

Current-Induced Reflectivity Effects in a Semiconductor*

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Recently, the effect produced on the optical absorption of a semiconductor by small dc fields ($\sim 10^3$ V/cm), which cause current but do not alter the band structure, was calculated. This calculation is herein extended to the reflectivity by use of the Kramers-Kronig and Fresnel relations. Reflectivity changes and polarization effects are found as functions of photon energy (0–0.4 eV) in InSb at 77°K. The effects for fundamental transitions are large ($\Delta R/R \sim 10^{-3}$), while the effects for intervalence band transitions are small but measurable ($\Delta R/R \sim 10^{-6}$). Uses of these effects are discussed.

I. INTRODUCTION

RECENTLY, the effect produced on the optical absorption of a semiconductor by small dc fields, which cause current but do not alter the band structure, was calculated.¹ Such a current-induced effect on the absorption implies a current-induced effect on the reflectivity, since the absorption coefficient α is related to the reflectivity R through the complex permittivity, Kramers-Kronig relations, and the Fresnel formula. Theoretically, the reflectivity effect might be useful, in a way similar to that suggested and demonstrated^{2,3} for the absorption effect, in determining the carrier distribution function and wave-function parameters. The reflectivity effect would enjoy an advantage over the absorption effect for often R is more easily measured than α in highly absorbing semiconductors. Therefore, we report here a calculation of the effect of current on the reflectivity of a semiconductor, and discuss means of obtaining the distribution function.

As in I, the calculation is performed for InSb, a typical member of one class of semiconductors. The current is described by a distribution function whose argument is the energy of carriers that are displaced in momentum space. Analysis necessary to the calculation is presented in Sec. II. Results for the current-induced reflectivity spectra over the energy range 0–0.4 eV for a lattice temperature of 77°K are presented and discussed in Sec. III.

II. ANALYSIS

Consider light of energy E incident normally on a linear isotropic homogeneous semiconductor. Electromagnetic theory and the principle of causality furnish relations between the absorption coefficient α and the complex permittivity ϵ ⁴:

$$\epsilon = \epsilon_1 + i\epsilon_2, \quad (2.1a)$$

$$\epsilon_2(E) = \hbar c n E^{-1} \alpha(E), \quad (2.1b)$$

$$\epsilon_1(E) = 1 + (2/\pi) P V \int_0^\infty E' \epsilon_2(E') (E'^2 - E^2)^{-1} dE'. \quad (2.1c)$$

Here, \hbar is Planck's constant divided by 2π , c is the speed of light in *vacuo*, n is the index of refraction of the semiconductor, and PV indicates that the principal value of the integral is taken. The last expression is invertible, and is known as a Kramers-Kronig relation.

By Fresnel's formula, the reflectivity R is given in terms of ϵ by

$$R = [B - (2B)^{1/2} - (\epsilon_1 - 1)] / [B + (2B)^{1/2} - (\epsilon_1 - 1)], \quad (2.2a)$$

$$B = \epsilon_1 + |\epsilon|. \quad (2.2b)$$

Placing the semiconductor in a small dc field \mathcal{E} changes α by $\Delta\alpha$, ϵ_2 by $\Delta\epsilon_2$, ϵ_1 by $\Delta\epsilon_1$, and R by ΔR . The fractional change in reflectivity is given by⁵

$$\Delta R/R = a(\epsilon_0)\Delta\epsilon_1 + b(\epsilon_0)\Delta\epsilon_2, \quad (2.3a)$$

where $\epsilon_0 = \epsilon_{10} + i\epsilon_{20}$ is the zero-field permittivity,^{5a} and

$$a \equiv C_1 [(\epsilon_{10} - 1)A_+ + \epsilon_{20}A_-], \quad (2.3b)$$

$$b \equiv C_2 [(\epsilon_{10} - 1)/A_+ - \epsilon_{20}/A_-], \quad (2.3c)$$

with

$$A_\pm \equiv \pm [2(|\epsilon_0| \pm \epsilon_{10})/|\epsilon_0|]^{1/2}, \quad (2.3d)$$

$$C_1 \equiv [(\epsilon_{10} - 1)^2 + \epsilon_{20}^2]^{-1}, \quad (2.3e)$$

$$C_2 \equiv 2\epsilon_{10}C_1|\epsilon_0|^{-2}. \quad (2.3f)$$

In case ϵ_{20} is negligibly small compared to ϵ_{10} , an application of L'Hospital's rule shows that

$$a = 2[(\epsilon_{10} - 1)\sqrt{\epsilon_{10}}]^{-1}, \quad (2.3g)$$

$$b = (\frac{1}{2}a)(\epsilon_{20}/\epsilon_{10})[\epsilon_{10}(1 - \sqrt{2}) - 1](\epsilon_{10} - 1)^{-1}. \quad (2.3h)$$

⁵ B. O. Seraphin and N. Bottka, Phys. Rev. **145**, 628 (1966).

^{5a} Values for ϵ_{10} were obtained from H. R. Philipp and H. Ehrenreich, Phys. Rev. **129**, 1550 (1963).

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† NASA trainee.

¹ C. A. Baumgardner and T. O. Woodruff, Phys. Rev. **173**, 746 (1968). This paper will hereafter be referred to as I.

² R. Bray and W. E. Pinson, Phys. Rev. Letters **11**, 268 (1963).

³ A. C. Baynham and E. G. S. Paige, Phys. Letters **6**, 7 (1963).

⁴ F. Stern, in *Solid State Physics—Advances in Research and Applications*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1963), Vol. 15, p. 299.

From I, α is given by

$$\alpha[E(k), \mathcal{E}, T] = \frac{\hbar}{2\pi c n} \left(\frac{e}{m} \right)^2 \sum_{u,l} \frac{k^2}{E(k)} \left| \frac{d}{dk} [E_u(k) - E_l(k)] \right|^{-1} \\ \times \int \sin\theta d\theta d\varphi |\langle \varphi_u(k) | \mathbf{a} \cdot \mathbf{p} | \varphi_l(k) \rangle|^2 \\ \times \{ f[E_l(|\mathbf{k} + \mathbf{d}|)] - f[E_u(|\mathbf{k} + \mathbf{d}|)] \}, \quad (2.4)$$

where T is the absolute temperature of the lattice, e and m are the charge and rest mass of an electron, respectively, and a carrier is described by momentum \mathbf{p} , wave vector \mathbf{k} , effective mass m^* , and mobility μ . The incident light is polarized in direction \mathbf{a} , and cgs units are used throughout. Expression (2.4) holds for direct transitions of wavevector \mathbf{k} between two states

of energies $E_u(k)$ and $E_l(k)$ ($E_u > E_l$) and corresponding wave functions $\phi_u(k)$ and $\phi_l(k)$, with distribution functions $f(E_u)$ and $f(E_l)$. The incident energy E is constrained to be a function of $k (= |\mathbf{k}|)$ by the conservation of energy:

$$E_u(k) - E_l(k) = E(k). \quad (2.5)$$

The field enters the calculation through the displacement wave vector \mathbf{d} given by

$$\hbar \mathbf{d} = m^* \mu \mathcal{E}, \quad (2.6)$$

so that for \mathcal{E} in the z direction and k given by spherical coordinates (k, θ, ϕ) , the distribution function depends on polar angle θ :

$$|\mathbf{k} + \mathbf{d}|^2 = k^2 + d^2 - 2kd \cos\theta. \quad (2.7)$$

Alternatively, ϵ_1 can be directly obtained from first principles.^{6,7} The result is

$$\epsilon_1(E) = 1 + 8\pi \hbar^2 \left(\frac{e}{m} \right)^2 \sum_{u,l} \sum_{\mathbf{k}} \frac{|\langle \varphi_u(k) | \mathbf{a} \cdot \mathbf{p} | \varphi_l(k) \rangle|^2 \{ f[E_l(|\mathbf{k} + \mathbf{d}|)] - f[E_u(|\mathbf{k} + \mathbf{d}|)] \}}{E_{ul}(k) [E_{ul}^2(k) - E^2]}, \quad (2.8)$$

where $E_{ul} = E_u - E_l$. Expression (2.8) is equivalent to Eq. (2.1c).

The distribution function in Eq. (2.4) is, in general, given by

$$f(E_i) = \{ 1 + \exp[(E_i - E_F)/k_B T] \}^{-1}, \quad (2.9)$$

which explains the dependence of α on T . Here, k_B is Boltzmann's constant and E_F is the Fermi level which depends on T , the concentration of carriers of both signs, and the energy-band structure of the semiconductor. Equation (2.9) is required for degenerate semiconductors ($|E_i - E_F| \approx k_B T$), but it may be approximated by the Boltzmann form of distribution function for nondegenerate semiconductors ($|E_i - E_F| \gg k_B T$):

$$f(E_i) \sim \exp[-(E_i - E_F)/k_B T]. \quad (2.10)$$

For the semiconductor under study (InSb), E_F is close to the conduction-band minimum. Thus, discussion of fundamental transitions (pairing each of the three valence bands with the conduction band) demands use of Eq. (2.9), whereas discussion of intervalence band transitions (pairing each of the three valence bands among themselves) permits use of Eq. (2.10).

The problem of determining E_F remains. In the degenerate calculation, E_F is found from⁸

$$2 \exp(\eta) = - (f - C) + [(f - C)^2 + (4f/\beta) \exp(E_d/k_B T)]^{1/2}, \quad (2.11a)$$

where

$$\eta = (E_F - E_{GT})/k_B T \quad (2.11b)$$

⁶ A. H. Wilson, *The Theory of Metals* (Cambridge University Press, London, 1936), p. 126 ff.

⁷ K. S. Viswanathan and J. Callaway, *Phys. Rev.* **143**, 564 (1966).

⁸ J. S. Blakemore, *Semiconductor Statistics* (Pergamon Press, Inc., New York, 1962), p. 120 ff. Equation (2.11) is the same as Eq. (321.18) in this reference.

is the reduced energy difference between E_F and the conduction-band minimum E_{GT} (see I), $f = N_c/N_d$ is the ratio of the effective density of states in the conduction band to donor impurity atoms, E_d is the ionization energy of donor-contributed electrons,⁹ and β is the impurity-level spin degeneracy (in the case of simple monovalent donors used here, $\beta = \frac{1}{2}$). The constant $C \approx 0.27$ is discussed in Appendix C of Ref. 8.

For the nondegenerate case, E_F is found from¹⁰

$$\exp(E_F/k_B T) = (\frac{1}{2}\rho_p)(2\pi\hbar^2/m_p^*k_B T)^{3/2}, \quad (2.12a)$$

where ρ_p is the density of holes, whose effective mass is given by

$$m_p^{*3/2} = m_1^{3/2} + m_2^{3/2}. \quad (2.12b)$$

The heavy-mass valence band has effective mass m_1 and the light-mass valence band m_2 . The resulting distribution function to be used in Eq. (2.4) is then

$$f(E_v) = 1 - 4\pi^3 \hbar^3 \rho_p \exp(E_v/k_B T) / [(2\pi k_B T)^{3/2} (m_1^{3/2} + m_2^{3/2})]. \quad (2.13)$$

III. CURRENT-INDUCED REFLECTIVITY EFFECTS

In performing the calculations, we use the energy bands and wave functions given by Kane¹¹ and used in I. The interval of integration used in evaluating $\Delta\epsilon_1$ by Eq. (2.1c) is truncated where calculations show $\Delta\epsilon_2$ to be insignificant.¹² For the sake of clarity, the current-induced reflectivity effects are presented for the two cases of direct fundamental transitions and direct

⁹ C. Hilsum and A. C. Rose-Innes, *Semiconducting III-V Compounds* (Pergamon Press, Inc., New York, 1961), p. 72.

¹⁰ A. H. Wilson, *The Theory of Metals* (Cambridge University Press, London, 1958), p. 231.

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

¹² B. O. Seraphin and N. Bottka, *Phys. Rev.* **139**, A560 (1965).

intervalence band transitions separately, although this separation cannot be made experimentally for photon energies for which both processes occur. Note also that in practice the electron temperature may be different from the lattice temperature due to the heating effect of the field. A means of accounting for this was discussed in Sec. V of I.

The matrix elements in Eq. (2.4) depend on the angle between \mathbf{a} and $\boldsymbol{\varepsilon}$. Thus, spectra of both absorption and reflectivity effects exhibit a polarization dependence. Three cases are studied here: $(\Delta R/R)_{\parallel}$ for $\mathbf{a} \parallel \boldsymbol{\varepsilon}$, $(\Delta R/R)_{\perp}$ for $\mathbf{a} \perp \boldsymbol{\varepsilon}$, and $(\Delta R/R)_{\text{pol}}$, which is the difference in these two changes. These changes are calculated by first finding the differences

$$\Delta\alpha_{\parallel} = \alpha[E(k), \boldsymbol{\varepsilon}, T] - \alpha[E(k), 0, T], \quad \mathbf{a} \parallel \boldsymbol{\varepsilon} \quad (3.1a)$$

$$\Delta\alpha_{\perp} = \alpha[E(k), \boldsymbol{\varepsilon}, T] - \alpha[E(k), 0, T], \quad \mathbf{a} \perp \boldsymbol{\varepsilon} \quad (3.1b)$$

$$\Delta\alpha_{\text{pol}} = \Delta\alpha_{\parallel} - \Delta\alpha_{\perp}, \quad (3.1c)$$

from Eq. (2.4), using the energies and wave functions mentioned above and the distribution functions discussed in Sec. II, and then applying Eqs. (2.1b), (2.1c), and (2.3). The results are shown in Figs. 1 and 2 for fundamental transitions and Figs. 3 and 4 for intervalence band transitions.

The reflectivity effects calculated here are comparable in magnitude to other electroreflectance effects pre-

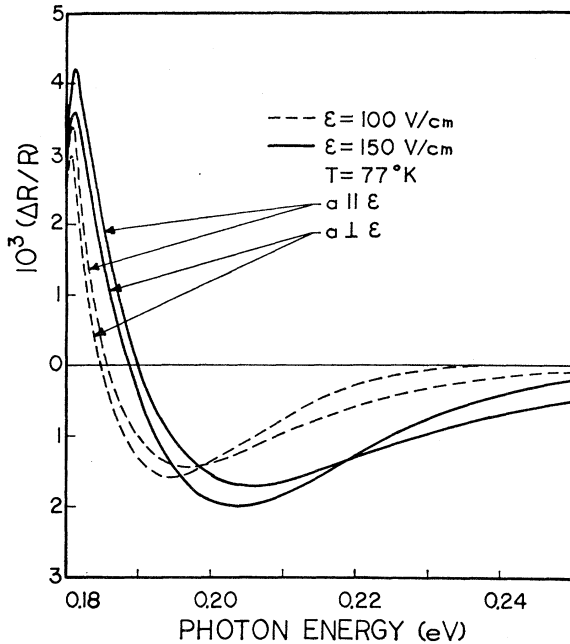


FIG. 1. Calculated current-induced fractional change in reflectivity versus photon energy for fundamental transitions in n -InSb, showing the dependence on polarization of incident light \mathbf{a} and imposed dc field $\boldsymbol{\varepsilon}$. Transitions between the split-off valence band and the conduction band are neglected. $E_F = 0.175$ eV, $N_d = 10^{16}$ cm $^{-3}$.

¹³ For an extensive list of references to both calculations and experiments, see D. E. Aspnes, P. Handler, and D. Blossey, Phys. Rev. 166, 921 (1968).

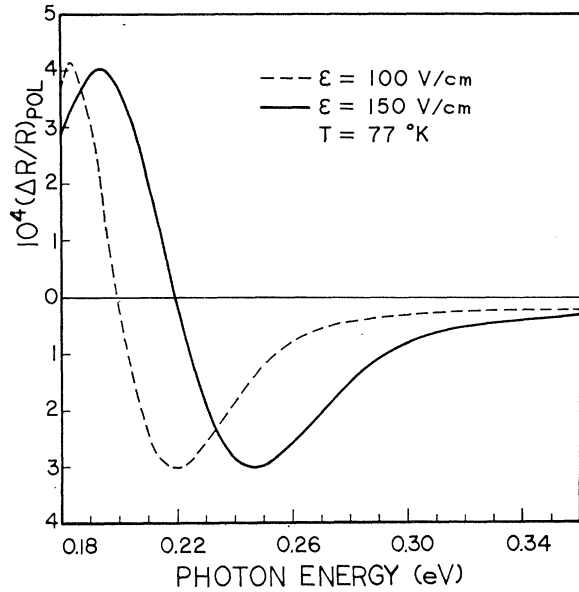


FIG. 2. Calculated current-induced fractional change in reflectivity polarization effect (light polarized parallel to field case less light polarized normal to field case) versus photon energy for fundamental transitions in n -InSb. Transitions between the split-off valence band and the conduction band are neglected. $E_F = 0.175$ eV, $N_d = 10^{16}$ cm $^{-3}$.

viously measured.¹³ Note that the effect for fundamental transitions at 77°K is fairly large. The calculation shows the magnitude of $\Delta\alpha$ in this case to be 10–100 times larger than for the similar calculation at 300°K performed in I. This behavior is readily understood from Eq. (2.9). The change in the number of carriers of energy E caused by the field is much greater for low temperatures than for high temperatures (E_F is about the same for both temperatures).

The field dependence of $\Delta\alpha$ was found in I to be \mathcal{E}^2 for transitions between parabolic bands. It follows from the linearity of Eqs. (2.1b), (2.1c), (2.2), and (2.3) that $\Delta R/R$ also varies as \mathcal{E}^2 with the field.

The sign of $(\Delta R/R)_{\text{pol}}$ follows from the sign of $\Delta\alpha_{\text{pol}}$, which was discussed in I. As pointed out there, this property depends on the symmetry properties of the wave functions. Experimental determination of $(\Delta R/R)_{\text{pol}}$ for a particular transition, thus, serves to check the theoretical values for the coefficients of the orbitals used in each wave function.

The polarization effect may be used to determine the distribution function as a function of k , assuming the wave functions to be used in the calculations are known. To do this, the difference of the distribution functions is expanded in a power series in $\mu = \cos\theta$;

$$\begin{aligned} f[E_l(|\mathbf{k}+\mathbf{d}|)] - f[E_u(|\mathbf{k}+\mathbf{d}|)] \\ &= \sum_{m=0}^{\infty} [H_l(k) - H_u(k)]_m \mu^m \\ &= \sum_{m=0}^{\infty} H_{lum}(k) \mu^m. \end{aligned} \quad (3.2)$$

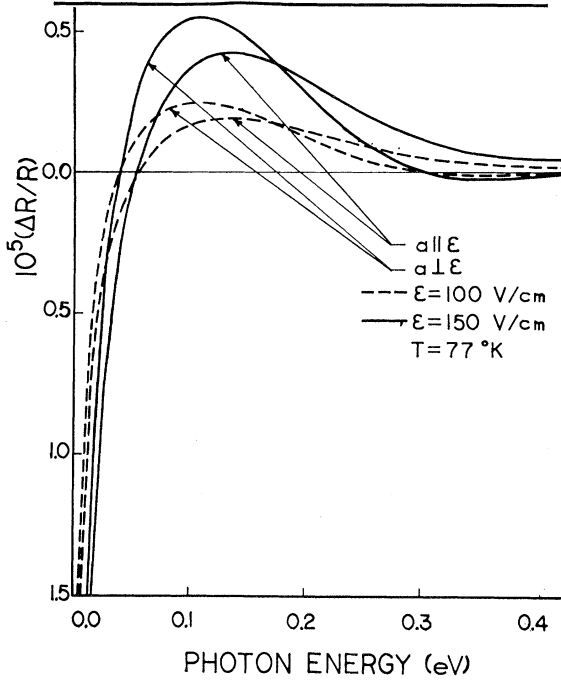


FIG. 3. Calculated current-induced fractional change in reflectivity versus photon energy for intervalence band transitions between the heavy-mass and light-mass valence bands in *p*-InSb, showing the dependence on polarization of incident light *a* and imposed dc field *E*. $\rho_p = 4 \times 10^{15} \text{ cm}^{-3}$, $\mu_p = 8 \times 10^3 \text{ cm}^2 \text{ V}^{-1} \text{ sec}^{-1}$.

This expression defines the expansion coefficients H_{lm} , H_{um} , and H_{lum} which can be determined to second order ($m \leq 2$) from the optical properties.² The second-order terms may be found by first relating $(\Delta R/R)_{\text{pol}}$ to $(\Delta \epsilon_2)_{\text{pol}}$ by a dispersion formula,^{14,15} i.e., the inversion of Eqs. (2.3a) and (2.1c). This is

$$(\Delta \epsilon_2)_{\text{pol}}(E) = \frac{b}{a^2 + b^2} \left(\frac{\Delta R}{R} \right)_{\text{pol}}(E) + \frac{a}{a^2 + b^2} \frac{2E}{\pi} PV \times \int_0^\infty \left(\frac{\Delta R}{R} \right)_{\text{pol}}(E') (E'^2 - E^2)^{-1/2} dE'. \quad (3.3)$$

Then, using Eqs. (2.1b) and (3.2) and the wave functions and notations of I, we obtain

$$(\Delta \epsilon_2)_{\text{pol}}[E(k)] = \frac{8}{15} e^2 P^2 \sum_{u,l} [G_{ul+}^2(k) - G_{ul-}^2(k)] \times \frac{k^2}{E(k)} \left| \frac{d}{dk} [E_u(k) - E_l(k)] \right|^{-1} H_{lu2}(k), \quad (3.4)$$

provided the series (3.2) is truncated at $m = 2$. Equating Eqs. (3.3) and (3.4) yields an equation for the H_{lu2} in terms of $(\Delta R/R)_{\text{pol}}$. If the changes in the reflectivity in certain regions of the spectrum can be attributed to a specific transition(s), a linear system of equations may be obtained. For each equation in the system, Eq. (3.3)

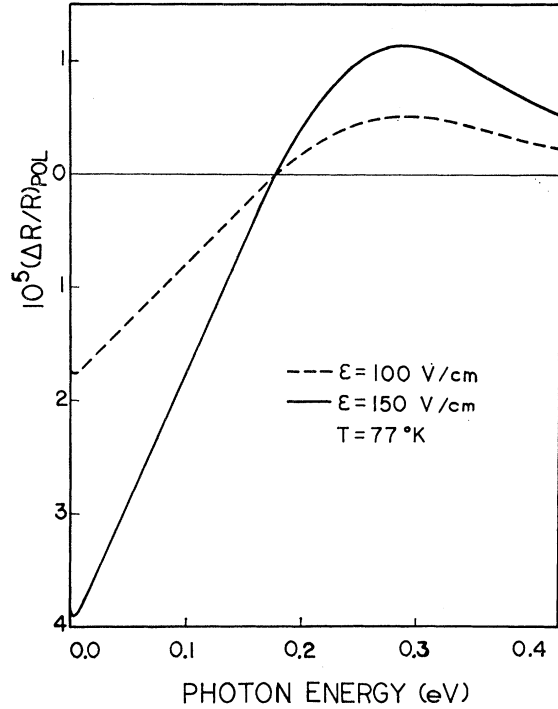


FIG. 4. Calculated current-induced fractional change in reflectivity polarization effect (light polarized parallel to field case less light polarized normal to field case) versus photon energy for intervalence band transitions between the heavy-mass and light-mass valence bands in *p*-InSb. $\rho_p = 4 \times 10^{15} \text{ cm}^{-3}$, $\mu_p = 8 \times 10^3 \text{ cm}^2 \text{ V}^{-1} \text{ sec}^{-1}$.

is equated to Eq. (3.4) separately, with the integral in Eq. (3.3) taken only over that energy range where the reflectivity change is attributed to the transition(s) appearing in Eq. (3.4). The system of equations may then be solved for the individual H_{lu2} .

It may be possible to go further and obtain H_{l2} and H_{u2} separately in either of two ways. The doping and temperature of the semiconductor can be chosen in such a way that the conductivity is due primarily to one band. Then the expansion coefficients for the other band(s) may be set equal to zero. Alternatively, a sufficient number of linear equations may be obtained to uniquely determine H_l and H_u .

Should the above analysis prove intractable for the semiconductor under study, a curve fitting procedure might be used to obtain information about the distribution function; e.g., the distribution functions in the theory of Sec. II could be expanded and the expansion coefficients adjusted until the theoretical curve fits the experimental curve.

Finally, it should be noted that, although the effects discussed herein are distinct from the electroreflectance effect caused by changes in the band structure (Franz-Keldysh effect in the reflectivity, i.e., Seraphin Effect), the results given above may be useful in interpreting small discrepancies between experiment and the theory of the latter effect if any currents are permitted during the experiments.

¹⁴ Y. Hamakawa, P. Handler, and F. A. Germano, Phys. Rev. **167**, 709 (1968).

¹⁵ F. C. Jahoda, Phys. Rev. **107**, 1261 (1957).