfrac{1}{2}$, the electric term does not play any role in the sound propagation or absorption.

5. **Summary and discussion.** — 5.1 SUMMARY. — It was shown in the last section that, in the vicinity of $\mathbf{q} = 0$, only non-electric terms (i.e. those uniquely involving electronic susceptibilities of the form

$\chi(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$ with both $\mathbf{G}$ and $\mathbf{G}'$ different from zero) play a role in the dynamical matrix of the acoustical phonons for a second type gapless semiconductor.

Using the notations of table IV, this matrix reads

$$Q = \left\| \begin{matrix} q^2[V^{\alpha\gamma,\beta\delta} + iq\,\tfrac{1}{2}\, V'^{\alpha\gamma,\beta\delta}]\,\hat{q}_\gamma\,\hat{q}_\delta - 2\,M\omega^2 & iq[J^{\alpha\gamma,\beta} + iq\,\tfrac{1}{2}\,J'^{\alpha\gamma,\beta}]\,\hat{q}_\gamma \\ -\,iq[J^{\alpha,\beta\delta} + iq\,\tfrac{1}{2}\,J'^{\alpha,\beta,\delta}]\,\hat{q}_\delta & C^{\alpha\beta} + iq\,\tfrac{1}{2}\,C'^{\alpha\beta} \end{matrix} \right\| \tag{5.1}$$

where the symmetry of those coefficients have been defined in (4.7) and where the non-hermitian terms exist only in the non-adiabatic regime, while the hermitian ones are identical in both regimes.

The folding of the matrix (5.1) into a 3 × 3 acoustical phonon matrix yields for the lowest order.

$$\| \hat{q}_\gamma[C^{\alpha\gamma,\beta\delta} + iq\,\tfrac{1}{2}\,C'^{\alpha\gamma,\beta\delta}]\,\hat{q}_\delta - 2\,Mv^2\,\delta_{\alpha\beta} \| = 0 \tag{5.2}$$

an expression in which v^2 is no longer self-consistently determined and where

$$C = V - JC^{-1}\,J^+ \tag{5.3a}$$

$$C' = V' - [J'\,C^{-1}\,J^+ + JC^{-1}\,J'^+ - JC^{-1}\,C'\,C^{-1}\,J^+] \tag{5.3b}$$

(here, we have used a matrix notation to have a more compact formula, as well as the form J, J^+ (or J', J'^+) to recall that those matrix are not symmetric).

(5.2) clearly shows that the sound velocity in α Sn has the same behaviour as in the other elements of the same series, and that the $iq\,\frac{1}{2}$ term leads to a $\omega\,\frac{1}{2}$ line width (or equivalently to a $q\,\frac{3}{2}$ attenuation). Furthermore, the analysis of C' (formula (5.3b)) with the rules (4.7) shows that there exist three independent absorption coefficients C'_{11}, C'_{12} and C'_{44}, only the latter being coupled to the internal relaxation of the atoms inside the primitive cell. Within the R.P.A. method, this attenuation is the only possible signature of a second type gapless semiconductor.

5.2 Discussion. — The search for such a sound absorption in α Sn is nevertheless meaningless for two types of reasons.

Firstly, our results are very sensitive to small deviations from the ideal case (0 K and absence of impurities). One easily finds that a temperature of 10^{-2} K or an impurity concentration of $10^{12}/\mathrm{cm}^3$ is sufficient to bring the Fermi level above $q_c^2/2\,\mu^*$ and thus transforming the second type gapless semiconductor into a more normal semimetal.

Secondly, the whole discussion has been based on the R.P.A. expressions of the susceptibility. On the other hand, Abrikosov [12] has recently shown that for $\omega \lesssim 10^{10}$ and $q \lesssim 10^4\ \mathrm{cm}^{-1}$, (which turn out to be of the same order of magnitude as $\omega = vq_c$ and q_c), this method was invalid, at least for the calculation of

$$\frac{1}{L(\mathbf{q}, \mathbf{q}, vq)}.$$

He finds that, when the many-body interaction is fully taken into account, this quantity behaves as $q^{3\left(1 - \frac{1}{\nu}\right)}$ with $\nu = 1.92$ instead of the R.P.A. value of 2. No results are yet available for the non-diagonal part of the susceptibility or for the diagonal one for $\mathbf{G}$ different from zero. Nevertheless, we believe that Abrikosov's results do not invalidate our conclusions concerning the single value of the sound velocity. They were indeed based largely on the fact that $3\left(1 - \frac{1}{\nu}\right)$ was positive, on symmetry properties, and on the analytic behaviour of $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$ for both $\mathbf{G}$ and $\mathbf{G}'$ different from zero. The two first properties are unchanged by the many body interaction. Furthermore, correlation effects will affect the value of $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega)$ but such changes should be identical in both the adiabatic and the non-adiabatic regimes. Thus, they should not result in a difference in the sound velocity between them. Nevertheless, correlations might affect the analytical behaviour of $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', 0)$. If that were the case, a new analysis of the sound-velocity problem would be necessary.

Similar conclusions are reached for the sound absorption discussed in the non-adiabatic regime. Abrikosov [13] and Gelmont [14] have indeed very recently argued that the electronic spectrum itself was profoundly modified, in the non-adiabatic region, with respect to the R.P.A. results. This suggests that the analytic behaviour of the imaginary part will be different from what we have found, even for $\chi^t(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', vq)$, so that the q dependence proposed for the non-adiabatic regime is unlikely to be correct.

APPENDIX

In this appendix, we shall briefly show that the three relations (4.8) are satisfied with $m = \frac{1}{2}$ in the non-adiabatic regime and $m = 1$ in the adiabatic one.

Indeed, table III shows that, while $Z_s^\beta(\mathbf{q}, vq)$ is at least of zero order in q, $1/L(\mathbf{q}, \mathbf{q}, \nu q)$ is proportional to $q^{\frac{1}{2}}$ for $q/q_c \ll 1$ and to q for $q/q_c \gg 1$. (4.8a) is then automatically satisfied, and the other two will be also, provided that

$$\lim_{\mathbf{q}\to 0} \sum_{s'} Z^{\beta}_{s'}(\mathbf{q}, \nu q) = O(q) . \qquad (A.1)$$

In order to prove (A.1) a combination of parity arguments with the charge neutrality sum rule (2, 4) is needed. Indeed, let us split the effective charge $Z^{\beta}_{s'}(\mathbf{q}, \nu q)$ into

$$Z^{\beta}_{s'}(\mathbf{q}, \nu q) = Z^{\beta(r)}_{s'(\mathbf{q})} + Z^{\beta(t)}_{s'(\mathbf{q})} \qquad (A.2)$$

with

$$Z^{\beta(I)}_{s'}(\mathbf{q}) = Z_{s'} \Bigg[q_{\beta}(1 - \delta_{I,c}) + \sum_{\mathbf{G},\mathbf{G}'} e^{i\mathbf{G}.\mathbf{R}_{s'}} \widehat{(\mathbf{q} + \mathbf{G})}_{\beta} \, ({}^{r}S)^{-1} \, (\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \nu q) \frac{4\pi}{|\mathbf{q} + \mathbf{G}'|} \times$$
$$\times \chi^{I}(\mathbf{q} + \mathbf{G}', \mathbf{q}, \nu q) \frac{1}{|\mathbf{q}|} \Bigg] \qquad (A.3)$$

with $I \equiv r$ or t.

Parity considerations are sufficient for showing that $Z^{\beta(t)}_{s'}(\mathbf{q})$ fulfils (A.1). Indeed, the only factor which enters this coefficient is $\sin(\mathbf{G}.\mathbf{R}_s)$ (see (3.10)) which is odd in $\mathbf{R}_s$. Applications of the same rules as for the non-electric part are then sufficient to obtain the desired results.

The proof that $Z^{\beta(r)}_{s'}(\mathbf{q})$ also fulfils (A.1), involves some considerations on the charge neutrality sum rule. Indeed, it can be inferred from [2] and [11] that the charge neutrality of a crystal in which every energy band is either completely full or completely empty may be written, within the R.P.A., as

$$O = \sum_{s'} Z^{\beta\gamma}_{s'} \equiv \sum_{s'} Z_{s'} \Bigg[\delta_{\beta\gamma} - \sum_{\mathbf{G},\mathbf{G}'}{}' e^{i\mathbf{G}.\mathbf{R}_{s'}} \hat{G}_{\beta}({}^{r}S)^{-1} (\mathbf{G}, \mathbf{G}') \frac{4\pi_i}{|G|} \sum_{\mathbf{k},\nu,\nu'} C^{\gamma}(\mathbf{G}, \mathbf{k}, \nu, \nu') \Bigg] \qquad (A.4)$$

with

$$C^{\gamma}(\mathbf{G}, \mathbf{k}, \nu, \nu') = \frac{1}{\Omega} [n_{\nu}(\mathbf{k}) - n_{\nu'}(\mathbf{k})] \frac{\langle \mathbf{k}, \nu' | e^{i\mathbf{G}'.\mathbf{r}} | \nu, \mathbf{k} \rangle \langle \mathbf{k}, \nu | r\gamma | \mathbf{k}, \nu' \rangle}{E_{\nu'}(\mathbf{k}) - E_{\nu}(\mathbf{k})} \qquad (A.5)$$

where $n_{\nu}(\mathbf{k})$ is the occupation number of an electronic state with energy $E_{\nu}(\mathbf{k})$ and wave function $| \nu, \mathbf{k} \rangle$.

Clearly, when the wave functions $| \nu, \mathbf{k} \rangle$ and $| \nu', \mathbf{k} \rangle$ are analytical functions of $\mathbf{k}$ one has

$$C^{\gamma}(\mathbf{G}, \mathbf{k}, \nu, \nu') = i \lim_{q\to 0} \frac{\partial}{\partial q\gamma} [n_{\nu}(\mathbf{k}) - n_{\nu'}(\mathbf{k} + \mathbf{q})] \frac{\langle \mathbf{k} + \mathbf{q}, \nu' | e^{i(\mathbf{q}+\mathbf{G}).\mathbf{r}} | \nu, \mathbf{k} \rangle \langle \mathbf{k}, \nu | e^{-i\mathbf{q}.\mathbf{r}} | \nu', \mathbf{k} + \mathbf{q} \rangle}{E_{\nu'}(\mathbf{k} + \mathbf{q}) - E_{\nu}(\mathbf{k})} \qquad (A.6)$$

and (A.6) is thus valid for all the matrix elements of type A (and also of type B as shown in [7]). But $C^{\gamma}(\mathbf{G}, \mathbf{k}, \nu, \nu')$ is equal to zero for a matrix element of type C because, due to (3.5a), such a matrix element involves a sum of terms of the form $\langle \varepsilon^{\alpha}(\mathbf{r}) | r_{\gamma} | \varepsilon^{\beta}(\mathbf{r}) \rangle$ which are equal to zero, $\varepsilon^{\alpha}(\mathbf{r})$ and $\varepsilon^{\beta}(\mathbf{r})$ having the same parity.

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