ARMY RESEARCH LABORATORY

Derivation of Effective-Mass Expressions for Electrons and Holes in the Anisotropic Multiband Semimetals Ar, Sb, and Bi

Frank J. Crowne

ARL-TR-2152

August 2000

Army Research Laboratory

Adelphi, MD 20783-1197

ARL-TR-2152 **August 2000**

Derivation of Effective-Mass Expressions for Electrons and Holes in the Anisotropic Multiband Semimetals Ar, Sb, and Bi

Frank J. Crowne

Sensors and Electron Devices Directorate

Abstract

In this report, certain properties of the multicomponent plasmas present in the group-V semimetals As, Sb, and Bi have been derived. Notable among these properties is anisotropy of the effective masses of both electrons and holes, which in turn leads to anisotropy in the plasma frequencies of these materials. Because the systems of interest are particles in a host matrix rather than bulk materials, it is likely that this anisotropy in the plasma response will be averaged out in some way; however, this problem must be examined in detail before such a conclusion is warranted.

Contents

Figures

1. Introduction

The electrodynamic properties of the semimetallic group-V elements (arsenic, antimony, and bismuth) are complex and ill-understood in many ways. This is primarily due to the complicated structures of their conduction and valence bands, which have many maxima and minima for the Fermi surface to intersect, resulting in multiple "pockets" of electrons and holes populated by carriers at all temperatures [1]. According to the Sommerfeld theory of metals, each minimum or maximum should give rise to a different species of electron or hole, so that the electrodynamic response of the material resembles that of a multicomponent plasma. To make matters worse, all these materials crystallize orthorhombically, so that their charge carriers (both electrons and holes) have anisotropic effective masses.

When nanometer-size samples of these materials (so-called *quantum dots*) are prepared, the resulting systems are expected to behave in unusual ways when probed by electromagnetic radiation. A particularly easy way to create such samples was discovered some 10 years ago, when researchers found that under certain conditions low-temperature growth of GaAs by molecular-beam epitaxy (MBE) resulted in material with large numbers of ultramicroscopic inclusions of As, up to 1 percent of the host volume [2], which arose from the aggregation of Ga_{As} antisite defects (i.e., lattice sites at which a gallium atom was replaced by an As atom). Although theories regarding their nature are still problematic, there are strong indications that these inclusions, which are roughly spherical in shape, consist of metallic arsenic. Similar behavior has been observed when InAs and GaSb are grown in this way.

There is ample reason to believe that these materials could be useful in device engineering. However, before this usefulness can be explored, the individual nanoparticles must be properly modeled with regard to interactions with electromagnetic waves. In this report, I derive an appropriate set of constitutive equations that can be used with the Maxwell equations to implement this modeling.

2. Boltzmann-Equation Calculation of Fermi Velocities in Group-V Semimetals

The most effective way to deal with metals and their interactions with electromagnetic radiation (light, microwaves, etc) is to use the Boltzmann-Vlasov equation to calculate momentum (k-space) distributions for the metallic charge carriers [3]. For semimetals, this naturally leads to a general multiband set of Boltzmann equations:

$$\partial_t f_j + v_\alpha^{(j)}(\vec{k})\partial_\alpha f_j + \frac{e}{\hbar}(\partial_\alpha \phi)\left(\frac{\partial}{\partial k_\alpha} f_j\right) = -\frac{1}{\tau_j}\left(f_j - \frac{n^{(j)}}{n_0^{(j)}} f_0^{(j)}(\vec{k})\right), \quad (1)$$

where $f^{(j)}(\vec{k}, \vec{x}, t)$ is the number distribution function for the jth carrier, $v_\alpha^{(j)}(\vec{k})$ is the semiclassical (hydrodynamic) velocity of such a carrier with momentum k, τ_j is its particle-number-conserving relaxation time, and $\phi(x, t)$ is any external (electrostatic) potential applied to the system. The hydrodynamic approximation introduces a parameterization of the solutions to these equations in terms of macroscopic variables such as density, drift velocity, etc, which are determined self-consistently as moments of the equations. If the particles are semiconducting with parabolic bands, we can use Maxwell-Boltzmann functions for the perturbed carrier distributions:

$$f^{(j)}(\vec{k}, \vec{x}, t) = 4\pi^3 n^{(j)}(\vec{x}, t)\left[m_l m_t^2\right]^{-1/2}\left(\frac{\hbar^2}{2\pi k_B T^{(j)}(\vec{x}, t)}\right)^{3/2} \exp\left\{-\frac{1}{kT^{(j)}(\vec{x}, t)} G^{(j)}(\vec{k}, \vec{x}, t)\right\}, \quad (2)$$

where

$$G^{(j)}(\vec{k}, \vec{x}, t) = \frac{\hbar^2}{2}\left(\vec{k} - \vec{k}_D^{(j)}(\vec{x}, t) - \vec{k}_{0j}\right)_\alpha \left[m_j^{-1}\right]_{\alpha\beta}\left(\vec{k} - \vec{k}_D^{(j)}(\vec{x}, t) - \vec{k}_{0j}\right)_\beta. \quad (3)$$

Here $n^{(j)}(\vec{x}, t)$ is the hydrodynamic density of carriers in the jth carrier pocket, $\vec{k}_D^{(j)}(\vec{x}, t)$ is the hydrodynamic drift momentum of carriers in this pocket, $k_0 j$ locates the center of the pocket in k-space, m_j^{-1} is the effective-mass tensor of the jth carrier type with principal values m_l and m_t (assuming the pockets are spheroidal), k_B is Boltzmann's constant, $T^{(j)}(\vec{x}, t)$ is the hydrodynamic temperature of the jth carrier type, and $\hbar$ is Planck's constant. The corresponding unperturbed distributions are

$$f_0^{(j)}(\vec{k}) = 4\pi^3 n_0^{(j)}\left[m_l m_t^2\right]^{-1/2}\left(\frac{\hbar^2}{2\pi k_B T}\right)^{3/2} \exp\left\{-\frac{\hbar^2}{2kT}\left(\vec{k} - \vec{k}_{0j}\right)_\alpha \left[m_j^{-1}\right]_{\alpha\beta}\left(\vec{k} - \vec{k}_{0j}\right)_\beta\right\}, \quad (4)$$

where $n_0^{(j)}$ is the equilibrium density of carriers in the jth carrier pocket, and T is the usual lattice temperature. For metallic particles, the correct distributions at low temperatures are perturbed Fermi distributions:

$$f^{(j)}(\vec{k},\vec{x},t) = \theta\left(\epsilon_F(\vec{x},t) - \epsilon_{Pj} - G^{(j)}(\vec{k},\vec{x},t)\right) , \tag{5}$$

where $\epsilon_F(\vec{x},t)$ is a position-dependent Fermi energy (imref) measured from some constant reference (e.g., vacuum), and ϵ_{Pj} marks the minimum energy of the jth pocket. The corresponding equilibrium distribution is

$$f_0^{(j)}(\vec{k}) = \theta\left(\epsilon_F - \epsilon_{Pj} - \frac{\hbar^2}{2}\left(\vec{k}-\vec{k}_{0j}\right)_\alpha \left[m_j^{-1}\right]_{\alpha\beta}\left(\vec{k}-\vec{k}_{0j}\right)_\beta\right) , \tag{6}$$

where ϵ_F is the equilibrium Fermi energy. We can relate the density $n_0^{(j)}$ to ϵ_F by introducing the density-of-states mass $\mu = \left[m_t^2 m_l\right]^{1/3}$ and the quantity $k_{Fj}^2 = 2\mu\Delta\epsilon_{Fj}/\hbar^2$, where $\Delta\epsilon_{Fj} = \epsilon_F - \epsilon_{Pj}$ (i.e., the Fermi wave vector of pocket j), and by integrating the distribution over k-space in the usual way. This gives

$$n_0^{(j)} = \frac{k_{Fj}^3}{3\pi^2} . \tag{7}$$

We can likewise define the deviation from equilibrium in the usual way:

$$\delta f^{(j)}(\vec{k},\vec{x},t) = f^{(j)}(\vec{k},\vec{x},t) - f_0^{(j)}(\vec{k}) . \tag{8}$$

By integrating only over k-space, we obtain the perturbed and unperturbed hydrodynamic particle densities and their difference:

$$\begin{aligned} n^{(j)}(\vec{x},t) &= \frac{2}{(2\pi)^3}\int d^3k f^{(j)}(\vec{k},\vec{x},t) , \\ n_0^{(j)} &= \frac{2}{(2\pi)^3}\int d^3k f_0^{(j)}(\vec{k}) , \\ \delta n^{(j)}(\vec{x},t) &= n^{(j)}(\vec{x},t) - n_0^{(j)} . \end{aligned} \tag{9}$$

Note that these also enter into the number-conserving collisional relaxation term and hence must be determined self-consistently. These equations couple to the Poisson equation in the usual way:

$$\nabla^2\phi = \frac{1}{\epsilon}\sum_j e_j \delta n^{(j)}(\vec{x},t) , \tag{10}$$

where the charge e_j = +1 for holes, −1 for electrons.

Let us linearize the Boltzmann equations around the unperturbed distributions:

$$\partial_t \delta f^{(j)} + v_\alpha^{(j)}(\vec{k})\partial_\alpha \delta f^{(j)} + \frac{e}{\hbar}(\partial_\alpha\phi)\left(\frac{\partial}{\partial k_\alpha} f_0^{(j)}(\vec{k})\right) = -\frac{1}{\tau_j}\left(\delta f^{(j)} - \frac{\delta n^{(j)}}{n_0^{(j)}} f_0^{(j)}(\vec{k})\right) , \tag{11}$$

where we neglect all spatial dependences to zero order. To solve these equations, we use the (wave) ansatz

$$
\begin{aligned}
\delta f^{(j)}(\vec{k},\vec{x},t) &= \delta f_q^{(j)}(\vec{k})e^{i(\vec{q}\cdot\vec{x}-\omega t)} , \\
\delta n^{(j)}(\vec{x},t) &= \delta n_q^{(j)}e^{i(\vec{q}\cdot\vec{x}-\omega t)} , \\
\phi_q &= -\frac{1}{\epsilon q^2}\sum_j e_j \delta n_q^{(j)} .
\end{aligned}
\tag{12}
$$

Then the equations for the perturbed system become

$$
\left(-i\omega+\frac{1}{\tau_j}\right)\delta f_q^{(j)}(\vec{k})+iq_\alpha v_\alpha^{(j)}(\vec{k})\delta f_q^{(j)}(\vec{k}) = -\frac{e_j}{\hbar}(iq_\alpha\phi_q)\left(\frac{\partial}{\partial k_\alpha}f_0^{(j)}(\vec{k})\right)+\frac{1}{\tau_j}\left(\frac{\delta n_q^{(j)}}{n_0^{(j)}}f_0^{(j)}(\vec{k})\right) , \tag{13}
$$

which are easily solved:

$$
\delta f_q^{(j)}(\vec{k}) = \frac{\frac{e_j}{\hbar}(q_\beta\phi_q)\left(\frac{\partial}{\partial k_\beta}f_0^{(j)}(\vec{k})\right)+\frac{i}{\tau_j}\left(\frac{1}{n_0^{(j)}}f_0^{(j)}(\vec{k})\right)\delta n_q^{(j)}}{\omega+\frac{i}{\tau_j}-q_\alpha v_\alpha^{(j)}(\vec{k})} . \tag{14}
$$

We can now substitute this expression back into the density expression

$$
\delta n_q^{(j)} = \frac{2}{(2\pi)^3}\int \delta f_q^{(j)}(\vec{k})\, d^3k \tag{15}
$$

to get

$$
\delta n_q^{(j)} = \frac{e_j}{\hbar}(q_\beta\phi_q)\frac{2}{(2\pi)^3}\int\frac{\frac{\partial}{\partial k_\beta}f_0^{(j)}(\vec{k})}{\omega+\frac{i}{\tau_j}-q_\alpha v_\alpha^{(j)}(\vec{k})}d^3k+\frac{i}{\tau_j}\frac{\delta n_q^{(j)}}{n_0^{(j)}}\frac{2}{(2\pi)^3}\int\frac{f_0^{(j)}(\vec{k})}{\omega+\frac{i}{\tau_j}-q_\alpha v_\alpha^{(j)}(\vec{k})}d^3k , \tag{16}
$$

which can be written

$$
\delta n_q^{(j)} = \frac{e_j}{\hbar}(q_\beta\phi_q)\Im_{1j}^\beta+\frac{i}{\tau_j}\frac{\delta n_q^{(j)}}{n_0^{(j)}}\Im_{2j} . \tag{17}
$$

The first term in this expression contains the vector coefficient

$$
\Im_{1j}^\beta = \frac{2}{(2\pi)^3}\int d^3k\frac{\frac{\partial}{\partial k_\beta}f_0^{(j)}(\vec{k})}{\omega+\frac{i}{\tau_j}-q_\alpha v_\alpha^{(j)}(\vec{k})} , \tag{18}
$$

while the second term contains the scalar coefficient

$$
\Im_{2j} = \frac{2}{(2\pi)^3}\int d^3\xi\frac{f_0^{(j)}(\vec{\xi})}{\omega+\frac{i}{\tau_j}-q_\alpha v_\alpha^{(j)}(\vec{\xi})} . \tag{19}
$$

Since each k-space pocket in the semimetal is ellipsoidal, the hydrodynamic velocities can be defined in terms of the effective mass tensors:

$$v_\alpha^{(j)}(\vec{k}) = \hbar \left[m_j^{-1}\right]_{\alpha\gamma} \left(\vec{k} - \vec{k}_{0j}\right)_\gamma \equiv \hbar \left[m_j^{-1}\right]_{\alpha\gamma} \xi_\gamma \,, \tag{20}$$

where $\vec{\xi}_\gamma$ is the deviation in k from the jth band minimum (or maximum). Then the scalar term becomes

$$\Im_{2j}^\beta = \frac{2}{(2\pi)^3} \int d^3\xi \frac{f_0^{(j)}(\vec{\xi})}{\omega + \frac{i}{\tau_j} - q_\alpha \hbar \left[m_j^{-1}\right]_{\alpha\gamma} \xi_\gamma} \,, \tag{21}$$

and the vector term becomes

$$\Im_{1j}^\beta = \frac{2}{(2\pi)^3} \int d^3\xi \frac{\frac{\partial}{\partial \xi_\beta} f_0^{(j)}(\vec{\xi})}{\omega + \frac{i}{\tau_j} - q_\alpha \hbar \left[m_j^{-1}\right]_{\alpha\gamma} \xi_\gamma} \,. \tag{22}$$

Using the Fermi distributions

$$f_0^{(j)}(\vec{\xi}) = \theta \left(\epsilon_F - \epsilon_{Pj} - \frac{\hbar^2}{2} \xi_\alpha \left[m_j^{-1}\right]_{\alpha\beta} \xi_\beta \right) \tag{23}$$

gives

$$\frac{\partial}{\partial \xi_\alpha} f_0^{(j)}(\vec{\xi}) = -\hbar^2 \left[m_j^{-1}\right]_{\alpha\beta} \xi_\beta \delta \left(\epsilon_F - \epsilon_{Pj} - \frac{\hbar^2}{2} \xi_\alpha \left[m_j^{-1}\right]_{\alpha\beta} \xi_\beta \right) \,. \tag{24}$$

Then $\Im_{1j}^\beta$ becomes

$$\Im_{1j}^\beta = -\hbar \frac{2}{(2\pi)^3} \int d^3\xi \frac{\hbar \left[m_j^{-1}\right]_{\beta\gamma} \epsilon_\gamma}{\omega + \frac{i}{\tau_j} - q_\alpha \hbar \left[m_j^{-1}\right]_{\alpha\gamma} \xi_\gamma} \delta(\epsilon_F - \epsilon_{\xi j}) \tag{25}$$

where

$$\epsilon_{\xi j} = \epsilon_{Pj} + \frac{\hbar^2}{2} \xi_\alpha \left[m_j^{-1}\right]_{\alpha\beta} \xi_\beta \,. \tag{26}$$

We can now solve the density equation

$$\left[1 - \frac{i}{\tau_j} \frac{\Im_{2j}}{n_0^{(j)}}\right] \delta n_q^{(j)} = \frac{e_j}{\hbar} (q_\beta \phi_q) \Im_{1j}^\beta \,, \tag{27}$$

and insert the results into Poisson's equation to get

$$\phi_q = -\frac{e^2}{\epsilon q^2} \phi_q \sum_j \left[1 - \frac{i}{\tau_j} \frac{\Im_{2j}}{n_0^{(j)}}\right]^{-1} \frac{1}{\hbar} q_\beta \Im_{1j}^\beta \,. \tag{28}$$

Note that $e_j^2 = e^2$ for solid-state systems. Equation (28) can only be true if

$$1 = -\frac{e^2}{\epsilon q^2} \sum_j \left[1 - \frac{i}{\tau_j} \frac{\Im_{2j}}{n_0^{(j)}}\right]^{-1} \frac{1}{\hbar} q_\beta \Im_{1j}^\beta \,, \tag{29}$$

where

$$q_\beta \Im_{1j}^\beta = -\hbar \frac{2}{(2\pi)^3} \int d^3\xi \frac{\hbar q_\beta \left[m_j^{-1}\right]_{\beta\gamma} \xi_\gamma}{\omega + \frac{i}{\tau_j} - \hbar q_\beta \left[m_j^{-1}\right]_{\beta\gamma} \xi_\gamma} \delta\left(\epsilon_F - \epsilon_{\xi j}\right) . \tag{30}$$

The roots of this equation define various dispersion relations for plasma waves $\omega^{(s)}(\vec{q})$.

Because of the δ-function, it is possible to evaluate expression (30) analytically. Write

$$\left[m_j^{-1}\right]_{\alpha\beta} = \bar{S}_{\alpha\lambda} D_{\lambda\nu} S_{\nu\beta} , \tag{31}$$

where the matrix S is a rotation chosen to diagonalize m_j^{-1}. Then

$$q_\beta \Im_{1j}^\beta = -\hbar \frac{2}{(2\pi)^3} \int d^3\xi \frac{\hbar q_\beta S_{\beta\lambda} D_{\lambda\nu} S_{\nu\gamma} \xi_\gamma}{\omega + \frac{i}{\tau_j} - \hbar q_\beta S_{\beta\lambda} D_{\lambda\nu} S_{\nu\gamma} \xi_\gamma} \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} \xi_\beta S_{\beta\lambda} D_{\lambda\nu} S_{\nu\gamma} \xi_\gamma\right) , \tag{32}$$

where $\Delta\epsilon_{Fj} = \epsilon_F - \epsilon_{Pj}$. Let $x_\nu = S_{\nu\gamma}\xi_\gamma$, $Q_\nu = S_{\nu\gamma} q_\gamma$. Then the Jacobian for this transformation is 1, and so

$$q_\beta \Im_{1j}^\beta = -\hbar \frac{2}{(2\pi)^3} \int d^3x \frac{\hbar Q_\lambda D_{\lambda\nu} x_\nu}{\omega + \frac{i}{\tau_j} - \hbar Q_\lambda D_{\lambda\nu} x_\nu} \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} x_\lambda D_{\lambda\nu} x_\nu\right) . \tag{33}$$

Now, since D is diagonal, we can easily define $D = D^{1/2} D^{1/2}$ as a scaling transformation. If $y_\nu = \left[D^{1/2}\right]_{\nu\gamma} x_\gamma$, $\Lambda_\nu = \hbar \left[D^{1/2}\right]_{\nu\gamma} Q_\gamma$, then

$$q_\beta \Im_{1j}^\beta = -\hbar \left[m_t^2 m_l\right]^{1/2} \frac{2}{(2\pi)^3} \int d^3y \frac{\Lambda_\nu y_\nu}{\omega + \frac{i}{\tau_j} - \Lambda_\nu y_\nu} \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} y^2\right) , \tag{34}$$

where the factor in front is the Jacobian of the scaling transformation. In spherical coordinates, this expression becomes

$$q_\beta \Im_{1j}^\beta = -\frac{\hbar}{2\pi^2} \left[m_t^2 m_l\right]^{1/2} \int_0^\infty y^2\, dy\, \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} y^2\right) \int_{-1}^1 d(\cos\theta) \frac{\Lambda y \cos\theta}{\omega + \frac{i}{\tau_j} - \Lambda y \cos\theta} , \tag{35}$$

where

$$\Lambda = \left[\hbar^2 \left(\frac{q_\perp^2}{m_t} + \frac{q_z^2}{m_l}\right)\right]^{1/2} = \left[\hbar^2 q_\alpha \left(m_j^{-1}\right)_{\alpha\beta} q_\beta\right]^{1/2} . \tag{36}$$

Here, $q_\perp$ and q_z are components of q perpendicular and parallel to the c-axis of the particle material in the principal-axis system of cylindrical coordinates. I have used the fact that as a scalar $|\Lambda|$ must be rotationally invariant. Introducing the density-of-states mass $\mu = \left[m_t^2 m_l\right]^{1/3}$ and the Fermi wave vector $k_{Fj}^2 = 2\mu\Delta\epsilon_{Fj}/\hbar^2$ for pocket j as we did above, we obtain

$$q_\beta \Im_{1j}^\beta = -\frac{\mu k_{Fj}}{2\pi^2\hbar} \int_{-1}^1 d\xi \frac{\xi}{\Gamma - \xi} , \tag{37}$$

where

$$\Gamma = \frac{\omega + \frac{1}{\tau_j}}{\left[2\Delta\epsilon_{Fj}\left(q_\alpha \left(m_j^{-1}\right)_{\alpha\beta} q_\beta\right)\right]^{1/2}} \tag{38}$$

contains the tensor nature of the effective mass both explicitly and implicitly through the Fermi energy. The integral is trivial:

$$q_\beta \Im_{1j}^\beta = \frac{\mu k_{Fj}}{2\pi^2\hbar}\left\{2 - \Gamma \ln\left(\frac{\Gamma+1}{\Gamma-1}\right)\right\} \equiv \frac{\mu k_{Fj}}{\pi^2\hbar} f_1(\Gamma) \; . \tag{39}$$

The quantity $\Im_{2j}$ can also be evaluated explicitly. Analysis similar to that given above leads to the double integral

$$\Im_{2j} = \frac{1}{2\pi^2}\left[m_t^2 m_l\right]^{1/2} \int_0^\infty y^2 \, dy \theta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2}y^2\right) \int_{-1}^{1} d(\cos\theta) \frac{1}{\omega + \frac{i}{\tau_j} - \Lambda y \cos\theta} \; . \tag{40}$$

Introducing the notation $y_F = \sqrt{\frac{2\Delta\epsilon_F}{\hbar^2}}$ and $\epsilon = \cos\theta$ as before, and using the properties of the Fermi function, we can rewrite the above as

$$\Im_{2j} = \frac{1}{2\pi^2}\left[m_t^2 m_l\right]^{1/2} \int_0^{y_F} y^2 \, dy \int_{-1}^{1} d\xi \frac{1}{\omega + \frac{i}{\tau_j} - \Lambda y \xi} \; . \tag{41}$$

Some algebra gives the following expression for this integral:

$$\Im_{2j} = \frac{3n_0^{(j)}}{2\left(\omega + \frac{i}{\tau_j}\right)}\left\{\Gamma^2 + \left(1 - \Gamma^2\right)\frac{\Gamma}{2}\ln\left(\frac{\Gamma+1}{\Gamma-1}\right)\right\} \equiv \frac{n_0^{(j)}}{\omega + \frac{i}{\tau_j}} f_2(\Gamma) \; , \tag{42}$$

where Γ is the quantity introduced above.

Let us solve the plasma dispersion relation to lowest order in q, i.e., the long-wavelength limit. To do so, we take the small-q limit of our explicit expressions in equations (30) and (42), which corresponds to $\Gamma \to \infty$. Some algebra shows that the function $f_2(\Gamma)$ defined in equation (42) goes to 1 in this limit, so to lowest order

$$\Im_{2j} = \frac{1}{\omega + \frac{i}{\tau_j}} \int d^3\xi f_0^{(j)}(\xi) = \frac{n_0^{(j)}}{\omega + \frac{i}{\tau_j}} \; . \tag{43}$$

The same limit for $q_\beta \Im_{1j}^\beta$ gives

$$q_\beta \Im_{1j}^\beta \approx \frac{\mu k_{Fj}}{\pi^2\hbar}\left\{-\frac{1}{3\Gamma^2}\right\} = -\frac{2\mu k_{Fj}}{3\pi^2\hbar}\left\{\frac{\Delta\epsilon_{Fj}\left(\frac{q_\perp^2}{m_t} + \frac{q_z^2}{m_l}\right)}{\left(\omega + i/\tau_j\right)^2}\right\} \; . \tag{44}$$

But

$$
\begin{aligned}
-\frac{2\mu\Delta\epsilon_{Fj}k_{Fj}}{3\pi^2\hbar}\left\{\frac{\frac{q_\perp^2}{m_t}+\frac{q_z^2}{m_l}}{(\omega+i/\tau_j)^2}\right\} &= -\hbar^2\frac{2\mu\Delta\epsilon_{Fj}}{\hbar^2}\frac{k_{FJ}}{3\pi^2}\left\{\frac{\frac{q_\perp^2}{m_t}+\frac{(q_z^2)}{m_l}}{(\omega+i/\tau_j)^2}\right\} \\
&= -\hbar\frac{k_{Fj}^3}{3\pi^2}\left\{\frac{q_\alpha\left[m_j^{-1}\right]_{\alpha\beta}q_\beta}{(\omega+i/\tau_j)^2}\right\} \\
&= -\hbar n_0^{(j)}\left\{\frac{q_\alpha\left[m_j^{-1}\right]_{\alpha\beta}q_\beta}{(\omega+i/\tau_j)^2}\right\}. \qquad (45)
\end{aligned}
$$

so that equation (29) becomes

$$
1=\frac{e^2}{\epsilon q^2}\sum_j\left[1-\frac{i}{\tau_j}\frac{1}{\omega+\frac{i}{\tau_j}}\right]^{-1}\frac{n_0^{(j)}}{\left(\omega+\frac{i}{\tau_j}\right)^2}q_\alpha\left[m_j^{-1}\right]_{\alpha\beta}q_\beta\,. \qquad (46)
$$

Assuming that the relaxation times are the same for all the pockets, we obtain

$$
1-\frac{e^2}{\epsilon q^2}\frac{1}{\omega\left(\omega+\frac{i}{\tau}\right)}q_\alpha\left\{\sum_j n_0^{(j)}\left[m_j^{-1}\right]\right\}_{\alpha\beta}q_\beta \qquad (47)
$$

or, introducing the unit vector $\hat{q}=\vec{q}/|\vec{q}|$,

$$
1-\frac{e^2}{\epsilon}\frac{1}{\omega\left(\omega+\frac{i}{\tau}\right)}\sum_j\left\{n_0^{(j)}\hat{q}_\alpha\left[m_j^{-1}\right]_{\alpha\beta}\hat{q}_\beta\right\}=0\,. \qquad (48)
$$

This expression, which is clearly in the form of a requirement that a "Drude"-type conductivity for the system should vanish, defines the "plasma frequency" of the multicomponent system as the sum in the numerator. In general this sum will depend on the direction of $\hat{q}$.

To derive an analogue of the linearized Thomas-Fermi equation and a corresponding screening length, we need to take these expansions to higher order in q. Saving next-order terms in $f_1(\Gamma)$ and $f_2(\Gamma)$ gives

$$
f_1(\Gamma)\approx-\frac{1}{3\Gamma^2}-\frac{1}{5\Gamma^4}\,.\quad f_2(\Gamma)\approx1+\frac{1}{5\Gamma^2}\,. \qquad (49)
$$

Let us rewrite equation (29) as

$$
1=-\frac{e^2}{\epsilon q^2}\sum_j\left[1-\frac{i}{\tau_j}\frac{f_2(\Gamma)}{\omega+\frac{i}{\tau_j}}\right]\frac{\mu k_{Fj}}{\pi^2\hbar}f_1(\Gamma) \qquad (50)
$$

and note that

$$
\frac{\mu k_{Fj}}{\pi^2\hbar}=\frac{3}{2}\frac{n_0^{(j)}}{\Delta\epsilon_{Fj}}\,. \qquad (51)
$$

Then equation (50) becomes

$$1 = -\frac{1}{q^2} \sum_j \lambda_j^2 \left[1 - \frac{i}{\tau_j} \frac{f_2(\Gamma)}{\omega + \frac{i}{\tau_j}} \right]^{-1} f_1(\Gamma) \,, \tag{52}$$

where λ_j^2 is the Thomas-Fermi screening length for carriers in the jth pocket:

$$\lambda_j^2 = \frac{3}{2\epsilon} \frac{n_0^{(j)} e^2}{\Delta\epsilon_{Fj}} \,. \tag{53}$$

With these results, we can easily derive the expression

$$1 = \sum_j \frac{n_0^{(j)} e^2}{\epsilon q^2} \frac{q_\alpha \left[m_j^{-1} \right]_{\alpha\beta} q_\beta}{\omega \left(\omega + \frac{i}{\tau_j} \right)} \left[1 + \frac{6}{5} \frac{\Delta\epsilon_{Fj}}{\left(\omega + \frac{i}{\tau_j} \right)^2} \left(1 + \frac{2}{3} \frac{i}{\omega\tau_j} \right) q_\alpha \left[m_j^{-1} \right]_{\alpha\beta} q_\beta \right] \,. \tag{54}$$

The peculiar fraction (6/5) that occurs in this expression derives from our linearization around a spatially independent zero-order distribution. A more careful linearization is needed to recover the true hydrodynamic value of this coefficient and, indeed, to recover any of the expressions encountered in classical fluid mechanics. This will be the subject of a subsequent report.

3. Calculations of Sums Over k-Space Minima for High-Symmetry Band Structures

3.1 Simple Cubic Band Structure

A simple cubic band structure is appropriate for elemental silicon (see fig. 1). In order to calculate the effective masses for this method, we assume that the densities in the carrier pockets are the same, and that the principal-axis projections are $\hat{x}\hat{x}$, $\hat{y}\hat{y}$, and $\hat{z}\hat{z}$. Since there are six pockets, each holds 1/6 of the electrons.

Let us write the effective masses as follows:

$$\begin{aligned}\left[m^{(1)}\right]^{-1} &= \left[m^{(-1)}\right]^{-1} = \frac{1}{m_l}\hat{x}\hat{x} + \frac{1}{m_t}\left(\hat{y}\hat{y} + \hat{z}\hat{z}\right) , \\ \left[m^{(2)}\right]^{-1} &= \left[m^{(-2)}\right]^{-1} = \frac{1}{m_l}\hat{y}\hat{y} + \frac{1}{m_t}\left(\hat{x}\hat{x} + \hat{z}\hat{z}\right) , \quad \text{and} \\ \left[m^{(3)}\right]^{-1} &= \left[m^{(-3)}\right]^{-1} = \frac{1}{m_l}\hat{z}\hat{z} + \frac{1}{m_t}\left(\hat{y}\hat{y} + \hat{x}\hat{x}\right) . \end{aligned} \tag{55}$$

Then the sum is simple:

$$\sum_j n_0^{(j)}\left[m_j^{-1}\right] = \frac{1}{6}n_0\left(\frac{1}{m_l} + \frac{2}{m_t}\right)2\left[\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}\right] = \frac{1}{3}n_0\left(\frac{1}{m_l} + \frac{2}{m_t}\right)\overleftrightarrow{1} , \tag{56}$$

where $\overleftrightarrow{1}$ is the identity matrix. This shows that the mass required is just the usual isotropic optical mass.

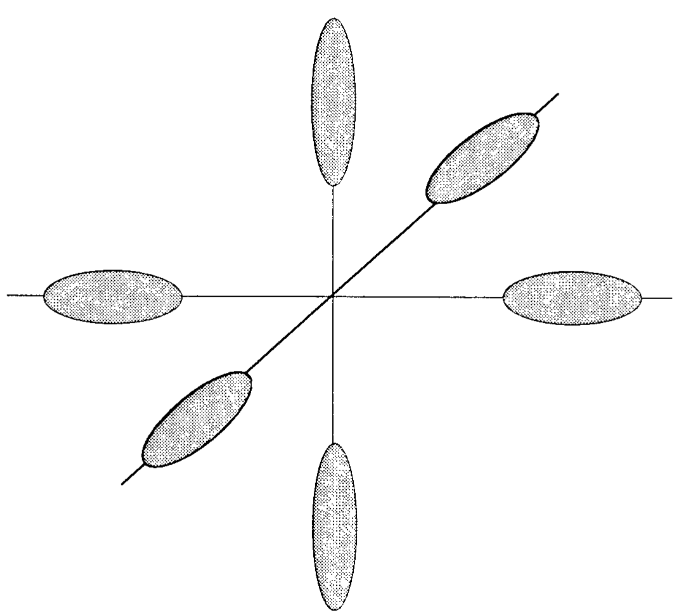

Figure 1. Conduction band minima (pockets) of silicon in k-space.

3.2 (111) Cubic Pockets (Tetrahedral Band Structure)

A tetrahedral band structure is appropriate for elemental germanium (see fig. 2). Here we have four pockets, at the vertices of a tetrahedron. The effective-mass tensors are

$$
\begin{aligned}
\left[m^{(1)}\right]^{-1} &= \left[m^{(-1)}\right]^{-1} = \frac{1}{m_l}\hat{e}_1\hat{e}_1 + \frac{1}{m_t}\left(\hat{s}_1\hat{s}_1 + \hat{t}_1\hat{t}_1\right) , \\
\left[m^{(2)}\right]^{-1} &= \left[m^{(-2)}\right]^{-1} = \frac{1}{m_l}\hat{e}_2\hat{e}_2 + \frac{1}{m_t}\left(\hat{s}_2\hat{s}_2 + \hat{t}_2\hat{t}_2\right) , \\
\left[m^{(3)}\right]^{-1} &= \left[m^{(-3)}\right]^{-1} = \frac{1}{m_l}\hat{e}_3\hat{e}_3 + \frac{1}{m_t}\left(\hat{s}_3\hat{s}_3 + \hat{t}_3\hat{t}_3\right) , \quad \text{and} \\
\left[m^{(4)}\right]^{-1} &= \left[m^{(-4)}\right]^{-1} = \frac{1}{m_l}\hat{e}_4\hat{e}_4 + \frac{1}{m_t}\left(\hat{s}_4\hat{s}_4 + \hat{t}_4\hat{t}_4\right) ,
\end{aligned}
\tag{57}
$$

where the vectors $\hat{e}_i, \hat{s}_i, \hat{t}_i \equiv \hat{e}_i \otimes \hat{s}_i$ mark the principal axes of the pocket ellipsoids:

$$
\begin{aligned}
\hat{e}_1 &= \tfrac{1}{\sqrt{3}}\left(\hat{x}+\hat{y}+\hat{z}\right) , & \hat{s}_1 &= \tfrac{1}{\sqrt{2}}\left(-\hat{x}+\hat{y}\right) , & \hat{t}_1 &= \tfrac{1}{\sqrt{6}}\left(-\hat{x}-\hat{y}+2\hat{z}\right) ; \\
\hat{e}_2 &= \tfrac{1}{\sqrt{3}}\left(-\hat{x}+\hat{y}-\hat{z}\right) , & \hat{s}_2 &= \tfrac{1}{\sqrt{2}}\left(-\hat{x}-\hat{y}\right) , & \hat{t}_2 &= \tfrac{1}{\sqrt{6}}\left(-\hat{x}+\hat{y}+2\hat{z}\right) ; \\
\hat{e}_3 &= \tfrac{1}{\sqrt{3}}\left(-\hat{x}-\hat{y}+\hat{z}\right) , & \hat{s}_3 &= \tfrac{1}{\sqrt{2}}\left(\hat{x}-\hat{y}\right) , & \hat{t}_3 &= \tfrac{1}{\sqrt{6}}\left(\hat{x}+\hat{y}+2\hat{z}\right) ; \quad \text{and} \\
\hat{e}_4 &= \tfrac{1}{\sqrt{3}}\left(\hat{x}-\hat{y}-\hat{z}\right) , & \hat{s}_4 &= \tfrac{1}{\sqrt{2}}\left(\hat{x}+\hat{y}\right) , & \hat{t}_4 &= \tfrac{1}{\sqrt{6}}\left(\hat{x}-\hat{y}+2\hat{z}\right) .
\end{aligned}
\tag{58}
$$

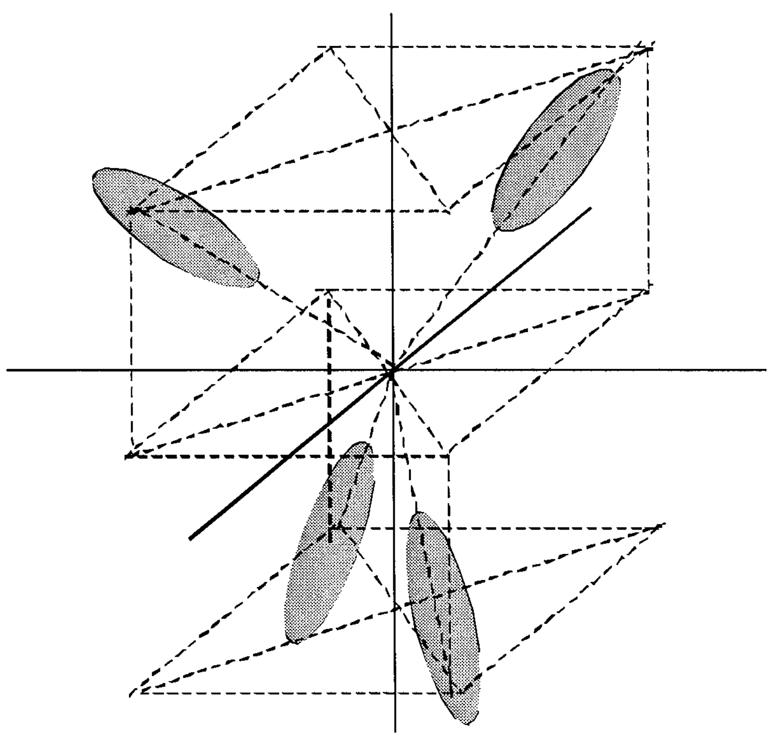

Figure 2. Conduction band minima (pockets) of germanium in k-space.

Then the dyadic products can be written in matrix form as follows:

$$
\begin{aligned}
\hat{e}_1\hat{e}_1 &= \tfrac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, &
\hat{s}_1\hat{s}_1 &= \tfrac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_1\hat{t}_1 &= \tfrac{1}{6}\begin{pmatrix} 1 & 1 & -2 \\ 1 & 1 & -2 \\ -2 & -2 & 4 \end{pmatrix}; \\
\hat{e}_2\hat{e}_2 &= \tfrac{1}{3}\begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix}, &
\hat{s}_2\hat{s}_2 &= \tfrac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_2\hat{t}_2 &= \tfrac{1}{6}\begin{pmatrix} 1 & -1 & -2 \\ -1 & 1 & 2 \\ -2 & 2 & 4 \end{pmatrix}; \\
\hat{e}_3\hat{e}_3 &= \tfrac{1}{3}\begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}, &
\hat{s}_3\hat{s}_3 &= \tfrac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_3\hat{t}_3 &= \tfrac{1}{6}\begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix}; \\
\hat{e}_4\hat{e}_4 &= \tfrac{1}{3}\begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix}, &
\hat{s}_4\hat{s}_4 &= \tfrac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_4\hat{t}_4 &= \tfrac{1}{6}\begin{pmatrix} 1 & -1 & 2 \\ -1 & 1 & -2 \\ 2 & -2 & 4 \end{pmatrix}.
\end{aligned}
\tag{59}
$$

Performing the summation once more, we obtain

$$
\begin{aligned}
\left[m^{(1)}\right]^{-1} &= \frac{1}{3m_l}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \frac{1}{m_t}\left\{\frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6}\begin{pmatrix} 1 & 1 & -2 \\ 1 & 1 & -2 \\ -2 & -2 & 4 \end{pmatrix}\right\} \\
&= \frac{1}{m_l}\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t}\begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix},
\end{aligned}
$$

$$
\begin{aligned}
\left[m^{(2)}\right]^{-1} &= \frac{1}{3m_l}\begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix} + \frac{1}{m_t}\left\{\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6}\begin{pmatrix} 1 & -1 & -2 \\ -1 & 1 & 2 \\ -2 & 2 & 4 \end{pmatrix}\right\} \\
&= \frac{1}{m_l}\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t}\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & \frac{2}{3} \end{pmatrix},
\end{aligned}
$$

$$
\begin{aligned}
\left[m^{(3)}\right]^{-1} &= \frac{1}{3m_l}\begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix} + \frac{1}{m_t}\left\{\frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6}\begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix}\right\} \\
&= \frac{1}{m_l}\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t}\begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{2}{3} \end{pmatrix}.
\end{aligned}
\tag{60}
$$

and so

$$\left[m^{(4)}\right]^{-1} = \frac{1}{3m_l}\begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix} + \frac{1}{m_t}\left\{\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6}\begin{pmatrix} 1 & -1 & 2 \\ -1 & 1 & -2 \\ 2 & -2 & 4 \end{pmatrix}\right\}$$

$$= \frac{1}{m_l}\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t}\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix} . \tag{61}$$

Each pocket holds 1/4 of the electrons. Then the total mass sum equals

$$\sum_j n_0^{(j)}\left[m_j^{-1}\right] = \frac{1}{4}n_0\left\{\frac{1}{m_l}\right\}\begin{pmatrix} \frac{4}{3} & 0 & 0 \\ 0 & \frac{4}{3} & 0 \\ 0 & 0 & \frac{4}{3} \end{pmatrix} + \frac{1}{m_t}\begin{pmatrix} \frac{8}{3} & 0 & 0 \\ 0 & \frac{8}{3} & 0 \\ 0 & 0 & \frac{8}{3} \end{pmatrix} = \frac{1}{3}n_0\left(\frac{1}{m_l} + \frac{2}{m_t}\right)\overleftrightarrow{1} , \tag{62}$$

which is again the isotropic optical mass.

4. Calculations of Sums Over k-space Minima for the Band Structures of Group-V Elements

The band structures of the group-V elements are described in detail by Lin and Falicov [4] and Shapira and Williamson [5]. For the conduction band, the pattern of ellipsoidal pockets shown in figure 3 is obtained; the angle with z-axis θ_C is material-dependent. I assume here that the valence band has a similar structure, although the actual Fermi surface of As is a single multiconnected surface rather than a collection of pockets.

Let

$$\sigma = \cos\theta_C\ , \quad \tau = \sin\theta_C\ . \tag{63}$$

Then the hexagonal symmetry in the basal plane motivates us to introduce the quantities

$$\alpha = 1/2\ , \quad \beta = \sqrt{3}/2\ . \tag{64}$$

This allows us to write the longitudinal-mass principal axis vectors as follows:

$$\begin{aligned}
\hat{e}_1 &= \tau\hat{x} + \sigma\hat{z}\ , \\
\hat{e}_2 &= \alpha\tau\hat{x} + \beta\tau\hat{y} - \sigma\hat{z}\ , \\
\hat{e}_3 &= -\alpha\tau\hat{x} + \beta\tau\hat{y} + \sigma\hat{z}\ , \\
\hat{e}_4 &= -\tau\hat{x} - \sigma\hat{z}\ , \\
\hat{e}_5 &= -\alpha\tau\hat{x} - \beta\tau\hat{y} + \sigma\hat{z}\ , \quad \text{and} \\
\hat{e}_6 &= \alpha\tau\hat{x} - \beta\tau\hat{y} - \sigma\hat{z}\ .
\end{aligned} \tag{65}$$

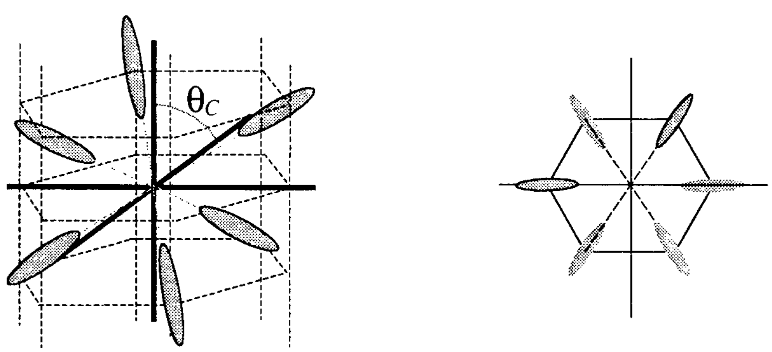

Figure 3. Conduction-band and valence-band minima (pockets) of As and Sb in k-space. Upper pockets are filled with electrons, lower ones with holes. (a) Three-dimensional view, and (b) view down c-axis (z-axis in (a)).

Then the other principal axes are

$$
\begin{array}{lll}
\hat{s}_1 = \hat{y} \,, & \hat{t}_1 = -\sigma\hat{x} + \tau\hat{z} \,; & \\
\hat{s}_2 = -\beta\hat{x} + \alpha\hat{y} \,, & \hat{t}_2 = \alpha\sigma\hat{x} + \beta\sigma\hat{y} + \tau\hat{z} \,; & \\
\hat{s}_3 = -\beta\hat{x} - \alpha\hat{y} \,, & \hat{t}_3 = -\alpha\sigma\hat{x} + \beta\sigma\hat{y} - \tau\hat{z} \,; & \\
\hat{s}_4 = -\hat{y} \,, & \hat{t}_4 = -\sigma\hat{x} + \tau\hat{z} \,; & \\
\hat{s}_5 = \beta\hat{x} - \alpha\hat{y} \,, & \hat{t}_5 = \alpha\sigma\hat{x} + \beta\sigma\hat{y} + \tau\hat{z} \,; & \text{and} \\
\hat{s}_6 = \beta\hat{x} + \alpha\hat{y} \,, & \hat{t}_2 = \alpha\sigma\hat{x} - \beta\sigma\hat{y} + \tau\hat{z} \,. &
\end{array}
\tag{66}
$$

As before, we find the projection operators

$$
\begin{array}{lll}
\hat{e}_1\hat{e}_1 = \begin{pmatrix} \tau^2 & 0 & \sigma\tau \\ 0 & 0 & 0 \\ \sigma\tau & 0 & \sigma^2 \end{pmatrix}, &
\hat{s}_1\hat{s}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_1\hat{t}_1 = \begin{pmatrix} \sigma^2 & 0 & -\sigma\tau \\ 0 & 0 & 0 \\ -\sigma\tau & 0 & \tau^2 \end{pmatrix}; \\
\hat{e}_2\hat{e}_2 = \begin{pmatrix} \alpha^2\tau^2 & \alpha\beta\tau^2 & -\alpha\tau\sigma \\ \alpha\beta\tau^2 & \beta^2\tau^2 & -\beta\tau\sigma \\ -\alpha\tau\sigma & -\beta\tau\sigma & \sigma^2 \end{pmatrix}, &
\hat{s}_2\hat{s}_2 = \begin{pmatrix} \beta^2 & -\alpha\beta & 0 \\ -\alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_2\hat{t}_2 = \begin{pmatrix} \alpha^2\sigma^2 & \alpha\beta\sigma^2 & \alpha\tau\sigma \\ \alpha\beta\sigma^2 & \beta^2\sigma^2 & \beta\tau\sigma \\ \alpha\tau\sigma & \beta\tau\sigma & \tau^2 \end{pmatrix}; \\
\hat{e}_3\hat{e}_3 = \begin{pmatrix} \alpha^2\tau^2 & -\alpha\beta\tau^2 & -\alpha\tau\sigma \\ -\alpha\beta\tau^2 & \beta^2\tau^2 & \beta\tau\sigma \\ -\alpha\tau\sigma & \beta\tau\sigma & \sigma^2 \end{pmatrix}, &
\hat{s}_3\hat{s}_3 = \begin{pmatrix} \beta^2 & \alpha\beta & 0 \\ \alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_3\hat{t}_3 = \begin{pmatrix} \alpha^2\sigma^2 & -\alpha\beta\sigma^2 & \alpha\tau\sigma \\ -\alpha\beta\sigma^2 & \beta^2\sigma^2 & -\beta\tau\sigma \\ \alpha\tau\sigma & -\beta\tau\sigma & \tau^2 \end{pmatrix}; \\
\hat{e}_4\hat{e}_4 = \begin{pmatrix} \tau^2 & 0 & \sigma\tau \\ 0 & 0 & 0 \\ \sigma\tau & 0 & \sigma^2 \end{pmatrix}, &
\hat{s}_4\hat{s}_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_4\hat{t}_4 = \begin{pmatrix} \sigma^2 & 0 & -\sigma\tau \\ 0 & 0 & 0 \\ -\sigma\tau & 0 & \tau^2 \end{pmatrix}; \\
\hat{e}_5\hat{e}_5 = \begin{pmatrix} \alpha^2\tau^2 & \alpha\beta\tau^2 & -\alpha\tau\sigma \\ \alpha\beta\tau^2 & \beta^2\tau^2 & -\beta\tau\sigma \\ -\alpha\tau\sigma & -\beta\tau\sigma & \sigma^2 \end{pmatrix}, &
\hat{s}_5\hat{s}_5 = \begin{pmatrix} \beta^2 & -\alpha\beta & 0 \\ -\alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_5\hat{t}_5 = \begin{pmatrix} \alpha^2\sigma^2 & \alpha\beta\sigma^2 & \alpha\tau\sigma \\ \alpha\beta\sigma^2 & \beta^2\sigma^2 & \beta\tau\sigma \\ \alpha\tau\sigma & \beta\tau\sigma & \tau^2 \end{pmatrix}; \\
\hat{e}_6\hat{e}_6 = \begin{pmatrix} \alpha^2\tau^2 & -\alpha\beta\tau^2 & -\alpha\tau\sigma \\ -\alpha\beta\tau^2 & \beta^2\tau^2 & \beta\tau\sigma \\ -\alpha\tau\sigma & \beta\tau\sigma & \sigma^2 \end{pmatrix}, &
\hat{s}_6\hat{s}_6 = \begin{pmatrix} \beta^2 & \alpha\beta & 0 \\ \alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, &
\hat{t}_6\hat{t}_6 = \begin{pmatrix} \alpha^2\sigma^2 & -\alpha\beta\sigma^2 & \alpha\tau\sigma \\ -\alpha\beta\sigma^2 & \beta^2\sigma^2 & -\beta\tau\sigma \\ \alpha\tau\sigma & -\beta\tau\sigma & \tau^2 \end{pmatrix}.
\end{array}
\tag{67}
$$

The dyadic sums are then

$$
\begin{aligned}
\sum_{i=1}^{6} \hat{e}_i\hat{e}_i &= \begin{pmatrix} 4\alpha^2\tau^2+2\tau^2 & 0 & 2(1-2\alpha)\tau\sigma \\ 0 & 4\beta^2\tau^2 & 0 \\ 2(1-2\alpha)\tau\sigma & 0 & 6\sigma^2 \end{pmatrix}, \\
\sum_{i=1}^{6} \hat{t}_i\hat{t}_i &= \begin{pmatrix} 4\alpha^2\sigma^2+2\sigma^2 & 0 & -2(1-2\alpha)\tau\sigma \\ 0 & 4\beta^2\sigma^2 & 0 \\ -2(1-2\alpha)\tau\sigma & 0 & 6\tau^2 \end{pmatrix}, \text{ and} \\
\sum_{i=1}^{6} \hat{s}_i\hat{s}_i &= \begin{pmatrix} 4\beta^2 & 0 & 0 \\ 0 & 4\alpha^2+2 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\end{aligned}
\tag{68}
$$

Hence,

$$
\sum_{i=1}^{6} \hat{s}_i\hat{s}_i + \hat{t}_i\hat{t}_i = \begin{pmatrix} 4\beta^2+4\alpha^2\sigma^2+2\sigma^2 & 0 & -2(1-2\alpha)\tau\sigma \\ 0 & 4\alpha^2+4\beta^2\sigma^2+2 & 0 \\ -2(1-2\alpha)\tau\sigma & 0 & 6\tau^2 \end{pmatrix}. \tag{69}
$$

Note that because $\alpha = 1/2$, this tensor is diagonal! Since $\beta^2 = 3/4$, the above becomes

$$\sum_{i=1}^{6} \hat{s}_i \hat{s}_i + \hat{t}_i \hat{t}_i = \begin{pmatrix} 3(1+\sigma^2) & 0 & 0 \\ 0 & 3(1+\sigma^2) & 0 \\ 0 & 0 & 6\tau^2 \end{pmatrix} . \tag{70}$$

Likewise, we have

$$\sum_{i=1}^{6} \hat{e}_i \hat{e}_i = \begin{pmatrix} 3\tau^2 & 0 & 0 \\ 0 & 3\tau^2 & 0 \\ 0 & 0 & 6\sigma^2 \end{pmatrix} \tag{71}$$

so that the averaged optical effective-mass tensor is

$$\begin{aligned} \sum_j n_0^{(j)} \left[m_j^{-1} \right] &= \frac{1}{6} n_0 \left\{ \frac{1}{m_l} \begin{pmatrix} 3\tau^2 & 0 & 0 \\ 0 & 3\tau^2 & 0 \\ 0 & 0 & 6\sigma^2 \end{pmatrix} + \frac{1}{m_t} \begin{pmatrix} 3\left(1+\sigma^2\right) & 0 & 0 \\ 0 & 3\left(1+\sigma^2\right) & 0 \\ 0 & 0 & 6\tau^2 \end{pmatrix} \right\} \\ &= \frac{1}{2} n_0 \begin{pmatrix} \frac{1}{m_l}\tau^2 + \frac{1}{m_t}\left(1+\ \sigma^2\right) & 0 & 0 \\ 0 & \frac{1}{m_l}\tau^2 + \frac{1}{m_t}\left(1+\ \sigma^2\right) & 0 \\ 0 & 0 & \frac{1}{m_l}\sigma^2 + \frac{1}{m_t}\tau^2 \end{pmatrix} . \end{aligned} \tag{72}$$

In keeping with our expectations, the effective mass tensor is somewhat anisotropic. However, there is an angle at which it becomes isotropic; this is

$$\cos 2\theta_C = \frac{m_l}{m_t - m_l} . \tag{73}$$

It is easy to show that the reported angles for the group-V materials do not satisfy this criterion, so that anisotropy will be a real issue in any study of their plasma response.

5. Conclusions

In this report, certain properties of the multicomponent plasmas present in the group-V semimetals As, Sb, and Bi have been derived. Notable among these properties is anisotropy of the effective masses of both electrons and holes, which in turn leads to anisotropy in the plasma frequencies of these materials. Because the systems of interest are particles in a host matrix rather than bulk materials, it is likely that this anisotropy in the plasma response will be averaged out in some way; however, this problem must be examined in detail before such a conclusion is warranted.

References

1. J. M. Ziman, *Principles of the Theory of Solids*, ch. 4, Cambridge University Press, Cambridge (1964).

2. Z. Liliental-Weber, A. Claverie, J. Washburn, F. Smith, and R. Calawa, "Microstructure of Annealed Low-Temperature-Grown GaAs Layers," *Appl. Phys.* A **53** (1991), 141.

3. K. Bløtekjær, "Transport Equations for Electrons in Two-Valley Semiconductors," IEEE *Trans. Electron Devices* **ED-17** (1970), 38.

4. P. J. Lin and L. M. Falicov, "Fermi Surface of Arsenic," *Phys. Rev.* **142** (1966), 441.

5. Y. Shapira and S. J. Williamson, "Quantum Oscillations in the Ultrasonic Attenuation and Magnetic Susceptibility of Arsenic," *Phys. Lett.* **14** (1965), 73.

Distribution

Admnstr
Defns Techl Info Ctr
Attn DTIC-OCP
8725 John J Kingman Rd Ste 0944
FT Belvoir VA 22060-6218

Ofc of the Secy of Defns
Attn ODDRE (R&AT)
The Pentagon
Washington DC 20301-3080

Ofc of the Secy of Defns
Attn OUSD(A&T)/ODDR&E(R) R J Trew
3080 Defense Pentagon
Washington DC 20301-7100

AMCOM MRDEC
Attn AMSMI-RD W C McCorkle
Redstone Arsenal AL 35898-5240

CECOM
Attn PM GPS COL S Young
FT Monmouth NJ 07703

DARPA
Attn DARPA/MTO E Martinez
3701 N Fairfax Dr
Arlington VA 22203-1714

Dir for MANPRINT
Ofc of the Deputy Chief of Staff for Prsnnl
Attn J Hiller
The Pentagon Rm 2C733
Washington DC 20301-0300

US Army ARDEC
Attn AMSTA-AR-TD M Fisette
Bldg 1
Picatinny Arsenal NJ 07806-5000

US Army Info Sys Engrg Cmnd
Attn ASQB-OTD F Jenia
FT Huachuca AZ 85613-5300

US Army Natick RDEC Acting Techl Dir
Attn SSCNC-T P Brandler
Natick MA 01760-5002

US Army Simulation, Train, & Instrmntn Cmnd
Attn J Stahl
12350 Research Parkway
Orlando FL 32826-3726

US Army Soldier & Biol Chem Cmnd Dir of Rsrch & Techlgy Dirctrt
Attn SMCCR-RS I G Resnick
Aberdeen Proving Ground MD 21010-5423

US Army Tank-Automtv Cmnd Rsrch, Dev, & Engrg Ctr
Attn AMSTA-TR J Chapin
Warren MI 48397-5000

US Army Train & Doctrine Cmnd
Battle Lab Integration & Techl Dirctrt
Attn ATCD-B J A Klevecz
FT Monroe VA 23651-5850

US Military Academy
Mathematical Sci Ctr of Excellence
Attn MDN-A LTC M D Phillips
Dept of Mathematical Sci Thayer Hall
West Point NY 10996-1786

Nav Surface Warfare Ctr
Attn Code B07 J Pennella
17320 Dahlgren Rd Bldg 1470 Rm 1101
Dahlgren VA 22448-5100

DARPA
Attn S Welby
3701 N Fairfax Dr
Arlington VA 22203-1714

Univ of Maryland Lab for Physical Sci
Attn K Ritter
Attn W Beard
College Park MD 20742

Hicks & Associates Inc
Attn G Singley III
1710 Goodrich Dr Ste 1300
McLean VA 22102

Distribution (cont'd)

Palisades Inst for Rsrch Svc Inc
Attn E Carr
1745 Jefferson Davis Hwy Ste 500
Arlington VA 22202-3402

US Army Rsrch Lab
Attn AMSRL-SL-BN J Soln
Aberdeen Proving Ground MD 21005

Director
US Army Rsrch Ofc
Attn H Everitt
Attn AMSRL-RO M Stroscio
Attn D Wolard
Attn J Harvey
Attn J Prater
Attn M Dutta
Attn AMSRL-RO-D JCI Chang
PO Box 12211
Research Triangle Park NC 27709

US Army Rsrch Lab
Attn AMSRL-DD J M Miller
Attn AMSRL-CI-AI-R Mail & Records Mgmt
Attn AMSRL-CI-AP Techl Pub (3 copies)
Attn AMSRL-CI-LL Techl Lib (3 copies)
Attn AMSRL-SE E Poindexter
Attn AMSRL-SE J M McGarrity
Attn AMSRL-SE J Pellegrino
Attn AMSRL-SE-DP A Bromborsky
Attn AMSRL-SE-DP H Brandt
Attn AMSRL-SE-DP R del Rosario
Attn AMSRL-SE-DS C Fazi
Attn AMSRL-SE-E H Pollehn
Attn AMSRL-SE-E J Mait
Attn AMSRL-SE-E W Clark
Attn AMSRL-SE-EE A Goldberg
Attn AMSRL-SE-EE D Beekman
Attn AMSRL-SE-EE M Patterson

US Army Rsrch Lab (cont'd)
Attn AMSRL-SE-EE S Kennerly
Attn AMSRL-SE-EE Z G Sztankay
Attn AMSRL-SE-EI B Beck
Attn AMSRL-SE-EI J Little
Attn AMSRL-SE-EI K K Choi
Attn AMSRL-SE-EI M Tidrow
Attn AMSRL-SE-EI N Dhar
Attn AMSRL-SE-EI R Leavitt
Attn AMSRL-SE-EI T Zheleva
Attn AMSRL-SE-EM G Simonis
Attn AMSRL-SE-EM J Pamulapati
Attn AMSRL-SE-EM M Tobin
Attn AMSRL-SE-EM P Shen
Attn AMSRL-SE-EM W Chang
Attn AMSRL-SE-EO N Gupta
Attn AMSRL-SE-EP D Wortman
Attn AMSRL-SE-EP J Bradshaw
Attn AMSRL-SE-EP J Bruno
Attn AMSRL-SE-EP M Wraback
Attn AMSRL-SE-EP P Folkes
Attn AMSRL-SE-EP R Tober
Attn AMSRL-SE-EP S Rudin
Attn AMSRL-SE-EP T B Bahder
Attn AMSRL-SE-EP T Oldham
Attn AMSRL-SE-R B Wallace
Attn AMSRL-SE-RE F Crowne (5 copies)
Attn AMSRL-SE-RE R Chase
Attn AMSRL-SE-RE R Kaul
Attn AMSRL-SE-RE S Tidrow
Attn AMSRL-SE-RL C Scozzie
Attn AMSRL-SE-RL A Lepore
Attn AMSRL-SE-RL M Dubey
Attn AMSRL-SE-RL S Svensson
Attn AMSRL-SE-SS K Jones
Adelphi MD 20783-1197

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE August 2000

3. REPORT TYPE AND DATES COVERED Interim, 1/99–9/99

4. TITLE AND SUBTITLE Derivation of Effective-Mass Expressions for Electrons and Holes in the Anisotropic Multiband Semimetals Ar, Sb, and Bi

5. FUNDING NUMBERS
DA PR: AH94
PE: 62120A

6. AUTHOR(S) Frank J. Crowne

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
U.S. Army Research Laboratory
Attn: AMSRL-SE-RE email: fcrown@arl.mil
2800 Powder Mill Road
Adelphi, MD 20783-1197

8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-TR-2152

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Laboratory
2800 Powder Mill Road
Adelphi, MD 20783-1197

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES
ARL PR: ONE6K1
AMS code: 622705.H94

12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

In this report, certain properties of the multicomponent plasmas present in the group-V semimetals As, Sb, and Bi have been derived. Notable among these properties is anisotropy of the effective masses of both electrons and holes, which in turn leads to anisotropy in the plasma frequencies of these materials. Because the systems of interest are particulates in a host matrix rather than bulk materials, it is likely that this anisotropy in the plasma response will be averaged out in some way; however, this problem must be examined in detail before such a conclusion is warranted.

14. SUBJECT TERMS Semimetals, effective mass, plasma frequency

15. NUMBER OF PAGES 26

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	UL

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102