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Influence of the Electron–Electron Scattering on the Kinetic Effects in Many-Valley Semiconductors

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The conductivity and magnetoresistance (MR) of a many-valley semiconductor are calculated for the case when electron scattering on impurities and on the electrons of the same and of the other valleys is characterized by different coupling constants. It is shown that, with increasing anisotropy of the ellipsoidal energy surfaces, the contribution of the electron–electron scattering grows rapidly and MR decreases. The ratio of the coupling constants may be determined unambiguously through analysing the stress dependence of the conductivity and of MR in these semiconductors. The piezomagnetoresistance is shown to increase along with growing electron–electron scattering.

Es werden Leitfähigkeit und Magnetowiderstand (MR) eines Vieltalhalbleiters für den Fall berechnet, wo die Elektronstreuung an Störstellen und mit Elektronen desselben und der anderen Täler durch unterschiedliche Kopplungskonstanten charakterisiert ist. Es wird gezeigt, daß mit steigender Anisotropie der ellipsoiden Energieflächen der Beitrag der Elektron–Elektronstreuung stark zunimmt und MR abnimmt. Das Verhältnis der Kopplungskonstanten läßt sich eindeutig durch eine Analyse der Spannungsabhängigkeit der Leitfähigkeit und der MR in diesen Halbleitern berechnen. Es wird gezeigt, daß der Piezo-Magnetowiderstand zusammen mit wachsender Elektron–Elektronstreuung zunimmt.

1. Introduction

Reference to a number of studies [1 to 6], concerned with calculations of the transport coefficients of heavily doped one-valley semiconductors, shows that one should necessarily take into account both electron–electron (e–e) scattering and that on impurities. The e–e scattering giving rise to a momentum exchange, its increase results in equalizing the electron momenta. Since the transverse MR is due to the counterflows directed perpendicularly to the current $\boldsymbol{J}$ and to the magnetic field $\boldsymbol{H}$, the e–e scattering essentially decreases MR, equalizing the transverse momenta (reducing their values and even nullifying them in the limit of intensive e–e scattering). Thus, as it was indicated in [6], MR is much more affected by e–e scattering than the conductivity, the latter being not very sensitive to the randomisation of electron momenta. A similar strong influence of intervalley e–e[1]) scattering on MR should be expected in many-valley semiconductors.

Actually with intense intravalley scattering and without intervalley one the electrons of each valley attain their specific momentum value; then MR stems

[1]) It is to be pointed out that here the intervalley e–e scattering is understood as that leading to a momentum transfer all electrons remaining in their valleys. Both the e–e and impurity scattering accompanied by intervalley electron transitions are neglected as they need much greater momentum transfer.

from the many-valley character of the band structure, i.e. from electron counterflows of different valleys in the transverse direction (perpendicular to $\boldsymbol{J}$ and to $\boldsymbol{H}$). The intervalley scattering which equalizes the electron momenta in different valleys reduces MR essentially. Therefore it may be possible to evaluate the intensities both of the intravalley and intervalley scattering knowing the magnitudes of MR and conductivity; a straightforward calculation of the latter is given below.

2. Solution of the Boltzmann Equation

In line with [5] we present the distribution function $f^{(\alpha)}(\boldsymbol{p})$ of electrons in the α valley in the form

$$f^{(\alpha)}(\boldsymbol{p}) = f_0(\varepsilon)\,[1 + F^{(\alpha)}(\boldsymbol{p})]; \quad |F^{(\alpha)}(\boldsymbol{p})| \ll 1\,, \tag{1}$$

where $f_0(\varepsilon)$ is the equilibrium Boltzmann distribution function, ε and $\boldsymbol{p}$ are the energy and the crystal momentum. The Coulomb scattering being dominant, one readily obtains, in the framework of ordinary routine, the Boltzmann equation for $F^{(\alpha)}(\boldsymbol{p})$:

$$-\,e\boldsymbol{E}\,\frac{\partial f_0}{\partial \boldsymbol{p}} - \frac{e}{c}\,[\boldsymbol{v}, \boldsymbol{H}]\,f_0(\varepsilon)\,\frac{\partial F^{(\alpha)}(\boldsymbol{p})}{\partial \boldsymbol{p}} = n_{np}B_{np}\sum_{i,j}\frac{\partial}{\partial p_i}\left[f_0(\varepsilon)\,\frac{\partial F^{(\alpha)}(\boldsymbol{p})}{\partial p_j}\,\frac{\partial^2 v}{\partial v_i \partial v_j}\right] -$$
$$-\sum_{i,j}\frac{\partial}{\partial p_i}\sum_{\beta=1}^{\lambda} B_{\alpha\beta}\int f_0(\varepsilon)\,f_0(\varepsilon')\left[\frac{\partial F^{(\beta)}(\boldsymbol{p}')}{\partial p_j'} - \frac{\partial F^{(\alpha)}(\boldsymbol{p})}{\partial p_j}\right]\frac{\partial^2(|\boldsymbol{v} - \boldsymbol{v}'|)}{\partial v_i \partial v_j}\,\mathrm{d}\boldsymbol{p}'. \tag{2}$$

Here $e = |e|$ stands for the electron charge, λ is the number of the valleys, n_{np} is the impurity concentration, $\boldsymbol{E}$ and $\boldsymbol{H}$ are the vectors of electric and magnetic fields. The terms on the right hand side of (2) describe the impurity scattering [5] and e–e scattering [5, 7], respectively. In contrast to [5, 7] where the same coupling constant $B = 2\pi e^4 \ln(h/b_0)$ (h is the radius of screening, $b_0 = e^2/(3kT)$) is attributed to the different above-mentioned scattering mechanisms, here the impurity scattering (B_{np}), the intravalley e–e scattering ($B_{\alpha\alpha}$) and the intervalley e–e scattering ($B_{\alpha\beta,\beta\neq\alpha}$) are described by different parameters. In this study we escape calculating the parameters B_{np} $B_{\alpha\alpha}$, and $B_{\alpha\beta}$ and discussing physical reasons for their difference, yet we shall indicate an experimental possibility of determining their ratios ($B_{\alpha\alpha}/B_{\alpha\beta}$, $B_{\alpha\alpha}/B_{np}$) by having estimated galvanomagnetic effects. Concerning the disparity between B_{np} and $B_{\alpha\alpha}$ arising from the difference of the static and h.f. dielectric permittivities, see, for instance, p. 113 in [9] and [10]; $B_{\alpha\alpha}$ and $B_{\alpha\beta}$ may differ only due to their being obtained by averaging the Coulomb interaction potential over the Bloch functions of a given valley ($B_{\alpha\alpha}$) or of different valleys ($B_{\alpha\beta}$).

For simplicity we confine ourselves to considering semiconductors of n-Si type where the valleys are situated on mutually perpendicular axes.[2]) The treatment of the Boltzmann equation in presence of the e–e scattering is discussed in detail in [5, 6]. In agreement with these studies, $F^{(\alpha)}(\boldsymbol{p})$ may be presented as follows:

$$F^{(\alpha)}(\boldsymbol{p}) = \frac{eE_x}{B_{np}n_{np}}\sqrt{\frac{\pi kT}{m_\perp}}\left(\boldsymbol{p}\cdot\boldsymbol{C}^{(\alpha)} + \boldsymbol{p}\cdot\boldsymbol{A}^{(\alpha)}\,\frac{\varepsilon}{kT}\right), \tag{3}$$

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[2]) Below two valleys ($\alpha\alpha'$) of a semiconductor such as n-Si arranged on the same axis $\langle 100\rangle$ one valley (α) are considered; hence, $B_{\alpha\alpha}$ and $B_{\alpha\beta}$ should be understood as $\frac{1}{2}(B_{\alpha\alpha} + B_{\alpha'\alpha'})$ and as $B_{\alpha\beta}$, $\beta \neq \alpha, \alpha', \beta'$.

where $\boldsymbol{C}^{(\alpha)}$ and $\boldsymbol{A}^{(\alpha)}$ are the unknown parameters of the distribution function, $m_\perp$ (and below $m_\parallel$) is the transverse (longitudinal) effective mass on the ellipsoidal isoenergetic surface. Then, multiplying (2) successively by v_k and $v_k\,\varepsilon/kT$ and integrating over all $\boldsymbol{p}$ in the system of $\langle 100\rangle$ axes, we get[3])

$$\left.\begin{aligned}
&\tilde{E}_k + \left[\left(\boldsymbol{C}^{(\alpha)} + \frac{5}{2}\boldsymbol{A}^{(\alpha)}\right), \tilde{\boldsymbol{H}}\right]_k = -\,(C_k^{(\alpha)} + A_k^{(\alpha)})\,T_{kk}^{(\alpha)} - \sum_{\beta\neq\alpha} M_{kk}^{\alpha\beta}(C_k^{(\alpha)} - C_k^{(\beta)}) - \\
&\qquad - \sum_{\beta\neq\alpha}(A_k^{(\alpha)}N_{kk}^{(\alpha\beta)} - A_k^{(\beta)}K_{kk}^{(\alpha,\beta)})\,; \\
&\tilde{E}_k + \left[\left(\boldsymbol{C}^{(\alpha)} + \frac{7}{2}\boldsymbol{A}^{(\alpha)}\right), \tilde{\boldsymbol{H}}\right]_k = -\left(C_k^{(\alpha)} + 2A_k^{(\alpha)}\right)\frac{2}{5}\,T_{kk}^{(\alpha)} - \\
&\qquad - A_k^{(\alpha)}\,L_{kk}^{(\alpha)} - \sum_{\beta\neq\alpha}(C_k^{(\alpha)} - C_k^{(\beta)})\,\varphi_{kk}^{(\alpha\beta)} - \sum_{\beta\neq\alpha}(A_k^{(\alpha)}\,\Psi_{kk}^{(\alpha\beta)} - A_k^{(\beta)}\Phi_{kk}^{(\alpha\beta)})\,.
\end{aligned}\right\} \quad (4)$$

Here $\tilde{E}_k = E_k/E_x$ (the current is assumed along the x-axis and E_x is the external field), $\tilde{\boldsymbol{H}} = e/c\,\boldsymbol{H}\,\sqrt{\pi/m_\perp}\,(kT)^{3/2}(B_{np}n_{np})^{-1}$.

The coefficients of (4) are presented in the Appendix. These equations should be supplemented by requiring absence of a transverse current: $j_\perp = 0$. The current $\boldsymbol{j} = \sum_\alpha \boldsymbol{j}_\alpha = -\,e\sum_{\alpha,\boldsymbol{p}} \boldsymbol{v}f^{(\alpha)}(\boldsymbol{p})$ is expressed in terms of $\boldsymbol{C}^{(\alpha)}$ and $\boldsymbol{A}^{(\alpha)}$ as follows:

$$\boldsymbol{j} = -\,e^2E_x\sqrt{\frac{\pi}{m_\perp}}\,\frac{(kT)^{3/2}}{B_{np}}\,\frac{1}{\lambda}\,\frac{n}{n_{np}}\sum_{\alpha=1}^{\lambda}\left(\boldsymbol{C}^{(\alpha)} + \frac{5}{2}\,\boldsymbol{A}^{(\alpha)}\right) \equiv \hat{\sigma}\boldsymbol{E}\,. \qquad (5)$$

Here n is the electron concentration.

3. Results

3.1 Many-valley semiconductor with isotropic valleys ($d \equiv m_\parallel/m_\perp = 1$)

To investigate the contribution of the intervally scattering to the galvanomagnetic effects, we consider, at first, a semiconductor with λ isotropic valleys. Using the equalities (A.2), the equations (4) are easily solved and the following expressions are obtained for the conductivity $\sigma_0 \equiv \sigma_{xx}$ ($H = 0$) and for the transverse MR $\Delta\sigma/\sigma_0 = (\sigma_0 - \sigma_H)/\sigma_0$ in weak magnetic field

$$V(d = 1, \lambda) = \left[1 + b\,\frac{4\sqrt{2}}{13}\,\frac{1 + (\lambda - 1)\,b'}{\lambda}\right]\left[1 + b\sqrt{2}\,\frac{1 + (\lambda - 1)\,b'}{\lambda}\right]^{-1}, \qquad (6)$$

$$W(d = 1, \lambda) = \left[1 + b\sqrt{2}\,\frac{1 + (\lambda - 1)\,b'}{\lambda}\right]^{-1}\left[1 + b\,\frac{4\sqrt{2}}{13}\,\frac{1 + (\lambda - 1)\,b'}{\lambda}\right]^{-2}. \qquad (7)$$

Hereafter $V = \sigma_0/\sigma_{np}$ is the conductivity and $W = \left(\frac{\Delta\sigma}{\sigma_0}\right)\Big/\left(\frac{\Delta\sigma}{\sigma_0}\right)_{np}$ is MR, measured respectively in units of

$$\sigma_{np} = \frac{39\sqrt{2}}{16}\,e^2\sqrt{\frac{\pi}{m_\perp}}\,\frac{(kT)^{3/2}}{B_{np}}\,\frac{n}{n_{np}}\,; \quad \left(\frac{\Delta\sigma}{\sigma_0}\right)_{np} = \frac{3600}{(169)^2}\left(\frac{\sigma_{np}H}{enc}\right)^2 \qquad (8)$$

with $b = (B_{\alpha\alpha}/B_{np})(n/n_{np})$, $b' = B_{\alpha\beta}/B_{\alpha\alpha}$ (see A.1). In the isotropic case $m_\perp$ in the expressions (8) is replaced by the isotropic effective mass $m_\perp = m^*$.

[3]) The equations (4) hold for semiconductors with isotropic and arbitrarily arranged valleys. For instance, in the $m_\parallel \to m_\perp$ approximation they may be applied to n- and p-type PbS possessing four roughly isotropic valleys both in the n- and p-bands.

Considering (6) and (7) leads to the following conclusion. 1. In the range of dominant Coulomb scattering the conductivity increases just as slowly as $\ln n$ (the ratio n/n_{np} is assumed constant), whereas MR decreases as fast as $(\ln n/n)^2$ (see also [6]). 2. MR is affected by e–e scattering far stronger than the conductivity. With b varying within a wide range of values from $b_1 \ll 1$, when the e–e scattering is negligible for instance, because of compensation $(n \ll n_{np})$ up to $b_2 \gg 1$, when e–e scattering prevails [9], the conductivity decreases 13/4 times and MR is reduced by a factor of $\left(\frac{4}{13}\right)^2 2\sqrt{2}\left[\frac{1+b'(\lambda-1)}{\lambda}\,b\right]^3 \gg 1$ and tends to zero as b^{-3}, 3. If $b' \neq 1$ the conductivity and MR depend on the number of isotropic valleys. Consequently, for investigating the intervalley e–e scattering, it is necessary to modify the number of populated valleys, other things being equal.

Since the number of populated valleys in a many-valley semiconductor can be changed by external pressure, below we shall calculate the conductivity and MR in a deformed semiconductor of n-Si type.

3.2 One-valley anisotropic semiconductor

Let a semiconductor such as n-Si be highly compressed along the x-axis $\left((\Delta\varepsilon_{2,3} - \Delta\varepsilon_1) \equiv \sum\limits_{i,k} (\delta_{i,k}^{(2,3)} - \delta_{i,k}^{(1)})\,\eta_{ik} \gg kT\right.$, where δ_{ik} and η_{ik} are the components of the deformation potential tensor in the α-valley and of the deformation tensor in the system of x, y, z-axes), respectively), so that it transforms into a one-valley ($\alpha = 1$) substance [11]. Then we get from (4) and (5)

$$\left.\begin{aligned} V(\lambda=1) &= \frac{8\sqrt{2}}{39}\,\frac{1.3\,T_2 + L_2}{T_2(0.4\,T_2 + L_2)}, \\ W(\lambda=1) &= \frac{4\cdot 169}{15\cdot 75}\,\frac{T_2}{(1.3\,T_1 + L_1)\,(1.3\,T_2 + L_2)\,(0.4\,T_2 + L_2)}. \end{aligned}\right\} \tag{9}$$

Analysing equation (9) reveals that, with increasing d-anisotropy of constant-energy surfaces, e–e scattering becomes progressively significant and for $d \gg b^{-1}$ it dominates $\left(L_2 \gg T_2\right.$, see (A1,) (A2)$\left.\right)$ determining the limiting values of $V = \frac{16}{39\pi} < V(d=1)$ and of $W = \frac{64\cdot 13}{9(db)^2}\left(1 + \frac{3\sqrt{2}}{13}\,b\right)^{-1}$, tending to zero as $(db)^{-2}$.

3.3 Two-valley semiconductor

For a two-valley semiconductor produced by strong dilatation $\left((\Delta\varepsilon_1 - \Delta\varepsilon_{2,3}) \gg kT\right)$ of a semiconductor such as n-Si along the x-axis (the current flows on the $\langle 100\rangle$ direction and the valleys situated on y, z-axes remain unaffected), we obtain from (4) and (5)

$$V(\lambda=2) = \frac{8\sqrt{2}}{39}\,\frac{1.3\,T_1 + L_1 + \Psi_1 - \Phi_1}{T_1(0.4\,T_1 + L_1 + \Psi_1 - \Phi_1)}, \tag{10}$$

$$W(\lambda=2) = \frac{4\cdot 169}{15\cdot 75}\,2T_1\,[\delta_1(0.4\,T_1 + L_1 + \Psi_1 - \Phi_1)\,(1.3\,T_1 + L_1 + \Psi_1 - \Phi_1)^{-1}]. \tag{11}$$

The explicit expression for δ_1 is presented in the Appendix (A.3). Here again, similarly to the one-valley case, with increasing d the contribution of e–e

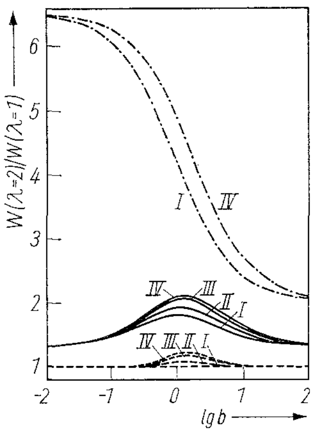

Fig. 1

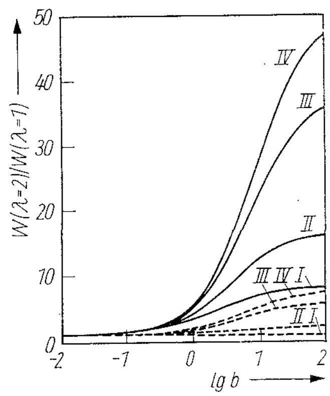

Fig. 2

Fig. 1. The ratio of the two-valley to one-valley conductivity $V(\lambda = 2)/V(\lambda = 1)$ versus the relative contribution of the e–e scattering b, for different values of the parameter b' determining the relative contribution of the intervalley e–e scattering: I. $b' = 1$; II. $b' = 0.5$; III. $b' = 0.1$; IV. $b' = 0$, solid, dashed, and dash-dotted curves correspond to $d = 4.68$ (n-Si), $d = 1$ (isotropic semiconductor), $d \gg 1, 1/b$ (high anisotropy case), respectively

Fig. 2. Ratio of the two-valley to one-valley MR $W(\lambda = 2)/W(\lambda = 1)$ versus b. The designation of curves here and in Fig. 3, 4 is the same as in Fig. 1

scattering grows progressively and for $d \gg 1$, $1/b$ $(L_2 \gg T_2)$ W tends to zero as $(db)^{-1}$.

Fig. 1 shows, for three values of d ($d = 1$ isotropic case, $d = 4.68$ the case of n-Si, and $d \gg 1$, $1/b$ the case of high anisotropy), the ratio $V(\lambda = 2)/V(\lambda = 1)$ of the conductivities of the two-valley and one-valley semiconductors versus $\lg b$ where b presents the relative contribution of e–e scattering which is taken as a parameter. Fig. 2 gives $W(\lambda = 2)/W(\lambda = 1)$ as a function of $\lg b$ only for two values of d, because $W(\lambda = 2)/W(\lambda = 1) \approx db \gg 1$, if $d \gg 1/b$.

3.4 Three-valley semiconductor

The formulae for the conductivity $V(\lambda = 3)$ and for MR $W(\lambda = 3)$ of an undeformed semiconductor such as n-Si can be easily derived from (4) and (5). These expressions being rather tedious, we limit ourselves to the plots of $V(\lambda{=}3)/V(\lambda = 1)$ (Fig. 3) and of $W(\lambda = 3)/W(\lambda = 1)$ Fig. (4), which are merely the piezoresistence and the piezo-MR for the case of strong compression along the x-axis (see Section 3.2). At high anisotropy the piezo-MR becomes very great

$$\left[\frac{W(\lambda = 3,\ d \gg 1,\ 1/b)}{W(\lambda = 1,\ d \gg 1,\ 1/b)}\right] \approx (db)^2 \gg 1$$

for this reason it is not plotted in Fig. 4. Analogous ratios $V(\lambda = 3)/V(\lambda = 2)$ and $W(\lambda = 3)/W(\lambda = 2)$, i.e. the piezoresistence and the piezo-MR in the case of strong dilation, can be easily obtained from Fig. 1, 3 and Fig. 2, 4.

4. Conclusions

From Fig. 4 it can be seen that the piezo-MR grows along with increasing e–e scattering and anisotropy of isoenergetic surfaces d. It should be noted that increasing d results in a relative enhancement of the contribution of e–e

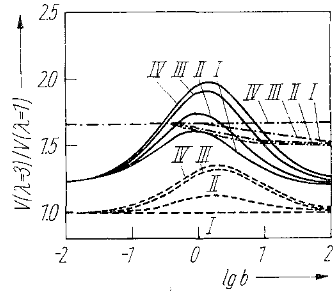

Fig. 3. Ratio of three-valley to one-valley conductivity versus b $V(\lambda = 3)/V(\lambda = 1)$. The curves correspond to those of the Fig. 1

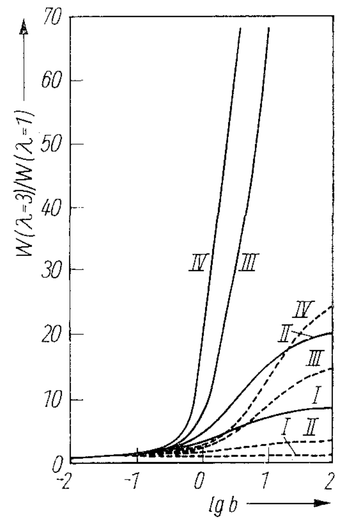

Fig. 4. Ratio of three-valley to one-valley MR versus b. The curves correspond to those of the Fig. 1. $W(\lambda = 3)/W(\lambda = 1)$

scattering (provided b and b' are invariable), since the coefficients L_2 and Ψ_2, which describe the intravalley and intervalley scattering, are proportional to d (see Appendix), while all other coefficients (including $T_{1,2}$) vary slightly with d. Therefore, with $db \gg 1$, the inequality $L_2 \gg T_{1,2}$ holds (with $dbb' \gg 1$, $\Psi_2 \gg T_{1,2}$) and e–e scattering becomes dominant. This being the case, $\boldsymbol{A}^{(\alpha)} \ll \boldsymbol{C}^{(\alpha)}$, as it follows from the second of equations (4); then only the first of equations (4), which describes the conservation of momentum, should be solved consistently with the requirement $j_\perp = 0$. In a one-valley semiconductor the condition $j_\perp = 0$ together with (5) results $C_\perp = 0$ and in vanishing MR ($W = 0$); then only C_x should be calculated from (4). In the two-valley case, from $j_\perp = 0$ it follows that $C_\perp^{(2)} + C_\perp^{(3)} = 0$ yet, (4) indicates the valleys 2 and 3 to be equivalent, and the situation appears similar to the one-valley case. In the three-valley case all the three $C_\perp^{(\alpha)}$ are different, therefore, the equality $\sum_\alpha C_\perp^{(\alpha)} = 0$ leads to $C_\perp^{(\alpha)} \neq 0$ and, with vanishing total transverse current, the current in each valley and MR differs from zero either. Thus, it is the many-valley band structure and the difference of Hall angles in the different values that give rise to MR and just in this situation as it is seen from Fig. 4, MR is badly affected by the intervalley e–e scattering.

Fig. 1 to 4 and equations (6) to (11) show that stress analysis of the conductivity and of MR seems rather advantageous for determining b and b' unambiguously, provided d is known. The magnitudes of the conductivity and of MR, which correspond to other orientations of the current (different from the $\boldsymbol{j} \parallel \langle 100 \rangle$ situation, discussed above), may be easily obtained using (4) and (5). Note that in the limiting case of classically strong magnetic fields the e–e scattering is eliminated at all. At $H \to \infty$ we have

$$V(d = 1, \lambda) = \frac{4}{13}, \quad V(\lambda = 1) = \frac{8\sqrt{2}}{39} \frac{1}{T_2},$$

$$V(\lambda = 2) = \frac{8\sqrt{2}}{39} \frac{1}{T_1}, \qquad V(\lambda = 3) = \frac{8\sqrt{2}}{39} \frac{3}{(2T_1 + T_2)},$$

respectively for an isotropic semiconductor with arbitrary number of valleys and for the one-valley, two-valley, and three-valley cases considered above.

Acknowledgement

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Appendix

The following relations hold between the coefficients of equations (4):

$$R_{xx}^{(1)} = R_{yy}^{(2)} = R_{zz}^{(3)} = R_2; \quad R_{yy}^{(1)} = R_{zz}^{(1)} = R_{xx}^{(2)} = R_{zz}^{(2)} = R_{xx}^{(3)} = R_{yy}^{(3)} = R_1,$$

$$S_{xx}^{(1,2)} = S_{xx}^{(1,3)} = S_{yy}^{(2,1)} = S_{yy}^{(2,3)} = S_{zz}^{(3,1)} = S_{zz}^{(3,2)} = S_3,$$

$$S_{yy}^{(1,2)} = S_{zz}^{(1,3)} = S_{xx}^{(2,1)} = S_{zz}^{(2,3)} = S_{yy}^{(3,2)} = S_{xx}^{(3,1)} = S_2,$$

$$S_{zz}^{(1,2)} = S_{yy}^{(1,3)} = S_{zz}^{(2,1)} = S_{xx}^{(2,3)} = S_{yy}^{(3,1)} = S_{xx}^{(3,2)} = S_1,$$

$$R \equiv L, T, \quad S \equiv K, M, N, \Phi, \Psi, \quad N_3 = K_2, \quad N_2 = K_3,$$

$$N_1 = K_1, \quad M_2 = M_3, \quad \Phi_2 = \Phi_3, \quad \varphi_i = \frac{2}{5} N_i .$$

Here the valleys 1, 2, 3 are oriented along the x, y, z-axis, respectively, and

$$\left.\begin{aligned}
&T_1 = \frac{a}{\sqrt{2}}\, g_1, \quad T_2 = a\sqrt{2} g_2, \quad L_1 = b\,\frac{a}{5\lambda}\left(g_1 + \frac{1}{2}\, g_2 + 1 - d^{-1}\right),\\
&L_2 = b\,\frac{2a}{5\lambda}\left(g_2 + \frac{1}{2}\, d g_1\right), \quad g_1 = 1 + \frac{d-2}{\sqrt{d-1}} \operatorname{arctg} \sqrt{d-1},\\
&g_2 = -1 + \frac{d}{\sqrt{d-1}} \operatorname{arctg} \sqrt{d-1},\\
&M_1 = b\,\frac{2a'}{\lambda}\, b' \left[1 - \frac{1}{4}\,(1+d)\,\varkappa\right], \quad M_2 = b\,\frac{a'}{\lambda}\, b' \left[-1 + (3d-1)\,\varkappa\right],\\
&K_1 = \frac{7}{4}\, M_1, \quad K_2 = b\,\frac{a'}{\lambda}\, b'\, \frac{19d+15}{8(d+1)} \left[-1 + \frac{49d-15}{19d+15}\,(1+d)\,\varkappa\right],\\
&K_3 = b\,\frac{a'}{\lambda}\, b'\, \frac{29d+17}{8(d+1)} \left[-1 + \frac{63d-17}{29d+17}\,(1+d)\,\varkappa\right],\\
&\Phi_1 = b\,\frac{a'}{5\lambda}\, b'\, \frac{11d^2 - 49d + 40}{8d(d+1)} \left[-1 + \frac{101d^3 - 38d^2 - 99d + 40}{11d^2 - 49d + 40}\,\varkappa\right],\\
&\Phi_2 = b\,\frac{a'}{5\lambda}\, b'\, \frac{21d^2 + 10d - 27}{16(d+1)^2} \left[1 - \frac{-153d^3 - 279d^2 + 413d + 27}{21d^2 + 10d - 27}\,\varkappa\right],\\
&\Psi_1 = b\,\frac{a'}{5\lambda}\, b'\, \frac{291d^2 - 283d - 4}{8d(d+1)^2} \left[1 - \frac{357d^3 + 566d^2 + 213d + 4}{291d^2 + 283d - 4}\,\varkappa\right],\\
&\Psi_2 = b\,\frac{a'}{5\lambda}\, b'\, \frac{56d^3 - 133d^2 + 166d + 211}{16(d+1)} \times\\
&\qquad \times \left[-1 + \frac{104d^4 + 17d^3 + 471d^2 + 283d - 275}{56d^3 - 133d^2 + 166d + 211}\,\varkappa\right],
\end{aligned}\right\} \quad (A.1)$$

$$\left.\begin{aligned}
\Psi_3 &= b\,\frac{a'}{5\lambda}\,b'\,\frac{695d^3 + 1054d^2 + 223d + 8}{16(d+1)^2}\,\times\\
&\quad\times\left[-1 + \frac{1309d^4 + 2307d^3 + 679d^2 - 327d - 8}{695d^3 + 1054d^2 + 223d + 8}\,\varkappa\right],\\
b &= \frac{n}{n_{np}}\,\frac{B_{\alpha\alpha}}{B_{np}};\quad b' = \frac{B_{\alpha\beta}}{B_{\alpha\alpha}},\quad a = \frac{\sqrt{d}}{d-1},\quad a' = \frac{d}{d-1},\quad d = \frac{m_{\|}}{m_{\perp}} \geqq 1,\\
\varkappa &= \frac{\sqrt{2}}{4\sqrt{d(d-1)}}\,\ln\left|\frac{\sqrt{2d} + \sqrt{d-1}}{\sqrt{2d} - \sqrt{d-1}}\right|.
\end{aligned}\right\}$$

Note that in the isotropic case ($d \equiv 1$) $R_{ii}^{(\alpha)} = R$; $S_{ii}^{\alpha\beta} = S$ and the coefficients are considerably simplified:

$$T_2 = \frac{2\sqrt{2}}{3},\quad L = \frac{8}{15\lambda}\,b,\quad M = b\,\frac{2b'}{3\lambda},\quad K = b\,\frac{7b'}{6\lambda},\quad \Psi - \Phi = Lb'. \tag{A2}$$

The parameter δ_1 entering (11) is given by

$$\left.\begin{aligned}
\delta_1 &= \frac{\eta_1(0.4\eta_3^2 - \eta_2\eta_4) + \xi_2(\xi_1\eta_4 - \xi_3\eta_3) + \xi_3(\xi_3\eta_2 - 0.4\xi_1\eta_3)}{0.4\eta_3^2 - \eta_2\eta_4};\\
\eta_1 &= \frac{1}{4}\,[1.3(T_1 + T_2) + L_1 + L_2 + \Psi_2 + \Psi_3 - 2\Phi_2];\quad \xi_1 = \frac{3}{8}\,(T_1 - T_2);\\
\eta_2 &= \frac{1}{4}\,(T_1 + T_2 + 4M_2);\quad \xi_2 = \frac{1}{4}\,[0.8(K_3 - K_2) - 0.6(T_1 - T_2)];\\
\eta_3 &= \frac{1}{4}\,(T_1 + T_2 + 2K_2 + 2K_3);\\
\xi_3 &= \frac{1}{4}\,(L_1 - L_2 + \Psi_2 - \Psi_3 - 0.2\,(T_1 - T_2));\\
\eta_4 &= \frac{1}{4}\,[0.8(T_1 + T_2) + L_1 + L_2 + \Psi_2 + \Psi_3 + 2\Phi_2].
\end{aligned}\right\} \tag{A3}$$

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