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Magnetic Field Dependence of the Hopping Transitions in Germanium and Silicon

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The influence of magnetic field on the phonon-induced hopping transitions leads to some galvanomagnetic effects in germanium and silicon crystals, e.g., magnetoresistivity in the impurity conduction. Here the probability of the hopping transitions between two donor centers in the presence of a weak magnetic field is calculated on the basis of the previous results of Myszkowski and Rogala. Only the adiabatic processes accompanied by emission or absorption of one phonon are considered. The exact form of the deformation potential is used, and both LA and TA phonons are taken into account. The theory is valid for donor centers situated on arbitrary substitutional sites in the crystal.

I. INTRODUCTION

The influence of magnetic field on the hopping phenomena in germanium and silicon was studied both theoretically[1-9] and experimentally.[10-17] The hopping phenomena are observed in crystals lightly doped with the impurities of both kinds, i.e., donors and acceptors. We consider only the n-type materials with the concentration of donors N_d higher than the concentration of acceptors N_a. Then the N_a electrons introduced by the donor centers occupy all the acceptor centers. Therefore, only $N_d - N_a$ donors are neutral. At sufficiently low temperature the electrons on these centers are not excited to the conduction band. If the concentration of the donors is sufficiently low, then the overlaps of one-center wave functions are small and the donor states are localized. These states have different energies because the randomly distributed acceptor centers produce the local electric fields. Moreover, the mutual interaction splits the states. Some of these states are ionized and some neutral; therefore, the electron transitions are possible. They are accompanied by absorption or emission of photons or phonons and called the "hopping transitions." External magnetic field influences these transitions changing their probability. It leads to some macroscopic effects induced by the magnetic field, e.g., magnetoresistivity in the hopping region.[1-4,10-12,15-17] In this paper we are interested in the case of the presence of an external, weak magnetic field.

The simplest microscopic model of the hopping transitions was given by Miller and Abrahams.[18] They considered the system of two donor centers and one electron in an external static electric field. This model was generalized by Trylski[8] to the case of external static electric and magnetic fields. The author assumed the wave functions of the two lowest states of the electron in the potential of two donor centers to be the linear combinations of the one-center wave functions, centered at the first and the second donor centers. Constructing the two-center wave functions, one takes into account only the lowest singlet state of an isolated donor center. This is justified if the splitting of the one-center states, caused by the central-cell potential ("chemical shift" potential), is higher than the energy difference between the two-center states.

Trylski obtained the coefficients in the two-center wave functions and the energy difference between the states using the variational procedure. Both centers of the donor pair were assumed to be on substitutional sites in the same sublattice of the crystal. However, the group-V donors in Ge and Si occupy substitutional sites in both sublattices and, for this reason, the treatment of Trylski was incomplete.

Gummel and Lax[19] gave the general theory of the transition probability between two nondegenerate electron states with simultaneous absorption or emission of phonons. They used the adiabatic approximation of Born and Oppenheimer and assumed the weak electron-lattice interaction. Then this theory was applied in a paper of Myszkowski and Rogala[20] (hereafter referred to as I) to consider the electron-lattice interaction in Ge and Si crystals. The authors assumed the wave functions of the electron in the initial and the final states in general forms. They determined the perturbing phonon operator on the basis of the deformation-potential theory and took into account the two independent deformation potential constants. The model of an isotropic continuous medium was used for the phonon spectrum of the crystal, including both LA and TA phonons. Under these assumptions the authors obtained the general formulas (24)–(26) for the phonon distribution functions which determine the transition probability.

The purpose of our work is to obtain the two-

center transition probability in the presence of an external magnetic field considering arbitrary substitutional positions of the centers.

In Sec. III we perform the transformation of the one-center wave function induced by the displacement of the donor center from the first sublattice of the crystal to the second. The method described in our previous work[21] (hereafter referred to as II) is applied here. Then the result is used to generalize the two-center wave functions of Trylski to the case of the donor centers on arbitrary substitutional sites in the crystal. The approximation of the weak magnetic field is discussed.

In Sec. IV the two-center wave functions in the presence of a weak magnetic field are substituted into the general phonon distribution functions of I. Only the "high-frequency" case (the wavelength of the involved phonon shorter than the distance between the centers) is considered here. All the assumptions introduced in II in the absence of the magnetic field are kept. Moreover, the electric field in the region of the donor pair is assumed to be approximately constant and its strength is limited. These assumptions are satisfied very well in practical applications. At concentrations of impurities at which the hopping phenomena are observed, the ionized acceptor centers are sufficiently far away from most of the donor pairs.

In the following part of this paper the two-center transition probability is averaged approximately over small regions around each of the actual positions of the donor centers, as was done in II in the absence of the magnetic field. The result is a slowly varying function of the distance between the centers and, for this reason, is more useful in the theories of the macroscopic hopping phenomena.

All the results of this paper are limited to the case of the adiabatic processes and of a weak magnetic field. They can be used in the theories of the macroscopic hopping phenomena induced by magnetic field, e.g., magnetoresistivity in the hopping region.[1-4,10-12,15-17]

II. GENERAL FORMALISM

Gummel and Lax[19] gave the general theory for the electron transitions induced by a weak phonon perturbation assuming the adiabatic Born-Oppenheimer approximation. The probability of the electron transition from the state a to the state b with simultaneous absorption or emission of only one phonon is

$$W_{ba}^{(1)} = 2\pi\hbar^{-2}\exp(-\alpha)[h(\omega_0) - \gamma^* g(\omega_0) - \gamma g^*(\omega_0) + |\gamma|^2 f(\omega_0)] \quad , \tag{1}$$

where

$$\alpha = \int_{-\infty}^{+\infty} f(\omega)d\omega \quad , \tag{2}$$

$$\gamma = \int_{-\infty}^{+\infty} g(\omega)d\omega \quad . \tag{3}$$

Here ω is the phonon frequency. Positive frequencies correspond to the emission and negative frequences to the absorption of a phonon. The function $h(\omega)$ is the distribution function of so-called "kinetic phonons" which arise because the energies of the electron states are different. Here the equilibrium positions of the crystal atoms are considered to be unaffected by the state of the electron. The functions $g(\omega)$ and $f(\omega)$ are connected with the "lattice relaxation" phonons which arise because of a local deformation of the crystal around the electron. This deformation consists of displacements of the equilibrium positions of the crystal atoms. The electron transition from one state to another may, therefore, induce a motion of the crystal lattice. Hence, emission or absorption of a phonon is possible. The one-phonon transitions, considered here, play a dominant role if $\alpha \ll 1$.[22-24] ω_0 is the frequency conserving the total energy of the system, being the sum of the two terms. The first term is the difference of the energy between the two electron states in a nondeformed crystal lattice. The other term is the difference of the electron-lattice interaction energy in these states. Because the second term is very small (of the order of magnitude of $E_{LR}S$)[5] for the two-center donor states (which are considered in this paper) one can assume

$$\hbar\omega_0 \simeq E_a(0) - E_b(0) = \Delta E_{ba} \quad , \tag{4}$$

where $E_a(0)$ and $E_b(0)$ are the energies of the electron in the states a and b, respectively, in nondeformed crystal lattice. The extension of that formalism on the nonadiabatic processes was done by Takeyama.[24]

In I the general Gummel-Lax theory was applied to the problem of the interaction of electrons with the acoustical phonons (both longitudinal and transverse) in Ge and Si crystals. The wave functions of the electron states were assumed in the general form

$$u_a(\vec{r}) = n^{-1/2}\sum_{i=1}^{n} F_a^{(i)}(\vec{r})\phi^{(i)}(\vec{r}) \quad , \tag{5}$$

$$u_b(\vec{r}) = n^{-1/2}\sum_{i=1}^{n} F_b^{(i)}(\vec{r})\phi^{(i)}(\vec{r}) \quad . \tag{6}$$

Here $\phi^{(i)}(\vec{r})$ is the Bloch function corresponding to the ith minimum of the conduction band. The functions $F_a^{(i)}(\vec{r})$ and $F_b^{(i)}(\vec{r})$ change slowly as compared with the Bloch functions. The sum is performed over all the minima of the conduction band (4 for Ge, 6 for Si). The crystal temperature was assumed to be very low as compared with the Debye temperature. This makes it possible to approximate the acoustical-phonon spectrum by the spectrum of an isotropic continuous medium. With

these assumptions the phonon distribution functions are given by Eqs. (24)–(26) of I. These formulas can be applied to arbitrary nondegenerate electron states in Ge and Si, if their wave functions are of the form (5) and (6). In particular, we are interested here in the two-center donor states in the presence of a magnetic field.

III. ELECTRON STATES IN PRESENCE OF EXTERNAL MAGNETIC FIELD

A. One-Center States

Van Huong[7] obtained the wave function of an electron bound to an isolated donor center in Ge or Si in the presence of a weak magnetic field $\vec{H}$. The chemical shift potential (the short-range potential of the impurity ion) splits the effective-mass one-center ground states. At sufficiently low temperature of the crystal only the lowest singlet state can be occupied by an electron. The corresponding wave function is[7]

$$u(\vec{r},\vec{H})=\sum_{i=1}^{n}\sigma^{(i)}(\vec{H})F^{(i)}(\vec{r},\vec{H})\phi^{(i)}(\vec{r}) \quad , \tag{7}$$

where $\phi^{(i)}(\vec{r})$ denote the Bloch functions. The envelopes $F^{(i)}(\vec{r},\vec{H})$ are used with the accuracy up to H^2. The valley phase factors $\sigma^{(i)}(\vec{H})$ are fixed by the chemical shift potential; for the weak magnetic field $\sigma^{(i)}(\vec{H})\simeq n^{-1/2}$.

Now we are interested in the one-center wave function corresponding to the position of the donor ion in the "second" sublattice. We apply the procedure described in II and limit our considerations to the case of the homogeneous magnetic field.

Using Eq. (7) and the symmetry properties of the envelopes

$$[F^{(i)}(\vec{r},\vec{H})=F^{(i)}(-\vec{r},\vec{H})=F^{(i)}(\vec{r},-\vec{H})]$$

and of the phase factors $[\sigma^{(i)}(\vec{H})=\sigma^{(i)}(-\vec{H})]$ one obtains for Ge

$$\tilde{u}'(\vec{r},\vec{H})=\exp\left(-\frac{ie}{2\hbar c}(\vec{H}\times\vec{t})\cdot\vec{r}\right)\tilde{u}(\vec{r},\vec{H}) \quad ,$$

$$\tilde{u}(\vec{r},\vec{H})=\exp(-\tfrac{3}{4}i\pi)\sum_{i=1}^{n}\sigma^{(i)}(\vec{H})F^{(i)}(\vec{r},\vec{H})\phi^{(i)}(\vec{r}+\vec{t})$$

$$\times\exp(i\vec{p}^{(i)}\cdot\vec{t}) \quad . \tag{8}$$

Here $\vec{p}^{(i)}$ is the vector from the center of the Brillouin zone to the ith minimum of the conduction band and $\vec{t}$ is the nonprimitive translation of the crystal lattice. The factor $\exp[-(ie/2\hbar c)(\vec{H}\times\vec{t})\cdot\vec{r}]$ arises from the performed transformation of the vector potential of the homogeneous magnetic field. The coordinate system is centered at the position of the "second" atom of the basis.

In the case of Si, $\sigma^{(i)}(\vec{H})=\sigma^{(j)}(\vec{H})$ for $\vec{p}^{(i)}=-\vec{p}^{(j)}$. The result of the transformation is

$$\tilde{u}'(\vec{r},\vec{H})=\exp\left(-\frac{ie}{2\hbar c}(\vec{H}\times\vec{t})\cdot\vec{r}\right)\tilde{u}(\vec{r},\vec{H}) \quad ,$$

$$\tilde{u}(\vec{r},\vec{H})=\sum_{i=1}^{n}\sigma^{(i)}(\vec{H})F^{(i)}(\vec{r},\vec{H})\phi^{(i)}(\vec{r}+\vec{t})$$

$$\times\exp(-i\vec{t}\cdot\vec{p}^{(i)}) \quad . \tag{9}$$

B. Two-Center States

Trylski[8] extended the Miller-Abrahams procedure[18] to the case of the presence of an external magnetic field. The two-center wave functions of the two lowest states of the electron are linear combinations of the one-center singlet wave functions centered on the first and on the second donor centers. As in the case of $H=0$ considered in II, the contributions to the two-center wave functions which come from the higher one-center states are neglected. These contributions arise because the electrostatic potential of one donor ion acts on the electron bound to the second center. Here we are interested only in the corrections to the two-center wave functions induced by the magnetic field. As in the case of $H=0$, the variational procedure is justified if the chemical shift splitting is much higher than the energy difference between the two-donor states and, moreover, the distance between the centers is sufficiently large.

Trylski performed the calculations assuming that both donor centers belong to the same sublattice. Here these results are extended to the case of the donor centers at arbitrary substitutional sites. The wave function of the electron in the lowest two-center state is of the form

$$u_b(\vec{r},\vec{H})=c_1^{-}(\vec{H})u_\xi(\vec{r},\vec{H})+c_2^{-}(\vec{H})\,u_\eta(\vec{r}-\vec{R},\vec{H})$$

$$\times\exp\left(-\frac{ie}{2\hbar c}(\vec{H}\times\vec{R})\cdot\vec{r}\right) \quad , \tag{10}$$

and in the higher state

$$u_a(\vec{r},\vec{H})=c_1^{+}(\vec{H})u_\xi(\vec{r},\vec{H})+c_2^{+}(\vec{H})u_\eta(\vec{r}-\vec{R},\vec{H})$$

$$\times\exp\left(-\frac{ie}{2\hbar c}(\vec{H}\times\vec{R})\cdot\vec{r}\right) \quad . \tag{11}$$

Here $\vec{R}$ is the vector from the first to the second donor center. The subscripts ξ and η denote the positions of the donor centers in the first or in the second sublattice of the crystal. They are independent and run over the values 1 and 2. We write $u_1(\vec{r},\vec{H})=u(\vec{r},\vec{H})$ and $u_2(\vec{r},\vec{H})=\tilde{u}(\vec{r},\vec{H})$. The phase factors induced by the magnetic field appear in Eqs. (10) and (11) only in the explicit form. The coordinate system is centered at the position of the first center, which is also the origin of the vector potential of the magnetic field. The displacement of the origin of the vector potential has no influence

on matrix elements of any potential.

Trylski obtained the coefficients in the form

$$c_1^{\pm}(\vec{H}) = z^{\pm}(\vec{H})\{1 + |z^{\pm}(\vec{H})|^2 + S(\vec{H})[z^{\pm}(\vec{H}) + z^{\pm}(\vec{H})^*]\}^{-1/2}, \quad (12)$$

$$c_2^{\pm}(\vec{H}) = \{1 + |z^{\pm}(\vec{H})|^2 + S(\vec{H})[z^{\pm}(\vec{H}) + z^{\pm}(\vec{H})^*]\}^{-1/2} \quad (13)$$

$$z^{\pm}(\vec{H}) = [\Delta(\vec{H}) + S(\vec{H})[W(\vec{H}) - W(\vec{H})^*] \pm (\{\Delta(\vec{H}) + S(\vec{H})[W(\vec{H}) + W(\vec{H})^*]\}^2 + 4|W(\vec{H})|^2 \times [1 - S(\vec{H})^2])^{1/2}]/2W(\vec{H})^* , \quad (14)$$

$$W(\vec{H}) = W_R(\vec{H}) - \tfrac{1}{2}S(\vec{H})\Delta(\vec{H}) + Z(\vec{H}) , \quad (15)$$

$$W_R(\vec{H}) = L(\vec{H}) - S(\vec{H})J(\vec{H}) , \quad (16)$$

$$L(\vec{H}) = \langle u_\xi(\vec{r}, \vec{H})|\, V_a\, |u_\eta(\vec{r} - \vec{R}, \vec{H}) \times \exp[-(ie/2\hbar c)(\vec{H} \times \vec{R}) \cdot \vec{r}]\rangle , \quad (17)$$

$$J(\vec{H}) = \langle u_\xi(\vec{r}, \vec{H})|\, V_b\, |u_\xi(\vec{r}, \vec{H})\rangle , \quad (18)$$

$$S(\vec{H}) = \langle u_\xi(\vec{r}, \vec{H})|u_\eta\ (\vec{r} - \vec{R}, \vec{H}) \times \exp[-(ie/2\hbar c)(\vec{H} \times \vec{R}) \cdot \vec{r}]\rangle , \quad (19)$$

$$Z(\vec{H}) = \langle u_\xi(\vec{r}, \vec{H})|\, V\, |u_\eta(\vec{r} - \vec{R}, \vec{H}) \times \exp[-(ie/2\hbar c)(\vec{H} \times \vec{R}) \cdot \vec{r}]\rangle - \tfrac{1}{2}S(\vec{H})[\langle u_\xi(\vec{r}, \vec{H})|\, V\, |u_\xi(\vec{r}, \vec{H})\rangle + \langle u_\eta(\vec{r} - \vec{R}, \vec{H})|\, V\, |u_\eta(\vec{r} - \vec{R}, \vec{H})\rangle] , \quad (20)$$

$$\Delta(\vec{H}) = \langle u_\xi(\vec{r}, \vec{H})|\, V\, |u_\xi(\vec{r}, \vec{H})\rangle - \langle u_\eta(\vec{r} - \vec{R}, \vec{H})|\, V\, |u_\eta(\vec{r} - \vec{R}, \vec{H})\rangle . \quad (21)$$

Here V_a and V_b are the energies of the electron in the Coulomb field of the donor ions a and b, respectively; V is the energy of the electron in the external electrostatic potential (we assume this energy to be lower at the center b). The energy difference between the two-center states a and b is

$$\Delta E_{ba}(\vec{H}) = [1 - S(\vec{H})^2]^{-1}(\{\Delta(\vec{H}) + S(\vec{H})[W(\vec{H}) + W(\vec{H})^*]\}^2 + 4|W(\vec{H})|^2[1 - S(\vec{H})^2])^{1/2} . \quad (22)$$

The quantities $W_R(\vec{H})$, $L(\vec{H})$, $J(\vec{H})$, $S(\vec{H})$ and $\Delta(\vec{H})$ defined by (16)–(19) and (21) are real. This property is used in (12)–(14). It results from the fact that the envelopes $F^{(i)}(\vec{r}, \vec{H})$ are real and invariant under the space inversion and, moreover, that the energy potential V_a in (17) can be replaced by V_b. The quantity $Z(\vec{H})$ is complex (unless $V = 0$) and, therefore, $W(\vec{H})$ and $c_1^{\pm}(\vec{H})$ are also complex. In this respect the problem in the presence of a magnetic field differs considerably from that in the absence of magnetic field. The treatment of Van Huong[7] is only an approximation.

At concentrations of impurities at which the hopping phenomena are observed the ionized acceptor centers are far away from most of the donor pairs. Their electric fields are approximately constant in the regions of the donor pairs, so that $\mathrm{Re}Z(\vec{H}) \simeq 0$, but $\mathrm{Im}Z(\vec{H}) = Z'(\vec{H}) \neq 0$.

If both centers belong to the same sublattice ($\xi = \eta$) Eqs. (7) and (16)–(19) yield

$$W_{R\,\mathrm{I\,Ge,Si}}(\vec{H}) \simeq -\frac{e^2}{n\epsilon R}\sum_{i=1}^{n}\exp(-R_i)\left\{\frac{R}{a}[R_i + 1] - [1 + R_i + \tfrac{1}{3}R_i^2] + \frac{e^2a^4}{720c^2\hbar^2(\beta+1)}[H^2 + \beta(\vec{k}^{(i)} \cdot \vec{H})^2] \times \left[\frac{R}{a}(-30R_i^4 - 135R_i^3 - 235R_i^2 + 360R_i + 360) + 10R_i^5 + 73R_i^4 + 233R_i^3 + 233R_i^2\right] + \frac{e^2a^2}{720c^2\hbar^2(\beta+1)}[(\vec{H} \cdot \vec{R}) + \beta(\vec{k}^{(i)} \cdot \vec{H})(\vec{k}^{(i)} \cdot \vec{R})]^2\left[\frac{R}{a}(30R_i^2 + 105R_i + 105) - 10R_i^3 - 63R_i^2 - 159R_i - 159\right]\right\}\cos(\vec{p}^{(i)} \cdot \vec{R}) . \quad (23)$$

Here $R_i = [R^2 + \beta(\vec{k}^{(i)} \cdot \vec{R})^2]^{1/2}/a$, a is the transverse radius of the envelopes, $\vec{k}^{(i)}$ is the unit vector in the direction of $\vec{p}^{(i)}$ (from the center of the Brillouin zone to the ith minimum of the conduction band), ϵ is the static dielectric constant of the crystal, and the constant $\beta = (m_l/m_t) - 1$ is connected with the anisotropy of the conduction band; $\beta = 18.8$ for Ge and $\beta = 4.2$ and Si. The same approximations in the integrals are used as in II and, moreover, $\sigma^{(i)}(\vec{H}) \simeq n^{-1/2}$. The functions $\cos(\vec{p}^{(i)} \cdot \vec{R})$ arise because of the performed displacement of the Bloch functions.

In the case of Ge and $\xi \neq \eta$ Eqs. (7), (8), and (16)–(19) yield the quantity $W_{R\,\mathrm{II\,Ge}}(\vec{H})$, which differs from (23) because the functions $\cos(\vec{p}^{(i)} \cdot \vec{R})$ are replaced by $\cos(\vec{p}^{(i)} \cdot \vec{R} \pm \frac{3}{4}\pi)$, as in the case of $H = 0$

(see II). Here the sign + refers to the configuration $\xi = 2$, $\eta = 1$ and the sign − to $\xi = 1$, $\eta = 2$. The vectors $\vec{p}^{(i)}$ are parallel to the nonprimitive translations $\vec{t}^{(i)}$ transforming the "first" sublattice into the "second" (the vector $\vec{t}$ is one of these translations).

In the case of Si and $\xi \neq \eta$ Eqs. (7), (9), and (16)–(19) yield the quantity $W_{RII\,Si}(\vec{H})$ of the same form as (23).

The magnetic field corrections to the function (23) should be relatively small compared with the zero-order term because of the assumption of the weak magnetic field. Assuming $\vec{H} \perp \vec{R}$ and taking the term with $\vec{k}^{(i)} \parallel \vec{H}$ (if such term does exist) one obtains

$$(e^2a^4H^2/16c^2\hbar^2)(R/a)^3 \ll 1 \ . \tag{24}$$

Here only the relevant values of R are considered (i.e., $R > 3a$). With the values of the transverse radii of the envelopes $a = 70.8$ Å for Ge and $a = 22.1$ Å for Si the resulting conditions are $H(R/a)^{3/2} < 5.3 \times 10^2$ kG for Ge and $H(R/a)^{3/2} < 5.4 \times 10^3$ kG for Si. These conditions are weaker than those of Van Huong.[7]

IV. TRANSITION PROBABILITY IN PRESENCE OF EXTERNAL MAGNETIC FIELD

Now we are interested in the transition probability between the two-donor states of electrons in the presence of an external weak magnetic field. The transition probability (1) involves the phonon distribution functions. They are given by the formulas (24)–(26) of I if the electron wave functions are of the general form (5) and (6). In the present problem the electron wave functions are (10) and (11). Comparing (5) and (6) with (10) and (11) and using (7) [with the approximation $\sigma^{(i)}(\vec{H}) \simeq n^{-1/2}$] one obtains for Ge and Si in the case of $\xi = \eta$ (both centers in the same sublattice)

$$F_a^{(i)}(\vec{r},\vec{H}) = c_1^+(\vec{H})F^{(i)}(\vec{r},\vec{H}) + c_2^+(\vec{H})\exp(-i\vec{p}^{(i)}\cdot\vec{R}) \times \exp\left(-\frac{ie}{2\hbar c}(\vec{H}\times\vec{R})\cdot\vec{r}\right) F^{(i)}(\vec{r}-\vec{R},\vec{H}) \ , \tag{25}$$

$$F_b^{(i)}(\vec{r},\vec{H}) = c_1^-(\vec{H})F^{(i)}(\vec{r},\vec{H}) + c_2^-(\vec{H})\exp(-i\vec{p}^{(i)}\cdot\vec{R}) \times \exp\left(-\frac{ie}{2\hbar c}(\vec{H}\times\vec{R})\cdot\vec{r}\right) F^{(i)}(\vec{r}-\vec{R},\vec{H}) \ . \tag{26}$$

Here the origin of the coordinate system is assumed to be at the position of the first center of the pair. The functions $\exp(-i\vec{p}^{(i)}\cdot\vec{R})$ arise because of the performed displacement of the Bloch functions.

Combining (25) and (26) with Eqs. (24)–(26) of I and using (12)–(15) we obtain the phonon distribution functions for the two-center transitions. However, even in this special case, these functions can not be calculated effectively because the matrix elements

$$\langle F^{(i)}(\vec{r}+\tfrac{1}{2}\vec{R},\vec{H})|\cos(\tau\cdot\vec{r})\cos\left[\frac{e}{2\hbar c}(\vec{H}\times\vec{R})\cdot\vec{r}\right] \times F^{(i)}|(\vec{r}-\tfrac{1}{2}\vec{R},\vec{H})\rangle \tag{27}$$

and

$$\langle F^{(i)}(\vec{r}+\tfrac{1}{2}\vec{R},\vec{H})|\sin(\tau\cdot\vec{r})\sin\left[\frac{e}{2\hbar c}(\vec{H}\times\vec{R})\cdot\vec{r}\right] \times |F^{(i)}(\vec{r}-\tfrac{1}{2}\vec{R},\vec{H})\rangle \tag{28}$$

(τ is the wave vector of the perturbing phonon) are involved. For this reason the following considerations are restricted to the "high-frequency" case only, in which the wavelength of the involved phonon is shorter than the distance between the centers (see I). We use also the assumption

$$S \ll 1 \ , \tag{29}$$

which is equivalent to the assumption $R \gg a$ justifying the procedure of Trylski, and the assumption

$$2W_R\,S \ll \Delta \ll 2W_R/S \ , \tag{30}$$

which is justified in most of the practical cases. However, in the presence of the magnetic field some additional assumptions are necessary to eliminate the complicated terms in the phonon distribution functions. One should assume

$$(e/2\hbar c)HR \ll \tau \tag{31}$$

in order to avoid substantial interference of the trigonometric functions in the matrix elements (27) and (28).

The quantities $W_R(\vec{H})$ and $S(\vec{H})$ have a similar magnetic field dependence. The quantity $\Delta(\vec{H})$ depends less strongly on the magnetic field, i.e.,

$$\left|\frac{\Delta(\vec{H})-\Delta(0)}{\Delta(0)}\right| < \left|\frac{W_R(\vec{H})-W_R(0)}{W_R(0)}\right| \tag{32}$$

according to the previous assumption that the electric field $\vec{E}$ is approximately constant in the region of the donor pair [for the constant electric field $\Delta(\vec{H}) = \Delta(0) = e\vec{R}\cdot\vec{E}$].

At usual concentrations of impurities in the crystal the electric fields of ionized acceptors are sufficiently weak in the regions of most of the donor pairs so that

$$Z'(\vec{H})^2 \ll |W_R(\vec{H})^2 - W_R(0)^2| \tag{33}$$

in practical applications of the theory.

The mentioned assumptions allow us to neglect

the terms proportional to the complicated matrix elements (27) and (28) in the phonon distribution functions. Moreover, we use the approximation

$$\langle F^{(i)}(\vec{r},\vec{H})|\exp(i\vec{\tau}\cdot\vec{r})|F^{(i)}(\vec{r},\vec{H})\rangle \simeq \left(1+\frac{11e^2a^4}{12c^2\hbar^2(\beta+1)}[H^2+\beta(\vec{H}\cdot\vec{k}^{(i)})^2]\right)$$
$$\times\langle F^{(i)}(\vec{r},0)|\exp(i\vec{\tau}\cdot\vec{r})|F^{(i)}(\vec{r},0)\rangle \qquad (34)$$

for the relevant values of τ ($\tau > a^{-1}$ for the adiabatic processes[21,24]). The magnetic field dependence of the matrix element (34) is much weaker than that of $W_R(\vec{H})$ and, in some cases, it can be neglected altogether.

Finally, we have simple formulas for the phonon distribution functions in the high-frequency case with the accuracy up to H^2:

$$f_\infty(\omega,\vec{H}) \simeq (16\pi^3\hbar d)^{-1}\theta(\omega)s(\omega)\left(1+\frac{11e^2a^4(\beta+3)}{18c^2\hbar^2(\beta+1)}H^2\right)\Delta(\vec{H})^2[4W_R(\vec{H})^2+\Delta(\vec{H})^2+4Z'(\vec{H})^2]^{-1}\ , \qquad (35)$$

$$\mathrm{Re}g_\infty(\omega,\vec{H}) \simeq (2\pi^2 d)^{-1}\theta(\omega)\hbar\omega^2 s(\omega)\left(1+\frac{11e^2a^4(\beta+3)}{18c^2\hbar^2(\beta+1)}H^2\right)[W_R(\vec{H})^2+Z'(\vec{H})^2]^{1/2}[4W_R(\vec{H})^2+\Delta(\vec{H})^2+4Z'(\vec{H})^2]^{-3/2}, \qquad (36)$$

$$h_\infty(\omega,\vec{H}) \simeq (2\pi^2 d)^{-1}\theta(\omega)\hbar^3\omega^4 s(\omega)\left(1+\frac{11e^2a^4(\beta+3)}{18c^2\hbar^2(\beta+1)}H^2\right)[W_R(\vec{H})^2+Z'(\vec{H})^2][4W_R(\vec{H})^2+\Delta(\vec{H})^2+4Z'(\vec{H})^2]^{-2}\ , \qquad (37)$$

where

$$\theta(\omega)=[2\sinh(\hbar\omega/2k_0T)]^{-1}\omega\exp(\hbar\omega/2k_0T)\ . \qquad (38)$$

T is the temperature of the crystal, d is the crystal density, and the function $s(\omega)$ is defined by the formula (31) of I. The function $\mathrm{Im}g_\infty(\omega,\vec{H})$ is negligible as compared with $\mathrm{Re}g_\infty(\omega,\vec{H})$.

Using the previous assumptions in (22) one obtains

$$\Delta E_{ba}(\vec{H}) \simeq [4W_R(\vec{H})^2+\Delta(\vec{H})^2+4Z'(\vec{H})^2]^{1/2}\ . \qquad (39)$$

The inequality (33) allows one to neglect $Z'(\vec{H})^2$ as compared with $W_R(\vec{H})^2$ in Eqs. (35)–(37) and (39). However, one can not neglect the magnetic field dependence of $\Delta(\vec{H})$ on the basis of (32).

Substituting Eqs. (4), (35)–(37), and (39) into (1)–(3) and neglecting $\mathrm{Im}g_\infty(\omega,\vec{H})$ one obtains in the high-frequency case

$$W^{(1)}_{ba\infty}(\vec{H}) \simeq [\pi\hbar^3 d]^{-1}\theta([4W_R(\vec{H})^2+\Delta(\vec{H})^2]^{1/2}/\hbar)s([4W_R(\vec{H})^2+\Delta(\vec{H})^2]^{1/2}/\hbar)W_R(\vec{H})^2\exp[-\alpha(\vec{H})][1-A_\infty(\vec{H})]^2\ , \qquad (40)$$

$$A_\infty(\vec{H}) \simeq \frac{\mathrm{Re}g_\infty(\vec{H})}{h_\infty(\vec{H})}\int_{-\infty}^{+\infty}\mathrm{Re}g_\infty(\omega,\vec{H})d\omega \simeq C\Delta(\vec{H})^2[4W_R(\vec{H})^2+\Delta(\vec{H})^2]^{-2}\left[1+\frac{11e^2a^4(\beta+3)}{18c^2\hbar^2(\beta+1)}H^2\right]\ , \qquad (41)$$

$$\alpha(\vec{H}) \simeq \int_{-\infty}^{+\infty}f_\infty(\omega,\vec{H})d\omega \simeq B\Delta(\vec{H})[4W_R(\vec{H})^2+\Delta(\vec{H})^2]^{-1}\left[1+\frac{11e^2a^4(\beta+3)}{18c^2\hbar^2(\beta+1)}H^2\right]\ . \qquad (42)$$

Here the same approximations under the integrals are used as in the case of $H=0$ (see I and II). The constants are $B=0.0083$, $C=0.0093$ (meV)^2 for Ge and $B=0.055$, $C=1.9$ (meV)^2 for Si.

The presented calculations of the transition probability are valid for both possible configurations of the donor centers. One should distinguish these configurations in the case of Ge using $W_{RI}(\vec{H})$ for $\xi=\eta$ and $W_{RII}(\vec{H})$ for $\xi\neq\eta$.

The probability of the reverse process $W^{(1)}_{ab}(\vec{H})$ (the transition from the state b to the state a connected with the absorption of a phonon) is given by the formula similar to (40) with the factor $\theta(-\Delta E_{ba}(\vec{H})/\hbar)$ instead of $\theta(\Delta E_{ba}(\vec{H})/\hbar)$.

For $H=0$, Eqs. (40)–(42) reduce to Eqs. (83)–(85) of I. The assumption of weak magnetic field is equivalent to (24) because $W_R(\vec{H})$ depends most strongly on the magnetic field. The condition (31) is weaker than (24) for the adiabatic processes and for the relevant values of R.

The obtained transition probability is a rapidly oscillating function of $\vec{R}$ because the quantity $W_R(\vec{H})$ involves factors $\cos(\vec{p}^{(i)}\cdot\vec{R})$ [or $\cos(\vec{p}^{(i)}\cdot\vec{R}\pm\frac{3}{4}\pi)$]. However, this oscillating part is unimportant in the theories of the macroscopic hopping phenomena in the crystal, involving transitions between a great number of randomly distributed donor centers. For this reason one can consider the "approximately averaged" transition probability, replacing $W_R(\vec{H})^2$ by its average $\langle W_R(\vec{H})^2\rangle$ in the transition

probability formula, as was done in II. With the simplifying assumption $\alpha(\vec{H})=0$ {the magnetic field dependence of the factor $\exp[-\alpha(\vec{H})]$ is negligible} the result is

$$\langle W^{(1)}_{ba\infty}(\vec{H})\rangle \simeq [\pi\hbar^3 d]^{-1}\theta([4\langle W_R(\vec{H})^2\rangle+\Delta(\vec{H})^2]^{1/2}/\hbar)s([4\langle W_R(\vec{H})^2\rangle+\Delta(\vec{H})^2]^{1/2}/\hbar)\langle W_R(\vec{H})^2\rangle$$
$$\times[1-C\Delta(\vec{H})^2[4\langle W_R(\vec{H})^2\rangle+\Delta(\vec{H})^2]^{-2}\ \{1+[11e^2a^4(\beta+3)/18c^2\hbar^2(\beta+1)]H^2\}\ ]^2\ . \tag{43}$$

Using the same procedure as in II one obtains on the basis of (23) for Ge and Si and for both configurations of the donor centers

$$\langle W_R(\vec{H})^2\rangle \simeq \left(\frac{e^2}{n\epsilon R}\right)^2\sum_{i=1}^{n}\exp(-2R_i)\left[\frac{R}{a}(R_i+1)-1-R_i-\tfrac{1}{3}R_i^2\right]\left\{\left[\frac{R}{a}(R_i+1)-1-R_i-\tfrac{1}{3}R_i^2\right]+\frac{e^2a^4}{360c^2\hbar^2(\beta+1)}\right.$$
$$\times[H^2+\beta(\vec{k}^{(i)}\cdot\vec{H})^2]\left[\frac{R}{a}(-30R_i^4-135R_i^3-235R_i^2+360R_i+360)\right.$$
$$\left.+10R_i^5+73R_i^4+233R_i^3+233R_i^2\right]+\frac{e^2a^2}{360c^2\hbar^2(\beta+1)}[(\vec{H}\cdot\vec{R})+\beta(\vec{k}^{(i)}\cdot\vec{H})(\vec{k}^{(i)}\cdot\vec{R})]^2$$
$$\left.\times\left[\frac{R}{a}(30R_i^2+105R_i+105)-10R_i^3-63R_i^2-159R_i-159\right]\right\} \tag{44}$$

with the accuracy up to H^2.

V. DISCUSSION OF RESULTS

In this paper the influence of the magnetic field on the phonon-induced hopping transitions in n-type Ge and Si is investigated. In particular, the system of the two donor centers and one electron in external, static, electric, and magnetic fields is considered. The two-center electron wave functions of Trylski[8] are generalized to the case of the donor centers on arbitrary substitutional sites in the crystal, i.e., not only in the same sublattice. These functions are linear combinations of the one-center wave functions,[7] centered on the first and the second donor center, respectively. They involve the overlap integral $S(\vec{H})$, the resonance energy $W_R(\vec{H})$, the difference of the averaged electrostatic energy of the electron on the isolated centers $\Delta(\vec{H})$ and some small quantity $Z'(\vec{H})$, which depend on the magnetic field and, in the case of Ge, also on the arrangement of the donor centers in the crystal.

The approximation of weak magnetic field is used here. The obtained condition (24) on the strength of this field is weaker than that of Van Huong.[7]

Then, the obtained two-center wave functions are used in the general formulas of I for the phonon distribution functions. Only the one-phonon transitions in the high-frequency case (the wavelength of the involved phonon shorter than the distance between the centers) are considered. With all the approximations used previously in I and II in the absence of magnetic field the resulting probability formula (40) is of a similar form. Clearly, it depends on the magnetic field because of the involved quantities $W_R(\vec{H})$, $\Delta(\vec{H})$, and of some additional factor involved in the functions $A_\infty(\vec{H})$ and $\alpha(\vec{H})$ [it arises because of the magnetic field dependence of the matrix element (34) which is, however, much weaker than that of $W_R(\vec{H})$]. In the case of Ge the transition probability depends also on the arrangement of the donor centers because of $W_R(\vec{H})$.

The electric field in the region of the donor pair is assumed to be weak and approximately constant because of the practical applications of the theory. The inequalities (32) and (33) and, also, the approximation $\mathrm{Re}Z(\vec{H})\simeq 0$ result from this assumption. The inequality (33) is equivalent to

$$E(R/a)^{3/2} < 1000\sqrt{3}(e/\epsilon a^2) \tag{45}$$

or $E(R/a)^{3/2} < 10^5\,\mathrm{V/cm}$ for Ge and $E(R/a)^{3/2} < 1.5\times10^6\,\mathrm{V/cm}$ for Si. It allows one to neglect $Z'(\vec{H})$ in the transition probability formula for most of the donor pairs in the crystal.

The two-center transition probability is averaged over small regions around each of the actual positions of the donor centers, as was done in I in the absence of the magnetic field. The resulting formula does not have the oscillating behavior and is more convenient in practical applications.

The results of this paper for the two-center transition probability are limited to the adiabatic processes and to the weak magnetic fields. They can be used in the theories of the macroscopic hop-

ping phenomena induced by the magnetic field, e.g., magnetoresistivity in the hopping region.[1-4,10-12,15-17]

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Trapping Effects and Acoustoelectric Current Saturation in ZnO Single Crystals

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Measurements of current-voltage characteristics for ZnO single crystals at temperatures between 77 and 640 °K are reported. Because of the buildup of an intense acoustic flux, a strong current saturation sets in when the trap-controlled electron drift velocity is equal to the velocity of sound. The temperature dependence of the saturated current is discussed in terms of a trapping model which includes nonlinear trapping effects. Our results indicate the presence of a shallow-donor level with an ionization energy of 50 meV and a deep-donor level approximately 230 meV below the conduction-band edge. The capture cross section for the shallow donors is determined to be about 5×10^{-12} cm^2 at 100 °K.

I. INTRODUCTION

The electronic properties of ZnO single crystals have been studied by Hutson,[1] who measured the Hall coefficient and the electrical conductivity at temperatures between 55 and 300 °K. By analyzing the temperature dependence of the free-electron density, Hutson obtained a donor ionization energy of 51 meV for hydrogen, zinc, and lithium donors.

Alternatively to Hall experiments, the electronic properties of piezoelectric semiconductors can be studied by means of the acoustoelectric current saturation.[2,3] This method was first employed by Moore and Smith[4] to investigate single crystals of semiconducting CdS. Subsequently, Rannestad[5] has determined the density and ionization energy of impurity states in photoconducting CdS by measuring the temperature dependence of the threshold field for current saturation. For ZnO, a preliminary discussion of the temperature dependence of the saturated current density was given by Meyer *et al.*[6] Below 200 °K, the experimental results could be explained in terms of the ionization of shallow donors with an activation energy between 40 and 70 meV. To account for the increase in saturated current at temperatures above 200 °K, the additional presence of a deep-donor level had to be assumed.