Parity nonconservation and photovoltaic effects in gases and semiconductors

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The effect of the weak electron-nucleon interaction on photovoltaic effects in gases and in crystals having inversion centers is discussed. Parity nonconservation in the weak interactions leads to the appearance of pseudovector components in the photocurrent. Parity nonconservation effects in the photoionization of hydrogen atoms in the $2S$ metastable state and in the photoexcitation of current carriers in germanium-type semiconductors are investigated in detail.

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I. INTRODUCTION

The purpose of this paper is to call attention to the possible manifestation of the weak interactions in photovoltaic phenomena in gases and in crystals having an inversion center. We shall be concerned with parity-nonconserving contributions to the photocurrent arising in homogeneous media under uniform illumination. The nonconservation of parity in the weak interactions leads to the appearance of both vector and pseudovector components in the photocurrent $\mathbf{j}$. Thus, in a homogeneous isotropic medium we have not only the usual drag current in the direction of the photon momentum $\mathbf{q}$, but also, as a result of parity nonconservation, a current in the direction of the photon spin $\mathbf{s} = i\mathbf{e}\times\mathbf{e}^*$ ($\mathbf{e}$ is the photon polarization vector):

$$\mathbf{j}=j_0\mathbf{q}/q+j_s\mathbf{s}.$$

The pseudovector current $j_s\mathbf{s}$ changes sign when the photon helicity flips and may therefore be investigated in experiments with circularly polarized photons. Effects due to parity nonconservation can also be detected in experiments with unpolarized photons in the case of polarization of atoms in gases or of current carriers in semiconductors, and also in experiments in which the application of an external magnetic field alters the electron spectrum in atoms or crystals. In that case the expression for the current will contain pseudovector terms proportional to $\mathbf{H}$ or to $\mathbf{q}(\mathbf{q}\cdot\mathbf{H})/q^2$, and to $\vec{\mathscr{P}}$ or to $\mathbf{q}(\mathbf{q}\vec{\mathscr{P}})/q^2$, ($\vec{\mathscr{P}}$ is the pseudovector that specifies the direction and degree of the polarization of the electrons in the initial state); these terms change sign when the direction of H or $\vec{\mathscr{P}}$ is changed. In all cases the photocurrent under consideration is, of course, proportional to the number of photons absorbed per unit time.

We shall consider photocurrents arising from parity nonconservation in two cases: a) in the photoionization of the metastable $2S$ state of the hydrogen atom, and b) in the photoexcitation of carriers in crystals with O_h symmetry having degenerate valence bands of the p-Ge type.

We consider the photocurrent in hydrogen for two reasons. First, the $2S$ state of hydrogen serves as a touchstone for such calculations, since closed analytic expressions can be obtained for the effects under consideration, and second, the effect in a magnetic field turns out to be "anomalously large" in hydrogen. The ratio of the current due to parity nonconservation to the drag current associated with momentum transfer from photons to electrons in a magnetic field is 2–3 orders of magnitude larger than in the case of ionization of fully spin-oriented $2S$ orders of magnitude larger than in the case of ionization of fully spin-oriented $2S$ states or in the case of excitation of Ge crystals by circularly polarized light. At the same time, in the case of ionization of $2S$ states of hydrogen by circularly polarized light the ratio of these currents is smaller than in the case of ionization of oriented $2S$ atoms by the factor $\alpha^2\sim 10^{-4}$, where α is the fine structure constant.

The effects under consideration are extremely small. However, the high accuracy of present-day measurements of electric current permits us to hope that they will be observable.

The results reported in Ref. 1, in which the circular photovoltaic effect in gyrotropic crystals[1)] was investigated, served as a stimulus to the present studies. A photocurrent $j_i = \gamma_{ik}s_k$ arises in gyrotropic crystals, where γ_{ik} is a pseudotensor analogous to the gyration tensor. This effect does not occur, i.e. $\gamma_{ik} = 0$, in nongyrotropic crystals, nor, in particular, in any crystals having a center of inversion. In principle, the weak interaction should give rise to nonvanishing components of γ_{ik} in all crystals.

II. THE PHOTOVOLTAIC EFFECT IN HYDROGEN

1. The photocurrent incident to the ionization of hydrogen by circularly polarized light

We shall begin our study of the effects of parity nonconservation on photovoltaic phenomena by considering the current that arises on ionization of hydrogen atoms in the $2S$ metastable state by circularly polarized light.

In the nonrelativistic approximation ($I\lesssim\omega\ll m$) the differential cross section for the photoeffect is given by the expression ($\hbar = c = 1$)

$$d\sigma=\frac{\alpha}{2\pi}\frac{mk}{\omega}|M|^2\,d\Omega, \tag{II.1}$$

the transition amplitude M having the form

$$M=-\frac{i}{m}\left\{\int d^3\mathbf{r}e^{i\mathbf{q}\mathbf{r}}\psi_f^+\mathbf{e}\nabla\psi_i+\frac{1}{2}\int d^3\mathbf{r}e^{i\mathbf{q}\mathbf{r}}\psi_f^+[\mathbf{q}\times\boldsymbol{\sigma}]\psi_i\right\}, \tag{II.2}$$

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Here k, m, and σ are the electron momentum, mass, and Pauli matrices; ω, $\mathbf{q}$, and $\mathbf{e}$ are the photon energy, momentum, and polarization vector (in the gauge $\mathbf{q}\cdot\mathbf{e}=0$), $I=\eta^2/8m$ is the ionization potential of the $2S$ level, $\eta=m\alpha$ is the Coulomb momentum ($\alpha=e^2=1/137$), and ψ_i and ψ_f are the nonrelativistic wave functions for the initial and final states.

The weak interaction resulting from the neutral currents leads to the following P-odd, T-invariant, nonrelativistic proton-electron interaction potential[6,7] (according to the standard Weinberg-Glashow-Salam model of the electroweak interaction):

$$V=\frac{G}{2^{3/2}m}\{\sigma\mathbf{p},\ (\varkappa_{1p}+\varkappa_{2p}\sigma\sigma_p)\delta(\mathbf{r})\}, \tag{II.3}$$

$$\varkappa_{1p}={}^1/_2(1-4\sin^2\theta_W),\quad \varkappa_{2p}=-\lambda\varkappa_{1p},\quad \lambda=g_A/g_V\approx 1.25,$$

where $\mathbf{p}$ is the momentum operator, the σ_p are the proton Pauli matrices, G is the Fermi constant, the angle θ_w is a model parameter, and $\{a,b\}$ denotes the anticommutator of the operators a and b.

As is well known, the weak-interaction potential (II.3) leads to mixing of stationary states of an atom that have the same total angular momentum J and opposite parities. Since the energies of the $(2S_{1/2})_J$ and $(2P_{1/2})_J$ bound states are very close together, the states being separated by an interval of the order of the Lamb shift, the "resonant" mixing of the states in the initial wave function ψ_i will play the dominant part. We shall therefore neglect the weak mixing in the final state and choose for ψ_f a Coulomb wave function in the continuous spectrum that contains an asymptotically plane wave and an incoming spherical wave[8]:

$$\psi_f=e^{\pi\xi/2}\Gamma(1+i\xi)e^{i\mathbf{kr}}F(-i\xi,\ 1,\ -i(\mathbf{kr}+kr))\chi_f, \tag{II.4}$$

where $\xi=\eta/k$ and χ_f is the final-state spin function for the electron-proton system.

In considering the P-odd effects in the absence of a magnetic field we shall neglect the hyperfine splitting. In that case the constant $\varkappa_{2p}$ that characterizes the P-odd interaction of the electron with the proton spin does not appear in the mixing factor for the $2S_{1/2}$ and $2P_{1/2}$ states and ψ_i becomes

$$\psi_i=\psi(2S_{1/2})+i\mathcal{F}\psi(2P_{1/2}),\qquad \mathcal{F}=-\sqrt{\frac{3}{2}}\frac{Gm^3\alpha^4}{32\pi\Delta_L}\varkappa_{1p}, \tag{II.5}$$

where Δ_L is the Lamb shift, $\psi(2S_{1/2})$ and $\psi(2P_{1/2})$ are the wave functions for the $2S_{1/2}$ and $2P_{1/2}$ states and are given by

$$\psi(2S_{1/2})=(\eta^3/8\pi)^{1/2}e^{-\eta r/2}(1-\eta r/2)\chi_i,$$
$$\psi(2P_{1/2})=-(\eta^5/96\pi)^{1/2}e^{-\eta r/2}\sigma\mathbf{r}\chi_i, \tag{II.6}$$

where χ_i is the initial spin function. Using the current experimental value of ~ 0.23 for $\sin^2\theta_W$ we obtain $\mathcal{F}\sim 0.5\times 10^{-12}$ for the mixing parameter; $\mathcal{F}$ is an order of magnitude larger in the deutron.

The transition amplitude M is

$$M=M_S+i\mathcal{F}M_P, \tag{II.7}$$

where M_S and M_P are the amplitudes for the photoeffects from the $2S_{1/2}$ and $2P_{1/2}$ states; they are given by (II.2) with ψ_i replaced by $\psi(2S_{1/2})$ and $\psi(2P_{1/2})$, respectively. The amplitude M_S is a scalar, while M_P is a pseudoscalar; it is the interference of these amplitudes that gives rise to P-odd effects in the differential cross section and current.

To determine M_S and M_P we resort to a multipole expansion, which is valid in our case since $I\lesssim\omega\ll m$ (the important quantities in the integrals are $r\sim 1/\eta$ and the multipole expansion parameter $\mathbf{q}\cdot\mathbf{r}\sim\omega/\eta\sim I/\eta\sim\alpha$, whereas the electron momentum may be large, $k/\eta\sim 1$). A standard calculation of the integrals (II.2) with confluent hypergeometric functions (see, e.g., Ref. 8) leads, within the necessary accuracy, to the following expressions for the amplitudes:

$$M_S=A_S\left\{(\mathbf{ek})+\frac{k^2(2-i\xi)}{2m^2\omega^2}(\mathbf{ek})\,(\mathbf{qk})+\frac{i}{2m\omega}(\mathbf{qk})\,([\mathbf{q}\times\mathbf{e}]\sigma)\right\}, \tag{II.8}$$

$$M_P=A_P\left\{ie\left(\sigma-\frac{4}{k^2}\frac{(1-i\xi)}{(2-i\xi)}(\sigma\mathbf{k})\mathbf{k}\right)\right.$$
$$\left.+\frac{2}{k^2m\omega}\frac{(1-i\xi)}{(2-i\xi)}(\mathbf{qk})\,([\mathbf{q}\times\mathbf{e}]\mathbf{k})\right\}, \tag{II.9}$$

where $2m\omega=k^2+(\eta/2)^2$,

$$A_S=\sqrt{\frac{\pi}{2}}\frac{\eta^{5/2}}{m^3\omega^2}e^{\pi\xi/2}\Gamma(2-i\xi)\left[\frac{i\xi+2}{i\xi-2}\right]^{-i\xi}, \tag{II.8a}$$

$$A_P=\frac{\eta}{2\sqrt{3}}\frac{(i\xi-2)}{(i\xi+2)(1-i\xi)}A_S. \tag{II.9a}$$

Let us discuss Eqs. (II.8) and (II.9). The first term in each of these equations represents the usual amplitude $(E1)_S$ or $(E1)_P$ for an electric dipole transition from the $2S_{1/2}$ or $2P_{1/2}$ state. These $E1$ amplitudes do not interfere in the differential cross section for photoionization of unpolarized atoms and do not lead to parity violating effects in the current. In this case the lack of interference between the leading terms of the multipole expansion is due to the fact that the $(E1)_S$ amplitude is spin independent while the $(E1)_P$ amplitude is linear[2)] in σ, and their product drops out of the cross section when it is averaged over the spins. Interference of the $(E1)_S$ and $(E1)_P$ amplitudes arises in the cross section for the photoeffect in the case of unpolarized photons on polarized hydrogen (see below) and leads, in addition, to polarization of the final electrons in the collision plane in the case of an unpolarized initial state.

Before discussing the remaining terms in Eqs. (II.8) and (II.9) we note that the amplitudes for magnetic dipole transitions are not among them. One can understand this by looking, for example, at the second term in (II.2). On replacing $\exp(i\mathbf{q}\cdot\mathbf{r})$ in this term by 1, the integral vanishes because of the orthogonality of the Coulomb wave functions for the continuous and discrete spectra (strongly forbidden $M1$ transitions).

The terms proportional to $(\mathbf{q}\cdot\mathbf{k})$ $(\mathbf{q}\times\mathbf{e}\cdot\sigma)$ and $(\mathbf{q}\cdot\mathbf{k})$ $(\mathbf{q}\times\mathbf{e}\cdot\mathbf{k})$ describe $(M2)_S$ and $(M2)_P$ magnetic quadrupole transitions (to be accurate, we note that the first of these terms contains the spin-orbit correction to the $E1$ transi-

tion). It is precisely because of the interference between the $(E1)_S$ and $(M2)_P$ transitions and between the $(E1)_P$ and $(M2)_S$ transitions that the P-odd dependence on the photon spin appears in the cross section and current.

Finally, the term of the form $(\mathbf{e}\cdot\mathbf{k})(\mathbf{q}\cdot\mathbf{k})$ describes the $(E2)_S$ transition. This term must be taken into account because the cross section for ionization from the $2S_{1/2}$ state is symmetric (in the $E1$ approximation[8]) under the substitution $\vartheta\to\pi-\vartheta$ (φ is the angle between the photon and electron momenta) and therefore does not give rise to the usual P-even current. Interference between the $(E1)_S$ and $(E2)_S$ transitions, however, leads to asymmetry of the cross section and to the appearance of a current.

Now let us consider the current. The usual calculations with the amplitudes (II.8) and (II.9) lead to the following expression for the average momentum transferred to an electron by a circularly polarized photon:

$$\langle\mathbf{k}\rangle=\frac{1}{\sigma(2S_{1/2})}\int\mathbf{k}\frac{d\sigma}{d\Omega}d\Omega=\frac{\alpha^2}{5}m\frac{(\omega_0-1)^2}{\omega_0}\mathbf{n}+\frac{\mathcal{F}\alpha^3}{80\sqrt{3}}m\frac{(\omega_0-1)(\omega_0-2)}{(\omega_0+3)}\mathbf{s},\qquad\text{(II.10)}$$

where $\omega_0=\omega/\mathbf{I}$, $\mathbf{n}=\mathbf{q}/q$, $\mathbf{s}=i\mathbf{e}\times\mathbf{e}^*$ is the photon spin, and $\sigma(2S_{1/2})$ is the total cross section for the photoeffect from the $2S_{1/2}$ state in the $E1$ approximation:

$$\sigma(2S_{1/2})=\frac{\alpha\pi^2}{3}\cdot2^{14}a^2\left(1+\frac{3}{\omega_0}\right)\left(\frac{1}{\omega_0}\right)^4\frac{\exp\{-4\xi\,\mathrm{arcctg}\,\xi/2\}}{1-e^{-2\pi\xi}},\qquad\text{(II.11)}$$

where $a=1/\eta$ is the Bohr radius.

Under steady-state conditions in the case of a gas that is not too highly rarefied, the photocurrent is related to the average momentum transferred to an electron by the formula

$$\mathbf{j}=\frac{e}{m}\langle\mathbf{k}\rangle\sigma(2S_{1/2})N\Phi\tau,\qquad\text{(II.12)}$$

where N is the concentration of $2S_{1/2}$ metastable atoms, Φ is the photon flux density, and τ is the electron momentum relaxation time. Using Eqs. (II.10) and (II.11), we obtain the following expression for the photocurrent produced by circularly polarized photons:

$$\mathbf{j}=j_0(\mathbf{n}+\varepsilon\mathbf{s}),\qquad\text{(II.13)}$$

$$j_0=e\frac{\alpha^2}{5}\frac{(\omega_0-1)^2}{\omega_0}\sigma(2S_{1/2})N\Phi\tau,\qquad\text{(II.14)}$$

$$\varepsilon=\mathcal{F}\frac{\alpha}{16\sqrt{3}}\frac{\omega_0(\omega_0-2)}{(\omega_0-1)(\omega_0+3)}.\qquad\text{(II.15)}$$

We note that the current, which is proportional to the photon spin $\mathbf{s}$, changes sign when the photon energy becomes equal to twice the ionization potential. Let us first discuss the drag photocurrent j_0 (for unpolarized photons). Its value naturally depends on the experimental conditions. If for an estimate we take $N\sim10^{10}\,\mathrm{cm}^{-3}$, $\tau\sim10^{-7}$ sec, and $\omega_0=1.25$ ($\lambda=292$ nm), we find that the photocurrent amounts to $\sim3\times10^{-11}$ ampere per watt of incident power.

The relative strength of the current that depends on the photon spin is very small in the case under consideration: $\varepsilon\sim10^{-3}\mathcal{F}\sim10^{-14}\varkappa_{ip}$. This is due to the fact that the $M2$ transition amplitudes, whose interference with the $E1$ amplitudes gives rise to the dependence of the current on the circular polarization of the photons, are small, being quadratic in $\mathbf{q}$. It therefore seems unlikely that an experimental study of this dependence would be fruitful in the case of hydrogen. A search for parity violating effects in the photocurrent arising from the orientation of the $2S$ electrons or from the presence of an external magnetic field would seem to be more promising in the case of hydrogen, and we now turn to the discussion of such effects.

2. Photocurrent incident to the polarization of atoms

In considering effects associated with the polarization of atoms, we may neglect the hyperfine structure of the $2S$ level. We write the polarization density matrix for the $2S$ state in the form

$$\rho=\tfrac{1}{2}(1+\vec{\mathcal{P}}\boldsymbol{\sigma}),\qquad\text{(II.16)}$$

where $\vec{\mathcal{P}}$ is a vector that defines the magnitude and direction of the polarization of the atom, i.e., the relative difference between the populations of the Zeeman sublevels with $m_j=\pm1/2$ (the α and β sublevels in Lamb's classification[9]). For simplicity we shall consider only the case in which the motion of the photon is either parallel or antiparallel to $\vec{\mathcal{P}}$, i.e., $n\|\vec{\mathcal{P}}$. Calculations similar to those presented above show that the expression for the photocurrent in the case of unpolarized photons can be written in the form

$$\mathbf{j}=j_0(\mathbf{n}+\zeta\vec{\mathcal{P}}).\qquad\text{(II.17)}$$

Here j_0 is the drag photocurrent (II.14). The relative magnitude of the parity violating component of the current is given, to the lowest order in ω/η by the formula

$$\zeta=-\frac{1}{2\sqrt{3}}\alpha\left(\frac{m}{k}\right)^2\mathcal{F},\qquad\text{(II.18)}$$

where k is the momentum of the ejected electron, m is its mass, and $\mathcal{F}$ is the mixing factor for the $2S_{1/2}$ and $2P_{1/2}$ levels [Eq. (II.5)]. For optical photons, $k\sim\alpha m$, so $\zeta\sim\alpha^{-1}\mathcal{F}$.

The parity violating effects under consideration are substantial when the degree of polarization is high: $\mathcal{P}\sim1$. Such high polarizations can be achieved in experiments with atomic beams, for example, by deexcitationof the β state ($m_j=-1/2$) in an electric field, and also by optical orientation of the atoms or by separating the $m_j=1/2$ and $m_j=-1/2$ states in a nonuniform magnetic field. But if the atoms are polarized in a uniform magnetic field so that the $2S_{1/2}$ levels are statistically populated, the degree of polarization of the atoms will be $\mathcal{P}\sim\mu H/T\sim10^{-4}$–$10^{-5}$ (at $T\approx300$°K) and the effect under discussion will be negligibly

small. In what follows, therefore, we shall neglect this small polarization when discussing the effect of a magnetic field.

3. The photocurrent in an external magnetic field

Now let us discuss the effects of parity nonconservation that arise as a result of the difference between the mixing factors for the Zeeman components of the $2S_{1/2}$ and $2P_{1/2}$ levels. This mechanism is specially important in the hydrogen atom,[10] when the $2S$ and $2P$ levels cross in comparatively weak magnetic fields. At the crossing points of the Zeeman components of the S and P levels, which have the same projection m_J of the total angular momentum of the atom, the mixing factors for these components are enhanced by the weak interaction by about an order of magnitude as compared with the other components. As a result of this, the admixed $2P_{1/2}$ state turns out to be strongly polarized. The polarization of the admixed P states, like the polarization of the S states in the preceding section, makes it possible for the leading terms in the photoeffect amplitude to interfere; these terms correspond to $E1$ transitions from S and P states [the $\mathbf{q}$-independent terms in Eqs. (II.8) and (II.9)], and the parity violation in the photoeffect turns out to be comparatively large. As was noted above, such interference does not take place in the case of unpolarized states because of the different electron-spin dependences of the corresponding parts of the amplitudes.

The range of variation of the magnetic field strength of greatest interest in connection with the photoeffect in hydrogen is the interval from 1.1 to 1.3 kG, in which there are two suitable crossing points of the S and P levels. The levels[3)] β_0 ($2S_{1/2}$, $m_j = -1/2$, $m_I = 1/2$) and f_0 ($2P_{1/2}$, $m_j = -1/2$, $m_I = 1/2$) cross at $H \approx 1.16$ kG, and the levels β_{-1} ($2S_{1/2}$, $m_j = -1/2$, $m_I = -1/2$) and f_{-1} ($2P_{1/2}$, $m_j = -1/2$, $m_I = -1/2$) cross at $H \approx 1.23$ kG (m_j is the projection of the electron angular momentum and m_I is that of the nuclear spin).

We can obtain an expression for the photocurrent in the presence of a magnetic field by using known calculations of the mixing factors for the $2S$ and $2P$ levels due to the weak interaction in a magnetic field,[10,11] together with Eqs. (II.8) and (II.9) for the photoeffect amplitudes. Since these formulas are very cumbersome in the general case, we present the final result for the special case of photons moving parallel or antiparallel to the magnetic field ($\mathbf{n} = \pm \mathbf{h}$, $\mathbf{h} = \mathbf{H}/H$) in the lowest approximation in ω/η:

$$\mathbf{j} = j_0(\mathbf{n} + \delta\mathbf{h}),$$

$$\delta = -\frac{\alpha m^2}{8\sqrt{3}\,k^2}\{2\,\mathrm{Re}\,\mathcal{F}(H) + \xi\,\mathrm{Im}\,\mathcal{F}(H)\},$$

$$\mathcal{F}(H) = -\sqrt{\frac{3}{2}}\frac{Gm^3\alpha^4}{64\pi}\left\{\frac{\varkappa_{1p}-\varkappa_{2p}}{\mathscr{E}_-(-H)} + \frac{\varkappa_{1p}+\varkappa_{2p}}{\mathscr{E}_+(-H)}\right\}, \qquad \text{(II.19)}$$

$$\mathscr{E}_\pm(-H) = \Delta_L - \frac{2}{3}\mu H + \frac{2}{9}\frac{(\mu H)^2}{\Delta_F} \pm \frac{1}{4}(\Delta_{HF}^S - \Delta_{HF}^P) + i\frac{\Gamma_P}{2}.$$

Here Δ_L is the Lamb shift, Δ_F is the fine-structure splitting of the $2P$ level, Δ_{HF}^S and Δ_{HF}^P are the hyperfine splittings of the $2S_{1/2}$ and $2P_{1/2}$ levels, respectively. Γ_P is the natural width of the $2P_{1/2}$ level, and μ is the Bohr magneton. The first term in the expression for $\mathcal{F}(H)$ corresponds to the mixing of the β_0 and f_0 states, while the second term corresponds to the mixing of the β_{-1} and f_{-1} states; we neglect the mixing of levels that do not cross. In the Weinberg-Glashow-Salam model we have $\varkappa_{1p} - \varkappa_{2p} \gg \varkappa_{1p} + \varkappa_{2p}$, so that β_0–f_0 mixing plays the dominant part.

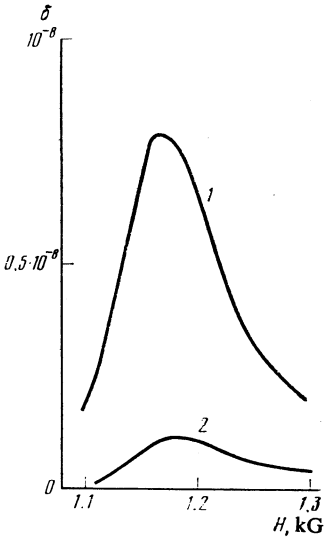

FIG. 1. The coefficient δ vs the magnetic field strength H for photon energies ω of 1.25 I (plot 1) and 2I (plot 2) (I is the ionization potential of the $2S$ state of hydrogen).

Figure 1 shows the relative magnitude of the parity violating effects in the photoeffect in a magnetic field. The figure shows the coefficient δ as a function of the magnetic field strength H near the crossing points of the $2S$ and $2P$ levels for two values of the incident photon energy: $\omega = 1.25I$ and $\omega = 2I$, where $I = m\alpha^2/8$ is the ionization potential of the $2S_{1/2}$ state. This dependence clearly exhibits resonance behavior at the crossing point of the β_0 and f_0 levels:

$$\mathrm{Re}\,\mathcal{F} \approx 0, \quad \mathrm{Im}\,\mathcal{F} \approx \sqrt{\frac{3}{2}}\frac{Gm^3\alpha^4}{32\pi}\frac{\varkappa_{1p}-\varkappa_{2p}}{\Gamma_P}. \qquad \text{(II.20)}$$

The relative magnitude of the effects associated with parity nonconservation rises rapidly on approaching the photoeffect threshold. It will be seen that, despite the fact that the e-p interaction constant is extremely small, it is quite reasonable to obtain the value $\delta \sim 10^{-8}$ for the current values of the Weinberg angle ($\sin^2\theta_w \approx 0.23$). The relative value of δ for the photoeffect in deuterium is about an order of magnitude larger.

Let us briefly consider another region of magnetic field strengths in which $H \sim 550$ G. The levels β_0 ($2S_{1/2}$, $m_j = -1.2$, $m_I = 1/2$) and e_0 ($2P_{1/2}$, $m_j = 1/2$, $m_I = -1/2$) cross in this region and their mixing ratio depends only on the weak constant $\varkappa_{2p}$. This region is of special interest in searching for effects associated with parity nonconservation in radio frequency transitions in hydrogen[12] since it makes it possible to distinguish effects associated with $\varkappa_{2p}$, but it offers no advantages in the case of the photoeffect. The point is that in radio frequency transitions the

nuclear spin has a definite projection in both the initial and the final states, whereas in the photoeffect one must sum over the final-state projections of the nuclear spin. However, the amplitudes M_S and M_P [Eqs. (II.8) and (II.9)] do not depend on the nuclear spin so that, in the lowest approximation, transitions from β_0 and e_0 do not interfere. Interference manifests itself only when the admixture of ($m_j = 1/2$, $m_I = -1/2$) states to β_0 and of ($m_j = -1/2$, $m_I = 1/2$) states to e_0 is taken into account, and this admixture is associated with the hyperfine interaction. In a magnetic field $H \approx 550$ G this admixture is small ($\sim \Delta^S_{HF}/4\mu H \sim 5\%$), so the crossing of the β_0 and e_0 levels does not enhance the parity violating effects, but simply makes a contribution comparable to that from levels that do not cross.

III. THE PHOTOVOLTAIC EFFECT IN GERMANIUM-TYPE CUBIC CRYSTALS

1. The effective Hamiltonian

The appearance of a photocurrent proportional to the photon spin **s** in crystals is due to the presence in the effective Hamiltonian of terms that are linear in the momentum **k**. The matrix elements of the effective Hamiltonian are given, to the second order of perturbation theory, by the formula

$$H_{mm'} = H'_{mm'} - \frac{1}{2}\sum_l H'_{ml}H'_{lm'}[(E_l - E_m)^{-1} + (E_l - E_{m'})^{-1}]. \tag{III.1}$$

In calculating the spectrum within the framework of the **k·p** method one usually takes the following term[13] as the perturbation H':

$$H_{\mathbf{k}} = \frac{k^2}{2m} + \frac{\mathbf{kp}}{m}, \tag{III.2}$$

where $\mathbf{p} = -i\nabla$ is the momentum operator. Taking the weak interactions into account in accordance with Eq. (II.3) leads to the appearance of another term in H':

$$V = g\sigma \sum_i [\mathbf{p}\delta(\mathbf{r} - \mathbf{R}_i) + \delta(\mathbf{r} - \mathbf{R}_i)\mathbf{p}], \tag{III.3}$$

where the summation is taken over the coordinates $\mathbf{R}_i$ of all the nuclei in the lattice, and

$$g = \frac{G\varkappa_1}{2^{3/2}m}, \quad \varkappa_1 = Z\varkappa_{1p} + (A - Z)\varkappa_{1n}. \tag{III.4}$$

Here Z and A are the nuclear charge and mass numbers, $\varkappa_{1p}$ is given by Eq. (II.3), and $\varkappa_{1n} = -1/2$. For Ge, using the value $\sin^2\theta_w = 0.23$, we obtain $\varkappa_1 = -19$. The matrix elements of H' are taken between Bloch functions at the extremal point; we write the Bloch functions in the form $\psi_{nk_0}(\mathbf{r})/N^{1/2}$, where N is the number of unit cells and the functions $\psi_{nk_0} = \exp(i\mathbf{k}_0\mathbf{r})u_{nk_0}$ are normalized to the volume Ω of a unit cell:

$$\int_\Omega dV \psi^*_{n\mathbf{k}_0}\psi_{n'\mathbf{k}_0} = \langle n\mathbf{k}_0 | n'\mathbf{k}_0\rangle = \delta_{nn'}. \tag{III.5}$$

Taking the periodicity of the crystal and the Bloch amplitudes $u_{n\mathbf{k}_0}(\mathbf{r})$ into account, we can write the matrix elements of the operator V in the form

$$V_{ms} = g\sum_a [(\mathbf{p}\psi_m)^+_{\mathbf{r}=\mathbf{R}_a}\sigma\psi_s(\mathbf{R}_a) + \psi_m{}^+(\mathbf{R}_a)\sigma(\mathbf{p}\psi_s)_{\mathbf{r}=\mathbf{R}_a}]. \tag{III.6}$$

The summation in (III.6), unlike that in (III.3), is taken over the coordinates $\mathbf{R}_a$ of the nuclei in a single unit cell.

For the coordinate wave functions at the point $\Gamma(\mathbf{k}_0 = 0)$, the values of $\psi_s(\mathbf{R}_a)$ differ from zero only for the representations $\Gamma_1(A_1^+)$ and $\Gamma'_2(A_1^-)$ of the group $O_h = T_d \times C_i$, while the values of $(\mathbf{p}\psi_s)_{\mathbf{r}=\mathbf{R}_a}$ differ from zero only for the representations $\Gamma'_{25}(F_2^+)$ and $\Gamma_{15}(F_2^-)$. Under an inversion that changes the places of the atoms in a unit cell of a crystal having the diamond lattice, the wave function changes sign, i.e., $\psi_s(\mathbf{R}_1) = -\psi_s(\mathbf{R}_2)$, for odd representations and remains unchanged, i.e., $\psi_s(\mathbf{R}_1) = \psi_s(\mathbf{R}_2)$ for even representations: the operator **p** is odd under inversion. Hence a matrix element of the operator V differs from zero only for the following pairs of single-valued representations: $\Gamma'_{25}, \Gamma'_2(F_2^+, A_1^-)$ and $\Gamma_{15}, \Gamma_1(F_2^-, A_1^+)$. The matrix element of the operator **p** in H_k [Eq. (III.2)] also differs from zero for these same pairs of representations. Since the operator V transforms according to the representation $\Gamma'_1(A_2^-)$ of the group O_h, its matrix elements V_{ms} for two-valued representations differ from zero only for the pairs Γ_7^-, Γ_7^+ $(E'_2{}^-, E'_1{}^+)$ and $\Gamma_6^-, \Gamma_6^+ (E'_1{}^-, E'_2{}^+)$, whose product contains Γ'_1.

In Ge, the wave functions of the valence band at the point Γ transform according to the representation Γ'_{25}, while those of the conduction band transform according to Γ'_2. When the spin-orbit interaction is taken into account, the representation Γ'_{25} splits into $\Gamma_7^+(E'_1{}^+)$ and $\Gamma_8^+(G'+)$, while Γ'_2 becomes $\Gamma_7^-(E'_2{}^-)$. The Hamiltonian $\mathscr{H}(\mathbf{k})$ for the electrons of the Γ_8^+ and Γ_7^+ bands, constructed in accordance with Eqs. (III.1), (III.2), and (III.6), can be written in the form

$$\mathscr{H}(\mathbf{k}) = \mathscr{H}_0(\mathbf{k}) + \mathscr{H}_1(\mathbf{k}), \tag{III.7a}$$

$$\mathscr{H}_0(\mathbf{k}) = (A + 2B)k^2 - 3B\sum_i J_i^2 k_i^2 - \frac{\sqrt{3}}{2}D\sum_{i\neq j}\{J_iJ_j\}k_ik_j + \frac{\Delta}{3}[(\mathbf{J}\sigma) - 1], \tag{III.7b}$$

$$\mathscr{H}_1(\mathbf{k}) = \gamma[2(\sigma\mathbf{k}) - (\mathbf{J}\sigma)(\mathbf{Jk}) - (\mathbf{Jk})(\mathbf{J}\sigma)]. \tag{III.7c}$$

Here $\mathbf{J}_i$ is the angular momentum operator in the basis $Y_m (m = 0 \pm 1)$, the σ_i are the electron Pauli matrices, $\{AB\} = (AB + BA)$, and

$$\gamma = -\frac{2g}{m}\sum_l S_l(\mathbf{R}_1)(p_xX)_{\mathbf{r}=\mathbf{R}_1}\langle X|p_x|S_l\rangle/E_{sl}. \tag{III.8}$$

The summation in (III.8) is taken over all the Γ'_2 bands, the S_1 are the wave functions of these bands, and X is one of the basis functions of the Γ'_{15} representation (the basis functions X, Y, and Z of the Γ'_{25} representation transform under the operations of the group O_h like yz, zx, and xy, respectively).

As was pointed out above, as a result of the spin-orbit interaction described by the last term in (III.7b), this representation splits into $\Gamma_8^+ (E(0)=0)$ and $\Gamma_7^+ (E(0)=-\Delta)$. It is assumed in (III.7) that the splitting Δ is much smaller than the width E_g of the forbidden band. In the spherical approximation, i.e., for $D = 3^{1/2}B$, when

$$\mathscr{H}_0(\mathbf{k}) = Ak^2 - 3B[(\mathbf{Jk})^2 - {}^2/_3 k^2] + {}^1/_3\Delta[(\mathbf{J\sigma}) - 1], \quad \text{(III.9)}$$

the spectra of the light and heavy holes near the extremum of the Γ_8^+ band are determined by the expressions

$$E(\mathbf{k}) = -(A \pm B)k^2. \quad \text{(III.10)}$$

while the spectrum of the holes in the Γ_7^+ band is determined by

$$E(\mathbf{k}) = -Ak^2 \pm 2\gamma k + \Delta. \quad \text{(III.11)}$$

In accordance with the group theoretical considerations presented above, the matrix $\mathscr{H}(\mathbf{k})$ for the Γ_8^+ band contains no terms linear in $\mathbf{k}$. This means that transitions between the branches of the Γ_8^+ band can give rise to a photocurrent associated with parity nonconservation only as a result of mixing of Γ_8^+ and Γ_7^+ states, and this becomes significant at high temperatures $T \approx \Delta$.[4)] In what follows, we shall therefore limit ourselves to a calculation of the photocurrent arising from the excitation of electrons from the Γ_7^+ band to the Γ_8^+ band (Fig. 2).

2. The photocurrent in $\Gamma_7^+ \to \Gamma_8^+$ transitions

The photocurrent arising from transitions between states i of the Γ_7^+ band and states j of the Γ_8^+ band is given by the formula

$$\mathbf{I} = -eK\Phi \int d^3\mathbf{k} \sum_{i,j} |M_{ij}|^2 f_{hj} \mathbf{v}_j \tau_j \delta(E_i + \omega - E_j) \times \left[\int d^3\mathbf{k} \sum_{i,j} |M_{ij}|^2 f_{hj} \delta(E_i + \omega - E_j) \right]^{-1}. \quad \text{(III.12)}$$

Here Φ is the light intensity, i.e. the number of photons incident on the specimen per second, K is the light absorption coefficient, $\mathbf{v}_j, \tau_j$, and f_{hj} are the velocity, momentum relaxation time, and distribution function, respectively, of the holes in branch j of the Γ_8^+ band, and M_{ij} is the transition matrix element. The current produced by photoholes in the Γ_7^+ band is not included in (III.12) because the lifetime of the photoholes in that band is very short. In a state of thermal equilibrium, the Γ_7^+ band is assumed to be completely filled by electrons. The transition matrix element M_{ij} is calculated from the eigenfunctions of the Hamiltonian $\mathscr{H}_0(\mathbf{k})$ [see (III.9)]. In this case it is convenient to take the quantization axis for the functions $Y_m^l (l = 3/2, 1/2)$ in the direction of the vector $\mathbf{k}$. We assume that $|\omega - \Delta| \ll \Delta$. In that case we may ignore the mixing of the basis functions for the Γ_8^+ and Γ_7^+ bands and determine them from the corresponding 4×4 and 2×2 determinants, neglecting the cross terms that determine the transition matrix elements M_{ij}.

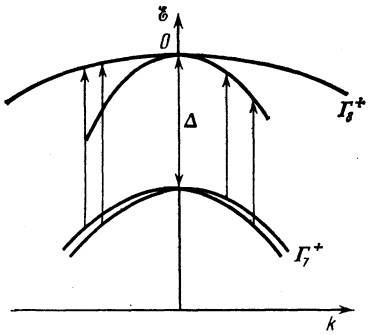

FIG. 2. Electron spectrum of the Γ_{25}' band in Ge (the arrows indicate transitions that give rise to a photocurrent associated with parity nonconservation)

In calculating the current associated with parity nonconservation, we may set the photon momentum $\mathbf{q}$ equal to zero. The contributions to this current come from two factors: first, from terms linear in $\mathbf{k}$ in the transition matrix elements, which lead to an anisotropic distribution of the electrons arising in the Γ_8^+ band, which gives rise to the current; and second, from terms linear in $\mathbf{k}$ in the energy of the Γ_7^+-band electrons [Eq. (III.11)], which occurs in the argument of the δ function. As a result, the energy of the electrons arising in the Γ_8^+ band depends on the direction of $\mathbf{k}$; moreover, $f_{hj}(\mathbf{k})$, the velocity $\mathbf{v}_j(\mathbf{k})$, and the relaxation time $\tau_j(\mathbf{k})$ also depend on the direction of $\mathbf{k}$, and so, therefore, in accordance with (III.12), does their contribution to the current.

It is evident from Eqs. (III.10) and (III.11) that when $\omega < \Delta$ only transitions of light holes into the band are possible, the holes leaving the Γ_8^+ band with the energy[5)]

$$\mathscr{E}_L = \frac{A+B}{B}(\Delta - \omega). \quad \text{(III.13)}$$

When $\omega > \Delta$, on the other hand, only transitions of heavy holes into the band are possible, the holes leaving the Γ_8^+ band with the energy

$$\mathscr{E}_H = \frac{A-B}{B}(\omega - \Delta). \quad \text{(III.14)}$$

Calculations using Eq. (III.12) lead to the following expression for the current:

$$\mathbf{I} = I_0(a\mathbf{n} + b\mathbf{s}), \quad \text{(III.15)}$$

where $\mathbf{n} = \mathbf{q}/q$.

When $\omega < \Delta$,

$$I_0 = eK_L\Phi(A+B)\tau_L q, \quad \text{(III.16)}$$

$$a = a_L = \frac{27}{85} + \frac{52}{85}\frac{A}{B}\left(\frac{5}{2} + Z_L\right), \quad \text{(III.17)}$$

$$b = b_L = \frac{3\gamma}{Bq}\left(1 + \frac{6}{17}Z_L\right), \quad \text{(III.18)}$$

$$Z_l = \frac{\partial \ln \tau_l}{\partial \ln \mathscr{E}_l} - \frac{\mathscr{E}_l}{T}, \quad \text{(III.19)}$$

$$K_l = -\frac{4BN_l e^2}{n\omega}\left(\frac{\pi \mathscr{E}_l}{T}\right)^{1/2} e^{-\mathscr{E}_l/T}, \quad \text{(III.20)}$$

where N_l is the concentration of holes of type l (in this case, light ones), $\mathscr{E}_l$ is the energy of those holes as given by Eq. (III.13), τ_l is the relaxation time, and n is the refractive index.

When $\omega > \Delta$, we have

$$I_0 = eK_H \Phi (A-B) \tau_H q, \tag{III.21}$$

$$a = a_H = \frac{3}{5} - \frac{A}{B}\left(\frac{5}{2} + Z_H\right), \tag{III.22}$$

$$b = b_H = \frac{2\gamma}{Bq}\left(\frac{3}{2} + Z_H\right), \tag{III.23}$$

where Z_H and K_H are given by Eqs. (III.19) and (III.20), and $\mathscr{E}_H$ is given by Eq. (III.14).

Estimates based on those formulas for Ge specimen with $\rho = 1.4\,\Omega$ cm $(N = N_L + N_H \approx 10^{14}$ cm$^{-3})$ at $T = 77$°K yield the following values for the drag current per unit incident power and absorption coefficient for light of frequency ω corresponding to the maximum absorption $(\mathscr{E}_H = (3/2)T)$:

$$\begin{aligned} &\text{a}\quad \omega = \Delta - \frac{3}{2}T\frac{B}{A+B}, \quad I_{drg} = 10^{-6}\ \text{A/W}, \\ &K_L = 8.4\cdot 10^{-4}\ \text{cm}^{-1}; \\ &\text{b}\quad \omega = \Delta + \frac{3}{2}T\frac{B}{A-B}, \quad I_{drg} = 3\cdot 10^{-8}\ \text{A/W}, \\ &K_H = 1.8\cdot 10^{-2}\ \text{cm}^{-1}. \end{aligned} \tag{III.24}$$

To estimate γ we must know the values of $F(\mathbf{R}_a)$ and $(p_x X)_{r=R_a}$. The main contribution to the sum in (III.8) comes from the nearest conduction band. According to Ref. (14), for this band we have

$$k_0 = |S(\mathbf{R}_a)|^2\Omega = (1.3-1.4)\cdot 10^4.$$

In accordance with the Bunyakovskiĭ-Schwarz inequality, we have

$$k = \left|\frac{S(\mathbf{R}_a)(p_x X)_{r=R_a}\Omega}{\langle S|p_x|X\rangle}\right| > \left|\frac{|S(\mathbf{R}_a)|^2 |p_x X|^2_{r=R_a}\Omega^2}{\langle |p_x X|^2\rangle}\right|^{1/2}.$$

Here it is supposed that $\langle |S|^2\rangle = 1$. We assume that

$$|p_x X|^2_{r=R_a}\Omega/\langle |p_x X|^2\rangle \approx k_0,$$

and for an estimate we set $k = k_0$. Then the ratio of the current associated with parity nonconservation (for $|s| = 1$) to the drag current is:

$$\begin{aligned} &\text{a}\quad \omega < \Delta \quad I_{PVE}/I_{drg} = 10^{-10}, \\ &\text{b}\quad \omega > \Delta \quad I_{PVE}/I_{drg} = 10^{-9}. \end{aligned} \tag{III.25}$$

This ratio is evidently of about the same order as in the case of excited hydrogen atoms with oriented $2S$ electrons.

Since the photocurrent associated with parity nonconservation appears in Ge in the zeroth order in $\mathbf{q}$, the current in a strong magnetic field that leads to orientation of the holes turns out to be of the same order as the current that arises from excitation by circularly polarized light.

3. The drag current that depends on the circular polarization of the light

The photocurrent associated with parity nonconservation may be masked by the drag current that depends on the polarization of the light. In cubic crystals having O_h symmetry, the photocurrent excited by plane polarized light depends on the propagation direction of the light and on the plane of polarization, even in the first order in $\mathbf{q}$.[5] Under excitation by circularly polarized light, the dependence on the degree of polarization appears in the third order in $\mathbf{q}$ and is given (for $\mathbf{s}\|\mathbf{q}$) by the formula

$$I_z = \alpha_1 \Phi \frac{(sq)}{q^2} q_x q_y (q_x^2 - q_y^2). \tag{III.26}$$

The current in the direction of $\mathbf{q}$ evidently always vanishes, and the current also vanishes when the light propagates in the direction of one of the principal axes (001), (111), or (110). If the angle between the vector $\mathbf{q}$ and the (001) axis is θ, the angle between the direction of the current and that axis is θ', the vectors $\mathbf{I}$ and $\mathbf{q}$ do not have the same direction, and both θ and θ' are very small as compared with unity, then

$$I_{drg} \sim \alpha_1 (sq)\, q^2 \theta\theta' \Phi.$$

This current is small as compared with the ordinary drag current by the parameter

$$\left|\frac{q}{mE_g}\langle S|p_x|X\rangle\right|^2 \theta\theta' \approx \frac{q^2\theta\theta'}{m^* E_g} \approx 10^{-6}\theta\theta'.$$

Here m^* is the effective mass of a Γ_7^--band electron. It is evident that if this current is not to exceed the current associated with parity nonconservation the specimen must be highly uniform and very precisely oriented and that the propagation direction of the light must also be very precisely oriented with respect to the crystallographic axes so that the product $\theta\theta'$ will be smaller than 10^{-4}, i.e. so that θ and θ' may not exceed 10′.

When the light-propagation and the current directions are along the other principal axes (111) and (110) the requirements on the orientations of $\mathbf{q}$ and $\mathbf{I}$ turn out to be even more rigid, and in these cases $\mathbf{I}_{drg} \sim (\theta - \theta')$.

In principle, a current associated with parity nonconservation could also be observed in crystals of the T_d class, in which the ordinary circular photovoltaic effect does not occur. Here, however, a drag current that depends on the degree of circular polarization of the light appears already in the second order in $\mathbf{q}$. When $\mathbf{s}\|\mathbf{q}$, this current is given by the formula

$$I_z = \alpha_2 \Phi \frac{(sq)}{q^2} q_z (q_x^2 - q_y^2). \tag{III.27}$$

In these crystals, therefore, the requirements on the orientations of $\mathbf{q}$ and $\mathbf{I}$ turn out to be extremely rigid. Moreover, it must be borne in mind that the linear photovoltaic effect appears in crystals of the T_d class in addition to the drag current. The corresponding current is independent of $\mathbf{q}$ and is given by the formula[5]

$$I_z = \Phi\chi(e_x e_y^* + e_y e_x^*). \tag{III.28}$$

For certain orientations this current also appears under excitation by unpolarized or circularly polarized light (but it does not depend on **s**).

In addition, there is another contribution to the photocurrent that must be considered, which depends on the sign of the circular polarization and is determined by the relation $\mathbf{I} \sim \mathbf{n} \times \mathbf{s}$, where **n** is the normal to the surface.[15,16] Since this current disappears only when $\mathbf{n} \| \mathbf{s}$, precise orientation of the specimen is required to eliminate it.

It follows from the calculations presented above that currents associated with parity nonconservation arise in both gases and crystals. These currents are extremely small. We shall not discuss the optimal conditions for possible experiments to detect these currents nor the requirements for those doubtless very complicated experiments. Experimental physicists are much better qualified to do that. We note only that, according to our estimates, the detection of these currents is not beyond the possibilities of present experimental techniques.

[1)]The circular photogalvanic effect has also been treated theoretically in Ref. 2 (for crystals having the so-called weak gyrotropy) and has been observed experimentally[3,4] in Te (also see the review article, Ref. 5).

[2)]Formally, σ appears in the $(E\,1)_p$ amplitude after substituting the expression (II.6) for $\psi(2P_{1/2})$ in (II.2) and ensures that it will be a pseudoscalar.

[3)]We neglect the small ($\sim 3\%$) admixture of states with $m_j = 1/2$, $m_l = -1/2$ in β_0 and f_0.

[4)]Although the current associated with a transition between branches of the Γ_8^+ band is smaller than the current associated with transitions from the Γ_7^+ by the parameter T/Δ, there may be some technical advantages in measuring it since a CO_2 laser could be used.

[5)]When the nonparabolicity is taken into account, the minimum separation between the Γ_7^+ band and the light-hole branch of the Γ_8^+ band, according to the isotropic model, is $(17/18)\Delta$. When k is increased further this separation again increases. The formulas below are therefore valid when $\Delta - \omega < \Delta/18$ and $T < (A+B)\Delta/18B = 374°\text{K}$. For transitions to the heavy-hole band for $\omega - \Delta > \Delta/18$ it is also necessary to take account of the mixing of the Γ_8^+ and Γ_7^+ bands.

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