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Dielectric function for a model, two-band semimetal

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An approximate expression for the frequency- and wave-vector-dependent random-phase-approximation longitudinal dielectric function at 0 °K, for a model, two-band semimetal, is derived. In the vicinity of electron and hole pockets, energy bands are assumed to be parabolic and ellipsoidal; the small-pocket approximation as well as the tight-binding approximation have been used for derivations. Contributions to the total polarizability due to interband (insulatorlike) transitions, intravalley (metal-like) transitions, and intervalley transitions, which are specific for a semimetal, have been given in a closed analytic form. The ellipsoidal symmetry of the carrier pockets does not destroy the isotropy of the Thomas-Fermi screening, whereas an anisotropy of interband polarizability does. Carrier transitions between different electron and hole valleys are shown to lead to small contributions to the total dielectric function, which are logarithmically sloped and rather localized in the $\vec{q}$ space. The multipocket plasma frequency in the $\vec{q}\to 0$ limit is anisotropic. A semiheuristic formula for the static dielectric matrix has also been derived with the aid of the generalized sum rule for oscillator strengths. Problems of inverting the dielectric matrix are reviewed.

I. INTRODUCTION

The self-consistent-field (SCF), or random-phase-approximation (RPA), longitudinal dielectric function without local-field corrections has the following form[1,2]:

$$\epsilon(\vec{q},\omega)=1-v_{\vec{q}}\sum_{\substack{n,n'\\ \vec{k},\vec{k}'}}\frac{f(E_{n,\vec{k}})-f(E_{n',\vec{k}'})}{E_{n,\vec{k}}-E_{n',\vec{k}'}+\hbar\omega+i\delta}\times|\langle n,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|n',\vec{k}'\rangle|^2\ . \tag{1}$$

By definition $\epsilon(\vec{q},\omega)=q^{-2}\sum_{ij}\epsilon_{ij}q_iq_j$, where $\epsilon_{ij}(\vec{q},\omega)$ is the dielectric tensor $\vec{D}=\overleftrightarrow{\epsilon}\cdot\vec{E}$, so that $\epsilon(\vec{q},\omega)$ (in general anisotropic in $\vec{q}$) describes the screening of the external potential by a system. $f(E_{n,\vec{k}})$ is the occupation number for the Bloch state $|n,\vec{k}\rangle=\Omega^{-1/2}e^{i\vec{k}\cdot\vec{r}}u_{n,\vec{k}}(\vec{r})$ with energy $E_{n,\vec{k}}$, $v_{\vec{q}}$ is the $\vec{q}$th Fourier transform of the electron potential, δ is an infinitesimal positive quantity, and the matrix element

$$\langle n,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|n',\vec{k}'\rangle=\delta_{\vec{k}',\vec{k}+\vec{q}}\,\Omega_a^{-1}\int u^*_{n,\vec{k}}(\vec{r})u_{n',\vec{k}+\vec{q}}(\vec{r})\,d^3r\ , \tag{2}$$

where the integration extends over the unit cell of the volume Ω_a.

The integrations involved in (1) have been done for a number of physically interesting situations. We should quote here Lindhard's expression for $\epsilon(\vec{q},\omega)$ for the free-electron gas,[3] the static $\epsilon(\vec{q},0)$ for a model isotropic two-band semiconductor of Penn,[4,5] the longitudinal sum-rule estimation of $\epsilon(\vec{q},0)$ for an insulator by Hermanson,[6] and the large-gap, tight-binding valence-band, and orthogonalized-plane-wave (OPW) conduction-band calculation of $\epsilon(\vec{q},0)$ for an insulator by Fry.[7,8] Lindhard's dielectric function is the usual starting point for attempts to go beyond RPA.[9–11] $\epsilon(\vec{q},\omega)$ may be treated as the diagonal part of the dielectric matrix $\epsilon(\vec{q}+\vec{K},\vec{q}+\vec{K}',\omega)$[12–14] ($\vec{K}$, $\vec{K}'$ are reciprocal-lattice vectors). It enables us to obtain the dielectric function with local-field corrections $1/\epsilon^{-1}(\vec{q},\vec{q},\omega)$.[13,14]

Equation (1) has also been applied to the case of a semiconductor with the symmetry-induced zero gap (Liu and Brust,[15] and Broerman[16] and the references quoted there). Cohen and collaborators have used the existing band-structure results to obtain $\epsilon(\vec{q},\omega)$ for a number of semiconducting systems by straightforward numerical computation (Ref. 17 and other references given there).

The purpose of the present paper is to establish the main features of the dielectric function for semimetals. Abrikosov[18,19] bases his formula for the dielectric tensor on realistic band-structure calculations for bismuthlike systems, but only for the case when $\vec{q}=0$. By some simplification of the band picture we have been able to calculate the longitudinal component of the dielectric tensor $\epsilon(\vec{q},\omega)$ and arrive at formulas that are relatively simple and transparent.

In Sec. II we discuss our model of a semimetal. In Sec. III a convenient modification of the initial formula (1) is given. Contributions to the polarizability due to intravalley carrier transitions are calculated in Sec. IV by using the "small-pocket approximation." The semiheuristic formula for the interband-transition polarizability is discussed in Sec. V. Intervalley transitions lead to small, irregular contributions to polarizability; they are investigated in Sec. VI. In Sec. VII the screening and plasma properties of our model semimetal are discussed. The sum rule for oscillator strengths is generalized and applied in Sec. VIII to derive an approximate semiheuristic formula for the static dielectric matrix for semimetals. Approxi-

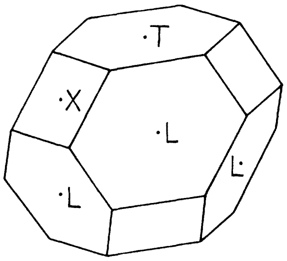

FIG. 1. Brillouin zone for antimony.

mate methods of inverting the matrix are discussed.

II. MODEL OF SEMIMETAL

Let us consider a typical semimetal—antimony. Conduction electrons occupy the states about points L of the Brillouin zone (BZ). Hole states are near points T of BZ (Fig. 1).[19] There are $\sim 10^{-3}$ conduction electrons per atom in electron pockets and the same number of holes in hole pockets. The energy bands at points L are shown in Fig. 2. The pockets are known to extend usually beyond the region of parabolic bands. Some authors suggest that the bands in the vicinity of the pockets are not ellipsoidal.[18,21]

In the present paper we choose a two-band model of a semimetal. It is convenient to treat it as dervied from the two-band model of a semiconductor or insulator (Fig. 3). The bands are separated by the direct energy gap for every wave vector $\vec{k}$ of the BZ. However, the bands overlap over small areas of the BZ, where they attain extreme values. If the states near the minimum of the conduction band are filled with electrons, we refer to a pocket in the electron valley. Empty states near the energy maximum of the valence band will be treated as occupied by holes; we then have a hole pocket in a hole valley.

We assume, for the sake of simplicity, that the energy bands near the pockets are both ellipsoidal and parabolic. The band about the nth pocket, i.e., the nth valley, centered at $\vec{k}_n$, can be written

$$E_{n,\vec{k}} - E_F = (\hbar^2/2m)\eta_n \mathcal{E}_{n,\vec{k}} ,$$
$$\mathcal{E}_{n,\vec{k}} = - D_n + (\vec{k} - \vec{k}_n)\overleftrightarrow{\Theta}_n(\vec{k} - \vec{k}_n) , \tag{3}$$

where $\eta_n \overleftrightarrow{\Theta}_n$ is the inverse effective-mass tensor, D_n is the "depth" of the nth valley, counted from the Fermi energy E_F and the valley character index $\eta_n = +1$ or -1, for electron and hole valleys, respectively. Now we put $\hbar^2/2m = 1$.

Each pocket is characterized by its position vector $\vec{k}_n$, tensor $\overleftrightarrow{\Theta}_n$, carrier concentration n_n, and carrier charge $\eta_n e$, where $\sum_n \eta_n n_n = 0$. The assumptions are that pocket carriers are degenerate (i.e., $T=0$), coupling with phonons is absent, and the pockets are far apart. The final results of our analysis may be useful also in the case of degenerate, many-valley semiconductors.

III. MODIFICATION OF THE POLARIZABILITY FORMULA

Formula (1) may be rewritten as follows:

$$\epsilon(\vec{q}, \omega) = 1 + 4\pi \sum_{n,n'} \alpha_{n,n'}(\vec{q}, \omega) \tag{4}$$

where the intraband $(n = n')$ and interband $(n \neq n')$ polarizabilities are

$$4\pi\alpha_{n,n'}(\vec{q}, \omega) = - v_{\vec{q}}\chi_{n,n'}(\vec{q}, \omega) ,$$
$$\chi_{n,n'}(\vec{q}, \omega) = \sum_{\vec{k},\vec{k}' \in \mathrm{BZ}} \frac{f(E_{n,\vec{k}}) - f(E_{n',\vec{k}'})}{E_{n,\vec{k}} - E_{n',\vec{k}'} + \hbar\omega + i\delta}$$
$$\times |\langle n, \vec{k}| e^{-i\vec{q}\cdot\vec{r}} | n', \vec{k}'\rangle|^2 . \tag{5}$$

The total polarizability is given by an additive form of functions $\chi_{n,n'}$, which will be called transition integrals. Some inter- and intraband transitions are shown in Fig. 3. The relevant transition integrals will be calculated or estimated below.

It is convenient to introduce an energy-shifted occupation number $\tilde{f}$, such that $\tilde{f}(E - E_F) = f(E)$. We have for the valleys (3)

$$f(E_{n,\vec{k}}) = \tfrac{1}{2}(1 - \eta_n) + \eta_n \tilde{f}(\mathcal{E}_{n,\vec{k}}) = \begin{cases} \tilde{f}(\mathcal{E}_{n,\vec{k}}) & \text{for the electron valley} \\ 1 - \tilde{f}(\mathcal{E}_{n,\vec{k}}) & \text{for the hole valley.} \end{cases} \tag{6}$$

In terms of it one can write a convenient formula for both inter- and intravalley transition integrals:

$$\chi_{n,n'}(\vec{q}, \omega) = \sum_{\vec{k},\vec{k}' \in \mathrm{BZ}} \frac{\eta_n \tilde{f}(\mathcal{E}_{n,\vec{k}}) - \eta_{n'} \tilde{f}(\mathcal{E}_{n',\vec{k}'}) - \frac{1}{2}(\eta_n - \eta_{n'})}{\eta_n \mathcal{E}_{n,\vec{k}} - \eta_{n'} \mathcal{E}_{n',\vec{k}'} + \hbar\omega + i\delta}$$
$$\times |\langle n, \vec{k}| e^{-i\vec{q}\cdot\vec{r}} | n', \vec{k}'\rangle|^2 . \tag{7}$$

IV. INTRAVALLEY TRANSITIONS

Let us concentrate now on the case $n = n'$. Introducing a new parameter γ, which takes the values $+1, -1$, and making use of specific properties of the Bloch states, we obtain after a short manipulation the following expression for intravalley transitions:

$$\chi_n(\vec{q}, \omega) = \sum_{\gamma=\pm 1} \sum_{\vec{k} \in \mathrm{BZ}} \tilde{f}(\mathcal{E}_{n,\vec{k}})$$
$$\times \frac{|\langle n, \vec{k}| e^{-i\gamma\vec{q}\cdot\vec{r}} | n, \vec{k} + \gamma\vec{q}\rangle|^2}{\mathcal{E}_{n,\vec{k}} - \mathcal{E}_{n,\vec{k}+\gamma\vec{q}} + \gamma\eta_n(\hbar\omega + i\delta)} . \tag{8}$$

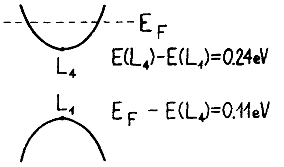

FIG. 2. Energy bands for antimony at point L of BZ (according to Ref. 20).

Calculation of the matrix elements in (8) is difficult. To avoid it, we assume that the effective region of $\vec{k}$ summation in (8) $[f(\mathcal{E}_{n,\vec{k}})=1]$ is small, compared with the BZ. We expect that even if the matrix elements vary significantly over the whole Brillouin zone, they are virtually constant both over electron and hole pockets, if these are sufficiently small. Therefore, within a "small-pocket approximation" we may write

$$\chi_n(\vec{q},\omega)=\sum_{\gamma=\pm 1}|\langle n,\vec{k}_n|e^{-i\gamma\vec{q}\cdot\vec{r}}|n,\vec{k}_n+\gamma\vec{q}\rangle|^2\mathfrak{L}_n(\gamma\vec{q},\gamma\eta_n\omega), \tag{9}$$

where $\vec{k}_n$ is the position vector of the center of nth pocket, and

$$\mathfrak{L}_n(\vec{q},\omega)=\sum_{\vec{k}\in \mathrm{BZ}}\frac{f(\mathcal{E}_{n,\vec{k}})}{\mathcal{E}_{n,\vec{k}}-\mathcal{E}_{n,\vec{k}+\vec{q}}+\hbar\omega+i\,\mathrm{sgn}(\omega)\delta}\,. \tag{10}$$

For the parabolic, ellipsoidal valleys the summations in (10) can be done analytically (see Appendix A). By neglecting for the sake of clarity the band index n, the result can be expressed as follows ($\mathfrak{L}'$ and $\mathfrak{L}''$ stand, respectively, for real and imaginary parts of $\mathfrak{L}$):

$$\mathfrak{L}'(\vec{q},\omega)=\frac{-1}{4\pi e^2}k^2_{\mathrm{TF}}\left\{\frac{1}{4}-\frac{\hbar\omega}{4\tilde{q}^2}+\frac{k_F}{4\tilde{q}}\left[1-\left(\frac{\hbar\omega-\tilde{q}^2}{2k_F\tilde{q}}\right)^2\right]\right.$$
$$\left.\times\ln\left|\frac{\tilde{q}^2+2k_F\tilde{q}-\hbar\omega}{\tilde{q}^2-2k_F\tilde{q}-\hbar\omega}\right|\right\},$$

$$\mathfrak{L}''(\vec{q},\omega)=-\,\mathrm{sgn}(\omega)\frac{1}{4\pi e^2}\frac{\pi}{4}k^2_{\mathrm{TF}}\frac{k_F}{\tilde{q}}$$
$$\times\begin{cases}1-\left(\dfrac{\hbar\omega-\tilde{q}^2}{2k_F\tilde{q}}\right)^2, & \left|\dfrac{\hbar\omega-\tilde{q}^2}{2k_F\tilde{q}}\right|\leqslant 1 \quad \text{(11a)}\\ 0\quad , & \left|\dfrac{\hbar\omega-\tilde{q}^2}{2k_F\tilde{q}}\right|>1\,, \quad \text{(11b)}\end{cases}$$

where

$$\begin{aligned}&\tilde{q}\equiv(\vec{q}\cdot\overleftrightarrow{\Theta}\cdot\vec{q})^{1/2}\quad, && |\overleftrightarrow{\Theta}|\equiv\det[\overleftrightarrow{\Theta}\,],\\ &k_F^2\equiv|\overleftrightarrow{\Theta}|^{1/3}(k_F^0)^2\quad, && k^2_{\mathrm{TF}}\equiv|\overleftrightarrow{\Theta}|^{-1/3}(k^0_{\mathrm{TF}})^2,\\ &k_F^0\equiv(3\pi^2 n)^{1/3}\quad, && (k^0_{\mathrm{TF}})^2=(4/\pi)a_B^{-1}k_F^0\,.\end{aligned} \tag{12}$$

The properties of a hypothetical ellipsoidal parabolic single-band system, which follow from (11), are summarized in Appendix B.

To gain some insight into the physics of the situation, let us estimate the matrix elements in (8) and (9) in the tight-binding approximation. Let $\varphi_n(\vec{r}-\vec{l})$ be the atomic or Wannier function localized on lattice site $\vec{l}$, and we have

$$\begin{aligned}&|n,\vec{k}\rangle=N^{-1/2}\sum_{\vec{l}}e^{i\vec{k}\cdot\vec{l}}\varphi_n(\vec{r}-\vec{l}),\\ &\langle n,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|n',\vec{k}+\vec{q}\rangle=\sum e^{-\vec{k}\cdot\vec{l}}M_{n,n'}(\vec{l},\vec{q}),\\ &M_{n,n'}(\vec{l},\vec{q})=\int\varphi_n^*(\vec{r}-\vec{l})\,e^{-i\vec{q}\cdot\vec{r}}\varphi_{n'}(\vec{r})\,d^3r\,.\end{aligned} \tag{13}$$

With a very sharp localization of $\varphi_n(\vec{r})$ ("very tight binding"), we obtain

$$\begin{aligned}&\langle n,k|e^{-i\vec{q}\cdot\vec{r}}|n',k+q\rangle\simeq M_{n,n'}(0,\vec{q}),\\ &M_{n,n}(0,\vec{q})=\rho_n(\vec{q}),\end{aligned} \tag{14}$$

where $\rho_n(\vec{q})$ is the atomic or Wannier form factor. If $\varphi_n(\vec{r})$ is the atomic function of s type, $\rho_n(\vec{q})$ decreases at large distances as q^{-4}. With this localization, therefore, the dielectric function tends to decrease with $\vec{q}$ more rapidly than in the plane-wave-like case, where $\langle n,k|e^{-i\vec{q}\cdot\vec{r}}|n,k+q\rangle=1$. With a moderate localization, the $\vec{l}\neq 0$ terms in (13) are not negligible and lead to anisotropy in $\vec{q}$ and dependence of $\chi_n(\vec{q},\omega)$ on the position vectors of pockets $\vec{k}_n$. In the long-wavelength limit the matrix elements in (8) become unity.

In principle, the tight-binding approximation is unsuitable for a system with the complicated electronic structure of a semimetal. We have been able, however, to derive the intravalley contributions to the polarizability without using it and it will serve only to estimate terms regarded as small, i.e., those due to intervalley transitions.

V. INTERBAND TRANSITIONS

Let us consider first nearly vertical small-$\vec{q}$ interband transitions, marked I in Fig. 3. In the present, the semimetal modifications of the semiconductor (insulator) two-band scheme [Fig. 3(a)] are assumed to concern only very small areas of the BZ. It follows that the principal contribution to polarizability is the same as in a semiconductor.

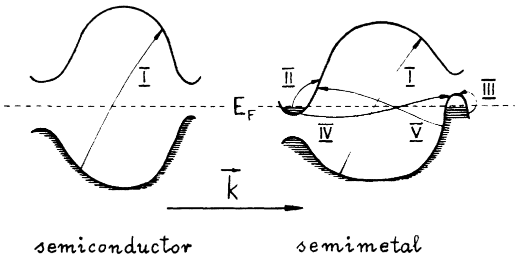

FIG. 3. Energy-band diagram for model two-band semimetal, as derived from the corresponding diagram for semiconductor or insulator. Arrows show various electron and hole transitions, contributing to the polarizability of the system.

In the static case ($\omega = 0$) it is rendered by the formula of Penn[4,5]:

$$4\pi\alpha_P(\vec{q}, 0) \simeq \left(\frac{h\Omega_v}{\mathcal{E}_g + \lambda q^2}\right)^2, \quad \mathcal{E}_g / E_F \ll 1$$
$$\chi_P(\vec{q}, 0) \simeq -\frac{q^2}{4\pi e^2}\left(\frac{\hbar\Omega_v}{\mathcal{E}_g + \lambda q^2}\right)^2, \tag{15}$$

where Ω_v is the plasma frequency for the lower (valence) band's electrons of density N, i.e., $\Omega_v^2 = 4\pi e^2 N/m$ and λ in the assumed units ($\hbar^2/2m = 1$) is close to 1. Within the small-pocket approximation N equals practically the number of all electrons $N + \frac{1}{2}n_0$ (where $n_0 = \sum_s n_s$), because $n_0 \ll N$; $\mathcal{E}_g$, the "average" energy gap between bands, is expected to be much larger than direct gaps in the pocket regions.

To gain some understanding of what the corresponding formula should be in the dynamical case ($\omega \neq 0$), let us consider a simple hypothetical system with two levels separated by $\mathcal{E}_g$. With N-fold degeneracy, the Kramers–Heisenberg dispersion formula (see, e.g., Ref. 22) gives us

$$4\pi\alpha'(0, \omega) = (\hbar\Omega_v)^2/[\mathcal{E}_g^2 - (\hbar\omega)^2]. \tag{16}$$

The imaginary part of the polarizability is $\sim \delta(\mathcal{E}_g - \hbar\omega) - \delta(\mathcal{E}_g + \hbar\omega)$. $\alpha'(0, \omega)$ matches the polarizability of Penn, Eq. (15), for $\omega = 0$ and is accurate in the limit $\omega \to \infty$. (In the intermediate, singular range of frequencies $\hbar\omega \sim \mathcal{E}_g$, we may possibly "smooth" it out, e.g., by the substitution $\alpha' \to \alpha'/(1 + \beta\alpha'^2)$, where β is a small adjustable quantity.)

Hence, it is expected that to include information about the dynamics of the system, the following, semiheuristic form of the small-$\vec{q}$ interband-transition integral may be useful:

$$\chi_P'(\vec{q}, \omega) \simeq -\frac{q^2}{4\pi e^2}\frac{(\hbar\Omega_v)^2}{(\mathcal{E}_g + \lambda q^2)^2 - (\hbar\omega)^2}, \tag{17}$$

the imaginary part having the two-δ-function form, as that for (16). For a noncubic crystal this formula should be further generalized, to include the anisotropy in $\vec{q}$.

VI. TRANSITIONS BETWEEN DIFFERENT VALLEYS

Besides the metal-like and insulatorlike transitions already considered, it is reasonable to distinguish in semimetals certain special transitions, which are just peculiar to them. These are the large-momentum-transfer (large-$\vec{q}$) transitions between states close to the Fermi level belonging to different valleys, nonequivalent with respect to the reciprocal-lattice translations. As an example we may take transitions IV and V between electron and hole valleys in Fig. 3(b), or the transitions between two electron valleys centered at different points L of the Brillouin zone (Fig. 1). Under the small-pocket approximation the corresponding contributions to the total polarizability should be considered small. However, owing to the step character of the occupation number and the zero denominators in (7), these transitions can contribute in an irregular way, and this effect should be therefore analyzed in detail.

This distinction of intervalley transitions is somewhat arbitrary; in an exact treatment they would be automatically included in the usual inter- or intraband transitions.

To clarify the nature of the expected irregular behavior, we shall apply the very-tight-binding approximation (14) and put also

$$M_{n,n'}(0, \vec{q}) = M_{n',n}(0, \vec{q}) = M_{n,n'}(0, \vec{q}). \tag{18}$$

In general, integrations for ellipsoidal valleys cannot be done analytically. We assume spherical valleys

$$\mathcal{E}_{n,\vec{k}} \equiv e_n(\vec{k} - \vec{k}_n) = -D_n^2 + d_n^2(k - k_n)^2, \tag{19}$$

where, for further convenience, the self-explanatory function $e_n(\vec{k})$ is introduced. Simple transformations of (7) give

$$\sum_{n \neq n'} \chi_{n,n'}(\vec{q}, \omega) = \sum_{n \neq n'} |M_{n,n'}(0, \vec{q})|^2$$
$$\times \{\eta_n[\mathcal{L}_{n,n'}(\vec{q} - k_{n,n'}, \omega, K_n)$$
$$+ \mathcal{L}_{n,n'}(-\vec{q} - \vec{k}_{n,n'}, -\omega, K_n)]$$
$$- \tfrac{1}{2}(\eta_n - \eta_{n'})\mathcal{L}_{n,n'}(\vec{q} - \vec{k}_{n,n'}, \omega, K_{\mathrm{BZ}})\}, \tag{20}$$

where the pocket separation vector $\vec{k}_{n,n'} = \vec{k}_{n'} - \vec{k}_n$, K_n is the radius of the nth pocket, i.e., $e_n(K_n - k_n) = 0$, K_{BZ} is a radius which is larger than the pocket's radii, and

$$\mathcal{L}_{n,n'}(\vec{Q}, \omega, K) = 2\frac{\Omega}{(2\pi)^3}\int_{|\vec{k}| \leq K}\frac{d^3k}{\eta_n e_n(\vec{k}) - \eta_{n'} e_{n'}(\vec{k} + \vec{Q}) + \hbar\omega + i\,\mathrm{sgn}(\omega)\delta}. \tag{21}$$

Here the $\vec{k}$ summation has already been substituted by integration. The following properties of the functions $\mathcal{L}$ should be noted:

$$\mathcal{L}_{n,n'}(\vec{Q}, \omega, K) = -\mathcal{L}_{n',n}(-\vec{Q}, -\omega, K),$$
$$\mathcal{L}_{n,n'}(\vec{Q}, \omega, K) = \mathcal{L}_{n,n'}(|\vec{Q}|, \omega, K). \tag{22}$$

Using $(x+i\delta)^{-1} = \mathcal{P}(1/x) - i\pi\delta(x)$, we can evaluate both the real and the imaginary parts of $\mathfrak{L} = \mathfrak{L}' + i\mathfrak{L}''$ by elementary methods. The result is

$$\mathfrak{L}'_{n,n'}(\vec{\mathrm{Q}}, \omega, K) = \frac{2\Omega}{(2\pi)^3}\,\frac{\pi}{2|\vec{\mathrm{B}}|}\Bigg[4KP + (2C/A + 2K^2 - P^2) \times \ln\left|\frac{(2K+P)^2 + 4C/A - P^2}{(2K-P)^2 + 4C/A - P^2}\right| - \begin{cases} 2WP\left(\operatorname{arctg}\dfrac{2K+P}{W} + \operatorname{arctg}\dfrac{2K-P}{W}\right)\Bigg], & W^2 > 0 \\ MP\ln\left|\dfrac{(2K+M)^2 - P^2}{(2K-M)^2 - P^2}\right|\Bigg], & M^2 > 0 \end{cases} \tag{23}$$

where by definition

$$4C/A - B^2/A^2 \equiv \begin{cases} W^2 & \text{for left-hand-side positive} \\ -M^2 & \text{for left-hand-side negative,} \end{cases} \tag{24}$$

and

$$P = |\vec{\mathrm{B}}|/A, \quad A = \eta_n d_n^2 - \eta_{n'} d_{n'}^2, \quad \vec{\mathrm{B}} = 2\eta_{n'} d_{n'}^2 \vec{\mathrm{Q}},$$
$$C = \hbar\omega - \eta_n D_n^2 + \eta_{n'} D_{n'}^2 - \eta_{n'} d_{n'} \vec{\mathrm{Q}}^2 . \tag{25}$$

Similarly

$$\mathfrak{L}''_{n,n'}(\vec{\mathrm{Q}}, \omega, K) = -\operatorname{sgn}(\omega)\pi\frac{2\Omega}{(2\pi)^3}\,\frac{\pi}{|\vec{\mathrm{B}}|}\begin{cases} k_2^2 - k_1^2, & k_2 < K, \quad \Delta \geqslant 0 \\ K^2 - k_1^2, & k_1 < K < k_2, \Delta \geqslant 0 \\ 0\,, & K < k_1, \quad \Delta \geqslant 0 \\ 0\,, & \Delta < 0\,, \end{cases} \tag{26}$$

where $\Delta = B^2 - 4AC$ and k_1, k_2 are

$$\begin{aligned} 2Ak_1 &= |\vec{\mathrm{B}}| - \Delta^{1/2} && \text{for } C > 0, \text{ all } A \\ &= -|\vec{\mathrm{B}}| + \Delta^{1/2} && \text{for } C < 0, \text{ all } A, \\ 2Ak_2 &= |\vec{\mathrm{B}}| + \Delta^{1/2} && \text{for } A > 0, \text{ all } C \\ &= -|\vec{\mathrm{B}}| - \Delta^{1/2} && \text{for } A < 0, \text{ all } C\,. \end{aligned} \tag{27}$$

Time-reversal symmetry requires that the band structure of a crystal has inversion symmetry. Let us consider the situation shown in Fig. 4. Pockets 1′ and 2′ are equivalent by inversion to 1 and 2, respectively. Transitions from pocket 1 to the empty states of valley 2 are accompanied by transitions from filled states of 2′ to empty states of 1′. An important point is that as a function of $\vec{\mathrm{q}}$ the sum of transition integrals $\chi_{1,2} + \chi_{2',1'}$ is, in general, more smooth than is each of its components separately.

Equation (20) should therefore be replaced as follows:

$$\sum_{n\neq n'} \chi_{n,n'}(\vec{\mathrm{q}}, \omega) = \sum_{n\neq n'} |M_{n,n'}(0, \vec{\mathrm{q}})|^2 \psi_{n,n'}(\vec{\mathrm{q}}, \omega), \tag{28}$$

where

$$\psi_{n,n'}(\vec{\mathrm{q}}, \omega) = \frac{1}{2}\sum_{\gamma=\pm1}\big[\eta_n \mathfrak{L}_{n,n'}(\gamma\vec{\mathrm{q}} - \vec{\mathrm{k}}_{n,n'}, \gamma\omega, K_n) + \eta_{n'}\mathfrak{L}_{n'n}(\gamma\vec{\mathrm{q}} - \vec{\mathrm{k}}_{n,n'}, \gamma\omega, K_{n'}) - \tfrac{1}{2}(\eta_n - \eta_{n'})\mathfrak{L}_{n,n'}(\vec{\mathrm{q}} - \vec{\mathrm{k}}_{n,n'}, \gamma\omega, K_{\mathrm{BZ}})\big], \tag{29}$$

in which the contributions due to transitions between the inversion-equivalent valleys have been explicitly added.

Using (22), we can write for the transitions between two valleys of the same character (i.e., $\eta_1 = \eta_2 = \eta$)

$$\psi_{1,2} = \tfrac{1}{2}\eta\sum_{\gamma=\pm1}\big[\mathfrak{L}_{1,2}(\gamma\vec{\mathrm{q}} - \vec{\mathrm{k}}_{1,2}, \gamma\omega, K_1) + \mathfrak{L}_{2,1}(\gamma\vec{\mathrm{q}} - k_{1,2}, \gamma\omega, K_2)\big], \tag{30}$$

and for transitions between the valleys of opposite character (i.e., $\eta_1 = \eta = -\eta_2$)

$$\psi_{1,2} = \tfrac{1}{2}\eta\sum_{\gamma=\pm1}\big[\mathfrak{L}_{1,2}(\gamma\vec{\mathrm{q}} - \vec{\mathrm{k}}_{1,2}, \gamma\omega, K_1) + \mathfrak{L}_{1,2}(\gamma\vec{\mathrm{q}} - \vec{\mathrm{k}}_{1,2}, -\gamma\omega, K_2) - \mathfrak{L}_{1,2}(\vec{\mathrm{q}} - \vec{\mathrm{k}}_{1,2}, \gamma\omega, K_{\mathrm{BZ}})\big]. \tag{31}$$

We shall study now the static contributions only. They appear to be independent of η.

A. Transitions between different electron valleys

Equation (30) gives

$$\psi_{1,2} = \frac{1}{2}\sum_{\vec{\mathrm{p}}=\vec{\mathrm{q}}\pm\vec{\mathrm{k}}_{1,2}}\big[\mathfrak{L}_{1,2}(\vec{\mathrm{p}}, 0, K_1) + \mathfrak{L}_{2,1}(\vec{\mathrm{p}}, 0, K_2)\big]. \tag{32}$$

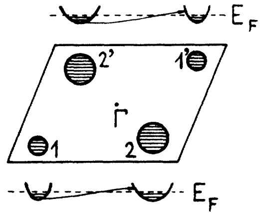

FIG. 4. Inversion property of the electronic band structure. Transitions between electron pockets 1 and 2 accompany the transitions between the inversion equivalent pockets 2′ and 1′.

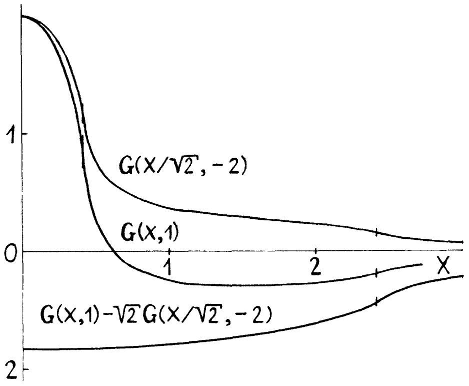

FIG. 5. Polarizability factors G, corresponding to transitions 1 → 2 and 2′ → 1′ between the electron valleys in Fig. 4 (upper curves) and full polarizability factor connected with these transitions, vs the reduced wave vector X. Vertical bars mark points of the logarithmic slope.

For the sake of simplicity we take both valleys as of the same depth, $D_1 = D_2 = D$. Equation (32) may be rewritten as follows:

$$\psi_{1,2} = \frac{1}{2}\,\frac{2\Omega}{(2\pi)^3}\,2\pi\,\frac{D}{(d_1 d_2)^{3/2}}\left[\mathcal{T}(X^+, s) + \mathcal{T}(X^-, s)\right], \tag{33}$$

where

$$X^{\pm} = |\vec{q} \pm \vec{k}_{1,2}|/K_1, \qquad s = d_2/d_1 = K_1/K_2, \tag{34}$$

and

$$\mathcal{T}(X, s) = \frac{s^{3/2}}{1-s^2}\left[G\left(X, \frac{s^2}{1-s^2}\right) - \frac{1}{s}\,G\left(sX, \frac{1}{s^2-1}\right)\right], \tag{35}$$

where

$$G(X, c) = 1 + \frac{1 - c(2c+1)X^2}{4cX}\ln\left|\frac{1+2cX-cX^2}{1-2cX-cX^2}\right| - \tfrac{1}{2}(c^2+c)^{1/2}X^2\ln\left|\frac{1+2(c^2+c)^{1/2}X+cX^2}{1-2(c^2+c)^{1/2}X+cX^2}\right| . \tag{36}$$

The slope of function $G(X, c)$ is logarithmic at two (positive) values of x: $1 \pm (1+1/c)^{1/2}$ (Fig. 5). The second term in the square bracket of (35) represents transitions between a pair of valleys equivalent by inversion to the pair contributing the first term (Fig. 4). In spite of the relative complexity of both terms separately, the sum is remarkably simple:

$$\mathcal{T}(X, s) = -2\,\frac{s^{1/2}}{1+s}\,f\left(\frac{sX}{1+s}\right), \tag{37}$$

where f is the Bardeen function[23]

$$f(y) = \tfrac{1}{2} + \frac{1-y^2}{4y}\ln\left|\frac{1+y}{1-y}\right| . \tag{38}$$

Hence, $\mathcal{T}(X, s)$ has a logarithmic slope only at $X = (1+s)/s$. This should be so also beyond the very-tight-binding approximation for the matrix elements (14) and (18) used here. If the curvatures of the two valleys are identical, $d_1 = d_2$, then $s = 1$ and $\mathcal{T}(X, 1) = -f(X/2)$, as for the intraband transitions in the free-electron case.

Going back to the initial nomenclature, the equation for logarithmic-slope surfaces can be written as follows:

$$|\vec{q} \pm \vec{k}_{n,n'}| = K_n + K_{n'} . \tag{39}$$

Away from these surfaces, the intervalley-transition integrals decrease rapidly with the distance. Consequently, in the $\vec{q}$ space, the meaningful contributions may be imagined as small hills well apart. For some directions of $\vec{q}$ they are absent and obviously do not contribute to the total polarizability.

B. Transitions between electron valleys and hole valleys

Equation (31) gives

$$\psi_{1,2} = \frac{\Omega}{(2\pi)^2}\,\frac{(D_1^2+D_2^2)^{1/2}}{(d_1^2+d_2^2)^{3/2}}\sum_{y=y^{\pm}}\left[F(y, \xi_1, c) + F(y, \xi_2, c) - F(y, \xi_{\mathrm{BZ}}, c)\right], \tag{40}$$

where

$$F(y, \xi, c) = \xi + \frac{\xi^2 - 1 + (1-c^2)y^2}{4y}\ln\left|\frac{(\xi+cy)^2 + a^2y^2 - 1}{(\xi-cy)^2 + a^2y^2 - 1}\right| - \begin{cases} (a^2y^2-1)^{1/2}\left[\operatorname{arctg}\dfrac{\xi+cy}{(a^2y^2-1)^{1/2}} + \operatorname{arctg}\dfrac{\xi-cy}{(a^2y^2-1)^{1/2}}\right], & a^2y^2 > 1 \\ \tfrac{1}{2}(1-a^2y^2)^{1/2}\ln\left|\dfrac{[\xi+(1-a^2y^2)^{1/2}]^2 - c^2y^2}{[\xi-(1-a^2y^2)^{1/2}]^2 - c^2y^2}\right|, & a^2y^2 < 1 \end{cases} \tag{41}$$

where

$$a^2 \equiv 2 - c^2, \quad c^2 = \frac{2d_2^2}{d_1^2+d_2^2}, \quad \xi_n^2 = K_n^2\,\frac{d_1^2+d_2^2}{D_1^2+D_2^2}, \quad n = 1, 2, \qquad y^2 = \frac{d_2^2 p^2}{2(D_1^2+D_2^2)}, \quad p^{\pm} \equiv |\vec{p}^{\pm}| = |\vec{q} \pm \vec{k}_{1,2}|, \quad \xi_{\mathrm{BZ}} > \xi_n . \tag{42}$$

Let us investigate in detail the slightly simpler case of equal curvature for both valleys, $d_1 = d_2 = 1$, i.e., $c=1$. Let $F(y, \xi, 1) \equiv F(y, \xi)$ and $y^{\pm} = p^{\pm}/(2D_1^2 + 2D_2^2)^{1/2}$, $\xi_1 = D_1/[(D_1^2+D_2^2)/2]^{1/2}$, $\xi_2 = D_2/[(D_1^2+D_2^2)/2]^{1/2}$; then $\xi_1^2+\xi_2^2=2$, and we have

$$\psi_{1,2} = \frac{\Omega}{(2\pi)^2} 2^{-3/2}(D_1^2+D_2^2)^{1/2}$$

$$\times \sum_{y=y^{\pm}} [F(y, \xi_1) + F(y, (2-\xi_1^2)^{1/2}) - F(y, \xi_{\mathrm{BZ}})] . \tag{43}$$

The slope of function F is logarithmic along certain lines in the $y-\xi$ plane, for $\xi < \sqrt{2}$, as shown in Fig. 6. Figure 7 shows the slopes of $F(y, 2)$, $F(y, \frac{31}{25})$ and $F(y, \frac{17}{25})$ [note: $(\frac{31}{25})^2 + (\frac{17}{25})^2 = 2$].

The square-root behavior at $y=1$ is a purely mathematical effect, which disappears completely in $F(y, \xi) + F(y, (2-\xi^2)^{1/2}) - F(y, \xi_{\mathrm{BZ}})$, the only function of physical importance, where $\xi_{\mathrm{BZ}} > \sqrt{2}$. The logarithmic slopes cancel each other at $y = \frac{1}{2}(\xi + (2-\xi^2)^{1/2})$, but add up at $y = \frac{1}{2}(\xi - (2-\xi^2)^{1/2})$.

With the situation considered in terms of the reduced transition vector $\vec{p}$ the slope is logarithmic when both electron and hole pockets are internally tangent (in the case of transitions between two electron valleys it is so when the pockets are externally tangent). A general form of the equation for the logarithmic slope surface, due to transitions between electron valley n and hole valley n' (and vice versa), is as follows:

$$|\vec{q} - \vec{k}_{n,n'}| = |K_n - K_{n'}| . \tag{44}$$

In this case also the logarithmic slope depends critically on the direction in the $\vec{q}$ space. If present, it occurs twice along the same direction, giving rise to an interesting volcano-type slope of the transition integral and polarizability (Fig. 8). Still, the formulas (40) and (43) have a rather illustrative character only, owing to the arbitrary choice of ξ_{BZ}.

In fact, these transitions are a part of the interband transitions I of Fig. 3, distinguished rather artificially to investigate the effect of transitions between states at the Fermi level. The irregular behavior analyzed above should therefore be manifest as small kinks imposed on Penn-like polarizability, Eq. (15).

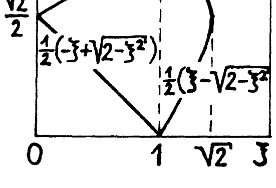

FIG. 6. Positions of the logarithmic-slope points of the function $F(y, \xi)$ in the $y-\xi$ plane; y is the reduced wave vector, whereas ξ depends on the characteristics of the electron and hole pockets.

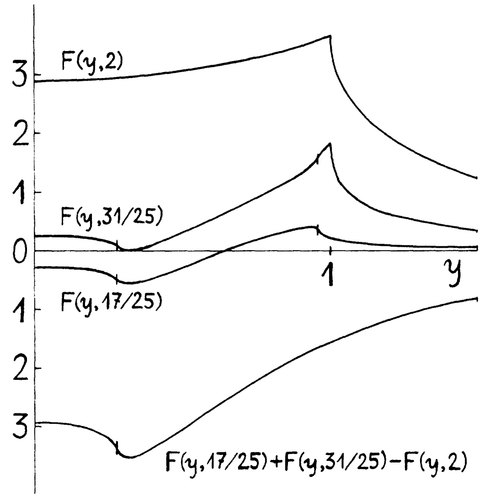

FIG. 7. Polarizability factors F connected with the transitions between electron and hole valleys vs the reduced wave vector y. The lowest curve represents the full polarizability factor. Vertical bars indicate the points of the logarithmic slope.

So far we have been able to express analytically (although with different degrees of accuracy) all polarizability contributions relevant for our model semimetal. Henceforth, we shall investigate its physical properties.

VII. SCREENING AND PLASMA PROPERTIES OF SEMIMETALS

A. Long-range screening

Let us consider $\epsilon(\vec{q}, \omega)$ for $\omega = 0$ and in the $q \to 0$ limit. From (9) and (15) we find

$$\epsilon(\vec{q}, 0) = \epsilon_P + \frac{1}{q^2} \sum_s k_{\mathrm{TF},s}^2 , \tag{45}$$

where

$$\epsilon_P = 1 + (\hbar \Omega_v / \mathcal{E}_g)^2 . \tag{46}$$

The intervalley contributions are neglected as small in comparison with ϵ_P, and the second term on the right-hand side of (45) summarizes all the intravalley contributions. With (45) treated as valid for all wave vectors $\vec{q}$, we arrive at a static screening of the Thomas–Fermi type. The screened Coulomb potential assumes the form

$$(1/\epsilon_P r)\, e^{-\kappa_{\mathrm{TF}} r} , \tag{47}$$

where κ_{TF} is the multipocket Thomas–Fermi screening factor

$$\kappa_{\mathrm{TF}}^2 \equiv \frac{1}{\epsilon_P} \sum_s k_{\mathrm{TF},s}^2 = \frac{4}{\pi a_B \epsilon_P} \sum_s |\overleftrightarrow{\Theta}_s|^{-1/3} (3\pi^2 n_s)^{1/3} . \tag{48}$$

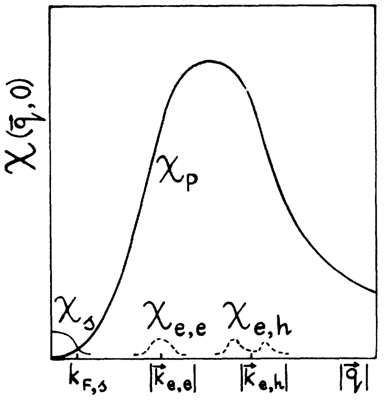

FIG. 8. Various transition integrals relevant for the model semimetal vs the wave vector q (static case, schematically): χ_s, intravalley, metal-like transitions (II and III in Fig. 3): χ_P, interband, insulatorlike transitions (I in Fig. 3): χ_{ee}, transitions between two electron (or hole) valleys: χ_{eh}, transitions between electron valley and hole valley (or vice versa, IV and V in Fig. 3). In both intervalley cases q is assumed as being parallel to the corresponding intervalley vectors k_{ee} or k_{eh}.

Three facts must be noted: (i) For a given density of pocket electrons and holes n_0, the screening factor κ_{TF} is larger when the number of pockets is higher, because $\sum_s n_s^{1/3} > (\sum_s n_s)^{1/3}$. (ii) The high value of the interband dielectric constant ϵ_P ($\simeq 100$ for Bi[24]) tends to increase the screening radius $\kappa_{\mathrm{TF}}^{-1}$, therefore favoring long-range interactions in semimetals. However, the concept of the Thomas-Fermi screening is not often applicable. (iii) Using the ellipsoidal valleys, we retain the spherical symmetry of the screened potential (47). However, in real systems, the interband polarizability [corresponding to $\alpha_P(\vec{q},0)$ in our case] is anisotropic, and this would make the screening so, too. In a system with the symmetry C_{3v} the equipotential surface around the point charge would be an ellipsoid of revolution around an axis parallel to the trigonal direction.

B. Static dielectric function–Kohn anomaly

In the static case,

$$\epsilon(\vec{q},0)=1-\frac{4\pi e^2}{q^2}\Big[\chi_P(\vec{q},0)+\sum_s\chi_s(\vec{q},0)+\sum_{s\neq s'}\chi_{s,s'}(\vec{q},0)\Big]. \tag{49}$$

The intravalley transition integral for the valley s is given by (9), with the appropriate inverse-effective-mass tensor $\overleftrightarrow{\Theta}_s$ and carrier density n_s. Since $\chi_s(\vec{q},0)$ incorporates

$$\mathcal{L}_s(\vec{q},0)=\frac{-1}{4\pi e^2}\frac{k_{\mathrm{TF},s}^2}{2}f\left(\frac{(\vec{q}\cdot\overleftrightarrow{\Theta}_s\cdot\vec{q})^{1/2}}{2k_{F,s}}\right) \tag{50}$$

[where $f(y)$ is defined by (38)], it has an infinite slope on the surface $\vec{q}\cdot\overleftrightarrow{\Theta}\cdot\vec{q}=4k_{\mathrm{F},s}^2$. It follows that the same behavior is displayed by function (49) at the set of surfaces corresponding to all the free-carrier pockets. The intervalley transitions, represented by $\chi_{s,s'}$, give rise to similar behavior at other surfaces in the $\vec{q}$ space [Eqs. (39) and (44)].

The Kohn effect therefore may, in principle, occur in the phonon dispersion curves[25,26] a number of times for every direction in the BZ. In practice, however, it can hardly be observed under the present experimental conditions, because its amplitude must be expected to be much smaller than for simple metals, especially under intervalley conditions.

It is not yet clear whether in calculating the phonon frequencies it is enough to screen the ionic interactions in the semimetal with the static dielectric function (49). It goes as q^{-2} for $\vec{q}\to 0$ and so the acoustic sum rule[27] is formally fulfilled, as it is for simple metals. However, the large amplitude of the semiconductor-type contribution to the polarizability (Fig. 8) suggests the need to use the full dielectric matrix $\epsilon(\vec{q}+\vec{K},\vec{q}+\vec{K}',0)$ rather than its diagonal version, Eq. (49). Related problems are discussed in Sec. VIII.

Various contributions to $\epsilon(\vec{q},0)$ are shown in Fig. 8. One sees that $\chi_P(\vec{q},0)$ dominates over the intravalley-transition integrals $\chi_s(\vec{q},0)$ [by the factor $\sim(h\Omega_v)^2/(\mathcal{E}_g k_{\mathrm{TF},s}^2)$], except in the small-$\vec{q}$ region. This is why the exact behavior of $\chi_s(\vec{q},0)$ at large $\vec{q}$ is not very important. Figure 8 shows also one of the contributions due to transitions between different electron valleys – χ_{ee}. Their maxima are in the region of large χ_P. Therefore, even if they are comparable with χ_P in amplitude, they seem to play a minor role. One should remember, however, that they have logarithmic slopes at certain surfaces in the $\vec{q}$ space. The same concerns also the volcano-type contributions χ_{eh} (Fig. 8) due to transitions between electron and hole valleys. It is interesting to note that electron and hole intravalley transitions contribute to $\epsilon(\vec{q},0)$ in the same way.

The above considerations show that for $|\vec{q}| < \min\{k_{F,s}\}$, the static dielectric function is dominated by the intravalley anisotropic contributions. If $|\vec{q}| > \max\{k_{F,s}\}$, it behaves much like the Penn dielectric function (15), with small logarithmic-slope kinks superimposed for some directions of $\vec{q}$ (Fig. 9).

C. Plasma oscillations

The dispersion relation for plasma frequencies of the system can be arrived at by solving the equation $\epsilon'(\vec{q},\omega)=0$. In semimetals we must expect in addition to the usual high-frequency plasma oscillations concerning all electrons also low-frequency plasma oscillations involving only free carriers in the pockets. Oscillations of this kind

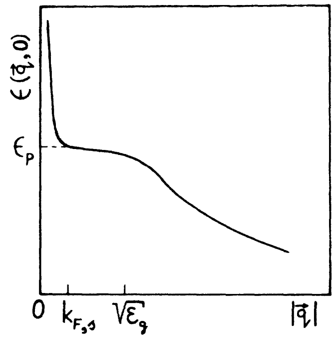

FIG. 9. Static dielectric function for semimetal vs wave vector $\vec{q}$ (schematically). Logarithmic-slope kinks are not shown.

have been first discussed by Pines.[28]

To simplify the final formulas we shall consider only the case $\vec{q}\to 0$ and assume that the plasma frequency is low enough as compared with $\mathcal{E}_g/\hbar$. Thus we can put $\omega=0$ in the formula for the interband polarizability (17). Its imaginary part then becomes 0. When $\vec{q}\to 0$ and $\omega>0$ $\mathcal{L}''(\vec{q},\omega)$ also disappears, and the damping of plasma oscillations may be neglected. We find easily

$$v_{\vec{q}}\chi_s'(\vec{q},\omega)\xrightarrow[\vec{q}\to 0]{}\frac{\omega_s^2}{\omega^2}\frac{\vec{q}\cdot\overleftrightarrow{\Theta}_s\cdot\vec{q}}{q^2}\,, \tag{51}$$

where $\omega_s^2=4\pi e^2 n_s/m$. Now we can write the expression for the real part of the dielectric function (neglecting for the sake of simplicity small terms, which are due to intervalley transitions):

$$\epsilon'(\vec{q},\omega)=\epsilon_P-\frac{1}{\omega^2 q^2}\sum_s \omega_s^2\vec{q}\cdot\overleftrightarrow{\Theta}_s\cdot\vec{q} \tag{52}$$

from which follows the formula for the multipocket plasma frequency for small $\vec{q}$,

$$\omega_{\mathrm{mp}}^2(\vec{q})=\frac{1}{\epsilon_P}\frac{\vec{q}\cdot\overleftrightarrow{\Theta}\cdot\vec{q}}{q^2}\,\omega_0^2,\quad \omega_0^2=\frac{4\pi e^2 n_0}{m}\ . \tag{53}$$

Summation s goes over all electron and hole pockets, and the multivalley inverse effective mass tensor is given by

$$\overleftrightarrow{\Theta}=\sum_s\frac{n_s}{n_0}\overleftrightarrow{\Theta}_s\ . \tag{54}$$

It follows from (53) that ω_{mp} can be anisotropic in $\vec{q}$. The number of independent parameters of the tensor $\overleftrightarrow{\Theta}$ follows from symmetry. For a cubic crystal there would be only one parameter (i.e., isotropy), but for the bismuth structure, for instance, there are two parameters. The previously mentioned anisotropy of $\alpha_P(\vec{q},\omega)$ for noncubic crystals may also contribute in (53).

Equation (52) may be compared with Abrikosov's result,[18] which, however, corresponds strictly to $\vec{q}=0$ and so does not show the anisotropy.

VIII. DIELECTRIC MATRIX–PROBLEM OF INVERSION

All the results obtained so far neglect local fields in crystals. Nevertheless, they may be useful for an approximate interpretation of optical experiments $[\epsilon(0,\omega)]$, or for calculating the screened potential of a charged impurity $[\epsilon(\vec{q},0)]$. The description of the collective phenomenon, the phonon in semimetals, requires the dielectric matrix it seems. In the SCF approximation it takes the form[12–14]

$$\epsilon(\vec{X},\vec{Y},\omega)=\delta_{\vec{X},\vec{Y}}+4\pi\sum_{n,n'}\alpha_{n,n'}(\vec{X},\vec{Y},\omega)\,, \tag{55}$$

$$\begin{aligned}
4\pi\alpha_{n,n'}(X,Y,\omega)&=-v(\vec{X})\chi_{n,n'}(\vec{X},\vec{Y},\omega)\,,\\
\chi_{n,n'}(\vec{X},\vec{Y},\omega)&=\sum_{\vec{K},\vec{K}'}f(E_{n,\vec{k}})\\
&\quad\times\left[\frac{\langle n,\vec{k}|e^{-i\vec{X}\cdot\vec{r}}|n',\vec{k}'\rangle\langle n',\vec{k}'|e^{i\vec{Y}\cdot\vec{r}}|n,\vec{k}\rangle}{E_{n,\vec{k}}-E_{n',\vec{k}'}+\hbar\omega+i\delta}\right.\\
&\quad\left.+\frac{\langle n,\vec{k}|e^{i\vec{Y}\cdot\vec{r}}|n',\vec{k}'\rangle\langle n',k'|e^{-i\vec{X}\cdot\vec{r}}|n,\vec{k}\rangle}{E_{n,\vec{k}}-E_{n',\vec{k}'}-\hbar\omega-i\delta}\right],
\end{aligned} \tag{56}$$

where $\vec{X}=\vec{K}+\vec{q}$, $\vec{Y}=\vec{K}'+\vec{q}$, $\vec{K}$, $\vec{K}'$ are reciprocal-lattice vectors, and

$$\begin{aligned}\langle n,\vec{k}|e^{-i(\vec{K}+\vec{q})\cdot\vec{r}}|n',\vec{k}'\rangle&=\delta_{\vec{k}',\vec{k}+\vec{q}+\vec{K}}\Omega_a^{-1}\int u_{n,\vec{K}}^*(\vec{r})u_{n',\vec{k}+\vec{q}}(\vec{r})\\
&\quad\times e^{-i\vec{K}\cdot\vec{r}}d^3r\ .\end{aligned} \tag{57}$$

The results for $\epsilon(\vec{q},\omega)$ suggest that only intravalley transitions II and III and interband transitions I (Fig. 3) play an important role in semimetals. The intravalley (metal-like) contribution may be calculated easily within the small-pocket approximation. Using $E_{n,\vec{k}+\vec{K}}=E_{n,\vec{K}}$ and $|n,\vec{k}+\vec{K}\rangle=|n,\vec{k}\rangle$ we obtain

$$\begin{aligned}\chi_n(\vec{X},\vec{Y},\omega)&=\langle n,\vec{k}_n|e^{-i\vec{X}\cdot\vec{r}}|n,\vec{k}_n+\vec{q}\rangle\\
&\quad\times\langle n,\vec{k}_n+\vec{q}|e^{i\vec{Y}\cdot\vec{r}}|n,\vec{k}_n\rangle\mathcal{L}_n(\vec{q},\omega)\\
&\quad+\langle n,\vec{k}_n|e^{i\vec{Y}\cdot\vec{r}}|n,\vec{k}_n-\vec{q}\rangle\\
&\quad\times\langle n,\vec{k}_n-\vec{q}|e^{-i\vec{X}\cdot\vec{r}}|n,\vec{k}_n\rangle\mathcal{L}_n(-\vec{q},-\omega)\,.\end{aligned} \tag{58}$$

In the very-tight-binding approximation [see (14)] the formula becomes simplified to

$$\begin{aligned}\chi_n(\vec{X},\vec{Y},\omega)&\simeq\rho_n(\vec{X})\rho_n^*(\vec{Y})\mathcal{L}_n(\vec{q},\omega)\\
&\quad+\rho_n^*(-\vec{X})\rho_n(-\vec{Y})\mathcal{L}_n(-\vec{q},-\omega)\ .\end{aligned} \tag{59}$$

Now let us take up the insulatorlike transitions I. To have at least some information about the contribution concerned we assume that both bands are very flat, so that $E_{c,\vec{k}}-E_{v,\vec{k}'}\simeq\mathcal{E}_g$ over the Jones zone (JZ), and concentrate on the static case. The following sum rule will be used:

$$\sum_t (E_t - E_s)[\langle s| e^{-i\vec{X}\cdot\vec{r}}| t\rangle\langle t| e^{i\vec{Y}\cdot\vec{r}}| s\rangle + \langle s| e^{i\vec{Y}\cdot\vec{r}}| t\rangle \times \langle t|e^{-i\vec{X}\cdot\vec{r}}| s\rangle] = (\hbar^2/m)\vec{X}\cdot\vec{Y}\langle s|e^{-i(\vec{X}-\vec{Y})\vec{r}}|s\rangle \ . \quad (60)$$

Its proof follows from an expansion of the expectation value of the double commutator $[[H, e^{-i\vec{X}\cdot\vec{r}}], e^{i\vec{Y}\cdot\vec{r}}]$ in the eigenstate $|s\rangle$ of $H=p^2/2m + V(\vec{r})$. Equation (60) is a generalization of the sum rule for the oscillator strengths.[29] For the two-flat-bands system the formula (60) can be approximately written as follows:

$$\mathcal{E}_g[\langle v, \vec{k}| e^{-i\vec{X}\cdot\vec{r}}| c, \vec{k}+\vec{X}\rangle\langle c, \vec{k}+\vec{X}| e^{i\vec{Y}\cdot\vec{r}}| v, \vec{k}\rangle + \langle v, \vec{k}| e^{i\vec{Y}\cdot\vec{r}}| c, \vec{k}-\vec{X}\rangle \langle c, \vec{k}-\vec{X}|e^{-i\vec{X}\cdot\vec{r}}|v, \vec{k}\rangle] \simeq (\hbar^2/m)\vec{X}\cdot\vec{Y}\langle v, \vec{k}| e^{-i(\vec{X}-\vec{Y})\vec{r}}| v, k\rangle \ . \quad (61)$$

Using it in the two-flat-band version of (55), we have

$$4\pi\alpha_P(\vec{X}, \vec{Y}, 0) \simeq \left(\frac{\hbar\Omega_v}{\mathcal{E}_g}\right)^2 \frac{\vec{X}\cdot\vec{Y}}{X^2}\rho_v(\vec{X}-\vec{Y}), \quad (62)$$

where $\rho_v(\vec{Q})$ is the form factor of the electron charge distribution for the lower (valence) band over the Jones zone

$$\rho_v(\vec{Q}) = N^{-1}\sum_{\vec{k}\in JZ} f(E_{v,\vec{k}})\langle v, \vec{k}| e^{-i\vec{Q}\cdot\vec{r}}| v, \vec{k}\rangle \ . \quad (63)$$

To make a suggestion, formula (62) may perhaps be applicable to real systems, when we treat $\rho_v(\vec{Q})$ as a sum of the Brillouin-zone form factors for all valence bands.

Formula (62) shows correct behavior in the $q\to 0$ limit.[27] The right formula for polarizability should converge to (15) on the main diagonal. Besides, by definition (55), $\chi_P(\vec{X}, \vec{Y}, 0)$ should be Hermitian in the indices $\vec{X}, \vec{Y}$. Therefore, the following form may be useful as the polarizability matrix for the insulatorlike transitions:

$$4\pi\alpha_P(\vec{X}, \vec{Y}, 0) \simeq \frac{\vec{X}\cdot\vec{Y}}{X^2} P(\vec{X})P(\vec{Y})\rho_v(\vec{X}-\vec{Y}), \quad (64)$$

where for cubic crystals $P(\vec{X}) = \hbar\Omega_v/(\mathcal{E}_g + \lambda X^2)$.

We assume in the present that the adiabatic approximation holds (although perhaps it does not for pocket carrier concentrations as low as, e.g., in Bi). Otherwise we would have to derive the dielectric matrix for a coupled electron-lattice system, which is very difficult. The phonon dynamical matrix in the adiabatic approximation has the following form[27, 30, 31]:

$$D^{\alpha,\beta}_{s,s'}(\vec{q}) = (M_sM_{s'})^{-1/2}[C^{\alpha\beta}_{s,s'}(\vec{q}) - \delta_{s,s'}\sum_{s''} C^{\alpha\beta}_{s,s''}(0)],$$
$$C^{\alpha\beta}_{s,s'}(\vec{q}) = Z_s Z_{s'}\frac{4\pi e^2}{\Omega}\sum_{\vec{K},\vec{K}'}\frac{(\vec{q}+\vec{K})^\alpha(\vec{q}+\vec{K}')^\beta}{|\vec{q}+\vec{K}|^2} \times\epsilon^{-1}(\vec{q}+\vec{K}, \vec{q}+\vec{K}', 0)\, e^{i(\vec{K}\cdot\vec{R}_s-\vec{K}'\cdot\vec{R}_{s'})} \ , \quad (65)$$

where Z_s is the charge of the nucleus at position $\vec{R}_s$ in the unit cell. If the charge neutrality of the system is to be preserved, the following sum rule must be fulfilled[27]:

$$\lim_{\vec{q}\to 0}\sum_{s,\vec{K}}\epsilon^{-1}(\vec{q}, \vec{q}+\vec{K}, 0)\frac{|\vec{q}|\,|\vec{q}+K|^\beta}{|\vec{q}+\vec{K}|^2} Z_s e^{-i\vec{K}\cdot\vec{R}_s} = 0 \ . \quad (66)$$

Both expressions depend on $\epsilon^{-1}(\vec{X}, \vec{Y}, 0)$, so there arises the problem of inverting the matrix $\epsilon(\vec{X}, \vec{Y},0)$. Essentially, for the infinite system considered, $\epsilon(\vec{q}+\vec{K}, \vec{q}+\vec{K}', 0) \equiv \epsilon_{\vec{K},\vec{K}'}(\vec{q})$ is an infinite matrix in $\vec{K}, \vec{K}'$. There seem to be no general criteria and prescriptions for the inversion procedure for infinite matrices.[32] The problem can be formulated as the "integral" equation for ϵ^{-1},[13] but it also is difficult to solve. We therefore have to concentrate on approximations suggested by physical intuition.

Hayashi and Shimizu,[33] Hanke and Bilz,[34] and Brown[35] have shown that the inverting of the dielectric matrix, rewritten in the representation of localized or Wannier functions, comes down to inverting a certain matrix indexed by lattice vectors. The more localized the functions, the lower becomes, in practice, the dimension of the matrix to be inverted.

Bertoni *et al.*[36] claim they have inverted the dielectric matrix for silicon analytically. It seems they have assumed the off-diagonal terms to be "small," so as to be able to write

$$\epsilon_{\vec{K},\vec{K}'} = \epsilon_{\vec{K}}\delta_{\vec{K},\vec{K}'} + \Delta_{\vec{K},\vec{K}'} \ ,$$
$$\epsilon^{-1}_{\vec{K},\vec{K}'} = \delta_{\vec{K},\vec{K}'}\frac{1}{\epsilon_{\vec{K}'}} - \frac{1}{\epsilon_{\vec{K}}}\Delta_{\vec{K},\vec{K}'}\frac{1}{\epsilon_{\vec{K}'}} \ . \quad (67)$$

This is exact to the first order in $\overleftrightarrow{\Delta}$.

The other approach, suggested by formula (64) [approximately, $\rho_v(\vec{Q})$ is large if the corresponding energy gap $\mathcal{E}_g(\vec{Q})$ is large], is to assume that there are only a few $\vec{K}$'s for which the external potential creates contributions to a total potential that are not negligible when $\vec{K}\neq\vec{K}'$. Let us put S for this set of "a few" reciprocal lattice vectors. One has the quasidiagonal form

$$\tilde{\epsilon}_{\vec{K},\vec{K}'} = \begin{cases} \epsilon_{\vec{K},\vec{K}'} \ , & \vec{K}, \vec{K}'\in S \\ 0 \ , & \vec{K}\in S, \vec{K}'\notin S \text{ or } \vec{K}\notin S, \ \vec{K}'\in S \\ \delta_{\vec{K},\vec{K}'}\epsilon_{\vec{K},\vec{K}} \ , & \vec{K}, \ \vec{K}'\notin S \end{cases} \quad (68)$$

the inverse being

$$\tilde{\epsilon}^{-1}_{\vec{K},\vec{K}'} = \begin{cases} \tilde{\epsilon}^{-1}_{\vec{K},\vec{K}'} \ , & \vec{K}, \vec{K}'\in S \\ 0 \ , & \vec{K}\in S, \ \ \vec{K}'\notin S \text{ or } \vec{K}\notin S, \ \vec{K}'\in S \\ \dfrac{1}{\epsilon_{\vec{K},\vec{K}}}\delta_{\vec{K},\vec{K}'} \ , & \vec{K}, \vec{K}'\notin S \end{cases} \quad (69)$$

with $\epsilon^{-1}_{\vec{K},\vec{K}'\in S}$ defined by the equation $\sum_{\vec{K}''\in S}\epsilon_{\vec{K},\vec{K}''}$

$\times \epsilon^{-1}_{\vec{K}'', \vec{K}'} = \delta_{\vec{K}, \vec{K}'}$.

In the consistent microscopic theory, (66) can be satisfied only if self-consistent band-structure calculations are carried out. To avoid this difficult step, Bertoni *et al.*[35] used (66) as an additional equation rather than as the consistency test. The off-diagonal elements of the dielectric matrix estimated previously within the pseudopotential approach have been made to satisfy (66) by multiplying them by a suitably chosen numerical factor.

In practice it is a convenient procedure, for it ensures that in the $\vec{q} \to 0$ limit acoustic-phonon frequencies tend to zero in spite of all the approximations made in the process of the derivation and inversion of the dielectric matrix. Basically, however, this procedure is far from satisfactory.

IX. CONCLUSIONS

The dielectric properties of a semimetal are rather close to those of a degenerate semiconductor. Only the intravalley (metal-like) electron transitions and interband (semiconductorlike) transitions seem to be important. They usually predominate over intervalley transitions, which are specific for a semimetal.

It has to be remembered, however, that both intra- and intervalley transitions produce, on certain surfaces in the $\vec{q}$ space, logarithmic slopes in the static dielectric function. For ellipsoidal carrier pockets these surfaces, owing to intravalley transitions, also have the shape of an ellipsoid, which is centered at $\vec{q} = 0$ but is twice as large as the pockets. Polarizability contributions for intervalley transitions have been estimated, for spherical pockets; in this case the logarithmic-slope surfaces have the shape of spheres centered on intervalley vectors. Such transitions introduce into the static dielectric function the hill-type (transitions between like valleys) and volcano-type (transitions between unlike valleys) contributions.

There may be the low-frequency plasma oscillation of all the pocket carriers in the system. The anisotropy of the energy bands within the valleys leads to an anisotropy of this multipocket plasma frequency, even in the $q \to 0$ limit. The additional anisotropy may come from the anisotropy of the interband (semiconductorlike) polarizability, which is possible for noncubic crystals. In the latter case even the static Thomas–Fermi screening would be anisotropic.

The generalization of the sum rule for the oscillator strengths has been given and applied to derive an approximate formula for the static dielectric matrix. It has shown the importance of the charge-distribution form factor for valence bands in the description of the semiconductorlike polarizability matrix. The formula obtained has a relatively simple form and the correct analytic properties in the $q \to 0$ limit. It is expected that it may be useful in calculating the phonon frequencies of some semiconductor or insulator systems.

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APPENDIX A: CALCULATION OF THE FUNCTION $\mathcal{L}(\vec{q},\omega)$

We fix the origin of the coordinate system at the center of the ellipsoid. We may write

$$\mathcal{L}(\vec{q}, \omega) = \frac{2\Omega}{(2\pi)^3} \int_{\vec{k}\cdot\overleftrightarrow{\Theta}\cdot\vec{k} \leq k_F^2} \frac{d^3k}{A - 2\vec{k}\cdot\overleftrightarrow{\Theta}\cdot\vec{q} + i\,\mathrm{sgn}(\omega)\delta}\,, \tag{A1}$$

where $A = \hbar\omega - \tilde{q}^2$, $\tilde{q}^2 \equiv \vec{q}\cdot\overleftrightarrow{\Theta}\cdot\vec{q}$, and the $\vec{k}$ integration goes over the volume of the ellipsoid, $\vec{k}\cdot\overleftrightarrow{\Theta}\cdot\vec{k} = k_F^2$. Now we rotate the coordinate system to coincide with the system of the principal axis of the ellipsoid and then rescale every dimension to transform the ellipsoid into the unit sphere. We obtain

$$\begin{aligned} \mathcal{L}'(\vec{q}, \omega) &= \frac{2\Omega}{(2\pi)^3} \frac{k_F^3}{|\overleftrightarrow{\Theta}|^{1/2}} \int_{|\vec{k}|\leq 1} \frac{d^3k}{A - 2\vec{Q}\cdot\vec{k}}\,, \\ \mathcal{L}''(\vec{q}, \omega) &= -\,\mathrm{sgn}(\omega)\pi \frac{2\Omega}{(2\pi)^3} \frac{k_F^3}{|\overleftrightarrow{\Theta}|^{1/2}} \int_{|\vec{k}|\leq 1} d^3k \\ &\quad \times \delta(A - 2\vec{Q}\cdot\vec{k})\,, \end{aligned} \tag{A2}$$

where $Q_i \equiv (\vec{q}\cdot\overleftrightarrow{\Theta}\cdot\overleftrightarrow{T})_i(\overleftrightarrow{T}^{-1}\cdot\overleftrightarrow{\Theta}\cdot\overleftrightarrow{T})_{ii}^{-1/2}k_F$ ($\overleftrightarrow{T}$ is the matrix of rotation) and the integration goes over the unit sphere. Introducing the spherical coordinates, we can easily calculate the integrals using

$$\begin{aligned} &\int_0^x dy\,y \ln \frac{y-a}{y+a} = \tfrac{1}{2}(x^2 - a^2)\ln\left|\frac{x-a}{x+a}\right| - xa\,, \\ &\int_0^\pi d\varphi \sin\varphi\, \delta(\cos\varphi - a) = \begin{cases} 1\,, & |a| \leq 1 \\ 0\,, & |a| > 1 \end{cases} \\ &|\vec{Q}| = k_F\tilde{q}\,, \end{aligned} \tag{A3}$$

with the final result (11).

APPENDIX B: PROPERTIES OF THE SINGLE, PARABOLIC, ELLIPSOIDAL BAND SYSTEM

Assuming that the matrix elements in (8) are unity, we have for the dielectric function in the one-band case the formula

$$\epsilon(\vec{q}, \omega) = 1 - (4\pi e^2/q^2)[\mathcal{L}(\vec{q}, \omega) + \mathcal{L}(\vec{q}, -\omega)]\,, \tag{B1}$$

which is identical with the Lindhard formula for the free-electron gas. The ellipsoidal character of the band enters only through the argument $\tilde{q}$ and the parameters scaled with $|\overleftrightarrow{\Theta}|^{1/3}$. $|\overleftrightarrow{\Theta}|^{-1/3}$, the geometric mean of effective masses, may be called the screening effective mass for the one-band system (in electron mass units).

Let us summarize the properties of the hypothetical system, characterized by the single, parabolic, ellipsoidal band: (i) The constant $\epsilon(\vec{q}, \omega)$ surfaces are ellipsoids given by the equation $\vec{q} \cdot \overleftrightarrow{\Theta} \cdot \vec{q} = \text{const}$. (ii) The surface of the logarithmic slope of $\epsilon(\vec{q}, 0)$ is rendered by the equation $\vec{q} \cdot \overleftrightarrow{\Theta} \cdot \vec{q} = 4k_F^2$ (or $\vec{q} = 2k_F$). (iii) The Thomas-Fermi screening is isotropic. (iv) The plasma frequency is an anisotropic function of $\vec{q}$ in the $\vec{q} \rightarrow 0$ limit:

$$\omega_p^2 = \frac{4\pi e^2 n}{m} \frac{\vec{q} \cdot \overleftrightarrow{\Theta} \cdot \vec{q}}{q^2} . \tag{B2}$$

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$$\sum_t (E_t - E_s)[\,|\langle s|e^{-\vec{q}\cdot\vec{r}}|t\rangle|^2 + |\langle s|e^{i\vec{q}\cdot\vec{r}}|t\rangle|^2] = \hbar^2 q^2/m .$$

Some authors (Refs. 6 and 22) used the simplified formula

$$\sum_t (E_t - E_s)\,|\langle s|e^{-i\vec{q}\cdot\vec{r}}|t\rangle|^2 = \hbar^2 q^2/2m ,$$

which is not appropriate if the eigenfunctions of H are complex (e.g., plane waves evidently obey the former, not the latter formula).

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