PHYSICAL REVIEW VOLUME 137, NUMBER 2A 18 JANUARY 1965

Faraday Effect in Solids

HERBERT S. BENNETT*
National Magnet Laboratory,† Massachusetts Institute of Technology, Cambridge, Massachusetts

AND

[EDWARD A. STERN‡
Physics Department, University of Maryland, College Park, Maryland

(Received 18 May 1964; revised manuscript received 21 August 1964)

Expressions for the weak-field Faraday effect in cubic materials are presented for the cases of transmission and reflection. These expressions contain the elements of the complex conductivity tensor. General quantum-mechanical expressions for the diagonal and off-diagonal elements of the frequency-dependent conductivity tensor are computed for arbitrary external magnetic fields and in the zero-wave-vector limit with the aid of dispersion relations. Sum rules for the conductivity tensor elements are also derived. The high-frequency limits of the conductivity elements are shown to reduce to the free-electron-gas results. A simple physical interpretation of the effect of the magnetic field on the conductivity tensor is given and this shows that two effects could contribute to the Faraday effect. These are the Zeeman splittings of the energy levels and the changes of the matrix elements. A calculation of the Faraday effect in the effective-mass approximation is performed. Special attention is given to the contribution of the spin-orbit interaction to first order and it is shown that for practically all nonferromagnetic metals this can be an appreciable effect on the interband part. The spin-orbit effect should be observed as a rapid variation in a comparatively small frequency range. The intraband part is not affected by spin-orbit effects to first order.

I. INTRODUCTION

THE Faraday effect involves the interaction of plane polarized electromagnetic waves with matter under the influence of a magnetic field. An electromagnetic wave propagating along the direction of an externally applied magnetic field and normally incident upon the surface of a solid will be partially transmitted through and/or partially reflected from the solid, depending upon the nature of the interaction. The transmitted or reflected wave is in general elliptically polarized with the major axis rotated from the plane of polarization of the incident wave. This rotation of the plane of polarization is known as the Faraday effect. When the external magnetic field H is weak and when the solid is not optically active, we can treat the Faraday effect as a first-order effect in H. We shall therefore restrict our considerations to solids which exhibit no optical activity.

Ever since it was first observed in the last century, the Faraday effect for gases, liquids and solids has captivated the interest of many persons.[1–6] However, we are not only interested in the Faraday effect by itself, but we also are interested in the application of the Faraday effect as a means by which we may acquire further information about solids. In particular, when the period of the incident electromagnetic wave is much smaller than the electron-lattice relaxation time, the Faraday effect can yield information on the band structure. This condition gives $\omega\tau \gg 1$, where ω is the angular frequency of the radiation and where τ is the electron-lattice relaxation time. The relaxation time for a typical conduction electron at room temperature is about 10^{-13}–10^{-14} sec.[7] Thus the effect will be useful for such purposes mainly in the infrared and optical frequency regions, that is, $\omega \gg 10^{14}$ (sec)$^{-1}$ or $\lambda \ll 10^{-3}$ cm, for which the photon energies, $\hbar\omega$, satisfy $\hbar\omega \gg 10^{-1}$ eV. The quantity λ is the wavelength of the radiation.

The usual method of measuring the Faraday effect by observing the rotation in transmission is not convenient in the case of most metals. In the visible and infrared regions, most metals are good reflectors and the light can transmit only through a very thin film. However, the Faraday rotation also occurs on reflection from nonferromagnetic metals with a magnetic field normal to the surface and we may use the information from this rotation to study the electron band structure. This effect is called the polar reflection Faraday effect.

We mention the magneto-optic Kerr effect here in order to prevent confusing this effect with the polar reflection Faraday effect. When the medium is a ferromagnetic material, there is also an elliptic polarization upon reflection with the axis rotated relative to the plane of polarization of the incident wave. This phenomenon, known as the magneto-optic Kerr effect, is

---

* Present address: Theoretical Physics Division, Atomic Energy Research Establishment Harwell, near Didcot, Berkshire, England.

† Supported by the U. S. Air Force Office of Scientific Research.

‡ Guggenheim Fellow, 1963–1964.

[1] S. D. Smith and T. S. Moss, *Solid State Conference, Brussels* (John Wiley & Sons, Inc., New York, 1958). See also T. S. Moss, S. D. Smith, and K. W. Taylor, Phys. Chem. Solids **8**, 323 (1959).

[2] E. A. Stern and R. D. Myers, Bull. Am. Phys. Soc. **3**, 416 (1958); E. A. Stern, *ibid.* **5**, 150 (1960); J. McGroddy and E. A. Stern, *ibid.* **8**, 392 (1963); see also Ref. 19.

[3] A. M. Portis, Phys. Chem. Solids **8**, 326 (1959).

[4] B. Lax and Y. Nishina, Phys. Rev. Letters **6**, 464 (1961).

[5] L. R. Ingersoll and D. H. Liebenberg, J. Opt. Soc. Am. **46**, 538 (1956).

[6] R. de Mallemann, F. Suhner, and J. Grange, Compt. Rend. **232**, 1049 (1951).

[7] F. Seitz, *The Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940), p. 639; J. R. Beattie and G. K. T. Conn, Phil. Mag. **46**, 989 (1955).

proportional to the net magnetization of the sample[8] and not to the external magnetic field, as is the case of a nonferromagnetic material. In the Kerr effect, the external magnetic field merely serves to align the spins and we neglect it in the calculation. Another difference between these materials is the order of magnitude of the effects. The rotation for a nonferromagnetic material in an external magnetic field is about 1/1000 of that for a ferromagnetic material in the same external magnetic field. For example, iron (Fe) at room temperature and in an external magnetic field H of 10^4 G exhibits an angle of rotation per centimeter of sample thickness θ, with $\theta \approx 1.3 \times 10^5$ (deg/cm); while aluminum under the same conditions has $\theta \approx 10^2$ (deg/cm). The discussion that follows shows that we can explain both the magneto-optic Kerr effect and the polar reflection Faraday effect by the electromagnetic vector potential-kinetic momentum interaction term of the Hamiltonian. We include both the spin-orbit interaction and the magnetic field vector potential in the kinetic momentum operator. For ferromagnetic materials the spin-orbit dominates while for nonferromagnetic materials the magnetic field vector potential is more important. However, spin-orbit effects will still be observable in nonferromagnetics.

All of the electrons in a solid, both conduction and "bound," plus the nuclei contribute to the Faraday effect. However, at optical and infrared frequencies, the largest contribution usually comes from the conduction electrons and sometimes an important contribution arises from the electrons in the next lower band. Early theoretical calculations of the Faraday effect in solids considered only the effect of the conduction electrons and then only in the case where the frequency of radiation is low enough so that band to band or interband effects can be neglected.[9] However, as we approach the optical region, the interband effects become more important.[10] For this reason, more recent calculations have included the effect of interband transitions on the Faraday effect.[4,11,12]

Section II contains the various preliminaries. We present the general form of the conductivity tensor in a magnetic field and assume the existence of an asymptotic expansion in H. We next give the expressions for the Faraday effect in terms of the conductivity tensor. After introducing the dispersion relations for the elements of the conductivity tensor, we then use them to derive a general quantum mechanical method for calculating these elements.

Section III reviews various expressions for the conductivity; namely the conductivity of classical electrons harmonically bound and the intraband contribution to the conductivity of solids with conduction electrons. We employ the dispersion relation method introduced in Sec. II to derive a general expression for the conductivity tensor. In Sec. IV we derive from this general expression the sum rules and the high- and low-frequency limits. We next calculate in Sec. V the Faraday effect for a solid in the effective mass approximation. We perform this calculation for a ferromagnetic solid and for a nonferromagnetic solid in order to show explicitly the difference between the magneto-optic Kerr effect and the polar reflection Faraday effect. In ferromagnetics, spin-orbit effects dominate, but even in nonferromagnetics these effects are appreciable. In Sec. VI, we give a summary and discussion of the paper.

The material in Secs. II, III, and IV of this paper was presented first in an abbreviated form[13] and later in an unpublished form.[14] Subsequently this material was employed by several authors in calculating the Faraday effect.[12,15] In view of the proven utility of this material, it was felt desirable to publish a coherent presentation of it and to include it in this paper even though parts of it have appeared in other published work as references from the original unpublished material.

II. THE CONDUCTIVITY TENSOR AND PRELIMINARIES

The interband effects are only important at frequencies greater than or of the order of magnitude of the interband frequencies of the solid. This means that it is sufficient to limit oneself to infrared and higher frequencies of radiation when considering the contribution of interband effects to the Faraday effect. The interaction between the electromagnetic wave and the spins of the electrons is negligible at these frequencies. The interaction of the magnetic field of the electromagnetic radiation with the orbital motion of the electrons is of the order of magnitude (v/c) times the interaction of the electric field of the electromagnetic radiation with the orbital motion of the electrons. Here, v is the velocity of electron, c is the velocity of light, and $(v/c) \approx 10^{-3}$ for thermal conduction electrons. Except for the innermost electrons of the heaviest elements, we may neglect the interaction of the magnetic field in the electromagnetic wave with the electrons. We will neglect it throughout this paper. Therefore, for our purposes, it is sufficient to consider the interaction of the electric field in the electromagnetic wave with the orbital motion of the electrons in the solid.

Various investigators have shown that the response of the electrons in a solid to an arbitrary electric field can be described in terms of a wave-number-dependent

---

[8] P. N. Argyres, Phys. Rev. **97**, 334 (1955).

[9] M. J. Stephen and A. B. Lidiard, Phys. Chem. Solids **9**, 43 (1958).

[10] S. D. Smith, T. S. Moss, and K. W. Taylor, Phys. Chem. Solids **11**, 131 (1959).

[11] J. Halpern, B. Lax, and Y. Nishina, Phys. Rev. **134**, A140 (1964); and L. M. Roth, *ibid.* **133**, A542 (1964).

[12] I. M. Boswarva, R. E. Howard, and A. B. Lidiard, Proc. Roy. Soc. (London) **A269**, 125 (1962).

[13] H. S. Bennett and E. A. Stern, Bull. Am. Phys. Soc. **5**, 279 (1960).

[14] H. S. Bennett and E. A. Stern, University of Maryland Technical Report No. 197, 1960 (unpublished).

[15] D. L. Mitchell and R. F. Wallis, Phys. Rev. **131**, 1965 (1963).

and frequency-dependent conductivity tensor, $\sigma_{ij}(\mathbf{k},\omega)$.[16] When an electric field that varies in space and time as,

$$\mathbf{E}(\mathbf{r},t)=\int \mathbf{E}(\mathbf{k},\omega)e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}d^3kd\omega\,, \tag{1}$$

exists by some means in the solid, then the induced current assumes the form,

$$J_i(\mathbf{r},t)=\sum_j \int \sigma_{ij}(\mathbf{r}t;\,\mathbf{r}'t')E_j(\mathbf{r}'t')dt'd^3r'\,, \tag{2}$$

where i and j refer to the Cartesian components. For a homogeneous time-dependent medium, the conductivity $\sigma_{ij}(\mathbf{r}t;\,\mathbf{r}'t')$ is invariant under displacements of position and time, i.e., $\sigma_{ij}(\mathbf{r}t;\,\mathbf{r}'t')=\sigma_{ij}(\mathbf{r}-\mathbf{r}';\,t-t')$. The transform of Eq. (2) then becomes,

$$J_i(\mathbf{k},\omega)=\sum_j \sigma_{ij}(\mathbf{k},\omega)E_j(\mathbf{k},\omega)\,. \tag{3}$$

A great simplication occurs for the long-wavelength limit $\mathbf{k}\rightarrow 0$. The long-wavelength limit is valid at optical frequencies for which the wavelength, $\lambda\approx 5\times 10^{-5}$ cm, is very much larger than interatomic distances, $d\approx 10^{-8}$ cm. The wavelength of light in a metal will be smaller than that in free space because of the skin-depth effect; but even in this case, the skin depth is much greater than atomic dimensions. In such situations, we may neglect the space dependence of the electric field experienced by both the "bound" and the conduction electrons and we may therefore approximate the problem by setting $\mathbf{k}=0$ in the electromagnetic field. We have then argued that the conductivity tensor $\sigma_{ij}(\mathbf{k}=0,\,\omega)$ adequately describes in the optical region the interaction between the electromagnetic wave and the solid.

In metals, because the skin depth causes a much more rapid variation of the electric field with position inside the metal than with position outside the metal, this approximation is valid for radiation between a few tenths of an electron volt and the x-ray region. The classical skin depth δ_{cl} occurs when $(v_0/\delta\omega)\ll 1$ and $(\sigma/\omega)\gg 1$, and is given by $\delta_{\mathrm{cl}}=c/(2\pi\omega\sigma)^{1/2}$. Here v_0 is the Fermi velocity and δ is the skin depth. Under these conditions the optical properties may be adequately described by $\sigma(0,\omega)$. However, at lower energies and at low temperatures in pure samples, anomalous skin effects become important and in order to treat these cases a knowledge of $\sigma(\mathbf{k},\omega)$ is required.

We will limit our considerations to solids with cubic symmetry, and will write the general form of the conductivity tensor in a magnetic field as determined by cubic symmetry alone. If the constant magnetic field points along z direction of the solid, and if this direction is also the positive z direction, then the conductivity tensor has the form[8,9]

$$\sigma(H)=\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ -\sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}. \tag{4}$$

The magnetic field is $H=(0,0,H)$ and the x and y directions coincide with the other two cubic axes of the solid.

We now present some analytic properties of the conductivity. From the conservation of energy for a sourceless medium and the principle of "strict causality" and by the use of the calculus of residues, we can prove that $\sigma_{ij}(\omega)$ must be an analytic function of ω in the upper half complex ω plane.[14,17] This statement then leads to dispersion relations between the real and the imaginary parts of σ_{ij}. Letting $\sigma_{ij}=\sigma_{1ij}+i\sigma_{2ij}$, where both σ_{1ij} and σ_{2ij} are real, we obtain the dispersion relations,

$$\sigma_{1ij}(\mathbf{k},\omega)=\frac{2}{\pi}P\int_0^\infty \frac{\omega'\sigma_{2ij}(\mathbf{k},\omega')}{(\omega'^2-\omega^2)}d\omega'\,, \tag{5}$$

and

$$\sigma_{2ij}(\mathbf{k},\omega)=\frac{-2}{\pi}\omega P\int_0^\infty \frac{\sigma_{1ij}(\mathbf{k},\omega')}{(\omega'^2-\omega^2)}d\omega'\,. \tag{6}$$

We have used the fact that $\sigma_{ij}(-\mathbf{k},\,-\omega)=\sigma_{ij}(\mathbf{k},\omega)^*$ and have assumed that σ_{ij} is even in $\mathbf{k}$ (i.e., that the crystal has inversion symmetry). The symbol P denotes the principal value of the integral. We are interested in calculating $\sigma_{ij}(\mathbf{k}\approx 0,\,\omega)$ and will use henceforth the simplified notation,

$$\sigma_{ij}(\mathbf{k}=0,\,\omega)\equiv\sigma_{ij}(\omega)\,.$$

We may reasonably expect that a representation of the conductivity tensor elements in terms of a power-series expansion in the magnetic field is meaningful at least in an asymptotic sense as long as the Landau quantization of energy levels plays a minor role. Accordingly, we write the asymptotic forms of the conductivity tensor:

$$\sigma_{xx}\approx\sigma_{xx}{}^{(0)}+\sum_{n=1}^{l}\frac{H^{2n}}{(2n)!}\sigma_{xx}{}^{(2n)}\,, \tag{7}$$

$$\sigma_{xy}\approx\sum_{n=0}^{l}\frac{H^{2n+1}}{(2n+1)}\sigma_{xy}{}^{(2n+1)}\,, \tag{8}$$

and

$$\sigma_{zz}\approx\sigma_{xx}{}^{(0)}+\sum_{n=1}^{l}\frac{H^{2n}}{(2n)!}\sigma_{zz}{}^{(2n)}\,. \tag{9}$$

---

[16] For example: J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **28**, No. 8 (1954); J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957).

[17] B. S. Gourary, J. Appl. Phys. **28**, 283 (1957). It should be noted that the condition of analyticity for $\sigma(\omega)$ requires the presence of some mechanism by which energy may be removed from the electronic system. For example, not withstanding the fact that we are interested in the $\omega\tau\gg 1$ region, τ is to be finite.

where $\sigma_{ij}^{(n)}$ is independent of H. The integer l is limited to values near one or to one only. Its specific value depends in part upon the model used to compute σ_{ij} and upon the value of H.

It is desirable to choose a representation that most conveniently expresses the relationship between the Faraday effect and the conductivity tensor. Therefore, we consider the incident plane wave to be the superposition of equal amplitude right and left circularly polarized waves. We define the two senses of circularly polarized electric fields as the real part of

$$\mathbf{E}_{\substack{r\\l}}=E(\omega)(\mathbf{x}\pm i\mathbf{y})e^{-i\omega t}. \tag{10}$$

The plus sign and the subscript r refer to right circularly polarized (RCP) electric fields and the minus sign and the subscript l refer to left circularly polarized (LCP) electric fields. The unit vectors in the x and y directions are denoted by $\mathbf{x}$ and $\mathbf{y}$, respectively. In a similar manner, we define the RCP and LCP currents as the real part of

$$\mathbf{J}_{\substack{r\\l}}=J(\omega)(\mathbf{x}\pm i\mathbf{y})e^{i\omega t}. \tag{11}$$

It is straightforward to show that the conductivity tensor in Eq. (4) gives the relationship

$$\mathbf{J}_{\substack{r\\l}}=\sigma_{\substack{r\\l}}\mathbf{E}_{\substack{r\\l}}, \tag{12}$$

where

$$\sigma_{\substack{r\\l}}=\sigma_{xx}\pm i\sigma_{xy} \tag{13}$$

is a simple scalar. Maxwell's field equations then relate the complex index of refraction, $(n+i\kappa)$, for RCP and LCP electric fields to the complex conductivity

$$(n_{\substack{r\\l}}+i\kappa_{\substack{r\\l}})^2=1+i(4\pi\sigma_{\substack{r\\l}}/\omega). \tag{14}$$

We now express the Faraday rotation θ in terms of the complex index of refraction. We divide the plane polarized incident radiation into RCP and LCP waves. Each sense of polarization has its own index of refraction. The angle θ is just one-half the phase angle change between the RCP and the LCP waves for both transmission and reflection. In transmission, the Faraday rotation is

$$\theta_{\text{trans}}=(\omega d/2c)(n_r-n_l), \tag{15}$$

where d is the distance propagated along the z axis in the medium. When $H\neq0$, we expand the quantity (n_r-n_l) in a power series in H using Eqs. (7), (8), (13), and (14). We will be interested in the weak field case and will calculate θ to first order in the magnetic field H. We find that to first order in H,

$$n_r-n_l=-(4\pi/\omega)(n^2+\kappa^2)^{-1}(\kappa\sigma_{2xy}^{(1)}+n\sigma_{1xy}^{(1)})H. \tag{16}$$

The quantities n and κ are the real and the imaginary parts of the complex index of refraction for $H=0$,

$$(n+i\kappa)^2=1+i(4\pi\sigma_{xx}^{(0)}/\omega). \tag{17}$$

To first order in H, the Faraday rotation becomes for transmission,

$$\theta_{\text{trans}}=VHd, \tag{18}$$

where

$$V=-(2\pi/c)(n^2+\kappa^2)^{-1}(\kappa\sigma_{2xy}^{(1)}+n\sigma_{1xy}^{(1)}) \tag{19}$$

is the Verdet constant.[18] Whenever $\kappa\sigma_{2xy}^{(1)}\ll n\sigma_{1xy}^{(1)}$, we have that

$$V\approx-(2\pi/cn)\sigma_{1xy}^{(1)}. \tag{20}$$

In the case of reflection of radiation normally incident from a region of vacuum upon a boundary between vacuum and the medium, we have the result,

$$\frac{E^{\text{reflected}}}{E^{\text{incident}}}=\frac{1-(n+i\kappa)}{1+(n+i\kappa)}. \tag{21}$$

Again, the difference in phase angle between RCP and LCP radiation is twice θ. Denoting the phase angle change on reflection by ρ, we have from Eq. (21) that

$$\rho=\tan^{-1}\{-2\kappa/(1-n^2-\kappa^2)\}, \tag{22}$$

and

$$\rho_r-\rho_l=2\theta=(\cos^2\rho)\left(\frac{\partial\tan\rho}{\partial\kappa}\Delta\kappa+\frac{\partial\tan\rho}{\partial n}\Delta n\right), \tag{23}$$

where $\Delta\kappa=\kappa_r-\kappa_l$ and $\Delta n=n_r-n_l$. By methods which are similar to those used to determine Δn, we find that

$$\Delta\kappa=(4\pi/\omega)(n^2+\kappa^2)^{-1}(\kappa\sigma_{1xy}^{(1)}-n\sigma_{2xy}^{(1)})H, \tag{24}$$

where the symbols with no subscripts refer to the values when $H=0$. Combining the results in Eqs. (16), (22), (23), and (24) we obtain to first order in H,

$$\theta_{\text{refl}}=FH, \tag{25}$$

where

$$F=\frac{4\pi}{\omega}\,\mathrm{Re}\left\{\frac{\sigma_{xy}^{(1)}}{(n+i\kappa)[1-(n+i\kappa)^2]}\right\}. \tag{26}$$

Here Re$\{\cdots\}$ means real part of $\{\cdots\}$.

We have tacitly assumed that a surface phenomenon like reflection can be described by the gross properties of the bulk medium. In metals this assumption should be valid because we expect with an ideal boundary that the bulk properties will prevail beyond a few angstroms from the boundary. This is due to the short shielding length in metals. Recent experiments with aluminum films[19] confirm that it is possible to produce such a sufficiently ideal boundary.

---

[18] F. A. Jenkins and H. E. White, *Fundamentals of Optics* (McGraw-Hill Book Company, Inc., New York, 1950), p. 597 and Chap. 28.

[19] E. A. Stern, J. C. McGroddy, and W. E. Harte (to be published).

Expressions (19) and (26) fulfill our goal of expressing the Faraday rotation in terms of the conductivity tensor. The only new quantities introduced by the presence of the magnetic field are the real and the imaginary parts of $\sigma_{xy}^{(1)}$. The literature already contains expressions for n and κ evaluated at zero magnetic field.[20] We will devote the next section to calculating σ_{xy}.

We have obtained the form of the conductivity tensor given in Eq. (4) by assuming that the Cartesian coordinate axes coincide with the [100] directions of the cubic crystal. To first order in H, $\sigma_{xx}=\sigma_{xx}^{(0)}$, and for such cubic solids this is independent of the orientation of the crystal axes.[14] Also, to first order in H, we have $\sigma_{xy}=H\sigma_{xy}^{(1)}$. By performing rotations on the third rank tensor $\sigma_{xy}^{(1)}$, we can show that $\sigma_{xy}^{(1)}$ is independent of the orientation of the crystal axes for cubic solids.[9] Thus, to first order in the magnetic field, the conductivity tensor of Eq. (4) is valid for any orientation of the crystal axes of cubic solids relative to the magnetic field. We must choose the Cartesian coordinates, however, so that the magnetic field is in the z direction. Since Eq. (4) is independent of the orientation of the cubic crystal axes to first order in the magnetic field, the weak-field Faraday effect is also independent of the orientation of the cubic crystal axes to first order in the magnetic field.

We conclude this section by relating the elements of the conductivity tensor to quantum-mechanical transition rates. It is most convenient to use plane polarized waves when computing the diagonal elements and circularly polarized waves when computing the transverse elements. The power P absorbed by a solid of volume V interacting with an electric field is given by,

$$P=\tfrac{1}{2}\int \mathrm{Re}\{\mathbf{J}^{*}\cdot\mathbf{E}dV\}. \tag{27}$$

Since we are neglecting the space variation of $\mathbf{E}$, Eq. (27) becomes

$$P=(\tfrac{1}{2}V)\ \mathrm{Re}\{\sum_{ij}\sigma_{ij}{}^{*}E_j{}^{*}E_i\}. \tag{28}$$

Hence, for the plane polarized electric field,

$$\mathbf{E}=\mathbf{x}\ \mathrm{Re}\{E(\omega)e^{-i\omega t}\}, \tag{29}$$

$$P_x=(\tfrac{1}{2}V)E^2\sigma_{1xx}; \tag{30}$$

while for circularly polarized electric fields,

$$P_{r_l}=(\tfrac{1}{2}V)E^2(\sigma_{1xx}\mp\sigma_{2xy}). \tag{31}$$

The minus and plus signs refer to RCP and LCP waves, respectively. From Eqs. (30) and (31), we obtain,

$$\sigma_{1xx}=(2P_x/VE^2)=\{(P_r+P_l)/VE^2\}, \tag{32}$$

and,

$$\sigma_{2xy}=\{(P_l-P_r)/VE^2\}. \tag{33}$$

And finally, we may compute the quantities P_x, P_l, and P_r from the relation

$$Pd\omega=\hbar\omega\sum_i W_i, \tag{34}$$

where W_i is the probability per unit time that a process i will occur which absorbs a quantum of energy in the range $\hbar\omega$ to $\hbar(\omega+d\omega)$. In the next section, we shall calculate W_i for plane polarized, RCP, and LCP electric waves.

III. CALCULATIONS OF THE CONDUCTIVITY TENSOR

In this section we review some of the models used to calculate the conductivity and then present our quantum-mechanical calculation.

Classical theories exist to calculate the conductivity. For example, we may use harmonically bound classical electrons with a finite relaxation time τ as a model of the solid upon which to base our discussion. We call this model a Hookean solid. The equation of motion for a Hookean solid electron is

$$m(d^2\mathbf{r}/dt^2)+(m/\tau)(d\mathbf{r}/dt)+m\omega_1{}^2\mathbf{r}=e\mathbf{E}+m\omega_0(d\mathbf{r}/dt)\times\mathbf{z}, \tag{35}$$

where $\omega_0=(eH/mc)$, ω_1 is the natural frequency of the system, and τ is the damping time. The $m\omega_1{}^2\mathbf{r}$ term of Eq. (35) effects a localization of the electron, and therefore, when $\omega_1=0$, Eq. (35) describes a conduction electron and when $\omega_1\neq 0$, Eq. (35) describes a bound electron. The equation of motion (35) then yields,

$$\sigma_{xx}=\frac{\sigma_0\{(1+\omega_2{}^2\tau^2+\omega_0{}^2\tau^2)+i\omega_2\tau(1+\omega_2{}^2\tau^2-\omega_0{}^2\tau^2)\}}{\{(1-\omega_2{}^2\tau^2+\omega_0{}^2\tau^2)^2+4\omega_2{}^2\tau^2\}}, \tag{36}$$

where $\omega_2=\omega\{1-(\omega_1/\omega)^2\}$, $\sigma_0=(\bar{n}e^2\tau/m)$, and where $\bar{n}$ is the number of electrons per unit volume. The transverse conductivity element is,

$$\sigma_{xy}=\frac{\sigma_0\omega_0\tau\{(1-\omega_2{}^2\tau^2+\omega_0{}^2\tau^2)+2i\omega_2\tau\}}{\{(1-\omega_2{}^2\tau^2+\omega_0{}^2\tau^2)^2+4\omega_2{}^2\tau^2\}}. \tag{37}$$

The semiclassical approach for the intraband contribution to the conductivity uses the linearized Boltzmann transport equation which inherently involves the wave-packet concept. For conduction electrons with arbitrary energy surfaces and a constant relaxation time, τ, the results are that[9,19]

$$\sigma_{xx}{}^{(0)a}=\frac{e^2I_{xx}\tau}{4\pi^3\hbar^2}\,\frac{(1+i\omega\tau)}{(1+\omega^2\tau^2)^2}, \tag{38}$$

and

$$\sigma_{xy}{}^{(1)a}=\frac{e^3I_{xy}\tau^2}{4\pi^3\hbar^4c}\,\frac{\{(\omega^2\tau^2-1)-i2\omega\tau\}}{(1+\omega^2\tau^2)^2}, \tag{39}$$

---

[20] See Chap. XVII of Ref. 7.

where a stands for intraband,

$$I_{xx}=\int_{S_f}\frac{\partial\epsilon}{\partial k_x}dk_ydk_z\,,$$

and

$$I_{xy}=\int_{S_f}\left\{\left(\frac{\partial\epsilon}{\partial k_x}\right)\frac{\partial^2\epsilon}{\partial k_y{}^2}-\left(\frac{\partial\epsilon}{\partial k_y}\right)\frac{\partial^2\epsilon}{\partial k_y\partial k_x}\right\}dk_ydk_z\,.$$

The quantities ϵ and $\mathbf{k}$ are, respectively, the energy and the wave vector of the conduction electron described by the Bloch function and $\int_{S_f}$ means an integration over the Fermi surface. In the derivation of Eqs. (38) and (39), we have neglected the quantization of the electron orbits in the magnetic field. This is justified as long as the quantity kT is much greater than the cyclotron energy.

At the present time there appear to be two nonfield-theoretic ways to carry out a quantum-mechanical calculation of the conductivity tensor. Both methods require the use of time-dependent perturbation theory. In one method, we explicitly evaluate the expression for the current density when charged particles move in an electromagnetic field; that is,

$$j=\frac{e}{m}\,\mathrm{Re}\left\{\Psi^*\left[\frac{\hbar}{i}\boldsymbol{\nabla}+\frac{e}{c}\mathbf{A}+\frac{\hbar}{4mc^2}\boldsymbol{\sigma}\times\boldsymbol{\nabla}V(r)\right]\Psi\right\}\,, \quad (40)$$

and we then identify the coefficients of the electric and magnetic fields with the respective conductivity tensor elements.[8,21]

The second method is based upon a more general formalism and turns out to be less laborious. One purpose of this paper is to present the physical concepts which are needed to justify the procedures used in this second method. The method contains two parts. This first part consists of a phenomenological approach to the Faraday effect and is the subject of the previous section. The second part involves the consideration of models from which we may obtain explicit expressions for the transition rate. This will be the subject of the present section.

We briefly state the principles that this second method incorporates. The analytic properties of the conductivity tensor give us integral equations which relate the real and the imaginary parts of the conductivity tensor, [see Eqs. (5) and (6)]. Hence, we only need either the real or the imaginary part of the conductivity tensor. The absorptive part of the conductivity tensor is easier to calculate since it is proportional to the probability per unit time for absorption processes to occur [see Eqs. (32), (33), and (34)]. A probability per unit time is less cumbersome to handle than a time-dependent wave function upon which the first method relies. The integral equations [Eq. (5)] then give us the dispersive part of the conductivity. Having thus obtained expressions for both the absorptive and dispersive parts of the conductivity, we will be able to treat the Faraday effect.

We will first calculate the transition probability W_i of Eq. (34), and then we will compute σ_{1xx} and σ_{2xy} by use of Eqs. (32) and (33), respectively. The semiclassical approximation for treating the interaction between electromagnetic radiation and the system of electrons is adequate for our purposes. The Hamiltonian denoting the system has the form

$$\mathcal{H}_s=\mathcal{H}_0+\sum_i\left\{\frac{e}{mc}\boldsymbol{\pi}_i\cdot\mathbf{A}_L(\mathbf{r}_i)+\frac{e^2}{2m^2c^2}\mathbf{A}_L{}^2(\mathbf{r}_i)\right\}\,, \quad (41)$$

where $\mathcal{H}_0$ is the Hamiltonian in the absence of the radiation field. The kinetic momentum operator, $\boldsymbol{\pi}_i=\mathbf{P}_i+(\hbar/4mc^2)(\boldsymbol{\sigma}_i\times\boldsymbol{\nabla}V(\mathbf{r}_i))$, satisfies the relation, $[\mathbf{r}_i,\mathcal{H}_0]=(i\hbar/m)\boldsymbol{\pi}_i$: where $\mathbf{P}_i=\mathbf{p}_i+(e/c)\mathbf{A}_M(\mathbf{r}_i)$, $\mathbf{p}_i$ is the canonical momentum operator, $\mathbf{A}_M(\mathbf{r}_i)$ is the vector potential of the uniform magnetic field, and $\mathbf{A}_L(\mathbf{r}_i)$ is the vector potential of the electric radiation field. The quantity $\boldsymbol{\sigma}_i$ is the Pauli spin operator; and the periodic potential $V(\mathbf{r}_i)$ is invariant under any transformation contained in the cubic point group of the crystal.

For the approximation of interest here, we may neglect that part of the Hamiltonian (41) which is second order in the vector potential $\mathbf{A}_L$. We shall also assume that the Coulomb interaction between the electrons, (e^2/r_{ij}), may be replaced by an effective one-body operator which maintains the lattice periodicity, and that to a good approximation the wave functions for electrons in the solid are product wave functions of single-electron wave functions. The Hamiltonian $\mathcal{H}_0$ under the above assumptions becomes a one-body operator

$$\mathcal{H}_0{}'=\textstyle\sum_i\mathcal{H}_{0i}{}'\,,$$

where

$$\mathcal{H}_{0i}{}'=\frac{P_i{}^2}{2m}+V(\mathbf{r}_i)+\frac{\hbar\mathbf{P}_i}{4m^2c^2}\cdot[\boldsymbol{\sigma}_i\times\boldsymbol{\nabla}V(\mathbf{r}_i)]+V_{\mathrm{eff}}(\mathbf{r}_i)\,. \quad (42)$$

The term containing the spin operator is the spin-orbit interaction.

Let us denote the eigenfunctions and the eigenvalues of $\mathcal{H}_{0i}{}'$ by χ_α and $\mathcal{E}_\alpha$, respectively;

$$\mathcal{H}_{0i}{}'\chi_\alpha=\mathcal{E}_\alpha\chi_\alpha\,, \quad (43)$$

where α includes all the quantum numbers associated with the symmetries of $\mathcal{H}_{0i}{}'$. The total Hamiltonian for the solid now assumes the form,

$$\mathcal{H}_s=\textstyle\sum_i\mathcal{H}_i=\sum_i(\mathcal{H}_{0i}{}'+\mathcal{H}_{Ri})\,, \quad (44)$$

where

$$\mathcal{H}_{Ri}=(e/mc)\boldsymbol{\pi}_i\cdot\mathbf{A}_L(\mathbf{r}_i)\,. \quad (45)$$

The term $\mathcal{H}_{Ri}$ represents the interaction between the electric field and an electron of the solid, and thereby,

---

[21] M. S. Dresselhaus and G. Dresselhaus, Phys. Rev. **125**, 499 (1962).

causes an electron initially in a state $|\alpha\rangle$ to make transitions to other states. We shall treat $\mathcal{H}_{Ri}$ as a small time-dependent perturbation.

The vector potential for the plane polarized electric field is

$$\mathbf{A}_L{}^p=\mathbf{x}c\,\mathrm{Re}\{(E(\omega)/i\omega)e^{-i\omega t}\}\,, \tag{46}$$

and for the RCP or LCP electric field it is

$$\mathbf{A}_L{}^{\substack{r\\l}}=c\,\mathrm{Re}\left\{\frac{E(\omega)}{i\omega\sqrt{2}}(\mathbf{x}\pm i\mathbf{y})e^{-i\omega t}\right\}\,. \tag{47}$$

Time-dependent perturbation theory gives us the transition probability per unit time from the state $|\alpha\rangle$ to the state $|\beta\rangle$;

$$W_{\beta\alpha}{}^p=\frac{2\pi}{\hbar}|\mathcal{H}_{R\beta\alpha}{}^p|^2\{\delta(\hbar\omega_{\beta\alpha}-\hbar\omega)+\delta(\hbar\omega_{\beta\alpha}+\hbar\omega)\}\,, \tag{48}$$

for plane waves; and

$$W_{\beta\alpha}{}^{\substack{r\\l}}=\frac{2\pi}{\hbar}\{|\mathcal{H}_{R\beta\alpha}{}^{\mp}|^2\delta(\hbar\omega_{\beta\alpha}+\hbar\omega)$$
$$+|\mathcal{H}_{R\beta\alpha}{}^{\mp}|^2\delta(\hbar\omega_{\beta\alpha}-\hbar\omega)\}\,, \tag{49}$$

for RCP and LCP waves, respectively. The respective absolute values squared of the indicated matrix elements are

$$|\mathcal{H}_{R\beta\alpha}{}^p|^2=\frac{E^*Ee^2}{4m^2\omega^2}|\langle\beta|\pi_x|\alpha\rangle|^2 \tag{50}$$

and

$$|\mathcal{H}_{R\beta\alpha}{}^{\pm}|^2=\frac{E^*Ee^2}{8m^2\omega^2}|\langle\beta|\pi^{\pm}|\alpha\rangle|^2\,, \tag{51}$$

where $\pi^{\pm}=\pi_x\pm i\pi_y$ and $\omega_{\beta\alpha}=\hbar^{-1}(\mathcal{E}_\beta-\mathcal{E}_\alpha)$.

Referring to Eqs. (32), (33), and (34), we obtain

$$\sigma_{1xx}=\frac{\pi e^2}{\hbar\omega m^2V}\sum_\beta{}''\sum_\alpha{}'|\langle\beta|\pi_x|\alpha\rangle|^2$$
$$\times\{\delta(\omega_{\beta\alpha}-\omega)+\delta(\omega_{\beta\alpha}+\omega)\} \tag{52}$$

and

$$\sigma_{2xy}=\frac{\pi e^2}{4\hbar\omega m^2V}\sum_\beta{}''\sum_\alpha{}'[|\langle\beta|\pi^-|\alpha\rangle|^2$$
$$\times\{\delta(\omega_{\beta\alpha}-\omega)+\delta(\omega_{\beta\alpha}+\omega)\}-|\langle\beta|\pi^+|\alpha\rangle|^2$$
$$\times\{\delta(\omega_{\beta\alpha}-\omega)+\delta(\omega_{\beta\alpha}+\omega)\}]\,, \tag{53}$$

where $\sum_\alpha{}'\{\cdots\}$ denotes a summation over the occupied states and $\sum_\beta{}''\{\cdots\}$ denotes a summation over the unoccupied states. The dispersion relations (5) and (6) then yield

$$\sigma_{2xx}=\frac{-2e^2\omega}{\hbar m^2V}\sum_\beta{}''\sum_\alpha{}'\frac{|\langle\beta|\pi_x|\alpha\rangle|^2}{|\omega_{\beta\alpha}|(\omega_{\beta\alpha}{}^2-\omega^2)} \tag{54}$$

and

$$\sigma_{1xy}=\frac{e^2}{2\hbar m^2V}\sum_\beta{}''\sum_\alpha{}'\left\{\frac{|\langle\beta|\pi^-|\alpha\rangle|^2}{(\omega_{\beta\alpha}{}^2-\omega^2)}-\frac{|\langle\beta|\pi^+|\alpha\rangle|^2}{(\omega_{\beta\alpha}{}^2-\omega^2)}\right\}\,. \tag{55}$$

Similar procedures show that σ_{2zz} has the same form as Eq. (54) with the subscripts x replaced by the subscripts z. Expressions (54) and (55) are exact to all orders in the external magnetic field H. However, since we have made no explicit statements concerning the states χ_α, these expressions are only formal solutions.

The asymptotic expansions of the conductivity tensor elements in Sec. II are valid only when the splitting of the energy levels due to the external magnetic field, $[(\hbar\omega_0/H)\approx 0.5\times10^{-8}(\mathrm{eV/G})]$, is much less than the gap energies $\mathcal{E}_g$ of the band structure. Most solids have gap energies of the order of magnitude of tenths of electron volts or more, $\mathcal{E}_g\sim 0.1$ eV, and this energy corresponds to a magnetic field of more than 10^8 G. Hence, we may assume that $\hbar\omega_0\ll\mathcal{E}_g$. Whenever $\hbar\omega_0\ll\mathcal{E}_g$, then we expect that the effects of H should be small and that the following inequalities apply to the interband frequencies of such solids:

$$\frac{\omega_{\beta\alpha}-\omega_{\beta\alpha}(0)}{\omega_{\beta\alpha}(0)}\ll 1 \tag{56}$$

and

$$\frac{|\langle\beta|\pi^{\pm}|\alpha\rangle|^2-|\langle\beta|\pi^{\pm}|\alpha\rangle_0|^2}{|\langle\beta|\pi^{\pm}|\alpha\rangle_0|^2}\ll 1\,, \tag{57}$$

where

$$\lim_{H\to0}\omega_{\beta\alpha}=\omega_{\beta\alpha}(0)$$

and

$$\lim_{H\to0}\langle\beta|\pi^{\pm}|\alpha\rangle=\langle\beta|\pi^{\pm}|\alpha\rangle_0\,.$$

The above limits imply a correspondence between states with a magnetic field present and states with no magnetic field present. This correspondence exists within the context of the effective mass approximation. In this paper, we shall not discuss whether it exists for other approximation schemes. Inequalities (56) and (57) and Eq. (55) allow us to write $\sigma_{xy}{}^{(1)}$ for nonferromagnetic solids as

$$\sigma_{1xy}{}^{(1)}=\frac{-e^2}{2\hbar m^2V}\sum_{\beta}{}''\sum_{\alpha}{}'\left[\left\{\frac{2|\langle\beta|\pi^-|\alpha\rangle|^2\omega^-{}_{\beta\alpha}}{(\omega^-{}_{\beta\alpha}{}^2-\omega^2)^2}\frac{\partial\omega^-{}_{\beta\alpha}}{\partial H}-\frac{1}{(\omega^-{}_{\beta\alpha}{}^2-\omega^2)}\frac{\partial}{\partial H}(|\langle\beta|\pi^-|\alpha\rangle|^2)\right\}\right.$$
$$\left.-\{\text{corresponding terms with the }+(\text{RCP})\text{ selection rules}\}\right]_{H=0}. \quad (58)$$

Here the quantities $\omega^{\pm}{}_{\beta\alpha}$ refer to those frequencies for which the matrix elements of $\pi^{\pm}$ with the states β and α are nonzero; i.e., $\langle\beta|\pi^{\pm}|\alpha\rangle\neq0$. In general, $\omega^+{}_{\beta\alpha}$ may be different from $\omega^-{}_{\beta\alpha}$. Also all terms are evaluated at $H=0$. From Eq. (58) we see that the weak field Faraday effect may be considered as being produced by two effects. One is the Zeeman splitting of the energy levels, the factor $\partial\omega^-{}_{\beta\alpha}/\partial H$; and the other one is the change of the square of the matrix element with H. The Zeeman splitting term produces a singularity of higher order near $\omega_{\beta\alpha}$ and we might expect this term to dominate near the absorption edge. For frequencies much higher than $\omega_{\beta\alpha}$ the term from the variation of the matrix element will dominate. At frequencies much less than $\omega_{\beta\alpha}$ both terms will be of the same order of magnitude.

Some metals have gap energies near 10^{-3} eV because of spin-orbit splitting or because of a point of accidental degeneracy near or at the Fermi surface. Under such conditions the inequality $\hbar\omega_0\ll\mathcal{E}_g$ may not necessarily be satisfied. For the case where $\hbar\omega_0\sim\mathcal{E}_g$, so called magnetic breakdown in the crystal occurs.[22] The above inequalities (56) and (57) are then violated and for such cases Eq. (58) will not be meaningful.

IV. SUM RULES AND LOW- AND HIGH-FREQUENCY LIMITS

In this section, we shall give the sum rules[23] and the limits satisfied by the elements of the conductivity tensor. The sum rule and high-frequency limits for the diagonal elements of the conductivity tensor are well known when $H=0$[20]; and for $H\neq0$, the same results also obtain. We will therefore only state the results here

$$\int_0^\infty\sigma_{1jj}(\omega)d\omega=\frac{\pi\bar{n}e^2}{2m}, \quad (59)$$

and

$$\lim_{\omega\to\infty}\sigma_{2jj}(\omega)=\frac{\bar{n}e^2}{m\omega}, \quad (60)$$

where j is either x, y, or z.

Deriving the sum rule and the high- and low-frequency limits for the off-diagonal element requires only the commutation relations and the completeness of the set of states for the one-body Hamiltonian. From Eq. (53), we have that

$$\int_0^\infty\omega\sigma_{2xy}(\omega)d\omega=\frac{-i\pi e^2}{2\hbar m^2V}\sum_{\beta}{}''\sum_{\alpha}{}'\{\langle\alpha|\pi_x|\beta\rangle\langle\beta|\pi_y|\alpha\rangle$$
$$-\langle\alpha|\pi_y|\beta\rangle\langle\beta|\pi_x|\alpha\rangle\}. \quad (61)$$

Let us denote the occupied states by the region $\alpha\leq\gamma$, and the unoccupied states by the region $\beta>\gamma$, where γ represents the quantum numbers of the highest occupied state. We then have the following relation,

$$\sum_{\beta>\gamma}{}''|\beta\rangle\langle\beta|=1-\sum_{\beta\leq\gamma}{}'|\beta\rangle\langle\beta|, \quad (62)$$

where we have used the fact that the solutions to the eigenvalue problem of Eq. (43) form a complete set. Inserting the relation (62) into Eq. (61) produces the result

$$\int_0^\infty\omega\sigma_{2xy}(\omega)d\omega=\frac{-i\pi e^2}{2\hbar m^2V}\sum_{\alpha\leq\gamma}{}'[\langle\alpha|[\pi_x,\pi_y]|\alpha\rangle$$
$$-\sum_{\beta\leq\gamma}{}'\{\langle\alpha|\pi_x|\beta\rangle\langle\beta|\pi_y|\alpha\rangle-\langle\alpha|\pi_y|\beta\rangle\langle\beta|\pi_x|\alpha\rangle\}]. \quad (63)$$

When the magnetic field is in the z direction, $\mathbf{H}=\mathbf{z}H$, then we may prove that

$$\langle\alpha|[\pi_x,\pi_y]|\alpha\rangle=(i\hbar eH/c)\langle\alpha|\alpha\rangle, \quad (64)$$

where the expectation value of the terms containing the spin operator $\boldsymbol{\sigma}$ is zero. The substitution of the commutator (64) into Eq. (63) gives,

$$\int_0^\infty\omega\sigma_{2xy}(\omega)d\omega=\frac{-i\pi e^2}{2\hbar m^2V}\left[\sum_{\alpha\leq\gamma}{}'\langle\alpha|\alpha\rangle\frac{i\hbar eH}{c}\right.$$
$$-\sum_{\alpha\leq\gamma}{}'\sum_{\beta\leq\gamma}{}'\{\langle\alpha|\pi_x|\beta\rangle\langle\beta|\pi_y|\alpha\rangle$$
$$\left.-\langle\alpha|\pi_y|\beta\rangle\langle\beta|\pi_x|\alpha\rangle\}\right]. \quad (65)$$

The second term of Eq. (65) is zero since it is antisymmetric in the dummy variables α and β which are both summed over the same region. Equation (65) then leads to the sum rule

$$\int_0^\infty\omega\sigma_{2xy}(\omega)d\omega=\frac{\pi e^3H\bar{n}}{2m^2c}, \quad (66)$$

---

[22] M. Cohen and L. Falicov, Phys. Rev. Letters **7**, 231 (1961).

[23] The reader should be aware that other proofs based upon field theoretic concepts exist for the sum rules. [See for example, P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959); and M. Ashkin, thesis, Harvard University, 1962 (unpublished).]

where $\bar{n}=(1/V)\sum'_{\alpha<\gamma}\langle\alpha|\alpha\rangle=N/V$. A term proportional to $\langle\sigma_z\nabla^2V\rangle$ would have appeared in Eqs. (65) and (66) if we had not dropped such a term in Eq. (64) by assuming $\langle\boldsymbol{\sigma}\rangle=0$. Sum rule (66) is thereby exact only for the case in which $\langle\boldsymbol{\sigma}\rangle=0$.

We compute the high-frequency limit of σ_{1xy} from Eq. (55),

$$\lim_{\omega\to\infty}\sigma_{1xy}(\omega)=\frac{-e^2}{2\hbar m^2\omega^2V}\sum_{\beta}{}''\sum_{\alpha}{}'\{|\langle\beta|\pi^-|\alpha\rangle|^2-|\langle\beta|\pi^+|\alpha\rangle|^2\}.\quad(67)$$

But the summation of Eq. (67) is just the summation of Eq. (61). Hence, we arrive at the high-frequency limit

$$\lim_{\omega\to\infty}\sigma_{1xy}(\omega)=\frac{-e^3H\bar{n}}{m^2\omega^2c}.\quad(68)$$

Equation (68) is the same as the free-electron-gas limit. The limit given in Eq. (68) is also equal to the limit obtained for the Hookean solid of Sec. III. The corresponding limit of Eq. (37) is

$$\lim_{\omega\to\infty}\sigma_{1xy}(\omega)=\frac{\sigma_0\omega_0}{\omega^2\tau}=\frac{-e^3H\bar{n}}{m^2\omega^2c}.\quad(69)$$

The sum rule and high-frequency limit given in Eqs. (66) and (68) have also been given elsewhere.[12]

A question arises as to how well the sum rule (66) and the limit (68) are satisfied when only conduction electrons are considered in the evaluation of σ. For this case, $\bar{n}$ is the number per unit volume of conduction electrons alone. The extent of agreement depends upon the smallness of the last terms in Eq. (65) which are summed between the core states and the conduction states.

In order to study the low-frequency behavior of σ_{1xy}, we write Eq. (55) in the form

$$\sigma_{1xy}(\omega)=\frac{e^2}{2\hbar m^2V}\sum_{\beta}{}''\sum_{\alpha}{}'\biggl[|\langle\beta|\pi^-|\alpha\rangle|^2\times\biggl\{\frac{1}{\omega_{\beta\alpha}{}^2}+\frac{\omega^2}{\omega_{\beta\alpha}{}^2(\omega_{\beta\alpha}{}^2-\omega^2)}\biggr\}-|\langle\beta|\pi^+|\alpha\rangle|^2\times\biggl\{\frac{1}{\omega_{\beta\alpha}{}^2}+\frac{\omega^2}{\omega_{\beta\alpha}{}^2(\omega_{\beta\alpha}{}^2-\omega^2)}\biggr\}\biggr]$$

$$\equiv G+\omega^2\sum_{\beta}{}''\sum_{\alpha}{}'F_{xy}(\omega^2;\alpha,\beta).\quad(70)$$

Observe that as $\omega\to0$, $\sigma_{1xy}(\omega)\to G$. To evaluate G let us write it as

$$G=\frac{e^2}{2\hbar m^2V}\sum_{\beta}{}''\sum_{\alpha}{}'\biggl\{\frac{\langle\alpha|\pi^+|\beta\rangle\langle\beta|\pi^-|\alpha\rangle}{\omega_{\beta\alpha}{}^2}-\frac{\langle\alpha|\pi^-|\beta\rangle\langle\beta|\pi^+|\alpha\rangle}{\omega_{\beta\alpha}{}^2}\biggr\}.\quad(71)$$

Since $[(x\pm iy),V(r)]=0$, we have

$$[(x\pm iy),\mathcal{H}_0']=i\hbar\pi^\pm/m.\quad(72)$$

The matrix element of the operator Eq. (72) leads to the equation

$$\langle\beta|(x\pm iy)|\alpha\rangle im\omega_{\beta\alpha}=\langle\beta|\pi^\pm|\alpha\rangle.\quad(73)$$

Applying Eq. (73) to Eq. (71) reduces G to the form

$$G=-\frac{ie^2}{\hbar V}\sum_{\beta}{}''\sum_{\alpha}{}'\{\langle\alpha|x|\beta\rangle\langle\beta|y|\alpha\rangle-\langle\alpha|y|\beta\rangle\langle\beta|x|\alpha\rangle\}.\quad(74)$$

We might be tempted to use Eq. (62) as the next step. However, in general, this is incorrect because not all states $|\beta\rangle$ are present as one might casually assume. For nonzero ω, transitions with $\omega_{\beta\alpha}=0$ contribute nothing to $G+\omega^2F_{xy}$. Hence, the transitions to unoccupied $|\beta'\rangle$ states for which $\omega_{\beta'\alpha}=0$ do not occur in the sum over states which gives Eq. (71). But in order to use the closure property (62) in the sum over the matrix elements of x and y, we must include the terms from these unoccupied states $|\beta'\rangle$. The matrix identity obtained from Eq. (72) clarifies the above:

$$\langle\beta|j|\alpha\rangle\hbar\omega_{\beta\alpha}=(-i\hbar/m)\langle\beta|\pi_j|\alpha\rangle,\quad(75)$$

where j can be either x or y. When $\omega_{\beta'\alpha}=0$, then it is possible to have $\langle\beta'|\pi_j|\alpha\rangle=0$ but $\langle\beta'|j|\alpha\rangle\neq0$. Such a possibility occurs in the case of free electrons in a magnetic field. This physically corresponds to the situation that in a uniform static electric field in the x or y direction no absorption occurs when collisional effects are negligible (the π matrix element is zero for $\omega_{\beta\alpha}=0$); but a current is produced (the x or y matrix element is nonzero corresponding to motion of the average position of the electrons). Adding and subtracting the matrix elements of x and y to these states $|\beta'\rangle$ and now using Eq. (62), we find

$$G=-(ie^2/\hbar V)\sum_{\alpha\leq\gamma}{}'\Bigl[\langle\alpha|[x,y]|\alpha\rangle-\sum_{\beta\leq\gamma}{}'\{\langle\alpha|x|\beta\rangle\langle\beta|y|\alpha\rangle-\langle\alpha|y|\beta\rangle\langle\beta|x|\alpha\rangle\}-\sum_{\beta'>\gamma}{}''\{\langle\alpha|x|\beta'\rangle\langle\beta'|y|\alpha\rangle-\langle\alpha|y|\beta'\rangle\langle\beta'|x|\alpha\rangle\}\Bigr].\quad(76)$$

The last sum in (76) now includes a sum over the states $|\beta'\rangle$. The first term of Eq. (76) is zero since $[x,y]=0$ and the second term of Eq. (76) is zero because it is antisymmetric in the dummy variables α and β. Hence, we have that

$$G=+(ie^2/\hbar V)\textstyle\sum_{\alpha\leq\gamma}{}'\sum_{\beta'>\gamma}{}''\{\langle\alpha|x|\beta'\rangle\langle\beta'|y|\alpha\rangle -\langle\alpha|y|\beta'\rangle\langle\beta'|x|\alpha\rangle\}\,, \quad (77)$$

where $|\beta'\rangle$ are all of those unoccupied states for which $\omega_{\beta'\alpha}=0$ and $\langle\alpha|\pi_j|\beta'\rangle=0$.

We may easily perform the evaluation of Eq. (77) by using the Boltzmann equation instead of directly calculating the matrix elements. The low-frequency limit of σ_{1xy} evaluated in this way for a solid with no open orbits is[24]

$$G=\lim_{\omega\to 0}\sigma_{1xy}=\frac{(\bar{n}_{-}-\bar{n}_{+})_{ec}}{H}\,, \quad (78)$$

where $\bar{n}_{-}$ is the number of electrons per unit volume and $\bar{n}_{+}$ is the number of holes per unit volume.

The low-frequency limit for σ_{1xy} has caused some confusion in the literature because a simple evaluation of Eq. (74) could easily assume that all possible matrix elements of x and y are present in G. In this case we would wrongly conclude that $G=0$. We see from Eq. (78) that $G=0$ only when there are no "free"carriers.

V. FERROMAGNETIC AND NONFERROMAGNETIC SOLIDS

So far we have made no distinction between ferromagnetic and nonferromagnetic solids. All statements apply equally well to both except where we explicitly state otherwise. In this section we consider the "effective mass approximation" model and calculate σ_{1xy} for a ferromagnetic and nonferromagnetic solid and illustrate the difference between the two. We use the formulation of the model given by Luttinger and Kohn.[25] The effective mass approximation assumes that only states of the band in the vicinity of a maximum or a minimum in energy are important. For this to be the case, the magnetic field must be weak enough so that the radius of the orbit of the electron is large compared to interatomic distances. This will be the case for usual fields. We choose the model for which all bands are simple and nondegenerate. Only the lowest band is occupied and all energy maxima or minima occur at $k=0$. We assume cubic symmetry about $k=0$ so that to order k^2 the energy for states in the nth band for $H=0$ are given by,

$$\mathcal{E}_{n'}(k)=(\hbar^2k^2/2m_{n'})+\mathcal{E}_{n'}(0)\,. \quad (79)$$

In what follows we find it convenient to set $\hbar=1$. We want to evaluate σ_{1xy} as given by Eq. (55) in the effective mass approximation. This requires the evaluation of the matrix elements of $\pi^{\pm}$. In order to evaluate σ_{1xy} asymptotically to the first order in H it is necessary to use the wave function[25] evaluated to the following order:

$$\psi_n(\mathbf{r})=F_{n,l}(\mathbf{r})U_{n0}(\mathbf{r}) +\boldsymbol{\nabla}_kU_{n0}(\mathbf{r})\cdot\mathbf{P}F_{n,l}(\mathbf{r})+\frac{s}{2}(\boldsymbol{\nabla}/i)(yF_{n,l}(\mathbf{r})) \cdot\sum_{\substack{r,t\\ r\neq t\, t\neq n}}\frac{(\mathbf{v}_{rt}v_{tn}{}^{x}+\mathbf{v}_{tn}v_{rt}{}^{x})}{\omega_{rt}\omega_{tn}}U_{r0}(\mathbf{r})\,, \quad (80)$$

where

$$\boldsymbol{\nabla}_kU_{n0}(\mathbf{r})=-\sum_{n'\neq n}\frac{U_{n'0}(\mathbf{r})\mathbf{v}_{n'n}}{m\omega_{n'n}}\,. \quad (81)$$

The subscript n refers to the band number, $U_{n0}(\mathbf{r})$ is the Bloch wave function in the nth band at $k=0$. Here,

$$\mathbf{P}=(\boldsymbol{\nabla}/i)+\mathbf{x}sy\,, \quad (82)$$

and

$$s=eH/c\,. \quad (83)$$

We have chosen a particular gauge to represent the magnetic field in the z direction.

Here also,

$$\mathbf{v}=(\boldsymbol{\nabla}/im)+(4m^2c^2)^{-1}(\boldsymbol{\sigma}\times\boldsymbol{\nabla}V(\mathbf{r}))\,, \quad (84)$$

and

$$\mathbf{v}_{rt}=\int U_{r0}{}^{*}(\mathbf{r})\mathbf{v}U_{t0}(\mathbf{r})d^3r_0\,. \quad (85)$$

The integration is over a unit cell and the $U_{r0}(\mathbf{r})$ are normalized in the unit cell. We also define

$$\omega_{rt}=\mathcal{E}_r(0)-\mathcal{E}_t(0)\,. \quad (86)$$

The wave function $F_{n,l}(\mathbf{r})$ is determined by the differential equation

$$\mathcal{E}_n(\mathbf{P})F_{n,l}(\mathbf{r})=\mathcal{E}_{nl}F_{n,l}(\mathbf{r})\,. \quad (87)$$

The subscript l denotes the quantum numbers required to specify the state. In order to estimate the order of magnitude of the various contributions to $\psi_n(\mathbf{r})$ we use the relations

$$\begin{gathered}\nabla_kU_{n0}\sim aU_{n0}\,,\\ PF_{n,l}\sim(F_{nl}/R)\,,\\ s\sim R^{-2}\,,\\ (v_{rt}/\omega_{rt})\sim a\,.\end{gathered} \quad (88)$$

Here a is of the order of interatomic dimensions and R is of the order of the radius of the electron orbit in the magnetic field and R is much larger than a. It is assumed as part of the effective mass approximation that the average momentum of an electron is of the order of $1/R$. We see that the second and third terms on the right-hand side of Eq. (80) give contributions to the wave

---

[24] A. B. Pippard, Rept. Progr. Phys. **23**, 202 (1960).

[25] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).

function of order a/R and a^2/R^2, respectively. However, as we will see, the contribution to σ_{1xy} is of order a^2/R^2 and we must use all of these terms. We have not included all terms of order a^2/R^2 in the wave function of Eq. (80). We have included those terms which contribute in the lowest order to σ_{1xy}.

Landau was the first one to give the solution of Eq. (87) in Cartesian coordinates[26]:

$$F_{n,l,k_x,k_y}(\mathbf{r})=(L_zL_x)^{-1/2}e^{i(k_xx+k_zz)}\lambda_l(y-y_0). \qquad (89)$$

Here $\lambda_l(y-y_0)$ is the normalized harmonic-oscillator function centered about the point $y_0=k_x/s$.

It is now a straightforward though tedious matter to use the wave function given in Eq. (80) to calculate σ_{1xy} from Eq. (55). To simplify the problem somewhat, we consider only the contribution from the n filled band inside the Fermi surface and the next higher empty band n'. The band edges may be either maximums or minimums of energy. We also limit the frequency $\omega<\omega_{n'n}$. We find

$$\begin{aligned}\langle n',l',k_x'k_z'|\pi^{\pm}|n,l,k_xk_z\rangle &=(2s)^{1/2}\delta_{n'n}\delta_{k_x'k_x}\delta_{k_z'k_z}\begin{Bmatrix} l^{1/2}\delta_{l;\,l-1} \\ (l+1)^{1/2}\delta_{l;\,l+1}\end{Bmatrix}+\delta_{k_x'k_x}\delta_{k_z'k_z}\delta_{l'l}\left[mv_{n'n}{}^{\pm}\mp s\frac{v_{n'n}{}^{\pm}}{\omega_{n'n}}-i(s/4)M_{n'n}{}^{\pm}+i(s/2)N_{n'n}{}^{\pm}\right] \\ &\quad+(2s)^{1/2}\delta_{k_x'k_x}\delta_{k_z'k_z}\begin{Bmatrix} l^{1/2}\delta_{l;\,l-1}\nabla_k{}^{-} \\ (l+1)^{1/2}\delta_{l;\,l+1}\nabla_k{}^{+}\end{Bmatrix}mv_{n'n}{}^{\pm}. \qquad (90)\end{aligned}$$

The upper terms in the brackets and the upper signs go with the π^+ matrix element and the lower terms and signs go with the π^- matrix elements. We also define:

$$\nabla_k{}^{\pm}=\partial/\partial k_x\pm i\partial/\partial k_y,\quad v_{n'n}{}^{\pm}=v_{n'n}{}^{x}\pm iv_{n'n}{}^{y},\quad M_{n'n}{}^{\pm}=M_{n'n}{}^{x}\pm iM_{n'n}{}^{y},\quad N_{n'n}{}^{\pm}=N_{n'n}{}^{x}\pm iN_{n'n}{}^{y},\quad \delta_{ab}=\begin{cases}1 & a=b\\ 0 & a\neq b,\end{cases}$$

$$\begin{aligned}M_{n'n}{}^{i}&=m\sum_{\substack{r,t\\ r\neq t\\ t\neq n\text{ or }n'}}\left\{\left(\frac{v_{rt}{}^{y}v_{tn}{}^{x}+v_{rt}{}^{x}v_{tn}{}^{y}}{\omega_{rt}\omega_{tn}}\right)v_{n'r}{}^{i}-\left(\frac{v_{rt}{}^{y}v_{tn'}{}^{x}+v_{rt}{}^{x}v_{tn'}{}^{y}}{\omega_{rt}\omega_{tn'}}\right)v_{nr}{}^{i}\right\}, \\ N_{n'n}{}^{i}&=m\sum_{\substack{r,t\\ r\neq n'\\ t\neq n}}\left(\frac{v_{rn'}{}^{x}v_{tn}{}^{y}-v_{rn'}{}^{y}v_{tn}{}^{x}}{\omega_{rn'}\omega_{tn}}\right)v_{rt}{}^{i}, \\ \boldsymbol{\nabla}_kv_{n'n}{}^{i}&=\sum_{\substack{r\\ r\neq n'\\ t\neq n\text{ or }n'}}\left(\frac{\mathbf{v}_{n'r}v_{rn}{}^{i}}{\omega_{n'r}}+\frac{\mathbf{v}_{rn}v_{n'r}{}^{i}}{\omega_{nr}}\right).\end{aligned} \qquad (91)$$

From Eqs. (55) and (90), and assuming *no* spin-orbit coupling, we find that the conductivity per unit volume and to first order in s becomes

$$\begin{aligned}\sigma_{1xy}=\frac{e^2s\bar{n}}{m_n{}^2(\omega_c{}^2-\omega^2)}+\frac{e^2s}{m^2}&\left\{\frac{2mv_{n'n}{}^{+}v_{n'n}{}^{-}}{\omega_{n'n}}-\frac{m}{2}M_{n'n}{}^{y}v_{n'n}{}^{x}\right. \\ &\left.+\frac{m}{2}M_{n'n}{}^{x}v_{n'n}{}^{y}+m^2(\nabla_k{}^{-}v_{n'n}{}^{+})(\nabla_k{}^{+}v_{n'n}{}^{-})+m^2(N_{n'n}{}^{y}v_{n'n}{}^{x}-N_{n'n}{}^{x}v_{n'n}{}^{y})\right\}\frac{2}{(2\pi)^3}\int\frac{d^3k}{(\omega_{n'n}{}^2(k)-\omega^2)}, \qquad (92)\end{aligned}$$

where the integral in Eq. (92) is over the interior of the Fermi surface, $\omega_c=eH/m_nc$, and $\omega_{n'n}(k)=\mathcal{E}_{n'}(k)-\mathcal{E}_n(k)$. Notice that the result for σ_{1xy} given in Eq. (92) has a frequency dependence which implies that only changes in matrix elements contribute and the Zeeman splitting effect does not contribute. We have used the property that with no spin-orbit coupling[25]

$$v_{n'n}{}^{i}=v_{nn'}{}^{i}=(v_{n'n}{}^{i})^{*}=(im)^{-1}\int U_{n'0}{}^{*}(\partial/\partial r^i)U_{n0}d^3r_0. \qquad (93)$$

---

[26] See, for example, Ref. 7, pp. 583–585.

We perform the integral over k by using Eq. (79),

$$\frac{2}{(2\pi)^3}\int\frac{d^3k}{\omega_{n'n}{}^2(k)-\omega^2}=\frac{1}{2\pi^2\omega\alpha^{3/2}}\left[(\omega_{n'n}+\omega)^{1/2}\tan^{-1}\left(\frac{\alpha^{1/2}k_0}{(\omega_{n'n}+\omega)^{1/2}}\right)-(\omega_{n'n}-\omega)^{1/2}\tan^{-1}\left(\frac{\alpha^{1/2}k_0}{(\omega_{n'n}-\omega)^{1/2}}\right)\right], \quad (94)$$

where

$$\alpha=(1/m_{n'})-(1/m_n),$$

and k_0 is the Fermi momentum.

The matrix element given in expression (90) has been previously calculated[27] but not to such high order in a/R. As can be seen in Eq. (92), every term in expression (90) contributes to σ_{1xy} to the same order even though they are of different order in expression (90). The reason for this is that when the matrix element of expression (90) is squared the term of zero order in a/R gets multiplied with the terms of order $(a/R)^2$ and the terms of order a/R multiply with themselves, all giving terms of the same order. The terms obtained by the square of the zero-order terms of expression (90) cancel.

Including the spin-orbit interaction *to first order* and neglecting terms of order of the spin-orbit interaction times the magnetic field, we find the following additional terms add to the expression for σ_{1xy} given in Eq. (92):

$$\sigma_{1xy}{}^{\text{s.o.}}=2e^2i\left\{\frac{1}{4m^2c^2}\left[v_{n'n}{}^x\left(\frac{\partial V(\mathbf{r})}{\partial x}\right)_{nn'}+v_{n'n}{}^y\left(\frac{\partial V(\mathbf{r})}{\partial y}\right)_{nn'}\right]+v_{n'n}{}^y\sum_{t\neq n}\left(\frac{H_{nt}'}{\omega_{tn}}v_{tn'}{}^x\right)-v_{n'n}{}^x\sum_{t\neq n}\left(\frac{H_{nt}'v_{tn'}{}^y}{\omega_{tn}}\right)\right.$$

$$\left.+v_{n'n}{}^y\sum_{t\neq n'}\left(\frac{H_{tn'}{}'v_{nt}{}^x}{\omega_{tn'}}\right)-v_{n'n}{}^x\sum_{t\neq n}\left(\frac{H_{tn'}{}'v_{nt}{}^y}{\omega_{tn'}}\right)\right\}\frac{2}{(2\pi)^3}\int\frac{d^3k\langle\sigma_z(k)\rangle}{(\omega_{n'n}{}^2(k)-\omega^2)};\quad n'\neq n, \quad (95)$$

$$\sigma_{1xy}{}^{\text{s.o.}}=0;\quad n'=n,$$

where

$$H_{nt}'=(4m^2c^2)^{-1}\int U_{n0}{}^*(\nabla V(r)\times\nabla/i)_zU_{t0}d^3r_0.$$

The U_{n0} used to evaluate all of the matrix elements of Eq. (95) are those for the spin-orbit interaction equal to zero. The $v_{n'n}{}^i$ are given by Eq. (93). The quantity $\langle\sigma_z\rangle$ means the average value of σ_z. In deriving Eq. (95), we have used the relations that,

$$(\nabla V(\mathbf{r}))_{n'n}{}^*=(\nabla V(\mathbf{r}))_{nn'}=-(\nabla V(\mathbf{r}))_{n'n},$$

and

$$(H_{tn'})^*=H_{nt'}=-H_{tn'}.$$

The terms given in Eq. (95) come from the first term in the parentheses of the second expression on the right-hand side of Eq. (90), i.e., the term proportional to $mv_{n'n}{}^{\pm}$. With no spin-orbit coupling the absolute magnitude squared of this term is the same for both + and − and does not contribute to σ_{1xy}. However, when the spin-orbit interaction is included then $|v_{n'n}{}^+|^2\neq|v_{n'n}{}^-|^2$ for two reasons; one, the wave function to first order becomes

$$U_{n0}'=U_{n0}-\langle\sigma_z\rangle\sum_{t\neq n}\frac{H_{tn}'U_{t0}}{\omega_{tn}}, \quad (96)$$

and two, $v_{n'n}$ contains the spin-orbit interaction as indicated by Eq. (84). The first two terms in the parentheses on the right-hand side of Eq. (95) come from the change in $v_{n'n}$ and the rest of the terms come from the change in wave function. Argyres[8] has also calculated the spin-orbit effect and his expression agrees with our Eq. (95) except that he does not have the terms that come from the change in $v_{n'n}$. We feel that these terms should be present. Notice that the spin-orbit interaction contributes only to the $n'\neq n$ term and does not contribute to the $n'=n$ term.

When the metal is ferromagnetic $\langle\sigma_z\rangle=-1$, and, as shown by Argyres,[8] the spin-orbit contribution of Eq. (95) dominates over the magnetic field contribution of Eq. (92). When the metal is nonferromagnetic and because of the Pauli spin paramagnetism χ_p, $\langle\sigma_z\rangle=0$ for all k except those values of k right at the Fermi surface where $\langle\sigma_z\rangle=-1$. The number of states per unit volume $N(H)$ for which $\langle\sigma_z\rangle=-1$ is given by

$$N(H)=2\mu_BHg(E_F), \quad (97)$$

where $\mu_B=e/2mc$ is the Bohr magneton, and $g(E_F)$ is the density of states per unit volume and unit energy at the Fermi energy E_F. For our model of unit volume,

$$g(E_F)=m_n{}^{3/2}(2E_F)^{3/2}\pi^{-2}, \quad (98)$$

where

$$E_F=k_0{}^2/2m_n.$$

We now estimate numerically the contribution of the spin-orbit interaction in *nonferromagnetic* metals and compare it with the magnetic contribution given by

---

[27] R. J. Elliot, J. P. McLean and G. G. MacFarlane, Proc. Phys. Soc. (London) **72**, 553 (1958); Corrigenda, *ibid.* **73**, 976 (1959).

Eq. (92). From Eqs. (92), (95), and (97), we take the ratio of the *interband* parts and find approximately that

$$\frac{\sigma_{1xy}{}^{\text{s.o.}}}{\sigma_{1xy}} \approx \frac{m^2 A \mu_B H g(E_F)}{sB\bar{n}}, \tag{99}$$

where $\bar{n}$ is the number of electrons per unit volume, A is i times the curly brackets in Eq. (95), and B is the term between the curly brackets in Eq. (92). We can estimate B from the high-frequency limit of σ_{1xy} given in Eq. (68). This limit shows that the *sum* of the interband terms are of the order of the intraband terms or

$$B \approx 1. \tag{100}$$

To estimate A we consider a typical term,

$$A \approx v_{n'n}{}^{y} \sum_{t\neq n} \left(\frac{H_{nt}'}{\omega_{tn}} v_{tn'}{}^{x}\right) \approx \left\langle \frac{1}{\omega_{tn}} \right\rangle v_{n'n}{}^{y} (H'v^{x})_{nn'}. \tag{101}$$

Here $\langle 1/\omega_{tn}\rangle$ is some average of the inverse of interband frequencies. After taking this out of the sum, we may sum the rest of the terms by closure. Since the missing term $(t=n)$ is zero we can sum over a complete set obtaining the result on the right-hand side. Just as in the estimate for B we estimated the sum of the interband terms, we will also estimate the sum of the interband terms to obtain an estimate of A. Summing over all $n'\neq n$ and remembering that the contribution for $n'=n$ is zero we obtain

$$A \approx \langle 1/\omega_{tn}\rangle (H'v^{x}v^{y})_{nn}. \tag{102}$$

In general we expect that $(H'v^{x}v^{y})_{nn}$ is nonzero. We know from the high-frequency limit of σ_{1xy} as given by Eq. (68) that A summed over all bands is strictly speaking zero. This is owing to a cancellation between the various terms. However, the method used here should be adequate to estimate the contribution from a single band for which the various terms are not expected to cancel one another. A rough order of magnitude estimate for the matrix element (102) is

$$(H'v^{x}v^{y})_{nn} \approx H_{\text{atomic}}{}' \hbar^2/m^2a^2, \tag{103}$$

where a is of the order of the lattice spacing and $H_{\text{atomic}}{}'$ is the atomic value of the spin-orbit interaction term. Inserting these various order of magnitude estimates back into Eq. (99) we obtain

$$\frac{\sigma_{1xy}{}^{\text{s.o.}}}{\sigma_{1xy}} \approx \frac{H_{\text{atomic}}{}' \hbar^2 \mu_B H g(E_F)}{a^2 s\bar{n}} \left\langle \frac{1}{\omega_{tn}} \right\rangle. \tag{99a}$$

Roughly speaking, for a metal $E_F g(E_F) \approx \bar{n}$ and $\mu_B H \approx s/m$. Also for a metal $E_F \approx \hbar^2/ma^2$. Inserting these estimates into (99a) gives

$$\sigma_{1xy}{}^{\text{s.o.}}/\sigma_{1xy} \approx H_{\text{atomic}}{}' \langle 1/\omega_{tn}\rangle. \tag{99b}$$

Typical interband energies are of the order of 1 eV. For materials around nuclear charge $z=30$, $H_{\text{atomic}}{}' \approx 0.1$ eV.[28]

The spin-orbit contribution in nonferromagnetics has a frequency dependence which differs from that of the magnetic field contribution. The magnetic field contribution comes from all electrons while the spin-orbit contribution comes from only those electrons in the vicinity of the Fermi surface where $\langle\sigma_z\rangle \neq 0$. The spread in energy of these electrons, $2\mu_B H$, is quite small compared to the Fermi energy, and this causes the energy denominator, $(\omega_{nn'}{}^2-\omega^2)^{-1}$, for these electrons to vary much more strongly than that for the magnetic field contribution for which the contributing electrons are spread over an energy range of the order of the Fermi energy. Because of this strong frequency dependence of the spin-orbit contribution, its effects should be noticeable even when the ratio in Eq. (99b) is small. For example,[28] for $z=10$, $H_{\text{atomic}}{}' \approx 0.01$ eV and the ratio in (99b) is about 0.01. However, because $(\mu_B H/E_F) \approx 10^{-4}$ in metals for $H \approx 10^4$ G, we expect that the spin-orbit contribution is concentrated in a much smaller frequency range than the magnetic-field contribution and that it should be observable as a comparatively rapid variation of the Faraday effect with frequency even for $z=10$ or smaller.

VI. DISCUSSION AND SUMMARY

We have presented a general formalism for calculating the Faraday effect in cubic materials. We base the formalism on dispersion relations which relate the real and imaginary parts of the elements of the conductivity tensor. A knowledge of the conductivity tensor permits a calculation of the Faraday effect from Eqs. (19) and (26). The imaginary part of the off-diagonal conductivity element σ_{xy} is proportional to the difference in absorption of right and left circularly polarized radiation. Once we calculate this, we may calculate the real part of the off-diagonal conductivity element by the dispersion relations.

After presenting the sum rules and the low- and high-frequency limits for the elements of the conductivity tensor, we obtain the physically reasonable result that at high frequencies the conductivity tensor becomes identical with the free electron result, i.e., at high enough frequencies the effects of the periodic potential disappear.

Paying particular attention to the role of the spin-orbit interaction, we perform a calculation of σ_{xy} for a solid in the effective mass approximation for nondegenerate bands. In ferromagnetic metals the spin-orbit interaction dominates and produces the large magneto-optic effects of ferromagnetism. Even in nonferromagnetic metals, the spin-orbit interaction contributes to the interband part of the conductivity tensor through the Pauli paramagnetism. The Pauli paramagnetism causes the electrons in the vicinity of the Fermi surface

---

[28] Y. Yafet, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1963), Vol. 14, pp. 8, 9.

to have a nonzero average value of spin. The spin-orbit interaction to first order produces effects proportional to the average value of spin. Because the spin-orbit contribution to σ_{xy} is concentrated in a much smaller frequency range than the magnetic field contribution, the former contribution should give, as an observable effect, a comparatively rapid variation with frequency. This rapid variation should occur even for metals with as small a nuclear charge as $z=10$. Large z materials will show correspondingly larger spin orbit effects since the spin-orbit interaction varies roughly as z^2. The intraband contribution to the conductivity is independent of spin-orbit effects to first order.

The general expression for the off-diagonal element of the conductivity tensor σ_{1xy} as given by Eqs. (55) and (58) shows us that two factors contribute to this element. One is the difference in matrix elements between RCP and LCP radiation and the other factor is the Zeeman splitting of the levels. In the effective mass approximation for cubic solids only the difference in matrix elements contributes to σ_{1xy}. The Zeeman splitting effect does not contribute. To first order in H, the Zeeman splitting is proportional to the average angular orbital momentum of the state. However, in cubic solids, the average angular orbital momentum is zero and thus we do not expect a Zeeman splitting effect to first order in H.

We base these conclusions on the assumption of nondegenerate bands and thus such conclusions are applicable to the usual case of a metal. However, for the case of degenerate bands such as in Si and Ge the situation can be quite different from the conclusions in this paper. For instance, a Zeeman splitting effect can exist via the spin-orbit coupling in the degenerate bands case.[11,12]

In real metals the division of σ_{1xy} into a frequency dependence produced by Zeeman splitting and one produced by a change in matrix element is not the most useful division because the finite lifetimes of the states in the metal cause the overlap of a very large number of states. We usually neglect this finite lifetime and assume an infinite lifetime of the states as we have done in Sec. V for the calculation of the Faraday effect. Using the general dispersion relations (5) and (6) we may treat the situation of finite lifetimes. In Eq. (5), σ_{2xy} is one-half the difference in absorption between LCP and RCP radiation. When the states have finite lifetimes, $\sigma_{2xy}(\omega)$ has contributions from all of the states within approximately the energy half-width of a single state. Each state within this energy range contributes to $\sigma_{2xy}(\omega)$ for two reasons. One is the change in matrix element to which $\sigma_{2xy}(\omega)$ is directly proportional, and the other is the Zeeman splitting of the levels, which is present when the orbital angular momentum is not quenched as in hexagonal metals. The Zeeman splitting contributes a term to $\sigma_{2xy}(\omega)$ which is proportional to the slope of the absorption versus frequency curve for either RCP or LCP radiation. Adding these various contributions to $\sigma_{2xy}(\omega)$, we may obtain $\sigma_{1xy}(\omega)$ from the dispersion relation (5) for which the frequency denominator is simply $(\omega_a{}^2-\omega^2)$.

The dispersion relations (5) and (6) plus the interpretation that σ_{2xy} is the difference in absorption between LCP and RCP radiation is a very powerful and general method to attack the calculation of the Faraday effect. Contrary to other calculations of the Faraday effect which are dependent on various assumptions such as an independent particle model, the dispersion relation approach is always valid regardless of the type of interaction between electrons and the nuclei or between the electrons themselves. It is valid in the relativistic or nonrelativistic limits, when spin-orbit interactions are present, etc. Another advantage of the dispersion relations approach is that it permits us to calculate σ_{2xy} or σ_{1xy} if we know the other over a wide enough frequency range by any means such as, for example, experimental measurements. Although we have limited the work in this paper to $\sigma_{xy}(0,\omega)$, the dispersion relations and the physical interpretation in terms of RCP and LCP radiation also hold for $\sigma_{xy}(\mathbf{k},\omega)$.

ACKNOWLEDGMENTS

The authors wish to thank Dr. A. B. Lidiard for correspondence and a helpful discussion and Dr. J. Halpern, Dr. B. Lax, Dr. Y. Nishina, Dr. L. Roth, and Dr. J. R. Anderson for useful discussions concerning this problem. We appreciate the helpful comments of Dr. A. Freeman and Dr. N. Horing pertaining to the manuscript. A question by Dr. P. N. Argyres on spin-orbit effects is also gratefully acknowledged.