

Theory of the Faraday Effect in Solids

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A calculation is made of the Faraday effect in solids. By the use of a modified Bloch representation developed for the problem of Bloch electrons in a magnetic field, the conductivity tensor is expanded to first order in the magnetic field. The result can be separated into the intraband or free carrier Faraday effect and contributions corresponding to direct interband transitions. The general form of the results is in agreement with previous expressions, but the present calculation enables one to predict the sign and order of magnitude of the effect from band-edge parameters. The results are applied to the case of the direct transition in Ge and III-V compounds.

I. INTRODUCTION

RECENT experimental investigation of Faraday rotation in semiconductors¹⁻³ has yielded information about interband as well as free carrier effects. While approximate theories⁴⁻⁶ have predicted the types of singularities to be expected for various interband transitions, there are questions such as the sign and magnitude of the effects for which a rigorous theoretical treatment is necessary. The groundwork for such a treatment has been laid by Bennett and Stern,⁷ who obtained a general expression for the conductivity tensor in a magnetic field [our Eq. (4)]. However, there are difficulties encountered in applying perturbation theory to magnetic effects on Bloch electrons, and it is not clear that Bennett and Stern's final results are entirely correct. In this paper, we shall make use of the author's modified Bloch representation⁸ for the magnetic problem. Using this representation, it is possible to expand the conductivity tensor to first order in the magnetic field. The result includes both the interband effects due to direct transitions, and the intraband or free-carrier Faraday effect. The latter has previously been treated by Stephen and Lidiard⁹ and others. We shall be mainly interested in the interband effects and shall evaluate both the low-frequency limit and the contribution near the singularity for simple and complicated models, the complicated model correspond-

ing to the direct transition in germanium and related materials. We shall not attempt to include exciton effects or to consider indirect transitions, and we shall limit ourselves to the low-magnetic field limit.

The result for the interband Faraday effect is found to consist essentially of two terms: one due to the Zeeman interaction and one due to the change of the matrix element for the transition due to the magnetic field. For the case of a direct transition between non-degenerate band edges, the singularity in the Faraday effect at frequencies near the energy gap is determined by the first term, in agreement with previous results, and in analogy with the atomic case. However, for degenerate band edges both terms contribute to the singularity, presumably due to quantum effects. The latter case is of interest in semiconductors, and the calculation enables one to predict the sign and order of magnitude of the effect from band-edge parameters.

II. THE CONDUCTIVITY TENSOR

The macroscopic theory of the Faraday effect has been developed by several authors,^{5,7} and the result we shall use is the relation between the angle θ of rotation of the plane of polarization per unit length and the conductivity tensor $\sigma_{\alpha\beta}$. For the magnetic field in the z direction, and for at least three-fold symmetry about this axis, we have

$$\theta = 2\pi\sigma_{xy}/nc, \quad (1)$$

where n is the refractive index, and where $\sigma_{xy} = -\sigma_{yx}$ is linear in the magnetic field for sufficiently small fields.

To calculate this, we begin as usual with the Hamiltonian for the problem of an electron in a periodic potential $V(\mathbf{r})$ and a magnetic field \mathbf{H} ,

$$\mathcal{H}(\mathbf{r}, \mathbf{P}, \mathbf{H}) = (1/2m)\mathbf{P}^2 + V(\mathbf{r}) + g\beta\mathbf{s} \cdot \mathbf{H}, \quad (2)$$

where

$$\mathbf{P} = \mathbf{p} + (1/2mc^2)\mathbf{s} \times \nabla V + e\mathbf{A}/c. \quad (3)$$

\mathbf{P} is the kinetic momentum operator, with \mathbf{A} the vector potential for the static magnetic field, and we have included spin-orbit effects by virtue of the second term.¹⁰ \mathbf{s} is the electron spin and the other symbols have their usual meanings. Now, using the methods of semi-

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classical radiation theory, the result for the conductivity tensor is

$$\sigma_{\alpha\beta} = \frac{e^2}{im\omega} \sum_{nn'} \left\{ \delta_{\alpha\beta} \delta_{nn'} f_n + \frac{1}{m} \frac{P_{nn'}^\beta P_{n'n}^\alpha f_{nn'}}{\mathcal{E}_{nn'} + \omega} \right\}. \quad (4)$$

Here, n and n' are eigenstates of Eq. (2), f_n is the Fermi distribution function for energy \mathcal{E}_n , $f_{nn'}$ is a shorthand notation for $f_n - f_{n'}$, likewise $\mathcal{E}_{nn'}$ for $\mathcal{E}_n - \mathcal{E}_{n'}$, α and β are vector components, and the frequency ω is assumed to have a small negative imaginary part.

The eigenstates of the magnetic Hamiltonian, Eq. (2), are rather complicated and we would rather not use them. At the same time, the Bloch representation is an inconvenient one because of the singular matrix elements of the vector potential. A much more convenient representation is the modified Bloch representation of R, which will be described briefly below. First let us rewrite the expression for the conductivity tensor, so that it is in the form of a trace,

$$\sigma_{\alpha\beta} = \frac{e^2}{im\omega} \text{tr} \left\{ \delta_{\alpha\beta} f(\mathcal{H}) + \frac{i}{m} \int_{-\infty}^0 \exp[i(\mathcal{H} + \omega)\tau] P^\beta \times \exp(-i\mathcal{H}\tau) [P^\alpha, f(\mathcal{H})] d\tau \right\}. \quad (5)$$

We are now free to use the desired representation due to the invariance of the trace.

We define the basis functions for the problem as follows. Let $v_{n\mathbf{k}}(\mathbf{r})$ be a periodic function of \mathbf{r} which reduces to the periodic part $u_{n\mathbf{k}}(\mathbf{r})$ of the Bloch function for zero magnetic field. (In R, $u_{n\mathbf{k}}$ was used instead of $v_{n\mathbf{k}}$, so that we are using a slight variation of the representation in R.) Let $\boldsymbol{\kappa} = \mathbf{k} + (e/c)\mathbf{A}(i\nabla_{\mathbf{k}})$ be the Fourier transform of the usual free-particle kinetic momentum operator. Then, the new basis functions are

$$\phi_{n\mathbf{k}} = v_{n\boldsymbol{\kappa}^*}(\mathbf{r}) \exp(i\mathbf{k}\cdot\mathbf{r}), \quad (6)$$

where $\boldsymbol{\kappa}^*$ is the complex conjugate of $\boldsymbol{\kappa}$ and operates on the \mathbf{k} in the plane wave. We must further specify the order of factors, since the different components of $\boldsymbol{\kappa}$ do not commute with each other, and we choose the completely symmetric combination. This definition of ϕ follows the treatment in Appendix II of R. The principal result of R is that using these basis functions and the Hamiltonian $\mathcal{H}(\mathbf{r}, \mathbf{p}, \mathbf{H})$ of Eq. (2), we obtain a crystal momentum space Hamiltonian

$$\mathcal{H}_{nn'}(\boldsymbol{\kappa}) = \int d\mathbf{r} v_{n\boldsymbol{\kappa}^\dagger} \mathcal{H}(\mathbf{r}, \mathbf{p}' + \boldsymbol{\kappa}, \mathbf{H}) v_{n'\boldsymbol{\kappa}}, \quad (7)$$

where \mathbf{p}' represents the first two terms of Eq. (3) and $v_{n\boldsymbol{\kappa}^\dagger}$ is the Hermitian conjugate of $v_{n\boldsymbol{\kappa}}$. The normalization of the basis set is determined by the normalization matrix

$$N_{nn'}(\boldsymbol{\kappa}) = \int d\mathbf{r} v_{n\boldsymbol{\kappa}^\dagger} v_{n'\boldsymbol{\kappa}}. \quad (8)$$

In Eqs. (7) and (8), we have products of symmetrized functions of $\boldsymbol{\kappa}$, which result in functions which are not symmetrized. It is possible to expand such products in powers of H , the coefficients of which are symmetrized, by using the following theorem proved in R. If $A(\boldsymbol{\kappa})$ and $B(\boldsymbol{\kappa})$ are symmetrized functions of $\boldsymbol{\kappa}$, then

$$A(\boldsymbol{\kappa})B(\boldsymbol{\kappa}) = C(\boldsymbol{\kappa}), \quad (9)$$

where $C(\boldsymbol{\kappa})$ is the symmetrized function formed from

$$C(\mathbf{k}) = \exp(-i\mathbf{h}\cdot\nabla_{\mathbf{k}} \times \nabla_{\mathbf{k}'} A(\mathbf{k}) B(\mathbf{k}') |_{\mathbf{k}=\mathbf{k}'} \\ = A(\mathbf{k}) B(\mathbf{k}) - i\mathbf{h}\cdot\nabla_{\mathbf{k}} A \times \nabla_{\mathbf{k}} B + \dots, \quad (10)$$

where $h = eH/2c$ (we are setting $\hbar = 1$). We need only carry out our expansions to first order in h for present purposes. Thus the normalization matrix is obtained from

$$N_{nn'}(\mathbf{k}) \cong \int d\mathbf{r} v_{n\mathbf{k}}^* v_{n'\mathbf{k}} - i\mathbf{h}\cdot \int d\mathbf{r} \nabla_{\mathbf{k}} v_{n\mathbf{k}}^* \times \nabla_{\mathbf{k}} v_{n'\mathbf{k}}. \quad (11)$$

In the present treatment, we shall choose v such that $N_{nn'}(\mathbf{k}) = \delta_{nn'}$, instead of simply setting v equal to u , as in R. This is because we want to take the trace with respect to a normalized representation. The simplest choice is

$$v_{n\mathbf{k}} \cong u_{n\mathbf{k}} + \frac{1}{2} \sum_{n'} u_{n'\mathbf{k}} i\mathbf{h}\cdot \int d\mathbf{r} \nabla_{\mathbf{k}} u_{n'\mathbf{k}}^* \times \nabla_{\mathbf{k}} u_{n\mathbf{k}}. \quad (12)$$

As in R, it is convenient to introduce the antisymmetric tensor

$$\epsilon_{\gamma\delta} = \epsilon_{\gamma\delta\lambda} h^\lambda / h, \quad (13)$$

where $\epsilon_{\gamma\delta\lambda}$ is the antisymmetric third rank tensor, and we use summation convention. We also define

$$x_{nn'}^\alpha = i \int d\mathbf{r} u_{n\mathbf{k}}^* \nabla_{\mathbf{k}}^\alpha u_{n'\mathbf{k}} = -i \int d\mathbf{r} (\nabla_{\mathbf{k}}^\alpha u_{n\mathbf{k}}^*) u_{n'\mathbf{k}}. \quad (14)$$

x is the part of the coordinate operator which is diagonal in \mathbf{k} . We can now write

$$v_{n\mathbf{k}} = u_{n\mathbf{k}} + \frac{1}{2} h \epsilon_{\gamma\delta} \sum_{n'} u_{n'\mathbf{k}} (x^\gamma x^\delta)_{n'n}. \quad (15)$$

Applying our product theorem, we expand the Hamiltonian to first order in h . The result is

$$\mathcal{H}_{nn'}(\boldsymbol{\kappa}) = \mathcal{E}_n(\boldsymbol{\kappa}) \delta_{nn'} + \mathcal{H}_{nn'}'(\boldsymbol{\kappa}), \quad (16)$$

$$\mathcal{H}'(\mathbf{k}) = h \epsilon_{\gamma\delta} [\{x^\gamma, (\pi^\delta + v^\delta)\} + s_{\gamma\delta}], \quad (17)$$

where

$$\pi_{nn'}^\delta = \frac{1}{m} \int u_{n\mathbf{k}}^* (\mathbf{p}' + \mathbf{k})^\delta u_{n'\mathbf{k}}, \quad (18)$$

$$v_{nn'}^\delta = \delta_{nn'} \pi_{nn}^\delta,$$

and the second term in Eq. (17) is the spin interaction. The first term of Eq. (17) reduced to $\beta \mathbf{L}\cdot\mathbf{H}$ in the tight-binding limit, since in this limit, \mathbf{x} becomes the

coordinate and $\mathbf{v} \rightarrow 0$. Equation (17) is the same as Eq. (54) of R, except for a normalization term.

To evaluate our trace, we also need to obtain \mathbf{P} in our representation

$$P_{nn'}^\alpha(\mathbf{\kappa}) = \int u_{n\mathbf{k}}^\dagger (\mathbf{p}' + \mathbf{\kappa})^\alpha u_{n'\mathbf{k}} \\ \cong (1/m) \{ \pi_{nn'}^\alpha(\mathbf{\kappa}) + \pi_{nn'}'^\alpha(\mathbf{\kappa}) \}. \quad (19)$$

Again, we can apply the multiplication theorem to obtain

$$\pi'^\alpha(\mathbf{k}) = h\epsilon_{\gamma\delta} [\{ x^\gamma, \nabla_{\mathbf{k}}^\delta \pi^\alpha \} + \delta_{\delta\alpha} (x^\alpha/m)]. \quad (20)$$

We now have the ingredients for evaluating the trace in Eq. (5); namely, \mathcal{H} and \mathbf{P} as symmetric functions of $\mathbf{\kappa}$ given to first order in h . We further need the fact, used in R, that the trace of a *symmetric* function of $\mathbf{\kappa}$ is the same as the trace of the same function of \mathbf{k} . We know how to symmetrize the products, but may be concerned over the fact that functions of \mathcal{H} appear which must be rearranged into symmetrized functions of $\mathbf{\kappa}$. However, it is readily shown that to first order in h , a function of $\mathcal{E}(\mathbf{\kappa})$ is symmetrized [for example in applying Eq. (10) to $(\mathcal{E}(\mathbf{\kappa}))^2$, the first-order term vanishes]. The magnetic part of the conductivity tensor then consists of three parts: $\sigma_{\alpha\beta}^{(1)}$ due to \mathcal{H}' , $\sigma_{\alpha\beta}^{(2)}$ due to π' , and $\sigma_{\alpha\beta}^{(3)}$ due to symmetrization.

Before calculating these, let us obtain some properties of the complete conductivity tensor from Eq. (4). If we interchange n and n' , we see that

$$\sigma_{\alpha\beta}(\omega) = -\sigma_{\beta\alpha}(-\omega), \quad (21)$$

where we reverse the imaginary as well as the real part of ω . The other relation we want is Onsager's relation, which we can prove from time reversal. The time-reversal operator is $-i\sigma_y \mathcal{C}$ where \mathcal{C} is the complex conjugation operator. Suppose we have the matrix element of an operator M between states 1 and 2. The matrix element of M between the time-reversed states is

$$(-i\sigma_y \psi_1^*, M(-i\sigma_y \psi_2^*)) = (\psi_1^*, i\sigma_y M(-i\sigma_y) \psi_2^*) \\ = (\psi_1, \bar{M} \psi_2) = (\psi_2, \bar{M}^\dagger \psi_1), \quad (22)$$

where \bar{M} is the time-reversed operator. Now without the magnetic field, the Hamiltonian is invariant under time reversal, so that the time reversed states are also eigenstates of the system. \mathbf{p} changes sign under time inversion, so we can see that using time reversed states simply interchanges α and β , showing that the conductivity tensor is symmetric for $H=0$. With the magnetic field, the time-reversed states are now the eigenstates of the Hamiltonian with the magnetic field reversed. Consequently, if we change the sign of H and time reverse the states, σ is unchanged. Therefore,

$$\sigma_{\alpha\beta}(\mathbf{H}) = \sigma_{\beta\alpha}(-\mathbf{H}). \quad (23)$$

The first-order term in H is therefore antisymmetric in α and β , and an even function of ω .

In calculating $\sigma_{\alpha\beta}^{(1)}$ and $\sigma_{\alpha\beta}^{(2)}$, we need not concern ourselves with symmetrization as H' and π' are already first order in H . For $\sigma_{\alpha\beta}^{(1)}$, we need the matrix element of a function of \mathcal{H} to first order in \mathcal{H}' . This can be shown to be

$$F(\mathcal{H}_0 + \mathcal{H}')_{nn'} \\ \cong F(\mathcal{E}_n) \delta_{nn'} \\ + \mathcal{H}'_{nn'} [F(\mathcal{E}_n) - F(\mathcal{E}_{n'}) / \mathcal{E}_n - \mathcal{E}_{n'}]. \quad (24)$$

It is understood that for $\mathcal{E}_n = \mathcal{E}_{n'}$, we take the limit, giving the derivative of F . With a little thought, we can apply this expansion directly to Eq. (4), first holding $\mathcal{E}_{n'}$ constant and letting

$$F(\mathcal{H}) = [f(\mathcal{H}) - f(\mathcal{E}_{n'}) / \mathcal{H} - \mathcal{E}_{n'} + \omega], \quad (25)$$

and then doing the same with \mathcal{E}_n constant and $\mathcal{E}_{n'}$ replaced by \mathcal{H} . This gives

$$\sigma_{\alpha\beta}^{(1)} = \frac{e^2}{i\omega} \sum_{nn'n''} \left\{ \mathcal{H}'_{nn''} \pi_{n'n''}^\beta \pi_{n'n}^\alpha \frac{1}{\mathcal{E}_{nn''}} \right. \\ \times \left(\frac{f_{nn'}}{\mathcal{E}_{nn'} + \omega} - \frac{f_{n'n'}}{\mathcal{E}_{n'n'} + \omega} \right) + \pi_{nn'}^\beta H'_{n'n'} \pi_{n'n}^\alpha \\ \left. \times \frac{1}{\mathcal{E}_{n'n'}} \left(\frac{f_{nn'}}{\mathcal{E}_{nn'} + \omega} - \frac{f_{n'n'}}{\mathcal{E}_{n'n'} + \omega} \right) \right\}. \quad (26)$$

In the first term we interchange n and n' , and in the second, we use time-reversed states which interchange α and β and changes the sign, since \mathcal{H}' changes sign under time inversion. This gives

$$\sigma_{\alpha\beta}^{(1)} = -2ie^2 \sum_{nn'n''} \pi_{nn'}^\alpha H_{n'n''} \pi_{n'n}^\beta \frac{1}{\mathcal{E}_{n'n''}} \\ \times \left\{ \frac{f_{nn'}}{\mathcal{E}_{nn'} - \omega^2} - \frac{f_{n'n''}}{\mathcal{E}_{n'n''} - \omega^2} \right\}. \quad (27)$$

For $\sigma_{\alpha\beta}^{(2)}$ we can also use Eq. (4) giving

$$\sigma_{\alpha\beta}^{(2)} = \frac{e^2}{i\omega} \sum_{nn'} (\pi_{nn'}^\beta \pi_{n'n}^\alpha + \pi_{n'n}^\beta \pi_{nn'}^\alpha) \frac{f_{nn'}}{\mathcal{E}_{nn'} + \omega}. \quad (28)$$

We now use this reversed states and interchange n and n' , which reverses ω , since π' remains the same under time inversion, while π changes sign. Averaging the two terms, we have

$$\sigma_{\alpha\beta}^{(2)} = -ie^2 \sum_{nn'} \pi_{nn'}^\alpha \pi_{n'n}^\beta \frac{f_{nn'}}{\mathcal{E}_{nn'} - \omega^2} - (\alpha \leftrightarrow \beta). \quad (29)$$

Here we have made use of the antisymmetry in α and β .

To evaluate $\sigma_{\alpha\beta}^{(3)}$, we must use Eq. (5). Let us write the integrand as

$$(f \exp[i(\mathcal{H} + \omega)\tau] P^\beta) (\exp(-i\mathcal{H}\tau) P^\alpha) \\ - (\exp[i(\mathcal{H} + \omega)\tau] P^\beta) (f \exp(-i\mathcal{H}\tau) P^\alpha). \quad (30)$$

Now looking at Eq. (10), we notice that the integral over \mathbf{k} of the first-order term in h vanishes, so that we can state that to this order, the trace of the product of two symmetric functions of \mathbf{k} is the same as the trace of the same functions of \mathbf{k} . Therefore, we need only symmetrize the quantities inside the parentheses in Eq. (30). Thus

$$f \exp[i(\mathcal{H}C + \omega)\tau] P^\beta \rightarrow f \exp[i(\mathcal{H}C + \omega)\tau] P^\beta - ih\epsilon_{\gamma\delta}(\nabla_{\mathbf{k}}^\gamma f + i\tau v_\gamma f) \exp[i(\mathcal{H}C + \omega)\tau] \nabla_{\mathbf{k}}^\delta P^\beta \quad (31)$$

and similarly for the other factors. Expanding to first order in h , regrouping terms and carrying out the integral over τ , we obtain

$$\begin{aligned} \sigma_{\alpha\beta}^{(3)} = & -\frac{e^2}{\omega} h \epsilon_{\gamma\delta} \sum_{nn'\mathbf{k}} \left\{ (\nabla_{\mathbf{k}}^\delta \pi_{nn'}^\beta) \pi_{n'n}^\alpha \frac{\nabla_{\mathbf{k}}^\gamma f_n}{\mathcal{E}_{nn'} + \omega} \right. \\ & - \pi_{nn'}^\beta (\nabla_{\mathbf{k}}^\delta \pi_{n'n}^\alpha) \frac{\nabla_{\mathbf{k}}^\gamma f_{n'}}{\mathcal{E}_{nn'} + \omega} - [v_{n'}^\gamma (\nabla_{\mathbf{k}}^\delta \pi_{nn'}^\beta) \pi_{n'n}^\alpha \\ & \left. - \pi_{nn'}^\beta (\nabla_{\mathbf{k}}^\delta \pi_{n'n}^\alpha) v_{n'}^\gamma] \frac{f_{nn'}}{(\mathcal{E}_{nn'} + \omega)^2} \right\}. \quad (32) \end{aligned}$$

By using time inversion and interchanging some indices, this can be written

$$\begin{aligned} \sigma_{\alpha\beta}^{(3)} = & e^2 h \epsilon_{\gamma\delta} \sum_{nn'\mathbf{k}} (\nabla_{\mathbf{k}}^\gamma \pi_{nn'}^\alpha) \pi_{n'n}^\beta \left(\frac{\frac{1}{2} \nabla_{\mathbf{k}}^\delta (f_n + f_{n'})}{\mathcal{E}_{nn'} - \omega^2} \right. \\ & \left. - \frac{f_{nn'} \mathcal{E}_{nn'} (v_n^\delta + v_{n'}^\delta)}{(\mathcal{E}_{nn'} - \omega^2)^2} \right) - (\alpha \leftrightarrow \beta). \quad (33) \end{aligned}$$

We have thus derived the first-order term in the conductivity tensor. We now wish to separate the free carrier and interband contributions, and also put the interband part into a simpler form. The free carrier contribution comes from $\sigma_{\alpha\beta}^{(3)}$, as it must, since the other terms involve the bands explicitly, and in fact is the term in Eq. (33) with $n = n'$. This is the only term which diverges as $\omega \rightarrow 0$. When $n = n'$, the matrix element of π is just v or the gradient of the energy. Let us calculate σ_{xy} , making use of $\epsilon_{\alpha\beta}$.

$$\begin{aligned} (\sigma_{xy})_{f.c.} = & -\frac{e^2 h}{\omega^2} \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nk} (\nabla_{\mathbf{k}}^\gamma \nabla_{\mathbf{k}}^\alpha \mathcal{E}_n) (\nabla_{\mathbf{k}}^\beta \mathcal{E}_n) \nabla_{\mathbf{k}}^\delta f(\mathcal{E}_n), \\ = & \frac{e^2 h}{\omega^2} \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nk} (\nabla_{\mathbf{k}}^\gamma \nabla_{\mathbf{k}}^\alpha \mathcal{E}_n) (\nabla_{\mathbf{k}}^\beta \nabla_{\mathbf{k}}^\delta \mathcal{E}_n) f(\mathcal{E}_n). \quad (34) \end{aligned}$$

The second form is obtained by integrating by parts. Equation (34) agrees with the result obtained by Stephen and Lidiard.⁹

To simplify the interband part, let us first take $\sigma_{xy}^{(2)}$ and substitute in our expression for π' from Eq. (20)

$$\begin{aligned} \sigma_{xy}^{(2)} = & -ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nn'\mathbf{k}} [\{x^\gamma, \nabla_{\mathbf{k}}^\delta \pi^\alpha\}_{nn'} + \delta_{\delta\alpha} x_{nn'}^\gamma] \\ & \times \pi_{n'n}^\beta \frac{f_{nn'}}{\mathcal{E}_{nn'} - \omega^2}. \quad (35) \end{aligned}$$

We can put π^α to the left of x^γ in this equation, as the two terms in the symmetric product go into each under the operation of time inversion plus interchange of n and n' , noting that \mathbf{k} changes sign. We now integrate the first term by parts, giving two contributions

$$\begin{aligned} \sigma_{xy}^{(2a)} = & ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nn'\mathbf{k}} [(\pi^\alpha (\nabla_{\mathbf{k}}^\delta x^\gamma - \delta_{\delta\alpha} x^\gamma))_{nn'} \pi_{n'n}^\beta \\ & + (\pi^\alpha x^\gamma)_{nn'} \nabla_{\mathbf{k}}^\delta \pi_{n'n}^\beta] \frac{f_{nn'}}{\mathcal{E}_{nn'} - \omega^2}, \quad (36) \end{aligned}$$

$$\sigma_{xy}^{(2b)} = ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nn'\mathbf{k}} (\pi^\alpha x^\gamma)_{nn'} \pi_{n'n}^\beta \nabla_{\mathbf{k}}^\delta \frac{f_{nn'}}{\mathcal{E}_{nn'} - \omega^2}, \quad (37)$$

where we have lumped the last part of Eq. (35) into $\sigma_{xy}^{(2a)}$. The gradients in $\sigma_{xy}^{(2a)}$ can now be expanded by the use of the following identities, proved from the definitions of x and π :

$$\nabla_{\mathbf{k}}^\delta x^\gamma - \nabla_{\mathbf{k}}^\gamma x^\delta = i[x^\delta, x^\gamma] \quad (38)$$

$$\nabla_{\mathbf{k}}^\delta \pi^\beta = i[x^\delta, \pi^\beta] + \frac{\delta_{\delta\beta}}{m}. \quad (39)$$

Thus, in the last part of Eq. (36)

$$\begin{aligned} (\pi^\alpha x^\gamma)_{nn'} \nabla_{\mathbf{k}}^\delta \pi_{n'n}^\beta = & (\pi^\alpha x^\gamma)_{nn'} \left[i(x^\delta \pi^\beta)_{n'n} \right. \\ & \left. - i(\pi^\beta x^\delta)_{n'n} + \frac{\delta_{\delta\beta}}{m} \delta_{n'n} \right]. \quad (40) \end{aligned}$$

For the second term in Eq. (40), interchanging n and n' results in the interchange of α and β , γ and δ , which leaves the sum in Eq. (36) unchanged. However, $f_{nn'}$ changes sign, so that this term vanishes, as does the last term in Eq. (40). What is left of $\sigma_{xy}^{(2a)}$ can be put in the form

$$\begin{aligned} \sigma_{xy}^{(2a)} = & -e^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nn'n'\mathbf{k}} (\pi^\alpha x^\gamma + i\delta_{\alpha\gamma})_{nn'} x_{n'n'}^\delta \pi_{n'n}^\beta \\ & \times \left\{ \frac{f_{nn'}}{\mathcal{E}_{nn'} - \omega^2} - \frac{f_{nn'}}{\mathcal{E}_{nn'} - \omega^2} \right\}. \quad (41) \end{aligned}$$

This is very similar to what appears in Eq. (27). We now have remaining $\sigma_{xy}^{(2b)}$ and $\sigma_{xy}^{(3b)}$, the interband part of $\sigma_{xy}^{(3)}$. The latter can be written from Eq. (39)

$$\begin{aligned} \sigma_{xy}^{(3b)} = & -ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nn'\mathbf{k}} (\pi^\alpha x^\gamma)_{nn'} \pi_{n'n}^\beta \\ & \times \left(\frac{\nabla_{\mathbf{k}}^\delta (f_n + f_{n'})}{\mathcal{E}_{nn'} - \omega^2} - \frac{2f_{nn'} \mathcal{E}_{nn'} (v_n^\delta + v_{n'}^\delta)}{(\mathcal{E}_{nn'} - \omega^2)^2} \right), \quad (42) \end{aligned}$$

where the prime indicates $n \neq n'$, and where we have used the fact that the two terms in the commutator give the same result, again from time inversion plus

$n \leftrightarrow n'$. This can be combined with $\sigma_{xy}^{(2b)}$ to give

$$\sigma_{xy}^{(2b)} + \sigma_{xy}^{(3b)} = 2ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum'_{nn'k} (\pi^\alpha x^\gamma)_{nn'} v_{n'}^\delta \pi_{n'}^\beta \times \frac{\partial}{\partial \mathcal{E}_{n'}} \frac{f_{nn'}}{\mathcal{E}_{nn'}^2 - \omega^2}. \quad (43)$$

Let us now compare this to Eq. (41), in which we make the substitution, valid if $\mathcal{E}_{n'} \neq \mathcal{E}_{n''}$,

$$x_{n'n''}^{\delta} = -i \frac{(\pi - v)_{n'n''}^{\delta}}{\mathcal{E}_{n'n''}}. \quad (44)$$

The derivative in Eq. (43) is just the limit of the last factor in Eq. (41), divided by $\mathcal{E}_{n'n''}$, as $\mathcal{E}_{n'} \rightarrow \mathcal{E}_{n''}$, so that the addition of Eq. (34) changes $\pi^\delta - v^\delta$ to $\pi^\delta + v^\delta$. We can now combine all this with $\sigma_{xy}^{(1)}$, in which we substitute the expression for \mathcal{H}' from Eq. (17), unsymmetrizing the product for now familiar reasons. The result is finally

$$\begin{aligned} \sigma_{xy}^{(1b)} &= -ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \\ &\times \sum'_{nn'n''k} \left[\pi_{nn'}^\alpha [x^\gamma (\pi^\delta + v^\delta) + s_{\gamma\delta}]_{n'n''} \pi_{n''}^\beta \right. \\ &\left. - \left(\pi^\alpha x^\gamma + i \frac{\delta_{\alpha\gamma}}{m} \right)_{nn'} (\pi^\delta + v^\delta)_{n'n''} \pi_{n''}^\beta \right] \frac{1}{\mathcal{E}_{n'n''}} \\ &\times \left\{ \frac{f_{nn'}}{\mathcal{E}_{nn'}^2 - \omega^2} - \frac{f_{n'n''}}{\mathcal{E}_{n'n''}^2 - \omega^2} \right\}, \quad (45) \end{aligned}$$

where the prime on the sum is to exclude the case where all three energies are equal.

Equation (45) is the principle result of this paper. It consists essentially of two terms, the first of which depends on the Zeeman interaction \mathcal{H}' of a band electron. This is divided into an orbital and spin part, just as in the atomic case. The momentum matrix elements π^α and π^β contribute to an oscillator strength for the transition. The second term in the square brackets is the contribution from the change in matrix elements due to the magnetic field and has its analog in the atomic case.

An important point to note in Eq. (45) is that all terms involving equal energy matrix elements of $x_{nn'}$ vanish from a cancellation between the two terms of Eq. (45). This is necessary as such matrix elements are not well defined and depend on the phase of the wave function, so that no physical quantity can depend on them.

III. LIMITING CASES

We shall now discuss the behavior of the Faraday effect for high and low frequencies, and in the tightly bound and free limits. For low frequencies and for bands which are completely filled or empty our expres-

sion for σ_{xy} vanishes as ω^2 . The proof, which we shall sketch briefly, is best begun from Eq. (27). In the limit as $\omega \rightarrow 0$ we can write for $\sigma_{xy}^{(1)}$:

$$\sigma_{xy}^{(10)} = -ie^2 \epsilon_{\alpha\beta} \sum_{nn'k} \pi_{nn'}^\alpha \mathcal{H}'_{n'n''} \pi_{n''}^\beta \frac{1}{\mathcal{E}_{nn'} \mathcal{E}_{n'n''}} \times \left\{ \frac{f_{nn'}}{\mathcal{E}_{nn'}} + \frac{f_{n'n''}}{\mathcal{E}_{n'n''}} - \frac{f_{n'n''}}{\mathcal{E}_{n'n''}} \right\}. \quad (46)$$

Using Eqs. (44) and (38), we obtain after an integration by parts and some interchanges of indices,

$$\begin{aligned} \sigma_{xy}^{(10)} &= -ie^2 \epsilon_{\alpha\beta} \sum_{nn'k} \{ [x^\alpha, \mathcal{H}'] \\ &+ i \nabla_k^\alpha \mathcal{H}' \}_{nn'} x_{n'n''}^\beta \frac{f_{nn'}}{\mathcal{E}_{nn'}}. \quad (47) \end{aligned}$$

Now, for $\sigma_{xy}^{(2)}$, we can write in the same limit, using the unsymmetric form of the product in Eq. (20)

$$\begin{aligned} \sigma_{xy}^{(20)} &= ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nn'k} \{ (\nabla^\gamma \pi^\alpha) x^\delta \\ &- \delta_{\delta\alpha} x^\gamma \}_{nn'} x_{n'n''}^\beta \frac{f_{nn'}}{\mathcal{E}_{nn'}}. \quad (48) \end{aligned}$$

Finally, in $\sigma_{xy}^{(3)}$, we use Eq. (44) for π^α , and notice that the term in which the energy denominator is differentiated vanishes, giving

$$\sigma_{xy}^{(30)} = -2e^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \sum_{nn'k} \{ \nabla_k^\gamma x^\alpha, v^\delta \}_{nn'} x_{n'n''}^\beta \frac{f_{nn'}}{\mathcal{E}_{nn'}}, \quad (49)$$

where we have again used time inversion to unsymmetrize the product. The three terms can now be combined and after considerable manipulation, the result is

$$\sigma_{xy}^{(0)} = ie^2 h \epsilon_{\alpha\beta} \epsilon_{\gamma\delta} \text{tr}[(\nabla^\gamma x^\alpha) x^\delta, x^\beta] f. \quad (50)$$

The commutator here, however, can be shown to be a gradient by making repeated use of Eq. (38), so that the integral over \mathbf{k} vanishes.

The high-frequency limit can be most readily proved from Eq. (4) by neglecting $\mathcal{E}_{nn'}$ in the denominator.

$$\sigma_{xy}^{(\infty)} = \frac{e^2}{im^2 \omega^2} \epsilon_{\alpha\beta} \text{tr}[P^\beta, P^\alpha] f = \frac{2e^2 h N}{m^2 \omega^2}, \quad (51)$$

where $N = \text{tr} f$, and we have used the commutation properties of the \mathbf{P} 's. This is the same as the free electron Faraday effect. The same result can be proved from Eq. (45), in which the final energy denominator becomes $f_{n'n''}/\mathcal{E}_{n'n''}\omega^2$, which does not depend on n . In the first term, therefore, were it not for the prime on the summation, we would have $(\pi^\alpha \pi^\beta)_{n'n''}$ after summing over n . However, the π 's commute, so that this vanishes from the antisymmetry between α and β . The same thing occurs for the part of the second term not involving $\delta_{\alpha\gamma}/m$. Therefore, for these two terms, we

replace the sum by the negative of the term with all three energies equal. After some manipulation, we arrive at

$$\sigma_{xy}^{(ib\infty)} = e^2 \hbar \frac{\epsilon_{\alpha\beta\epsilon\gamma\delta}}{\omega^2} \times \sum \left[-\nabla^\alpha \nabla^\gamma \mathcal{E}_n \nabla^\beta \nabla^\delta \mathcal{E}_n + \frac{\delta_{\alpha\gamma} \delta_{\beta\delta}}{m} \right] f_n, \quad (52)$$

which simply subtracts off the free-carrier effect and replaces it by the free-electron result.

The tight-binding result can be obtained by letting x actually become the coordinate, and by ignoring the dependence of all quantities on \mathbf{k} . The Zeeman interaction in Eq. (17) becomes simply $\beta(\mathbf{L} + g_0 \mathbf{s}) \cdot \mathbf{H}$, and for π' , we keep only the second term, which is the vector potential in the symmetric gauge.

IV. APPLICATION TO BAND MODELS

We begin with the simplest possible model, consisting of two spherical bands, one of which, the valence band, is occupied and the other of which is empty. If spin-orbit interaction is present, it is possible to have an allowed transition between two such bands, and the rotation comes about from the Zeeman interaction for each band, which is characterized by a g factor.

In Eq. (45), when ω approaches the energy gap, the dominant energy dependence comes from the terms with $n' = n''$, in which case σ_{xy} goes as $(\mathcal{E}_g - \omega)^{-1/2}$.^{1,2,4} We shall initially include only these terms and furthermore evaluate the quantities in the curly bracket at the band edge. The second quantity in the curly bracket (which is due essentially to the effect of the magnetic field on the transition probabilities) vanishes at $k=0$, and the first term can be interpreted in terms of the energy difference between levels due to the Zeeman interaction. Using these approximations and also using Eq. (44), we have

$$\sigma_{xy}^{(ib)} \cong e^2 \hbar \epsilon_{\alpha\beta\epsilon\gamma\delta} \sum'_{n'n''} [(x^\gamma \pi^\delta + x^\delta \pi^\gamma)_{n'n''} \times x_{n''n'} \pi_{n'n''}^\beta \mathcal{E}_{n''n'}]_{k=0} \frac{2f_{n'n'} \mathcal{E}_{n'n'}}{(\mathcal{E}_{n'n'} - \omega^2)^2}. \quad (53)$$

Writing the Zeeman interaction as $g(\mathbf{s} \cdot \mathbf{h}/m)$ for the $n'n''$ pair of bands, we see that the next two factors represent the contribution to the g factor from band n , which we shall denote by g' . This gives, using a matrix notation for the pairs of bands, and now letting n and n' go over conduction and valence bands,

$$\begin{aligned} \sigma_{xy}^{(ib)} &\cong \frac{e^2}{m^2 \hbar} \text{tr} \sum_{n'n'k} [[g_{n'} \mathbf{s} \cdot \mathbf{h}][g_{n'}' \mathbf{s} \cdot \mathbf{h}] \mathcal{E}_{n'n'}]_{k=0} \\ &\quad \times \frac{2f_{n'n'} \mathcal{E}_{n'n'}}{(\mathcal{E}_{n'n'} - \omega^2)^2} \\ &= \frac{e^2 \hbar}{2m^2} \mathcal{E}_g (g_c g_{c'} - g_v g_{v'}) \sum_{\mathbf{k}} \frac{2\mathcal{E}_{cv}}{(\mathcal{E}_{cv} - \omega^2)^2}. \end{aligned} \quad (54)$$

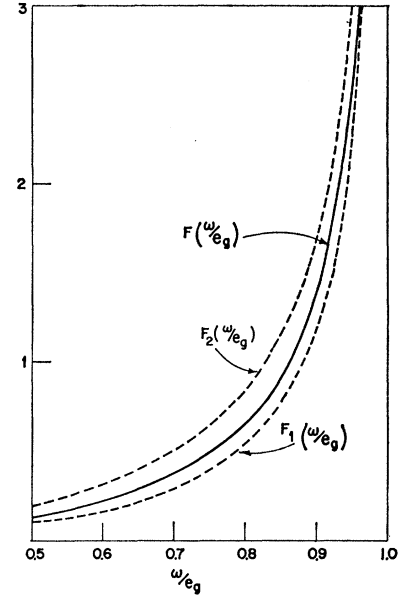


FIG. 1. Comparison of functions F_1 , F_2 , and F .

We now have the problem that the frequency dependence of Eq. (54) is not correct for small ω , as σ_{xy} should vanish as ω^2 . This can be remedied by subtracting off the $\omega=0$ term as was done by Boswawa, Howard, and Lidiard,⁵ but it seems more natural to subtract off a term depending on $(\mathcal{E}_{cv} - \omega^2)^{-1}$, as such terms do appear in Eq. (45). In doing this, we are assuming that no other bands are involved, as well as evaluating certain elements at the band edge. The appropriate term to subtract in the summation over k in Eq. (54) is $2/\mathcal{E}_{cv}(\mathcal{E}_{cv} - \omega^2)$. The sum over k is then

$$\sum_{\mathbf{k}} \frac{2\omega^2}{\mathcal{E}_{cv}(\mathcal{E}_{cv} - \omega^2)^2} = \left(\frac{2\mu}{\mathcal{E}_g}\right)^{3/2} \frac{1}{16\pi} F_1\left(\frac{\omega}{\mathcal{E}_g}\right). \quad (55)$$

$$F_1(x) = \frac{1}{x} \left(\frac{1}{(1-x)^{1/2}} - \frac{1}{(1+x)^{1/2}} \right) - \frac{4}{x^2} [2 - (1-x)^{1/2} - (1+x)^{1/2}]. \quad (56)$$

Here we have assumed parabolic bands, and μ is the reduced effective mass. This expression is the same as that obtained by Kolodziejczak, Lax and Nishina,⁴ which was obtained from a semiclassical argument. The function $F_1(x)$ approaches $(1-x)^{-1/2}$ as x approaches 1, and goes to zero as $5x^2/16$. The corresponding function $F_2(x)$, obtained by subtracting the zero frequency term from Eq. (54), is given by Eq. (56) with the second term replaced by -1 . F_2 goes to zero as $\frac{5}{2}x^2$, so that at low frequencies, it is twice $F_1(x)$. The functions F_1 and F_2 are plotted in Fig. 1 along with another function described below. It is interesting to note that the functions fall off much more rapidly than $1/(1-x)^{-1/2}$ below the gap.

Above the gap, $(1-x)^{1/2}$ becomes imaginary, and we take the real part of F_1 , which is negative near $x=1$, and approaches about -3 at $x=1$. The function then has a dispersion-like character, although it is unsymmetrical.

The Faraday rotation from these two bands is given by

$$\theta = \frac{e^2 h}{4nc(2m\mathcal{E}_g)^{1/2}} \left(\frac{\mu}{m}\right)^{3/2} (g_c g_c' - g_v g_v') F_1\left(\frac{\omega}{\mathcal{E}_g}\right). \quad (57)$$

It can be seen that the sign of the Faraday rotation depends on the g factor and the contribution of the relevant band to the g factor.

An attempt to study the low-frequency behavior would seem logical at this point, and it would be reasonable to consider the case in which only the two bands interacted. However, in this case $g_c' = -g_v'$, and if we neglected the spin contribution to the g factor, the primed and unprimed g factors are the same and the leading term vanishes. It, therefore, seems appropriate to consider a more complicated model. It has been found possible to solve exactly the case of an s -like conduction band and a p -like valence band without spin-orbit interaction when the two are close enough that all other bands can be neglected, and also the free-electron effective masses and g factor can be ignored. The band-edge basis functions are S for the conduction band, and iX , iY , iZ for the valence band,¹¹ and the $k \cdot p$ Hamiltonian in this representation is

$$\mathcal{H} = \begin{pmatrix} \mathcal{E}_g/2 & k_x P/m & k_y P/m & k_z P/m \\ k_x P/m & -\mathcal{E}_g/2 & 0 & 0 \\ k_y P/m & 0 & -\mathcal{E}_g/2 & 0 \\ k_z P/m & 0 & 0 & -\mathcal{E}_g/2 \end{pmatrix}, \quad (58)$$

where

$$P = i \int d\mathbf{r} S p_x X, \quad (59)$$

with P assumed to be positive.

To diagonalize the Hamiltonian, we first transform to a representation with one basis function

$$i(r_x X + r_y Y + r_z Z), \quad (60)$$

where $\mathbf{r} = \mathbf{k}/k$, and two other basis functions in which \mathbf{r} is replaced by \mathbf{s} and \mathbf{t} , which are unit vectors perpendicular to \mathbf{r} and to each other, and which we need not specify otherwise. In the new representation, the Hamiltonian breaks up into a 2×2 block

$$\mathcal{H}_{2 \times 2}' = \begin{bmatrix} \mathcal{E}_g/2 & kP/m \\ kP/m & -\mathcal{E}_g/2 \end{bmatrix}, \quad (61)$$

which is uncoupled from the remaining two bands which are degenerate and flat with energy $-\mathcal{E}_g/2$. We next make a unitary transformation to diagonalize

Eq. (61). Defining

$$\begin{aligned} \mathcal{E}_g/2 &= a, \\ kP/m &= b > 0, \\ c &= (a^2 + b^2)^{1/2}, \end{aligned} \quad (62)$$

we have for this transformation

$$U_{2 \times 2} = \begin{bmatrix} u_+ & u_- \\ u_- & u_+ \end{bmatrix}; \quad (63)$$

$$u_{\pm} = (c \pm a/2c)^{1/2}.$$

The eigenvalues of \mathcal{H} are $\pm c$. We need the matrix element of π in the new representation

$$\pi = \frac{P}{m} \begin{pmatrix} \frac{b\mathbf{r}}{c} & \frac{a\mathbf{r}}{c} & s u_+ & t u_+ \\ \frac{a\mathbf{r}}{c} & \frac{-b\mathbf{r}}{c} & -s u_- & -t u_- \\ s u_+ & -s u_- & 0 & 0 \\ t u_+ & -t u_- & 0 & 0 \end{pmatrix}. \quad (64)$$

We are now in a position to evaluate Eq. (45), if we use Eq. (44) for x . The result before summing over k is

$$\sigma_{xy} = \frac{2}{3} c^2 h \left(\frac{P}{m}\right)^4 \sum_{\mathbf{k}} \left\{ \frac{1}{2c(c-a)} \frac{1}{(c+a)^2 - \omega^2} - \frac{a(2c^2 - a^2)}{c^3 b^2} \frac{1}{(2c)^2 - \omega^2} - \frac{8a}{c} \frac{1}{((2c)^2 - \omega^2)^2} \right\}. \quad (65)$$

The integrals can be done exactly and the resulting expression for the Faraday rotation is

$$\theta = -\frac{(\sqrt{2}-1)e^2 h}{3nc} \frac{P}{m\mathcal{E}_g} F\left(\frac{\omega}{\mathcal{E}_g}\right), \quad (66)$$

where

$$F(x) = \frac{2}{\pi(\sqrt{2}-1)} \left\{ \frac{2}{x(1-x^2)^{1/2}} \tan^{-1} \frac{x}{(1-x^2)^{1/2}} - \frac{1}{[x(1-x)]^{1/2}} \tan^{-1} \left(\frac{x}{1-x}\right)^{1/2} - \frac{1}{[x(1+x)]^{1/2}} \right\} \times \ln[(1+x)^{1/2} + (x)^{1/2}]. \quad (67)$$

$F(x)$ approaches $(1-x)^{-1/2}$ as $x \rightarrow 1$, as was true of the previous energy functions F_1 and F_2 . For low frequencies, we have

$$F(x) \sim \frac{8}{15\pi(\sqrt{2}-1)} x^2 = 0.41x^2. \quad (68)$$

Notice that $F(x)$ correctly goes to zero for low fre-

¹¹ E. O. Kane, Phys. Chem. Solids **1**, 249 (1957).

quencies, although this is not true for the integrand in Eq. (65).

In Fig. 1, the functions F_1 , F_2 , and F are compared. We would have arrived at F_1 or F_2 for this model if we had used essentially the same approximations as in the simple band case, so that it is heartening to note that the three functions do not differ drastically. In applying the formalism to a more realistic case, as we do in the next section, we shall make use of F_1 , which is a little better for this model than F_2 .

An interesting feature of θ in this case is that it is negative, whereas in the corresponding atomic case, θ would be positive. This appears to be due to the reversal in sign of the Zeeman interaction (\mathcal{H}') for the valence band, when it is dominated by the interaction with the nearby band above it. In the atomic case, there is a sum rule; or, in other words, L is a good quantum number for a spherical atom with no spin. In several semiconductors, the sign of θ is reversed for interband transitions.

V. APPLICATION TO SEMICONDUCTORS

A more realistic model to which we now apply the above formalism is that of an s -like conduction band and a spin-orbit split valence band as is found in Ge and some III-V compounds. In this case, we will evaluate only the most singular term, as this itself turns out to be rather complicated.

The complexity comes about because we are dealing with a degenerate band edge, the $J_{3/2}$ valence band edge. In Eq. (45), the second term in the square brackets will now be finite at $k=0$, and so must be considered. The reason for this is that there exist intervalence band matrix elements of x which go as $1/k$ as $k \rightarrow 0$. In Eq. (45), the energy denominator goes as k^2 , and the numerator as k , giving $1/k$. In the terms with n' and n'' in the valence band and n in the conduction band, these singular matrix elements always occur with matrix elements of π or v going as k , so that the result is finite for $k \rightarrow 0$. As was pointed out earlier, we need not concern ourselves with matrix elements of x between states of equal energy, as these cancel between the two terms.

We shall outline the calculation for the case in which anisotropy can be neglected, since this avoids a rather lengthy calculation, but shall state that with an appropriate choice of parameters, the result is good to first order in the anisotropy of the valence band. The treatment of the valence band is based on that of

Luttinger¹² and Dresselhaus, Kip and Kittel,¹³ although we shall use a slightly different representation. The basis functions for the valence band are

$$\begin{aligned}\phi_1 &= i(X+iY)\alpha, \\ \phi_2 &= i(X-iY)\beta, \\ \phi_3 &= (i/\sqrt{6})[(X+iY)\beta - 2Z\alpha], \\ \phi_4 &= (i/\sqrt{6})[-(X-iY)\alpha - 2Z\beta],\end{aligned}\quad (69)$$

with the conduction band functions given by $S\alpha$ and $S\beta$.

The effective mass Hamiltonian for the valence band is given in this representation by

$$\mathcal{H}_{em} = - \begin{pmatrix} w-v & 0 & t & u \\ 0 & w-v & -u^* & t^* \\ t^* & -u & w+v & 0 \\ u^* & t & 0 & w+v \end{pmatrix}, \quad (70)$$

where

$$\begin{aligned}w &= \frac{\gamma_1 k^2}{2m}, \\ v &= \bar{\gamma} \frac{3k_z^2 - k^2}{2m}, \\ t &= -\sqrt{3}\bar{\gamma}(k_x - ik_y)k_z, \\ u &= -(\sqrt{3}/2)\bar{\gamma}(k_x - ik_y)^2.\end{aligned}\quad (71)$$

Here γ_1 and $\bar{\gamma} \cong \gamma_2 \cong \gamma_3$ are the parameters used by Luttinger.¹² We will need matrix elements of

$$\begin{aligned}\pi &\cong \pi_0 + \pi_1, \\ \bar{x} &\cong \bar{x}_0 + \bar{x}_{-1},\end{aligned}\quad (72)$$

where the index gives the order in k , and where the bar over x indicates that we omit equal energy matrix elements. π_0 and, hence, \bar{x}_0 are obtained by using zero-order basis functions. π_1 is given by $\nabla_k \mathcal{H}_{em}$, and \bar{x}_{-1} is obtained from π_1 through Eq. (44).

We now wish to transform to a representation in which k is in the z direction, as we did in the last section. This is simple for \mathcal{H}_{em} , for which we merely replace the unit vectors $\mathbf{i}, \mathbf{j}, \mathbf{k}$, by $\mathbf{s}, \mathbf{t}, \mathbf{r}$, and assume the spins to be quantized in the \mathbf{r} direction. The new effective-mass Hamiltonian is then diagonal with eigenvalues $-(\gamma_1 \mp 2\bar{\gamma})k^2/2m$. For π_1 , we take the gradient of \mathcal{H}_{em} in the *original* representation and then replace $\mathbf{i}, \mathbf{j}, \mathbf{k}$ by $\mathbf{s}, \mathbf{t}, \mathbf{r}$. We cannot simply differentiate the new \mathcal{H}_{em} , as the coefficients of the transformation depend on \mathbf{k} . The 4×4 result is

$$\pi_1 = \frac{k}{m} \begin{pmatrix} (\gamma_1 - 2\bar{\gamma})\mathbf{r} & 0 & -\sqrt{3}\bar{\gamma}(\mathbf{s} - i\mathbf{t}) & 0 \\ 0 & (\gamma_1 - 2\bar{\gamma})\mathbf{r} & 0 & -\sqrt{3}\bar{\gamma}(\mathbf{s} + i\mathbf{t}) \\ -\sqrt{3}\bar{\gamma}(\mathbf{s} + i\mathbf{t}) & 0 & (\gamma_1 + 2\bar{\gamma})\mathbf{r} & 0 \\ 0 & -\sqrt{3}\bar{\gamma}(\mathbf{s} - i\mathbf{t}) & 0 & (\gamma_1 + 2\bar{\gamma})\mathbf{r} \end{pmatrix}, \quad (73)$$

¹² J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).

¹³ G. Dresselhaus, A. Kip, and C. Kittel, Phys. Rev. **98**, 368 (1955).

with \bar{x}_{-1} given again by Eq. (45). In the Zeeman interaction \mathcal{H}' , we can now write down the part involving \bar{x}_{-1} , but the part involving x_0 and π_0 involves another band parameter κ introduced by Luttinger.¹² The matrix of the interband contribution to the Zeeman interaction for the valence band is

$$-\frac{\kappa}{m} \begin{pmatrix} 3\mathbf{h}\cdot\mathbf{r} & 0 & \sqrt{3}\mathbf{h}\cdot(\mathbf{s}-i\mathbf{t}) & 0 \\ 0 & -3\mathbf{h}\cdot\mathbf{r} & 0 & -\sqrt{3}\mathbf{h}\cdot(\mathbf{s}+i\mathbf{t}) \\ \sqrt{3}\mathbf{h}\cdot(\mathbf{s}+i\mathbf{t}) & 0 & \mathbf{h}\cdot\mathbf{r} & 2\mathbf{h}\cdot(\mathbf{s}-i\mathbf{t}) \\ 0 & -\sqrt{3}\mathbf{h}\cdot(\mathbf{s}-i\mathbf{t}) & 2\mathbf{h}\cdot(\mathbf{s}-i\mathbf{t}) & -\mathbf{h}\cdot\mathbf{r} \end{pmatrix}. \quad (74)$$

Finally, the (6×6) matrix of π_0 is readily obtained from the new basis functions. This gives us the information for the term in which n is in the conduction band and n' and n'' are in the valence band. For the opposite case, we need the Zeeman interaction for the conduction band which is simply $g_c\mathbf{s}\cdot\mathbf{h}/m$. We can now evaluate the most singular term in Eq. (45), which comes out

$$\sigma_{xy} \cong \frac{e^2\hbar P^2}{3m^3} \sum_{\mathbf{k}} \left[-(g_c+10\kappa+10\bar{\gamma})F_{ll} + (-g_c-10\kappa+10\bar{\gamma})F_{hh} - 4(\gamma_1-\bar{\gamma}-\kappa)(F_{hh}+F_{ll}-2F_{hl}) \right], \quad (75)$$

where

$$F_{ij} = \mathcal{E}_i + \mathcal{E}_j / [(\mathcal{E}_i + \mathcal{E}_j)^2 - \omega^2]^2, \quad (76)$$

i and j run over h for heavy and l for light. The energies are

$$\mathcal{E}_i = \mathcal{E}_g + \frac{\hbar^2 k^2}{2\mu_i}, \quad (77)$$

where μ_i is the reduced mass obtained from α_c and $\gamma_1 \pm 2\bar{\gamma}$, the reciprocal effective masses for the conduction and valence bands.

Carrying out the sum over \mathbf{k} , we arrive at expressions involving the first term of F_1 , Eq. (56). As in the previous section, we correct the low-frequency dependence by including the second term of F_1 . The Faraday rotation is now given by

$$\theta = \theta_0 H F_1(\omega/\mathcal{E}_g), \quad (78)$$

$$\theta_0 H = \frac{e^2\hbar P^2}{24cnm^3} \left(\frac{2}{\mathcal{E}_g} \right)^{3/2} (\mu_h^{3/2} + \mu_l^{3/2}) g_{\text{eff}}. \quad (79)$$

$$g_{\text{eff}} = \left[-(g_c+10\kappa) + 10\bar{\gamma}(x^3-1)/(x^3+1) - 4(\gamma_1-\bar{\gamma}-\kappa)(x^3-1)(x-1)/(x^3+1)(x+1) \right], \quad (80)$$

where

$$x = (\mu_h/\mu_l)^{1/2} > 1. \quad (81)$$

We have written this in terms of g_{eff} to conform with previous theories.³ We see immediately that g_{eff} can be of either sign, depending on which parameters dominate. The last term in g_{eff} is usually small and vanishes for the Kane model,¹¹ in which case $\bar{\gamma} = \kappa = \frac{1}{2}\gamma_1$.

We can now relate the various quantities to band parameters of semiconductors. We must first define the average $\bar{\gamma}$ of γ_2 and γ_3 :

$$\bar{\gamma} = (2\gamma_2 + 3\gamma_3)/5. \quad (82)$$

This particular average is obtained by averaging $\mathcal{E}(\mathbf{k})$ ¹³ over the direction of \mathbf{k} to first order in the anisotropy, and as stated earlier, actually gives the Faraday effect correctly to first order in the anisotropy. We now have¹²⁻¹⁴

$$\gamma_1 = (f+2g+2h_1-3)/3, \quad (83)$$

$$\bar{\gamma} = (5f+g+h_1)/30, \quad (84)$$

$$\kappa = (f-g-h_1-2)/6, \quad (85)$$

$$P^2/m\mathcal{E}_g = (f/2), \quad (86)$$

$$\alpha_c = 1 + f[(3\mathcal{E}_g + 2\Delta)/3(\mathcal{E}_g + \Delta)], \quad (87)$$

$$g_c = 2 - f[2\Delta/3(\mathcal{E}_g + \Delta)]. \quad (88)$$

Here $f, g, h_1 > 0$ are the magnitudes of $F, G,$ and H_1 of Ref. 13, expressed in units of $1/2m$. We are assuming $H_2 = 0$. For α_c and g_c , we are assuming that the conduction band interacts only with the valence bands and the split-off band. Δ is the spin-orbit splitting. Notice that with our choice of $\bar{\gamma}$, there are only two parameters outside of energy gaps which enter.

The above parameters are actually applicable to semiconductors possessing inversion symmetry, and applying them to III-V compounds as we shall, implies the assumption that certain antisymmetric¹¹ parameters are negligible.

The theory has been applied to several semiconductors, as shown in Table I and Fig. 2. Inserting numbers into Eq. (79), we can write

$$\theta_0 = (5.17f/n\sqrt{\mathcal{E}_g}) [(\mu_h/m)^{3/2} + (\mu_l/m)^{3/2}] g_{\text{eff}}, \quad (89)$$

in deg/cm-kG, where \mathcal{E}_g is in eV. In calculating g_{eff} and θ_0 , band parameters were used as given in the table. The parameters used were low-temperature values, since the room-temperature values are not known. However, the room-temperature energy gap was used to normalize the frequency in $F_1(\omega/\mathcal{E}_g)$.

¹⁴ L. M. Roth, B. Lax, and S. Zwerdling, Phys. Rev. **114**, 90 (1959).

TABLE I. Comparison of theory and experiment for θ_0 and g_{eff} . The experimental data are the room-temperature results in Fig. 1, except for the starred entry for InSb, which was the 77°K result of Smith, Pidgeon and Prosser.^a

	ε_g (eV)		Δ (eV)	f	$g+h_1$	Theory		Experiment	
	300°K	0°K				θ_0 deg/cm-kG	g_{eff}	θ_0 deg/cm-kG	g_{eff}
InSb	0.18 ^b	0.23 ^c	0.9 ^e	91 ^e	10 ^e	-16	-30	{-30 -20*	{-57 -38*
InAs	0.36 ^b	0.41 ^d	0.43 ^d	51 ^d	6 ^d	-12	-22.5	-10.5	19.5
Ge	0.80 ^b	0.90 ^b	0.29 ^e	29 ^f	7 ^f	-4.2	-12.6	-2.6	-7.8
GaAs	1.41 ^g	1.53 ^h	0.33 ⁱ	14 ^j	{5 ⁱ 7 9	{-1.4 -0.15 +1.1	{-3.7 -0.4 +2.9	+1.33	+3.6

^a See Ref. 18.

^b S. Zwerdling, B. Lax, and L. M. Roth, Phys. Rev. 108, 1402 (1957).

^c S. Zwerdling, W. H. Kleiner, and J. P. Theriault, Suppl. J. Appl. Phys. 32, 2118 (1961).

^d See Ref. 15.

^e A. H. Hahn, Phys. Rev. 97, 1647 (1955).

^f J. J. Stickler, H. J. Zeiger, and G. S. Heller, Phys. Rev. 127, 1077 (1962).

^g T. S. Moss, Suppl. J. Appl. Phys. 32, 2136 (1961).

^h M. A. Sturge, Phys. Rev. 127, 768 (1962).

ⁱ See Ref. 16.

^j See Ref. 2.

For Ge and InSb, the band parameters are well known. For InAs and GaAs, f was determined from the electron mass and energy gaps through Eq. (87), while $g+h_1$ was obtained from intervalence band optical absorption measurement of Matossi and Stern¹⁵ and Braunstein.¹⁶ For GaAs, this corresponds to the lowest value of $g+h_1$ given. The others are included in order to obtain the experimental sign of the effect, as will be discussed below.

The experimental points in Fig. 2 are obtained by subtracting off the free carrier Faraday effect and normalizing by the value of θ_0 , given in the table under "experimental." In Ge, a constant value of 4°/kG-cm was subtracted off from the data, to account for some additional rotation which has been attributed to an L point transition.¹⁷ In GaAs, a constant rotation of 0.62°/kG-cm was subtracted off. The free carrier Faraday effect for this case actually appears to extrapolate to a finite value at zero wavelength (see Ref. 2, Fig. 2). This may be due to interconduction band transitions. For InSb, we have also included the 77°K results of Smith, Pidgeon and Prosser.¹⁸ Their fit was to $F_2(x_1)$, and we merely fitted $F_1(x)$ at one point ($\frac{3}{4}\omega_g$) to obtain θ_0 .

VI. DISCUSSION

The theoretical and experimental values of θ_0 follow the same general trend with energy gap, and for the first three materials, the sign and order of magnitude of the effect are predicted by the theory, the latter to better than a factor of two. From the theoretical result for g_{eff} , we expect that as the gap increases and the

parameter f becomes smaller with respect to $g+h_1$, the Faraday effect becomes positive. For GaAs, with $g+h_1=5$, the theory does not yet give the sign change. This will be discussed further below. However, we can understand in the light of this the fact that larger gap semiconductors have positive interband rotations. InP, GaP, AlSb, CdS, and Si all have positive

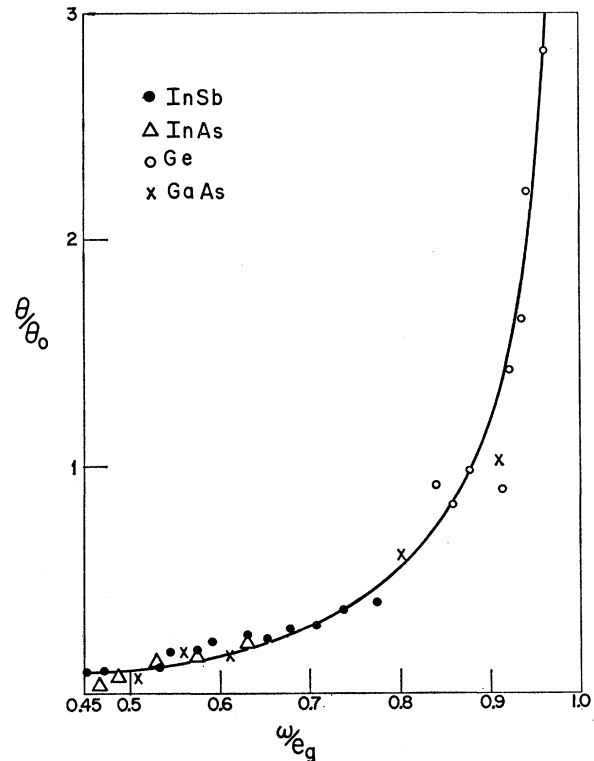


FIG. 2. Room-temperature experimental data fit to the function $F_1(\omega/\varepsilon_g)$. The value of θ_0 used is given in Table I. The sources of the results are given in Refs. 1 (InSb), 2 (InAs and GaAs), and 3 (Ge).

¹⁵ F. Matossi and F. Stern, Phys. Rev. 111, 472 (1958).

¹⁶ R. Braunstein, Phys. Chem. Solids 8, 280 (1959).

¹⁷ I. M. Boswarva and A. B. Lidiard, in *Proceedings of the International Conference on Physics of Semiconductors, Exeter* (The Institute of Physics and the Physical Society, London, 1962), p. 308.

¹⁸ S. D. Smith, C. R. Pidgeon, and V. Prosser, in Ref. 17, p. 301.

rotations¹⁹⁻²¹ (Si has a different $k=0$ conduction band structure, and so is perhaps not comparable except in a general way). Since not much information is available as to the parameters for these materials, we have made no attempt at a detailed fit. The only one of these with a smaller gap than GaAs (1.29 eV at 0°K) is InP, for which the rotation is similar in magnitude to that in GaAs.

It is clear from our results that the negative sign is due to the reversed sign of the Zeeman interaction in the valence band, due to the close interaction with the conduction band. It is not due to the negative g factor in the conduction band, as suggested by Cardona,² since Eq. (80) shows that a negative g_c gives a positive contribution to g_{eff} (due to a negative g_c').

Uncertainties in the calculation include the approximation leading to the function F_1 , and the use of low-temperature valence band parameters. In this connection, we should note that better agreement is obtained from the 77° data of Smith, Pidgeon, and Prosser,¹⁸ although their 5° data seem to give a larger g_{eff} . There is an additional uncertainty in the expression for g_{eff} , due to the fact that there are terms of both signs in it, which are 3 or 4 times the magnitude of the final result.

One thing we have neglected in the calculation is exciton effects. Wallis and Mitchell¹⁷ have presented evidence that these effects are important in the interband Faraday effect in Ge. However, Wallis and Mitchell's results are concerned mainly with effects quite near the energy gap. It seems reasonable to neglect them at energies less than a few times the binding energy, which is the range we are dealing with here.

We have also neglected the contribution from the split-off band in Ge and GaAs, although this is probably partly taken care of by the constant rotation which was subtracted. This contribution is difficult to estimate because cross terms between the valence bands are important, and for this reason, we suspect that the relative contribution of the split-off band plus cross terms, while important, is less than that calculated by Boswarva and Lidiard.¹⁷

Boswarva and Lidiard have also calculated the interband Faraday effect for Ge due to the first two valence bands. Their calculation involves summing the contribution of the valence band Landau levels, and should be equivalent to ours, although their method is more difficult to apply than ours. Their final numerical result does not seem to agree with ours, but this appears to be a matter of units.

The case of GaAs deserves special discussion. It had been hoped that the theory could predict the reversal of sign for this compound as compared with smaller gap

semiconductors. However, while the order of magnitude is predicted, the sign is sensitive to the value of $g+h_1$, and a rather large value (~ 9) is necessary to give the correct sign. [The variation of g_{eff} with $(g+h_1)$ is mainly through κ , and $dg_{\text{eff}}/d(g+h_1)$ is approximately 5/3.] Although the uncertainty involved in subtracting two larger numbers (~ 10) to obtain the theoretical g_{eff} would not lead us to take the result too seriously, it is interesting to speculate on the consequences of such a large value.

First, let us clarify the experimental evidence on this parameter, which is related to the heavy hole mass by

$$m/m_h = (3/5)(g+h_1) - 1. \quad (90)$$

Ehrenreich²³ has obtained the values 0.68 and 0.12 for the heavy and light masses from the electron mass and from the intervalence band optical absorption results of Braunstein¹⁵ which give the mass ratios $m_h/m_s = 3.38$ and $m_s/m_l = 1.7$, where m_s is the mass of the split-off band. The latter is given by γ_1 except that f should be decreased in proportion to the increased gap. Ehrenreich neglected $g+h_1$ in calculating m_l , so that his result is probably too large. We can calculate $g+h_1$ from f and the mass ratios using Eqs. (86) and (87). In fact, we have too much information, but a value of $g+h_1$ of about 5 seems to be the most consistent, giving $m_h/m_s = 3.2$, $m_s/m_l = 1.85$, and also $m_l/m = 0.085$, $m_h/m = 0.50$. This value of $g+h_1$ is the first entry in the table, and results in a negative g_{eff} .

The parameter h_1 , which we assume much larger than g ,¹³ is determined by the interaction of the valence band with the Γ_{15} conduction band. A value of h_1 smaller than that in Ge is expected according to the calculation of Callaway,²⁴ because the antisymmetric potential present in the compound would repel the Γ_{15} conduction band relative to the valence band. Callaway predicts this gap to be 4.5 eV compared with 3.2 for Ge interpreted from optical data.²⁵

A value of 9 for $g+h_1$ would imply a smaller value for this gap, perhaps as small as 2 eV. There is in fact some optical data which could support such a small gap. There is structure between 2 and 3 eV in the reflectivity of GaAs as measured by Greenaway,²⁶ which has been tentatively assigned to an L -point transition. There is also the absorption measured in n -type GaAs by Spitzer and Whelan,²⁷ beginning at 0.25 eV and leveling off at 0.5 eV. This could be partly due to a direct transition²⁸ between Γ_2 and Γ_{15} as it varies little with temperature. Pressure measurements could shed light on this matter.²⁸ If such measurements were to imply

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²⁸ W. Paul, Suppl. J. Appl. Phys. **32**, 2082 (1961) (and personal communication).

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a value for the valence band to Γ_{15} gap of the order of 2 eV, this would certainly improve our agreement for the Faraday effect, although it would raise some theoretical questions.

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Spontaneous and Stimulated Recombination Radiation in Semiconductors*

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Spectral line shapes of the radiation produced by band-to-band recombination of excess carriers in semiconductors are calculated under the assumption that the momentum matrix element is the same for all initial and final states, i.e., that there is no momentum selection rule. The peak of the stimulated radiation falls at a lower photon energy than does the peak of the spontaneous radiation, except when $T=0^\circ\text{K}$. Some numerical results are given for simple parabolic bands, specifically for the case of electron injection into p -type GaAs, and are used to deduce the temperature dependence of the forward current which is necessary to maintain a fixed gain in the active region of a diode. The result is closely related to the temperature dependence of the threshold current in an injection laser, and gives reasonable agreement with experiment. The effect of a conduction band tail is briefly considered.

I. INTRODUCTION

RADIATIVE recombination is one of the principal processes by which electrons and holes present in excess of the thermal equilibrium concentrations can recombine in semiconductors, and has been extensively studied.¹⁻⁸ In most cases considered heretofore the radiative recombination has been primarily spontaneous radiation. However, the discovery of injection lasers⁹⁻¹¹

has confirmed the conjecture that photon populations can be high enough to give a substantial amount of stimulated emission.^{12,13} In this paper, we calculate, on the basis of a simple model, the spectral line shape of the spontaneous and stimulated radiation emitted in band-to-band recombination. The actual line shape of the radiation emitted depends on the boundary conditions and the operating conditions of a particular experiment, and is illustrated by a number of examples.

We restrict our attention to the case of band-to-band transitions, because we believe this case to be the best approximation in semiconductors in which substantial concentrations of shallow impurities are present, causing the impurity levels to merge with adjacent bands. Other models can, of course, be more applicable in other cases. For example, transitions between states of isolated impurities are responsible for the red emission of the ruby laser, and such systems have been studied in considerable detail.¹⁴ Transitions between a band and one or more impurity levels may also be important, and results for this case have been obtained by Eagles¹⁵ and by Dumke.¹⁶

In the next section we give some general results concerning the spontaneous and stimulated spectral functions, and in Sec. III we give more specific results for the case of transitions with no selection rule between simple parabolic conduction and valence bands with

* A brief account of this work was presented at the American Physical Society Meeting in St. Louis, Missouri, in March, 1963 [Bull. Am. Phys. Soc. 8, 201 (1963)].

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