

## Theory of the Damping of Alfvén Waves in Bismuth Metal\*†

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The theory of the relaxation frequency tensor for an ellipsoidal conduction band is developed, and calculated for the case of the electron and hole bands in bismuth assuming ionized impurity scattering. The theory of Alfvén-wave propagation is developed, and the ratios of relaxation times for several different field orientations are calculated. The results are compared with McLachlan's data. Possible mechanisms for the damping, including Frenkel defects, are discussed.

### I. INTRODUCTION

IN a previous paper<sup>1</sup> (hereafter called I) the theory of the screening charge and potential of an ionized impurity in bismuth has been developed. The purpose of the present work is to apply the impurity potential derived in I to the damping of Alfvén waves in bismuth, using the Boltzmann equation with the scattering included via the Born approximation.

Alfvén waves are magnetohydrodynamic waves in a plasma consisting of equal numbers of positive and negative carriers. Their existence in interstellar space was first proposed by Alfvén<sup>2</sup>; however, Buchsbaum and Galt<sup>3</sup> were first to interpret certain experimental data in bismuth in terms of Alfvén waves. The waves themselves were first produced in transmission through a bismuth slab by Williams,<sup>4</sup> and since then a number of workers have reported Alfvén wave experiments in bismuth<sup>5</sup> and antimony.<sup>6</sup> In the case of bismuth, there is a great deal of inconsistency in the results of different workers. Disagreements of, say, 50% in the measured values of Alfvén-wave velocity for a given static  $\mathbf{H}$  field, microwave  $\mathbf{E}$  field, and wave propagation vector are not uncommon. There is no discernible pattern in the experimental discrepancies; however, differences in experimental geometry are almost certainly responsible.<sup>7</sup>

We shall compare our results with the experimental data of McLachlan,<sup>8</sup> who measured Alfvén-wave relaxation times in bismuth at low temperatures (4.2°K) and "intermediate" magnetic fields (i.e., fields small enough so that quantum oscillations in measured quantities are small, but sufficiently high so that Landau damping is absent).

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<sup>1</sup> D. H. Brownell, Jr., and E. H. Hygh, *Phys. Rev.* **164**, 909 (1967).

<sup>2</sup> H. Alfvén, *Nature* **150**, 405 (1942).

<sup>3</sup> S. J. Buchsbaum and J. K. Galt, *Phys. Fluids* **4**, 1514 (1961).

<sup>4</sup> G. A. Williams, *Bull. Am. Phys. Soc.* **7**, 409 (1962).

<sup>5</sup> For a bibliography of experiments, see Ref. 8.

<sup>6</sup> G. A. Williams, *Bull. Am. Phys. Soc.* **9**, 353 (1963).

<sup>7</sup> G. A. Williams (private communication).

<sup>8</sup> D. S. McLachlan, *Phys. Rev.* **147**, 368 (1966).

We begin in Sec. II by developing the theory of the magnetoconductivity tensor an ellipsoidal carrier band in the equation-of-motion formalism, postulating a relaxation frequency tensor. In Sec. III we use the Boltzmann equation and the results of I to obtain results equivalent to those of Sec. II for long relaxation times. The propagation of Alfvén waves is discussed in Sec. IV, and the theory compared with experiment in Sec. V.

### II. THEORY: EQUATION-OF-MOTION APPROACH

We consider an ellipsoidal band ( $i$ ) of carriers of charge  $q_i$ , density  $n_i$  per unit volume, and mass tensor  $\mathbf{m}$ ; in Sec. III we find that  $\mathbf{m}$  is the tensor which connects velocity and momentum at the Fermi surface:

$$\mathbf{p} = \mathbf{m}\mathbf{v}, \quad \epsilon_p = \epsilon_F. \quad (1)$$

In the case of a nonparabolic band,  $\mathbf{m}$  is in general not the tensor which connects force and acceleration. We assume the system is at  $T=0$ , so the formalism is simplified for a nonparabolic band.

In the presence of a static magnetic field  $\mathbf{H}$ , an electric field of the form  $\mathbf{E} \exp(-i\omega t)$ , and a relaxation mechanism described phenomenologically by a relaxation frequency tensor<sup>9</sup>  $\mathbf{v}$ , the equation of motion is, in cgs Gaussian units,

$$\mathbf{m}\dot{\mathbf{v}} = -i\omega\mathbf{m}\mathbf{v} = q_i[\mathbf{E} - (1/c)\mathbf{H} \times \mathbf{v}] - \mathbf{m}\mathbf{v}\mathbf{v}. \quad (2)$$

This may be solved for  $\mathbf{v}$ :

$$\mathbf{v} = q_i \mathbf{T}^{-1} \mathbf{E}, \quad (3)$$

where

$$\mathbf{T} = -i\omega\mathbf{m} + \mathbf{m}\mathbf{v}\mathbf{v} + (q_i/c)\mathbf{H} \times \mathbf{I}, \quad (4)$$

with

$$(\mathbf{H} \times \mathbf{I})_{ij} = \sum_k \epsilon_{ikj} H_k. \quad (5)$$

Using the relations

$$\mathbf{j} = n_i q_i \mathbf{v} = \boldsymbol{\sigma}^{(i)} \mathbf{E}, \quad (6)$$

we obtain

$$\boldsymbol{\sigma}^{(i)} = n_i q_i^2 \mathbf{T}^{-1}. \quad (7)$$

<sup>9</sup> C. Herring and E. Vogt, *Phys. Rev.* **101**, 944 (1956).

With  $\mathbf{v}=0$ , this is equivalent to the result quoted by Lax, Button, Zeiger, and Roth.<sup>10</sup>

### III. THEORY: BOLTZMANN EQUATION APPROACH

The method of Sec. II, while giving results equivalent to those of the present section for  $|\nu_{ij}| \ll \omega$ , of course gives no information about  $\mathbf{v}$  itself. We now proceed to a Boltzmann (kinetic) equation formalism and calculate  $\mathbf{v}$  from the properties of the relaxation mechanism. We assume that the system is at  $T=0$ , that only ionized impurities (charge  $Ze$ , density  $N$  per unit volume) contribute to the damping, and that the effect of the scattering may be regarded as a small perturbation.

We assume an ellipsoidal band of carriers in plane-wave states  $\exp(i\mathbf{p}\cdot\mathbf{x}/\hbar)$ , normalized to unit volume, for which

$$F(\epsilon) = \frac{1}{2}\mathbf{p}\cdot\boldsymbol{\alpha}_b\cdot\mathbf{p}, \quad (8)$$

where  $\epsilon$  is energy and  $\mathbf{p}$  momentum, both measured from the band minimum.  $\boldsymbol{\alpha}_b$  is the inverse-mass tensor "at the bottom of the band," and  $F(\epsilon) \approx \epsilon$  as  $\epsilon \rightarrow 0$ . In the case of a parabolic band,  $F(\epsilon) = \epsilon$ . Velocity and momentum are related at the Fermi energy by

$$\mathbf{v} = \boldsymbol{\alpha}\mathbf{p}, \quad (9)$$

where

$$\boldsymbol{\alpha} = \left( \frac{dF}{d\epsilon} \bigg|_{\epsilon=\epsilon_F} \right)^{-1} \boldsymbol{\alpha}_b \equiv \mathbf{m}^{-1}. \quad (10)$$

Thus at  $\epsilon = \epsilon_F$  we have

$$\begin{aligned} G &= \text{constant} \\ &= \frac{1}{2}\mathbf{p}\cdot\boldsymbol{\alpha}\cdot\mathbf{p} \\ &= \left( \frac{dF}{d\epsilon} \bigg|_{\epsilon=\epsilon_F} \right)^{-1} F(\epsilon_F). \end{aligned} \quad (11)$$

Throughout this paper,  $\mathbf{m}$  and  $\boldsymbol{\alpha}$  will be the mass tensor and its inverse at the Fermi surface.

The Boltzmann equation<sup>11</sup> for the distribution function  $f$  is, omitting diffusion,

$$\dot{f} = \dot{f}_{\text{fields}} + \dot{f}_{\text{scattering}}. \quad (12)$$

Suppose a static magnetic field  $\mathbf{H}$  is present, and an electromagnetic wave of the form

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}e^{i(\mathbf{K}\cdot\mathbf{x} - \omega t)} \quad (13)$$

is propagating through the solid. In a damped wave,  $\mathbf{K}$  will be complex. We assume the distribution function is of the form

$$f(\mathbf{x}, \mathbf{p}) = f_0(\epsilon_p) + f_1(\mathbf{p})e^{i(\mathbf{K}\cdot\mathbf{x} - \omega t)}, \quad (14)$$

where  $\mathbf{p}$  includes the spin index, and

$$\begin{aligned} f_0(\epsilon) &= 1, & \epsilon \leq \epsilon_F, \\ f_0(\epsilon) &= 0, & \epsilon > \epsilon_F. \end{aligned} \quad (15)$$

There will be present a scattering transition probability  $W_{\mathbf{p}\mathbf{p}'}$  per unit time, for the carriers to scatter from state  $\mathbf{p}$  to state  $\mathbf{p}'$ . Using the fact that

$$W_{\mathbf{p}\mathbf{p}'} = W_{\mathbf{p}'\mathbf{p}}, \quad (16)$$

and the fact that the scattering is elastic, Eq. (12) becomes

$$\begin{aligned} -i\omega f_1(\mathbf{p}) &= -q_i\mathbf{v}\cdot\mathbf{E}\frac{df_0}{d\epsilon} + \frac{q_i}{c}\mathbf{H}\cdot(\mathbf{v}\times\nabla_{\mathbf{p}})f_1(\mathbf{p}) \\ &+ \lambda \sum_{\mathbf{p}'} W_{\mathbf{p}\mathbf{p}'} [f_1(\mathbf{p}') - f_1(\mathbf{p})], \end{aligned} \quad (17)$$

where  $\lambda$  indicates the scattering is to be considered a small perturbation; ultimately we set  $\lambda=1$ . We seek a solution of the form

$$f_1(\mathbf{p}) = f_{11}(\mathbf{p}) + \lambda f_{12}(\mathbf{p}), \quad (18)$$

where  $f_{11}$  and  $f_{12}$  are linear in  $\mathbf{E}$ .

Equations (17) and (18) then give

$$-i\omega f_{11}(\mathbf{p}) = -q_i\mathbf{v}\cdot\mathbf{E}\frac{df_0}{d\epsilon} + \frac{q_i}{c}\mathbf{H}\cdot(\mathbf{v}\times\nabla_{\mathbf{p}})f_{11}(\mathbf{p}), \quad (19)$$

and

$$\begin{aligned} -i\omega f_{12}(\mathbf{p}) &= \frac{q_i}{c}\mathbf{H}\cdot(\mathbf{v}\times\nabla_{\mathbf{p}})f_{12}(\mathbf{p}) \\ &+ \sum_{\mathbf{p}'} W_{\mathbf{p}\mathbf{p}'} [f_{11}(\mathbf{p}') - f_{11}(\mathbf{p})]. \end{aligned} \quad (20)$$

It is easily shown that a solution to Eq. (19) is

$$f_{11}(\mathbf{p}) = -q_i\frac{df_0}{d\epsilon}\mathbf{v}\cdot(\mathbf{m}\mathbf{T}_0^{-1})\cdot\mathbf{E}, \quad (21)$$

where, referring to Eq. (4), we have set

$$\mathbf{T} \equiv \mathbf{T}_0 + \mathbf{m}\mathbf{v} \quad (22)$$

with

$$\mathbf{T}_0 = -i\omega\mathbf{m} + (q_i/c)\mathbf{H}\times\mathbf{I}. \quad (23)$$

Writing the current as

$$\begin{aligned} \mathbf{j} &= \mathbf{j}_1 + \lambda\mathbf{j}_2 \\ &= (\boldsymbol{\sigma}_1^{(i)} + \lambda\boldsymbol{\sigma}_2^{(i)})\mathbf{E}, \end{aligned} \quad (24)$$

we obtain for the first quantity on the right-hand side

$$\begin{aligned} \mathbf{j}_1 &= \sum_{\mathbf{p}} q_i f_{11}(\mathbf{p})\mathbf{v} \\ &= -\frac{q_i^2}{4\pi^3\hbar^3} \int \frac{df_0}{d\epsilon} \mathbf{v} [\mathbf{v}\cdot(\mathbf{m}\mathbf{T}_0^{-1})\cdot\mathbf{E}] d\epsilon \frac{dA}{v}. \end{aligned} \quad (25)$$

We have made use of Eq. (21) and the fact that

$$d\mathbf{p} = d\epsilon \frac{dA}{v} \quad (26)$$

<sup>10</sup> B. Lax, K. J. Button, H. J. Zeiger, and L. M. Roth, Phys. Rev. **102**, 715 (1956).

<sup>11</sup> J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, England, 1960), Sec. 7.3.

where  $dA$  is the area element on the surface  $\epsilon = \text{constant}$ . Since

$$df_0/d\epsilon = -\delta(\epsilon - \epsilon_F) \quad (27)$$

at  $T=0$ , we have

$$\mathbf{j}_i = \frac{q_i^2}{4\pi^3\hbar^3} \int_{\epsilon=\epsilon_F} \mathbf{v} [\mathbf{v} \cdot (\mathbf{m}\mathbf{T}_0^{-1}) \cdot \mathbf{E}] \frac{dA}{v}, \quad (28)$$

so that

$$\boldsymbol{\alpha}_1^{(i)} = \frac{q_i^2}{4\pi^3\hbar^3} \int (\mathbf{v}\mathbf{v}) (\mathbf{m}\mathbf{T}_0^{-1}) \frac{dA}{v}. \quad (29)$$

Now it is easily shown that

$$\int_{\epsilon=\epsilon_F} \frac{\mathbf{v}\mathbf{v}}{v} dA = V_{Fi} \boldsymbol{\alpha}, \quad (30)$$

where  $V_{Fi} = 4\pi^3\hbar^3 n_i$  is the volume in  $\mathbf{p}$  space enclosed by the Fermi surface. Thus

$$\boldsymbol{\alpha}_1^{(i)} = n_i q_i^2 \mathbf{T}_0^{-1}, \quad (31)$$

in agreement with Eq. (7) for  $\mathbf{v}=0$ .

We now treat Eq. (20). Assuming that  $f_{12}(\mathbf{p})$  is restricted to the Fermi surface, we make use of an expansion of  $f_{12}$  in Chambers coordinates.<sup>12</sup> If  $p_z$  is the polar axis (which need not be along the direction of  $\mathbf{H}$ ), the coordinates are  $\epsilon$ ,  $p_z$ , and  $\varphi$ , and the volume element is

$$d\mathbf{p} = m^* d\epsilon dp_z d\varphi, \quad (32)$$

where  $m^* = m^*(\epsilon)$  is the cyclotron mass about the polar axis. Hence,

$$\begin{aligned} dA/v &= m^* dp_z d\varphi \\ &= m^* p_{z \max} d\mu d\varphi, \end{aligned} \quad (33)$$

where  $p_{z \max}$  is the maximum value of  $p_z$  on the surface  $\epsilon = \text{constant}$ , and

$$p_z = p_{z \max} \mu, \quad -1 \leq \mu \leq 1. \quad (34)$$

The use of such coordinates may at first seem cumbersome; however, their worth can easily be established in our present study. For example, in Chambers coordinates on an ellipsoidal Fermi surface, we have the following spherical harmonic expansion:

$$v_i = \sum_{m=-1}^1 a_{im} Y_{1m}(\mu, \varphi). \quad (35)$$

The value of such a relation becomes clear when we expand  $f_{12}$  in spherical coordinate form on the Fermi surface:

$$f_{12}(\mathbf{p}) = q_i \frac{df_0}{d\epsilon} [\mathbf{v} \cdot (\mathbf{m}\boldsymbol{\beta}) \cdot \mathbf{E} + \sum_{\substack{l=0 \\ l \neq 1}}^{\infty} \sum_{m=-l}^l b_{lm} Y_{lm}(\mu, \varphi)]. \quad (36)$$

The tensor  $\boldsymbol{\beta}$  of course is to be determined. It can now easily be seen from the above considerations that we

<sup>12</sup> J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, England, 1960), Sec. 12.7.

immediately have

$$\boldsymbol{\alpha}_2^{(i)} = -n_i q_i^2 \boldsymbol{\beta}, \quad (37)$$

since the integration over the surface of  $\mathbf{v} Y_{lm}$  for  $l \neq 1$  gives zero contribution.

If we now let the polar axis  $p_z$  coincide with the direction of  $\mathbf{H}$ , we have

$$\frac{q_i}{c} \mathbf{H} \cdot (\mathbf{v} \times \nabla_{\mathbf{p}}) = \Omega \frac{\partial}{\partial \varphi}, \quad (38)$$

where  $\Omega$  is the cyclotron frequency:

$$\Omega = \frac{q_i H}{m^* c}. \quad (39)$$

Using the familiar property of spherical harmonics,

$$\frac{\partial}{\partial \varphi} Y_{lm} = i m Y_{lm}, \quad (40)$$

after inserting expressions (36) and (21) into Eq. (20), we obtain the result

$$\begin{aligned} i\omega q_i \frac{df_0(\epsilon)}{d\epsilon} \mathbf{v} \cdot (\mathbf{m}\boldsymbol{\beta}) \cdot \mathbf{E} &= -\frac{q_i^2}{c} \frac{df_0(\epsilon)}{d\epsilon} \mathbf{H} \cdot (\mathbf{v} \times \nabla_{\mathbf{p}}) [\mathbf{v} \cdot (\mathbf{m}\boldsymbol{\beta}) \cdot \mathbf{E}] \\ &+ q_i \sum_{\mathbf{p}'} W_{\mathbf{p}\mathbf{p}'} \frac{df_0(\epsilon')}{d\epsilon'} (\mathbf{v}' - \mathbf{v}) \cdot (\mathbf{m}\mathbf{T}_0^{-1}) \cdot \mathbf{E} \\ &+ \frac{df_0(\epsilon)}{d\epsilon} \sum_{\substack{l=0 \\ l \neq 1}}^{\infty} \sum_{m=-l}^l c_{lm} Y_{lm}(\mu, \varphi), \end{aligned} \quad (41)$$

where the  $c_{lm}$  are constants linear in  $\mathbf{E}$ .

We now use the results of first-order time-dependent perturbation theory for the transition probability<sup>13</sup>:

$$W_{\mathbf{p}\mathbf{p}'} = \frac{2\pi N}{\hbar} |V_{\mathbf{p}-\mathbf{p}'}|^2 \delta(\epsilon - \epsilon') \delta_{\sigma\sigma'}, \quad (42)$$

where  $V_{\mathbf{p}-\mathbf{p}'}$  is the matrix element of the potential of one impurity,  $\sigma$  and  $\sigma'$  are the spins of states  $\mathbf{p}$  and  $\mathbf{p}'$ , and  $N$  is the density of impurities. For an ionized impurity of charge  $Ze$  in bismuth,  $V_{\mathbf{p}-\mathbf{p}'}$  is given by Eq. (28) of I:

$$V_{\mathbf{p}-\mathbf{p}'} = V_{0\mathbf{p}-\mathbf{p}'} \left[ 1 - \frac{4\pi e^2 \hbar^2}{(\mathbf{p}-\mathbf{p}') \cdot \boldsymbol{\epsilon}_l \cdot (\mathbf{p}-\mathbf{p}')} \sum_i R_{i, \mathbf{p}-\mathbf{p}'} \right]^{-1}, \quad (43)$$

<sup>13</sup> J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, England, 1960), Sec. 3.1. The criteria for the applicability of this formula are the same as those for the Born approximation, to which it is equivalent. It is easily shown that the conditions are satisfied in the case of a screened charge in bismuth. See L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), Sec. 26.

with

$$V_{0\mathbf{p}-\mathbf{p}'} = \frac{4\pi Z e q_i \hbar^2}{(\mathbf{p}-\mathbf{p}') \cdot \boldsymbol{\varepsilon}_i \cdot (\mathbf{p}-\mathbf{p}')}. \quad (44)$$

Here  $\boldsymbol{\varepsilon}_i$  is the lattice dielectric tensor of the solid, and  $R_{i,\mathbf{p}-\mathbf{p}'}$  is defined by Eq. (29) of I. Substituting expression (42) into Eq. (41), and integrating with respect to  $\mathbf{v}(dA/v)d\epsilon$ , the terms in  $Y_{lm}$ , for  $l \neq 1$ , give zero contribution, and we obtain

$$\boldsymbol{\beta} = \mathbf{T}_0^{-1} \mathbf{s} \mathbf{T}_0^{-1}, \quad (45)$$

where

$$s_{ij} = s_{ji} = \frac{N}{16\pi^5 \hbar^3 n_i} \iint |V_{\mathbf{p}-\mathbf{p}'}|^2 p_i (p_j - p_j') \frac{dA'}{v'} \frac{dA}{v}. \quad (46)$$

The connection of  $\mathbf{s}$ , which is independent of  $\mathbf{H}$  and  $\omega$ , with  $\mathbf{v}$  of Sec. II is immediate. Referring to Eq. (22),

$$\begin{aligned} \boldsymbol{\sigma}^{(i)} &= n_i q_i^2 (\mathbf{T}_0 + \mathbf{m}\mathbf{v})^{-1} \\ &\approx n_i q_i^2 (\mathbf{T}_0^{-1} - \mathbf{T}_0^{-1} \mathbf{m}\mathbf{v} \mathbf{T}_0^{-1}) \end{aligned} \quad (47)$$

for sufficiently small  $\nu_{ij}$ . Comparing this with the result of the present section,

$$\boldsymbol{\sigma}^{(i)} \approx \boldsymbol{\sigma}_1^{(i)} + \boldsymbol{\sigma}_2^{(i)} = n_i q_i^2 (\mathbf{T}_0^{-1} - \mathbf{T}_0^{-1} \mathbf{s} \mathbf{T}_0^{-1}), \quad (48)$$

we see that

$$\mathbf{s} = \mathbf{m}\mathbf{v}. \quad (49)$$

Thus we have established the validity of a relaxation frequency tensor (dependent only on the band parameters and the properties of the scattering) for Alfvén-wave propagation with sufficiently small damping.

Finally, in a solid such as bismuth, with several ellipsoidal carrier bands, the total magnetoconductivity tensor is given by

$$\boldsymbol{\sigma} = \sum_i \boldsymbol{\sigma}^{(i)}, \quad (50)$$

where  $i$  ranges over all the carrier bands.

#### IV. ALFVÉN-WAVE PROPAGATION

We now consider Alfvén-wave propagation in the "intermediate" field region, i.e., we have  $|\mathbf{K} \cdot \mathbf{v}| \ll \omega \ll \Omega$ , but  $H$  (and hence  $\Omega$ ) are sufficiently small that quantum oscillations in the density of states near the Fermi surface are negligible. In practice these oscillations are always present; however, in the region under consideration, they are easily averaged over in the data to obtain such quantities as Alfvén-wave velocities and relaxation times.<sup>8</sup>

Maxwell's equations, neglecting displacement currents, lead to the equation

$$\mathbf{j} = (ic^2/4\pi\omega) \mathbf{K} \times (\mathbf{K} \times \mathbf{E}) = \boldsymbol{\sigma} \mathbf{E}, \quad (51)$$

so that the dispersion relation of the wave is the determinantal equation

$$|\sigma_{ik} + (ic^2/4\pi\omega)(K^2 \delta_{ik} - K_i K_k)| = 0. \quad (52)$$

The presence of anisotropic relaxation greatly complicates the form of  $\boldsymbol{\sigma}$ , so the solution of Eq. (52) is rather cumbersome. Following Kaner and Skobov,<sup>14</sup> we go to a two-dimensional formalism with the following choice of axes:

Let  $z$  be the direction of  $\mathbf{K}$ ; this is consistent with the discussion of the previous section since we will be comparing our results with data for the situation  $\mathbf{K} \parallel \mathbf{H}$ . Then we can eliminate  $E_z$  from the equations since, from Eq. (51),

$$\mathbf{K} \cdot \mathbf{j} = 0. \quad (53)$$

The result is then the secular equation of a  $2 \times 2$  matrix:

$$\left| \sigma_{\alpha\beta}' - \frac{c^2 K^2}{4\pi i \omega} \delta_{\alpha\beta} \right| = 0, \quad (54)$$

where  $\alpha, \beta = x, y$ , and

$$\sigma_{\alpha\beta}' = \sigma_{\alpha\beta} - \sigma_{\alpha z} \sigma_{z\beta} / \sigma_{zz}. \quad (55)$$

When  $\mathbf{H}$  is along the trigonal axis,  $\boldsymbol{\sigma}$  is diagonal, and when  $\mathbf{H}$  and  $\mathbf{K}$  are along a binary axis, we have  $|\sigma_{\alpha z} \sigma_{z\beta}| \ll |\sigma_{\alpha\beta} \sigma_{zz}|$ . Thus in both these cases, we have  $\sigma_{\alpha\beta}' \approx \sigma_{\alpha\beta}$ . There is no such simplification of  $\boldsymbol{\sigma}'$  when  $\mathbf{H}$  and  $\mathbf{K}$  are along a bisectrix axis.

The anticipated result for the observed Alfvén-wave velocity  $v_A$  is, in the limit of small  $\nu_{ij}$ ,

$$v_A = \omega/K_1 = H[4\pi n f(m)(1+1/4\omega^2\tau^2)]^{-1/2}, \quad (56)$$

where  $f(m)$  is a function of the carrier masses,  $n$  is the electron (and hole) density, and we have set

$$K = K_1 + iK_2. \quad (57)$$

Here  $n f(m)$  is the so-called "mass density," and  $\tau$  plays the role of a relaxation time.

In the absence of damping, and with  $\Omega \gg \omega$ , an ellipsoidal carrier band ( $i$ ) with  $\mathbf{H}$  along the  $z$  direction has the following conductivity tensor<sup>10</sup>:

$$\boldsymbol{\sigma}_1^{(i)} = -\frac{i\omega n_i c^2}{H^2} \begin{bmatrix} \mu_{xx} & \mu_{xy} + b_i & -\eta_{xz} b_i \\ \mu_{xy} - b_i & \mu_{yy} & \eta_{yz} b_i \\ \eta_{xz} b_i & -\eta_{yz} b_i & b_i^2/m_{zz} \end{bmatrix}, \quad (58)$$

where we have kept only terms of highest order (except in  $\sigma_{xy}$  and  $\sigma_{yx}$ , where the terms in  $b_i$  cancel out in the total conductivity tensor). Here,

$$\begin{aligned} \mu_{xx} &= m_{yy} - m_{yz}^2/m_{zz}, \\ \mu_{xy} &= m_{xz} m_{yz}/m_{zz} - m_{xy}, \\ \mu_{yy} &= m_{xx} - m_{xz}^2/m_{zz}, \\ \eta_{xz} &= m_{yz}/m_{zz}, \\ \eta_{yz} &= m_{xz}/m_{zz}, \\ b_i &= iq_i H/\omega c. \end{aligned} \quad (59)$$

<sup>14</sup> E. A. Kaner and V. G. Skobov, Zh. Eksperim. i Teor. Fiz. 45, 610 (1963) [English transl.: Soviet Phys.—JETP 18, 419 (1964)].

The condition  $\Omega \gg \omega$  implies that

$$|b_i| \gg |\mu_{ij}|. \quad (60)$$

Now using Eqs. (58), (59), and (48), we obtain for the single carrier ellipsoid

$$\sigma_2^{(i)} = \frac{n_i c^2}{H^2} \begin{pmatrix} \xi_{xx} & \xi_{xy} & -\zeta_{xz} b_i \\ \xi_{xy} & \xi_{yy} & \zeta_{yz} b_i \\ \zeta_{xz} b_i & -\zeta_{yz} b_i & \lambda_{zz} b_i^2 \end{pmatrix}, \quad (61)$$

where again we have kept only terms of highest order, and

$$\begin{aligned} \xi_{xx} &= s_{yy} - 2s_{yz}\eta_{xz} + s_{zz}\eta_{xz}^2, \\ \xi_{xy} &= -s_{xy} + s_{yz}\eta_{yz} + s_{xz}\eta_{xz} - s_{zz}\eta_{xz}\eta_{yz}, \\ \xi_{yy} &= s_{xx} - 2s_{xz}\eta_{yz} + s_{zz}\eta_{yz}^2, \\ \zeta_{xz} &= (s_{yz} - s_{zz}\eta_{xz})/m_{zz}, \\ \zeta_{yz} &= (s_{xz} - s_{zz}\eta_{yz})/m_{zz}, \\ \lambda_{zz} &= -s_{zz}/m_{zz}^2. \end{aligned} \quad (62)$$

Now when the  $\sigma^{(i)}$  are summed over all carrier bands, and transformed according to Eq. (55), the result is

$$\sigma' = \sigma_1' + \sigma_2', \quad (63)$$

where  $\sigma_1'$  and  $\sigma_2'$  are of the form

$$\sigma_1' = -\frac{i\omega n c^2}{H^2} \begin{pmatrix} \mu_{xx}' & \mu_{xy}' \\ \mu_{xy}' & \mu_{yy}' \end{pmatrix}, \quad (64)$$

and

$$\sigma_2' = \frac{n c^2}{H^2} \begin{pmatrix} \xi_{xx}' & \xi_{xy}' \\ \xi_{xy}' & \xi_{yy}' \end{pmatrix}, \quad (65)$$

[ $n$  is now the total electron (or hole) density]. The dispersion relation, Eq. (54), then yields

$$\begin{aligned} K^2 &= K_1^2 - K_2^2 + 2iK_1K_2 \\ &= \frac{4\pi\omega^2 n}{H^2} f(m) + \frac{4\pi i\omega n}{H^2} g(s, m), \end{aligned} \quad (66)$$

where  $f(m)$  is a function of the  $m_{ij}$ , and  $g(s, m)$  is a function of the  $s_{ij}$  and  $m_{ij}$ .

When  $|K_1| \gg |K_2|$ , we obtain

$$K_1 = [(4\pi\omega^2 n/H^2)f(m)]^{1/2} [1 + g^2(s, m)/8\omega^2 f^2(m)], \quad (67)$$

so that, from Eq. (56),

$$v_A = H \{4\pi n f(m) [1 + g^2(s, m)/4\omega^2 f^2(m)]\}^{-1/2}. \quad (68)$$

Thus, the effective relaxation time  $\tau$  is

$$\tau = f(m)/g(s, m). \quad (69)$$

The application of perturbation theory to the Boltzmann equation, of course, depends on the condition

$$\omega\tau \gg 1. \quad (70)$$

When  $\sigma_1'$  is diagonal, we have for the normal modes

either

$$f(m) = \mu_{xx}', g(s, m) = \xi_{xx}', \mathbf{E} \| x, \quad (71)$$

or

$$f(m) = \mu_{yy}', g(s, m) = \xi_{yy}', \mathbf{E} \| y. \quad (72)$$

Actually,  $\mathbf{E}$  has a small component in the  $z$  direction unless  $\sigma_{\alpha\beta}' = \sigma_{\alpha\beta}$ . When  $\sigma_1'$  is not diagonal,  $\mathbf{E}$  will have nonzero  $x$  and  $y$  components in a normal mode; in this case the secular equation (54) must be worked out and compared with Eq. (66) to obtain  $f(m)$  and  $g(s, m)$ . Expressions for the  $\mu_{\alpha\beta}'$  and  $\xi_{\alpha\beta}'$  for each of the experimental arrangements under consideration are given in Table I, in terms of the mass tensor for ellipsoid  $A$ :

$$\mathbf{m}^{(A)} = \begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & m_4 \\ 0 & m_4 & m_3 \end{pmatrix}, \quad (73)$$

the hole mass tensor,

$$\mathbf{m}^{(H)} = \begin{pmatrix} M_1 & 0 & 0 \\ 0 & M_1 & 0 \\ 0 & 0 & M_3 \end{pmatrix}, \quad (74)$$

the  $\mathbf{s}$  tensor of ellipsoid  $A$ ,

$$\mathbf{s}^{(A)} = \begin{pmatrix} s_1 & 0 & 0 \\ 0 & s_2 & s_4 \\ 0 & s_4 & s_3 \end{pmatrix}, \quad (75)$$

and the  $\mathbf{s}$  tensor for the holes,

$$\mathbf{s}^{(H)} = \begin{pmatrix} S_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_3 \end{pmatrix}. \quad (76)$$

These tensors are given in the crystal system 1 = binary, 2 = bisectrix, 3 = trigonal; their form is determined by crystal symmetry.

## V. CALCULATIONS AND DISCUSSION

The calculation of  $\mathbf{s}$ , Eq. (46), was done on the Univac 1108 computer using the band parameters of Smith, Baraff, and Rowell (SBR).<sup>15</sup> The calculation was carried out in dimensionless  $\mathbf{P}$  space as described in the discussion in I, Sec. III. The results for  $\mathbf{s}^{(A)}$  and  $\mathbf{s}^{(H)}$  are as follows:  $s_1 = 2.95$ ,  $s_2 = 24.1$ ,  $s_3 = 5.89$ ,  $s_4 = -1.38$ ,  $S_1 = 69.3$ ,  $S_3 = 151.0 Z^2 N \times 10^{-36} \text{ g sec}^{-1}$ , where  $N$  is in units of  $\text{cm}^{-3}$ . These values and the SBR mass parameters may be used in the expressions of Table I to obtain the ratios of the various  $\tau$ 's for the different experimental arrangements of Ref. 8. The result is as follows:  $\tau(\mathbf{H} \| 1, \mathbf{E} \| 2) : \tau(\mathbf{H} \| 1, \mathbf{E} \| 3) : \tau(\mathbf{H} \| 2, \mathbf{E} \| 1) : \tau(\mathbf{H} \| 2, \mathbf{E} \| 3) : \tau(\mathbf{H} \| 3, \mathbf{E} \| 1 \text{ or } 2) = 1.29 : 1.68 : 1.28 : 0.29 : 1.00$ .

The relaxation times of Ref. 8 are shown in Fig. 1 together with a fit of the above calculated relaxation times. The fit appears good, as least by the standards of typical theory-experiment fits for bismuth. This fit corresponds to a value of  $Z^2 N = 1.16 \times 10^{16} \text{ cm}^{-3}$ . If we assume that  $|Z| = 1$ , the concentration of ionized im-

<sup>15</sup> G. E. Smith, G. A. Baraff, and J. M. Rowell, Phys. Rev. **135**, A1118 (1964).

purities would be about 4.2% of the electron (or hole) concentration. Unless the sample contained very nearly equal numbers of acceptor or donor impurities, then it would have been uncompensated far too much for pure Alfvén-wave behavior to result, in the range of magnetic fields (5–20 kG) and microwave frequencies (300–2000 Mc/sec) used in the experiment.

TABLE I. The  $\mu_{\alpha\beta'}$  and  $\xi_{\alpha\beta'}$  for three different experimental geometries. The  $\alpha$  and  $\beta$  here refer to principal crystal axes: 1=binary, 2=bisectrix, 3=trigonal.

$$\begin{aligned} \mathbf{k} \parallel \mathbf{H} \parallel \text{trigonal: } \mu_{11}' &= \mu_{22}' = \frac{1}{2}(m_1 + m_2) - \frac{1}{2}(m_4^2/m_3) + M_1 \\ \xi_{11}' &= \xi_{22}' = \frac{1}{2}(s_1 + s_2) - s_4(m_4/m_3) + \frac{1}{2}s_3(m_4^2/m_3^2) + S_1 \\ \mathbf{k} \parallel \mathbf{H} \parallel \text{binary: } \mu_{22}' &= m_3 - \frac{2m_4^2}{m_1 + 3m_2} + M_3 \\ \mu_{33}' &= \frac{m_2}{3} + \frac{8}{3} \frac{m_1 m_2}{m_1 + 3m_2} + M_1 \\ \mu_{23}' &= m_4 \frac{m_1 - m_2}{m_1 + 3m_2} \\ \xi_{22}' &= s_3 - 4s_4 \frac{m_4}{m_1 + 3m_2} + 2(s_1 + 3s_2) \left( \frac{m_4}{m_1 + 3m_2} \right)^2 + S_3 \\ \xi_{33}' &= \frac{1}{2}(s_1 + s_2) - (s_1 - s_2) \frac{m_1 - m_2}{m_1 + 3m_2} + \frac{1}{2}(s_1 + 3s_2) \left( \frac{m_1 - m_2}{m_1 + 3m_2} \right)^2 + S_1 \\ \xi_{23}' &= s_4 \frac{m_1 - m_2}{m_1 + 3m_2} + (s_1 - s_2) \frac{m_4}{m_1 + 3m_2} - (s_1 + 3s_2) \frac{m_4(m_1 - m_2)}{(m_1 + 3m_2)^2} \\ \mathbf{k} \parallel \mathbf{H} \parallel \text{bisectrix: } \mu_{33}' &= \frac{m_1}{3} + \frac{8}{3} \frac{m_1 m_2}{3m_1 + m_2} + M_1 \\ \xi_{33}' &= \frac{1}{2}(s_1 + s_2) - (s_1 - s_2) \frac{m_1 - m_2}{3m_1 + m_2} + \frac{1}{2}(3s_1 + s_2) \left( \frac{m_1 - m_2}{3m_1 + m_2} \right)^2 + S_1 \\ \mu_{11}' &= m_2 - \frac{m_4^2}{3m_2} - \frac{2}{3} \frac{m_4^2}{3m_1 + m_2} + M_3 \\ &+ \left( \frac{4}{3} \frac{m_4}{3m_1 + m_2} - \frac{m_4}{3m_2} \right)^2 \left( \frac{1}{3m_2} + \frac{1}{3(3m_1 + m_2)} + \frac{1}{M_1} \right)^{-1} \\ \xi_{11}' &= s_3 - \frac{2}{3}s_4 \frac{m_4}{m_2} - \frac{4}{3}s_4 \frac{m_4}{3m_1 + m_2} + \frac{1}{3}s_2 \frac{m_4^2}{m_2^2} \\ &+ \frac{2}{3}(3s_1 + s_2) \left( \frac{m_4}{3m_1 + m_2} \right)^2 + S_3 + 2 \left( \frac{4}{3} \frac{m_4}{3m_1 + m_2} - \frac{m_4}{3m_2} \right) \\ &\times \left[ \frac{m_4}{\frac{1}{2}s_2} \frac{m_4}{m_2^2} - \frac{4}{3}(3s_1 + s_2) \frac{m_4}{(3m_1 + m_2)^2} - \frac{s_4}{3m_2} + \frac{4}{3} \frac{s_4}{3m_1 + m_2} \right] \\ &\times \left( \frac{1}{3m_2} + \frac{8}{3(3m_1 + m_2)} + \frac{1}{M_1} \right)^{-1} + \left[ \frac{s_2}{3m_2^2} + \frac{8}{3(3m_1 + m_2)^2} + \frac{S_1}{M_1^2} \right] \\ &\times \left( \frac{4}{3} \frac{m_4}{3m_1 + m_2} - \frac{m_4}{3m_2} \right)^2 \left( \frac{1}{3m_2} + \frac{8}{3(3m_1 + m_2)} + \frac{1}{M_1} \right)^{-2} \end{aligned}$$

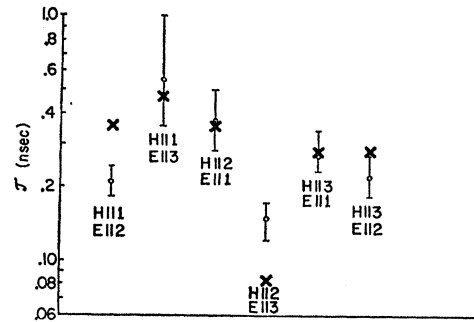


FIG. 1. Fit of calculated relaxation times with the data of Ref. 8. Points with error bars, Ref. 8;  $\times$ , calculated.

As it is highly unlikely that ionized impurities are responsible for the observed damping of Alfvén waves, the other possibilities are (a) neutral impurities, (b) dislocations, and (c) Frenkel defects. Lattice vacancies (or interstitials) alone are ruled out since they act as acceptors (or donors) in Bi. If the above relaxation times were due to lattice vacancies, this would correspond to an excess concentration of holes over electrons of about 0.84% of the electron concentration, which is still far too high for pure Alfvén-wave behavior.

Neutral impurities, being of very short range, would be expected to yield far more nearly isotropic relaxation frequency tensors than the ones which are consistent with the data of Ref. 8.<sup>16</sup> Dislocations in bismuth would be expected to act either as donors, acceptors or dipoles. If they act as donors or acceptors, they are ruled out as the dominant mechanism in Alfvén-wave damping by the arguments applying to ionized impurities. It is difficult to estimate the scattering properties of dislocations which act as dipoles of unknown moment; therefore this mechanism for Alfvén-wave damping cannot be ruled out.

Suppose for the sake of argument that the damping is due to Frenkel defects. We first need to estimate the energy of formation  $\epsilon_f$  and the activation energy  $\epsilon_+$  for these defects in bismuth. The vacancy left by a Frenkel defect in bismuth acts as a charged scatterer of  $Z = -5$ , and the interstitial acts as a charged scatterer of  $Z = +5$ , and thus the defect has no net effect on the electron or hole density in the plasma. Furthermore, the number of Frenkel defects,  $n_F$ , is equal to  $\frac{1}{2}$  the number  $N$  of scatterers with  $|Z| = 5$  in the crystal. If  $N'$  is the number of atoms in the crystal, and  $N''$  the number of possible interstitial sites, we may use the formula for the equilibrium concentration of Frenkel defects<sup>17</sup>:

$$n_F = (N'N'')^{1/2} \exp(-\epsilon_f/2kT). \quad (77)$$

If we assume the sample at cryogenic temperatures contains a concentration of defects equal to the equilibrium concentration at  $\frac{1}{2}$  the melting point of bismuth (which

<sup>16</sup> C. Herring, Bell System Tech. J. 34, 237 (1955).

<sup>17</sup> C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, Inc., New York, 1966), 3rd ed., Ch. 18.

is 545°K), we obtain, for the sample of Ref. 8, the value  $\epsilon_j = 0.87$  eV. If we make the approximation that the jump frequency  $\omega_j$  is given by

$$\omega_j \approx \omega_D \exp(-\epsilon_+/kT), \quad (78)$$

where  $\omega_D \approx 120^\circ\text{K}$  is the Debye frequency of bismuth, and if we assume a jump frequency of one cps at  $T = \frac{1}{2}$  the melting point, we obtain the value  $\epsilon_+ = 0.68$  eV.

The above analysis corresponds to the following physical situation: The defects are frozen in the solid at a temperature not far below room temperature. The energy of formation is somewhat lower than that usually found in solids, corresponding to the somewhat loose packing of the atoms in bismuth. The activation energy is lower than the energy of formation, which is always the case in a solid.

## VI. CONCLUDING REMARKS

We conclude that serious consideration must be given to the possibility of Frenkel defects being the dominant scattering centers in very pure, well-annealed bismuth single crystals at cryogenic temperatures. This possibility suggests the desirability of carrying out galvanomagnetic studies, including Alfvén-wave experiments, on irradiated and/or quenched bismuth single crystals.

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## Phonon Frequencies in Copper at 49 and 298°K\*

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Phonon frequencies for wave vectors along the principal symmetry directions in copper have been determined at 49 and 298°K from neutron inelastic-scattering measurements. In general, the temperature dependences of the frequencies were found to be smaller for the higher-frequency modes. For the lower frequencies ( $\nu \lesssim 3 \times 10^{12}$  cps), the frequency changes measured are consistent with the 3–4% changes estimated from the isothermal elastic constants. For higher frequencies the relative changes are much smaller, often being 1% or less. Axially symmetric force models, which included interactions to the sixth nearest neighbors, were fitted to the data and have been used to calculate a frequency distribution function  $g(\nu)$  at each temperature. A comparison of the temperature dependences of the moments of these distributions with various Grüneisen parameters leads to the conclusion that Cu does not satisfy the assumption of the quasi-harmonic model. The Debye temperature  $\theta_C$  versus temperature curve calculated with the 49°K  $g(\nu)$  is in excellent agreement with results from specific-heat measurements in the entire 0 to 298°K range. A fairly strong temperature dependence for the widths of some well-focused phonons was observed.

## INTRODUCTION

MEASUREMENTS of the coherent inelastic scattering of neutrons by solids can give directly the phonon dispersion relations  $\nu(q)$  and, in principle, considerable information about interatomic forces.<sup>1</sup> However, the analyses of such measurements are always made on the basis of a harmonic theory, whereas the measurements are usually obtained under conditions in which anharmonic effects are not negligible. Although one expects a harmonic analysis of the data to yield qualitatively correct conclusions, the development of a truly quantitative description of the interatomic forces

requires a better understanding of anharmonicity. Even the most accurate interpolation formula for the dispersion relations will yield a frequency distribution function  $g(\nu)$  of dubious value, because anharmonicity affects differently the various physical properties that, in a harmonic theory, depend on  $g(\nu)$ .<sup>2</sup> To take a proper account of anharmonicity in a force model analysis of dispersion curve data is prohibitively complex, however, judging from the theoretical work in the literature.<sup>3–5</sup> Thus, at the present time it seems that a more fruitful examination of anharmonicity involves the measurement of the temperature (and pressure) dependences of the energies and lifetimes of phonons as well as the

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<sup>1</sup> See for example, G. Dolling and A. D. B. Woods, in *Thermal Neutron Scattering*, edited by P. A. Egelstaff (Academic Press Inc., New York, 1965), Chap. 5.

<sup>2</sup> T. H. K. Barron, in *Proceedings of the International Conference on Lattice Dynamics at Copenhagen, 1963*, edited by R. F. Wallis (Pergamon Press, Inc., New York, 1963), p. 247.

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<sup>5</sup> E. R. Cowley and R. A. Cowley, *Proc. Roy. Soc. (London)* **287**, 259 (1965).