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Strong-Field Magnetoresistance of Impurity Conduction in *n*-Type Germanium*

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A simple theory is given of the strong-field magnetoresistance in the phonon-induced hopping region of impurity conduction in *n*-type germanium. It is shown to be convenient to consider separately the effect of a magnetic field in three cases: the weak, the moderately strong, and the extremely strong field case. In a moderately strong field the shrinking of a donor wave function and the phase difference produced by the magnetic field between two neighboring donors lead to a formula qualitatively identical with the empirical formula found experimentally by Sladek and Keyes. The magnetoresistance in an extremely strong magnetic field is also discussed, in which the wave function in the plane perpendicular to the field becomes similar to the free-electron wave function in a magnetic field.

I. INTRODUCTION

RECENTLY, Sladek and Keyes[1,2] measured the strong-field magnetoresistance in the phonon-induced hopping region of impurity conduction in *n*-type germanium. They found the order of magnitude, the magnetic-field dependence, and the anisotropy of the magnetoresistance remarkably different from those of conduction electrons in the usual energy bands. They have proposed an empirical formula to describe their results and suggested a possible phenomenological interpretation based on the shrinking of a donor wave function by the magnetic field, which was first treated by Yafet, Keyes, and Adams.[3]

On the other hand, we have shown in a preceding paper[4] that the characteristic properties of the weak-field magnetoresistance in the hopping region[5] can be explained, at least qualitatively, by considering two mechanisms: the shrinking of each donor wave function by the magnetic field, and the phase difference produced by the field between two neighboring donors. The effect of the phase difference, which is represented by the Lorentz force in band conduction, contributes the same order of magnitude as the shrinking effect.

In this paper we shall show that two such mechanisms contribute the same order of magnitude to the magnetoresistance in any strong magnetic field. In Sec. II we discuss the effect of the shrinking of a donor wave function on impurity conduction. It is shown to be convenient to consider separately the effect of a magnetic field in three cases: the weak, the moderately strong, and the extremely strong field case. The experiment by SK corresponds to the moderately strong-field case and can be explained in part by the shrinking effect. In Sec. III the effect of the phase difference between two neighboring donors will be discussed in a moderately strong field case. We shall derive a formula, from the shrinking and the phase-factor effects, qualitatively identical with the empirical formula of SK. The last section is devoted to the discussion of the magnetoresistance in an extremely strong field.

II. SHRINKING OF A DONOR WAVE FUNCTION

As is well known,[6] the ground-state wave function of donors in *n*-type germanium is written as the sum of contributions from four valleys of the conduction band,

$$\Psi(\mathbf{r})=\sum_{p=1}^{4}\alpha_pF_p(\mathbf{r})\phi_p(\mathbf{r}), \tag{2.1}$$

where $\phi_p(\mathbf{r})$ is the Bloch function for the pth conduction band minimum and $\alpha_p=\frac{1}{2}$ for all valleys in zero magnetic field. The envelope function is given by

$$F_p(\mathbf{r})=(\pi a^2b)^{-1/2}\exp\{-[(x^2+y^2)/a^2+z^2/b^2]^{1/2}\}, \tag{2.2}$$

the change of which, by a magnetic field, will be discussed in this section. In (2.2) the z axis is chosen in the valley axis direction.

In general, an arbitrarily oriented magnetic field gives rise to a very complex change of the shape of the spheroidal hydrogenlike wave function (2.2). As discussed in I, however, one can approximate to the actual situation in *n*-type germanium by taking into account only the decrease of the transverse spatial extent in (2.2) by the magnetic field component parallel to the valley axis direction because of the strong mass anisotropy of the conduction electrons. According to the model used in I,[4,7–9] the conductivity

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[1] R. J. Sladek and R. W. Keyes, Phys. Rev. **122**, 437 (1961), hereafter referred to as SK.
[2] In this paper we do not consider the experiment on the strong-field magnetoresistance in InSb [R. J. Sladek, J. Phys. Chem. Solids **5**, 157 (1958)], since the experiment was performed at impurity concentrations considerably higher than those in the hopping region.
[3] Y. Yafet, R. W. Keyes and E. N. Adams, J. Phys. Chem. Solids **1**, 137 (1956).
[4] N. Mikoshiba and S. Gonda, preceding paper [Phys. Rev. **127**, 1954 (1962)], hereafter referred to as I.
[5] C. Yamanouchi and W. Sasaki (private communication).
[6] W. Kohn, *Solid-State Physics* edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 5, p. 257.
[7] T. Kasuya and S. Koide, J. Phys. Soc. Japan **13**, 1287 (1958).
[8] A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).
[9] N. F. Mott and W. D. Twose, *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1961), Vol. 10, p. 107.

for impurity conduction in the hopping region is proportional to the weighted angular average of the square of the resonance energy W,

$$\begin{aligned} &W=L-SJ,\\ &L\equiv(\Psi_i,\ (-e^2/\kappa r_j)\Psi_j),\\ &S\equiv(\Psi_i,\Psi_j),\\ &J\equiv(\Psi_i,\ (-e^2/\kappa r_j)\Psi_i),\end{aligned} \tag{2.3}$$

where the suffixes i and j denote the occupied and unoccupied donor sites, respectively, and r_j is the distance between the position of an electron and the site j. The square of the resonance energy W in n-type germanium has the following properties[4]: (1) $|W|^2$ is given by the sum of contributions from four valleys, $|W|^2=\sum_{p=1}^4 |W_p|^2$, and (2) the main contributions to each $|W_p|^2$ come from donor pairs in the plane perpendicular to the pth valley axis. The latter results directly from the strong anisotropy of the effective mass. These two properties of $|W|^2$ are essentially equivalent to the first and second conditions for the empirical formula of SK. The last condition for the SK formula is equivalent to the relation,

$$\langle|W_p|^2\rangle_{\mathrm{av}}=\langle|W_{p0}|^2\rangle_{\mathrm{av}} \times\exp\left\{-(\gamma+\delta|\cos\phi_p|)\frac{\kappa R^3H^2}{m_t^*c^2}\right\}, \tag{2.4}$$

for the components of conductivity perpendicular to the valley axis, where $\langle\ \rangle_{\mathrm{av}}$ denotes the weighted angular average, ϕ_p is the angle between the pth valley axis and the magnetic field direction, γ and δ are numerical constants ($\gamma=1.4\times10^{-2}$ and $\delta=2.9\times10^{-2}$ from experiment at $T=2.26$°K), m_t^* is the transverse effective mass, R is the average donor separation, and κ is the dielectric constant.

Since the actual situation is still fairly complicated in n-type germanium even if we adopt the approximations already mentioned, we first estimate the effect of a magnetic field on a hydrogen wave function. Moreover, we make here two approximations: (1) neglect of the linear Zeeman term as in I, and (2) neglect of the angular dependence of the quadratic Zeeman term. Such approximations are good to within a numerical factor of order unity as long as we are concerned only with the change in the wave function in the plane perpendicular to the magnetic field. The Schrödinger equation is therefore written in a simple form,

$$\frac{1}{r^2}\cdot\frac{d}{dr}\left(r^2\frac{d\Psi}{dr}\right)=-\frac{2m^*}{\hbar^2}\left(E+\frac{e^2}{\kappa r}-\frac{e^2H^2r^2}{8m^*c^2}\right)\Psi, \tag{2.5}$$

where E is the energy eigenvalue and H is the magnetic field. In the absence of the magnetic field Eq. (2.5) has a solution of the $1s$-like function,

$$\Psi=N^{-1/2}\exp(-r/a) \tag{2.6a}$$

with

$$E=-e^2/2\kappa a,\quad a=\kappa\hbar^2/m^*e^2, \tag{2.6b}$$

where N is the normalization constant.

In the presence of a magnetic field, it is convenient to consider separately three cases: the weak, the moderately strong, and the extremely strong field case. Let us first consider that the magnetic field is weak so that the energy eigenvalue E is approximately given by (2.6b) or by

$$E=E_0\left(1-\frac{\kappa a^3H^2}{2m^*c^2}\right), \tag{2.7a}$$

with

$$\kappa a^3H^2/2m^*c^2\ll1 \tag{2.7b}$$

from the perturbation theory.[4,10] Using the WKB method[11] we obtain the solution of (2.5):

$$\Psi\cong N^{-1/2}\exp\left(-\frac{r}{a}\right)\exp\left(-\frac{1}{24}\frac{\kappa H^2}{m^*c^2}r^3\right), \tag{2.8}$$

under the conditions

$$r/a\gg1, \tag{2.9a}$$

$$\kappa H^2r^3/4m^*c^2\ll r/a. \tag{2.9b}$$

Since the resonance energy in the hopping region is determined by the wave function at large distances (several Bohr radii) from the donor atom, the condition (2.9a) holds in the present problem.

A. Weak Field Case

We now define the weak field case in which the energy eigenvalue is approximated by (2.6b) or (2.7a), and the expansion of the wave function (2.8) to H^2 is a good approximation, i.e.,

$$\Psi\cong N^{-1/2}e^{-r/a}\left(1-\frac{1}{24}\frac{\kappa H^2}{m^*c^2}r^3\right). \tag{2.10}$$

[10] A. Miller [thesis, Rutgers University, 1960 (unpublished)] calculated the shrinking effect using a variational method and obtained $\Psi=N^{-1/2}e^{-r/a}$, $a=a_0[1-(\kappa a_0^3/2m^*c^2)H^2]$. If we use this function for the calculation of the resonance energy, we obtain $|W|^2=|W_0|^2\exp[-(\kappa a_0^2R/m^*c^2)H^2]$, in place of (2.21). This means that the simple variational calculation does not give information about the shape of the wave function at large distances from the nucleus.

[11] The WKB method suggests the form of the wave function,

$$\Psi=(C/r\sqrt{|p|})\exp\{-(1/\hbar)\textstyle\int|p|dr\}$$

in the classically inaccessible parts of space, where the classical momentum p in the present problem is given by

$$p=[2m^*(E+e^2/\kappa r-e^2H^2r^2/8m^*c^2)]^{1/2}.$$

[See, for instance, L. D. Landau and E. M. Lifshitz, *Quantum Mechanics, Nonrelativistic Theory* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1958, p. 159).] If we regard the Coulomb potential and the magnetic perturbation as small quantities compared with E, we obtain

$$|p|\cong(\hbar/a)(1-a/r+\kappa aH^2r^2/8m^*c^2),$$

which leads to (2.8).

The wave function (2.10) is identical with that derived by the Schwartz perturbation method[4] except for the angular part and leads to a magnetoresistance proportional to H^2.

B. Moderately Strong Field Case

There is a moderately strong field case in which the situation is different from the weak field case only because the expansion of the wave function (2.8) to H^2 is no longer a good approximation. In other words, the conditions

$$\frac{1}{2}\frac{\kappa a^3}{m^*c^2}H^2 \ll 1, \tag{2.11a}$$

$$\frac{1}{12}\left(\frac{r}{a}\right)^3\left(\frac{1}{2}\frac{\kappa a^3}{m^*c^2}H^2\right) \gtrsim 1 \tag{2.11b}$$

hold in this case. We can see the compatibility of (2.11b) with the condition (2.9b) used in solving the Schrödinger equation.

C. Extremely Strong Field Case

In sufficiently strong fields $E(H)$ and $a(H)$ determined by a variational method[3] are no longer approximated by zero-field values. When we neglect the terms $E(H)$ and $e^2/\kappa r$ in (2.5), the Schrödinger equation has a solution

$$\Psi \cong N^{-1/2}\exp(-r^2/4a_f^2), \tag{2.12}$$

$a_f \equiv (\hbar c/eH)^{1/2}$ being the spatial extent of the free-electron wave function in a magnetic field. If we formally write

$$E(H) = -e^2/2\kappa a^*(H), \tag{2.13}$$

the condition for obtaining (2.12) is written in a form similar to (2.9), i.e.,

$$\begin{gathered} r/a_f \gg 1, \\ \kappa H^2 r^3/4m^*c^2 \gg r/a^*(H). \end{gathered} \tag{2.14}$$

We define the extremely strong field case as the range in which the wave function at large distances from the donor atom is given by (2.12). It should be remarked in passing that the classification into three cases depends not only on the magnetic field strength but also on the average donor separation.

One can calculate the resonance energy in a moderately strong field by the use of (2.8) for the donor wave functions. As will be seen in the next section, the effect of the phase difference gives a similar change in the pair of wave functions. Strictly speaking, we must therefore calculate both effects on the resonance energy at the same time. However, we cannot develop the quantitative theory owing to the complicated donor wave functions in n-type germanium. We approximate to the actual situation by calculating one effect while neglecting the other; i.e., treating the other effect as independent of r.

Using (2.3), (2.8), and elliptic coordinates (μ,ν,φ), we obtain for one pair of donors

$$\begin{aligned} L &= -\frac{\pi e^2R^2}{2\kappa N}\int_1^\infty d\mu\int_{-1}^1 d\nu\,(\mu-\nu) \\ &\qquad\times\exp[-\beta\mu-k(\mu^3+3\mu\nu^2)], \\ S &= \frac{\pi R^3}{4N}\int_1^\infty d\mu\int_{-1}^1 d\nu\,(\mu^2-\nu^2) \\ &\qquad\times\exp[-\beta\mu-k(\mu^3+3\mu\nu^2)], \end{aligned} \tag{2.15}$$

while $J \cong -e^2/\kappa R$ remains approximately unchanged. Here we put for brevity

$$\beta \equiv R/a, \quad k \equiv \kappa H^2R^3/96m^*c^2. \tag{2.16}$$

Equations (2.15) are rewritten as

$$L = -\frac{\pi e^2R^2}{\kappa N}\int_0^1 d\nu\, I_1, \quad S = \frac{\pi R^3}{2N}\int_0^1 d\nu (I_2-\nu^2I_0), \tag{2.17}$$

where

$$\begin{aligned} I_n &= e^{-(\beta+k+3k\nu^2)}\int_0^\infty dt(1+t)^n e^{-(\beta+3k\nu^2+3k)t-3kt^2-kt^3} \\ &\cong \beta^{-1}e^{-(\beta+k+3k\nu^2)}. \end{aligned} \tag{2.18}$$

In evaluating (2.18), we use the approximations that $\beta \gg 1$ and $\beta \gg 3k$. Thus, we obtain

$$\begin{aligned} L &\cong -\frac{\pi e^2Ra}{\kappa N}e^{-(\beta+k)}\Phi_0(H,m^*), \\ S &\cong \frac{\pi R^2a}{2N}e^{-(\beta+k)}[\Phi_0(H,m^*)-\Phi_2(H,m^*)], \end{aligned} \tag{2.19}$$

where we define the integrals,

$$\Phi_n(H,m^*) \equiv \int_0^1 d\nu\,\nu^n\exp\left(-\frac{1}{32}\frac{\kappa H^2R^3}{m^*c^2}\nu^2\right). \tag{2.20}$$

(Φ_n can be evaluated by the table of error functions.) The square of the resonance energy is therefore written in the form

$$|W|^2 = |W_0|^2\exp\left\{-\frac{1}{48}\frac{\kappa H^2R^3}{m^*c^2}\right\}f(H,m^*), \tag{2.21a}$$

$$f(H,m^*) \equiv \frac{9}{16}[\Phi_0(H,m^*)+\Phi_2(H,m^*)]^2. \tag{2.21b}$$

We now assume that an expression similar to (2.21) can be used in the resonance energy for our complicated wave function (2.1) and (2.2), because the main contri-

butions to $|W|^2$ come from pairs in the plane perpendicular to the valley axis, i.e., to the *effective* magnetic field in our approximations. We thus obtain the expression for "single-valley" conductivity corresponding to the empirical formula of SK,

$$\langle|W_p|^2\rangle_{\rm av}=\langle|W_{p0}|^2\rangle_{\rm av}\times\exp\left\{-\frac{1}{48}\frac{\kappa R^3}{m_t^*c^2}H^2\cos^2\phi_p\right\}\times f(H\cos\phi_p,m_t^*). \quad (2.22)$$

We compare the formula (2.22) with the empirical one (2.4) in the following way.

(1) The order of magnitude of the magnetoresistance. We tentatively choose the magnetic field satisfying $\kappa H^2R^3/32m_t^*c^2=1$. In the case in which the magnetic field is parallel to the valley axis, the empirical formula gives

$$\rho_0/\rho=\langle|W_p|^2\rangle_{\rm av}/\langle|W_{p0}|^2\rangle_{\rm av}=0.253,$$

while the formula (2.22) gives the same value. The agreement appears to be good if we accept the simple relation $R=sN_D^{-1/3}$ with $s=1$ (N_D: donor concentration), which has been used by SK to derive the empirical formula. We expect s is somewhat smaller than unity[12] so that the formula (2.22) gives a somewhat smaller magnetoresistance than (2.4).

(2) The dependence of the magnetoresistance on the average donor separation is in close agreement with experiment.

(3) The anisotropy of the magnetoresistance. We again take the value $\kappa H^2R^3/32m_t^*c^2=1$ and plot ρ_0/ρ against ϕ in Fig. 1. We should remark that the difference between the theoretical and empirical curves becomes largest at $\phi=\pi/2$, where the effect of the shrinking vanishes in our approximation. One could conclude that the experiment by SK is explained *in part* by the effect of the shrinking of each donor wave function.

III. EFFECT OF PHASE DIFFERENCE BETWEEN TWO DONORS

The effect of the phase factor on impurity conduction produced by the magnetic field between two neighboring donors has been discussed in the case of weak-field magnetoresistance by Miller[10] and in detail in I.[13] When we fix the origin of the vector potential, for example, at the donor site i, the donor wave function at the site j is modified by a phase factor,

$$\exp\left[\frac{ieH}{2c\hbar}(x_{ij}'y'-y_{ij}'x')\right], \quad (3.1)$$

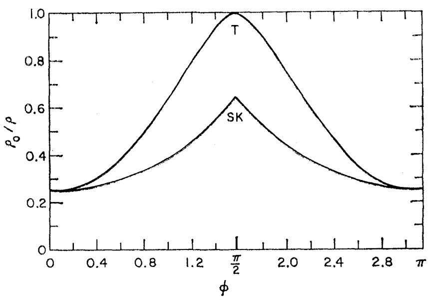

FIG. 1. The anisotropy of the "single valley" magnetoresistance due to the shrinking effect in a moderately strong field. The curve T represents the theoretical values of ρ_0/ρ. We tentatively put $\kappa H^2R^3/32m_t^*c^2=1$. The curve SK represents the corresponding empirical formula.

where the coordinate system is so chosen that the z' axis is in the magnetic field direction and the symmetric gauge of the vector potential is used. In this section we discuss the effect of the phase factor on the magnetoresistance in a moderately strong field case, neglecting the effect of the shrinking of each donor wave function.

When we take the z axis in the donor pair direction, the phase factor of (3.1) can be simply expressed as[14]

$$\exp\left(-\frac{ieH}{2c\hbar}Rx\sin\omega\right), \quad (3.2)$$

where ω is the angle between the magnetic field and the donor pair directions. We now calculate the resonance energy of (2.3) using elliptic coordinates (μ,ν,φ). For the wave function (2.1) and (2.2), we obtain

$$L\cong-\frac{e^2}{\kappa\pi a^3}\sum_{p=1}^{4}|\alpha_p|^2e^{-i\mathbf{p}\cdot\mathbf{R}}L_1,\qquad S\cong\frac{1}{\pi a^3}\sum_{p=1}^{4}|\alpha_p|^2e^{-i\mathbf{p}\cdot\mathbf{R}}S_1, \quad (3.3)$$

where

$$L_1=\frac{R_p^2}{4}\int_{-1}^{1}d\nu\int_1^\infty d\mu\int_0^{2\pi}d\varphi\,\mu\times\exp[-\beta\mu-ik\cos\varphi(1-\nu^2)^{1/2}(\mu^2-1)^{1/2}],$$
$$S_1=\frac{R_p^3}{8}\int_{-1}^{1}d\nu\int_1^\infty d\mu\int_0^{2\pi}d\varphi(\mu^2-\nu^2)\times\exp[-\beta\mu-ik\cos\varphi(1-\nu^2)^{1/2}(\mu^2-1)^{1/2}], \quad (3.4)$$

while $J\cong-e^2/\kappa R$ is not affected by the phase factor. Here $\mathbf{p}$ is the wave number vector of the Bloch function

[12] In the absence of the magnetic field, the observed resistivity can be fitted by $s\sim0.7$ in the Mott-Twose theory (reference 9, p. 149). See also H. Fritzsche and M. Cuevas, Phys. Rev. **119**, 1238 (1960).

[13] See also T. Holstein, Phys. Rev. **124**, 1329 (1961).

[14] It is possible to take y in place of x in the exponential. The result does not depend on such an ambiguity.

at the pth minimum and we put for brevity

$$\beta \equiv R_p/a, \quad k \equiv (eRR_p/4c\hbar)H \sin\omega, \tag{3.5}$$

$$\begin{aligned} R_p &\equiv a[(x_{ij}^2+y_{ij}^2)/a^2+z_{ij}^2/b^2]^{1/2} \\ &= R(1+\alpha\cos^2\theta_p)^{1/2}, \end{aligned} \tag{3.6}$$

where $\alpha=(a^2/b^2)-1\cong 20$ in n-type germanium, θ_p the angle between the pth valley axis and the direction of the donor pair $(i)-(j)$. Integration over φ in (3.4) gives

$$\begin{aligned} L_1 &= \pi R_p^2 \int_0^1 d\nu \int_1^\infty d\mu\, \mu e^{-\beta\mu} \\ &\qquad \times J_0[k(1-\nu^2)^{1/2}(\mu^2-1)^{1/2}], \\ S_1 &= \frac{\pi R_p^3}{2} \int_0^1 d\nu \int_1^\infty d\mu (\mu^2-\nu^2) e^{-\beta\mu} \\ &\qquad \times J_0[k(1-\nu^2)^{1/2}(\mu^2-1)^{1/2}], \end{aligned} \tag{3.7}$$

where $J_0(x)$ is the Bessel function of the first kind. The integral over μ can be readily performed by changing the variable into t ($t^2=\mu^2-1$) and with the aid of the Hankel transform formula,[15]

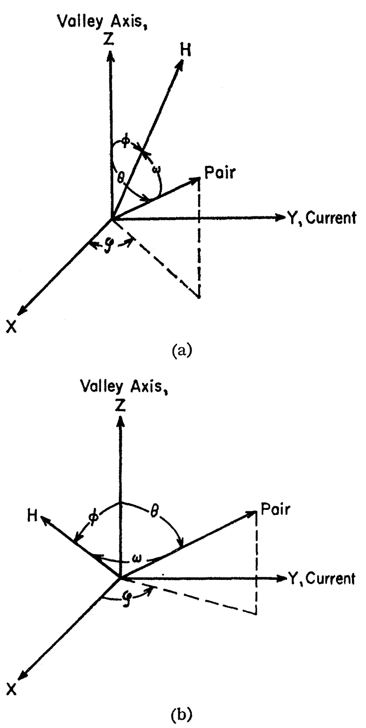

FIG. 2. The coordinate system used in taking the weighted angular average of the square of the resonance energy in Sec. III. (a) The case (A) in which the current flows in the y direction and the magnetic field is in the yz plane. (b) The case (B) in which the current flows in the y direction but **H** in the xz plane. In both cases the weight of the pair is $\sin^2\theta \sin^2\varphi$, and the angular average is taken over the right hemisphere.

$$\int_0^\infty (x^2+y^2)^{-1/2} x e^{-a(x^2+y^2)^{1/2}} J_0(bx)dx = (a^2+b^2)^{-1/2} e^{-y(a^2+b^2)^{1/2}}. \tag{3.8}$$

The results are

$$\begin{aligned} L_1 &= \pi R_p^2 \int_0^1 d\nu \left[\frac{\beta}{(\beta^2+\xi^2)}+\frac{\beta}{(\beta^2+\xi^2)^{3/2}}\right] \\ &\qquad \times \exp[-(\beta^2+\xi^2)^{1/2}], \\ S_1 &= \frac{\pi R_p^3}{2} \int_0^1 d\nu \left[-\frac{1}{(\beta^2+\xi^2)}+\frac{\beta^2-1}{(\beta^2+\xi^2)^{3/2}}+\frac{3\beta^2}{(\beta^2+\xi^2)^2}\right. \\ &\qquad \left. +\frac{3\beta^2}{(\beta^2+\xi^2)^{5/2}}-\frac{\nu^2}{(\beta^2+\xi^2)^{1/2}}\right] \exp[-(\beta^2+\xi^2)^{1/2}], \end{aligned} \tag{3.9}$$

where we have put $\xi^2\equiv k^2(1-\nu^2)$.

We now use an approximation suitable for the moderately strong field case,

$$\beta^2 \gg k^2, \tag{3.10}$$

for the evaluation of the integrals in (3.9). The approximation (3.10) is rewritten as

$$\epsilon\kappa R^3 H^2/16 m_t^* c^2 \ll R/a, \tag{3.11}$$

making use of the relation[4]

$$(\epsilon\kappa a^3/m_t^* c^2) = (ea^2/\hbar c)^2, \tag{3.12}$$

where $\epsilon\cong 0.67$ for Sb-doped Ge and $\cong 0.56$ for As-doped Ge, if we take $a(\mathrm{Sb})=69.3$ Å and $a(\mathrm{As})=58.1$ Å. This approximation is consistent with the definition of the moderately strong field case, (2.9). Using (3.10), the main terms of L_1 and S_1 are given by

$$\begin{aligned} L_1 &\cong \pi R_p a \exp\left(-\frac{R_p}{a}-\frac{1}{2}\frac{ak^2}{R_p}\right), \\ S_1 &\cong \frac{\pi}{3} R_p^2 a \exp\left(-\frac{R_p}{a}-\frac{1}{2}\frac{ak^2}{R_p}\right). \end{aligned} \tag{3.13}$$

Thus, using (2.3), (3.3), and (3.13), we finally obtain[16]

$$\begin{aligned} |W_p|^2 &\cong \frac{1}{16}\left(\frac{2e^2}{3\kappa a^2}\right)^2 R^2(1+\alpha\cos^2\theta) \\ &\quad \times \exp\left[-\frac{2R}{a}(1+\alpha\cos^2\theta)^{1/2}\right] \\ &\quad \times \exp\left[-\frac{\epsilon\kappa R^3 H^2}{16 m_t^* c^2}\sin^2\omega(1+\alpha\cos^2\theta)^{1/2}\right]. \end{aligned} \tag{3.14}$$

[15] Eredelyi, Magnus, Oberhettinger, and Tricomi, *Tables of Integral Transforms* (McGraw-Hill Book Company, New York, 1954), Vol. 2, p. 9.

[16] Eq. (3.14) does not give the correct formula for the weak field case, because we have neglected the small H-dependent factor in front of the exponential term.

For the comparison with the empirical formula (2.4), we must take the weighted angular average of (3.14) for the current in the direction perpendicular to the valley axis, z. As in I, we assume that (1) the vacant sites (j) are distributed with equal probability around the occupied site (i) on a sphere with the radius R and (2) the weight of the pair can be taken into account by multiplying by the square of the direction cosine of the angle between the pair and the current directions. Moreover, we assume here, as we did in the case of zero magnetic field, that the main contribution to the current comes from the donor pair in the direction perpendicular to the valley axis, i.e., in (3.14)

$$\alpha\cos^2\theta\ll 1,\quad \cos\theta\cong 0. \tag{3.15}$$

This is consistent with negligible conductivity in the direction of the valley axis in the empirical formula of SK.

It will be sufficient to consider the following special cases: case (A) in which the current flows in the y direction and the magnetic field is in the yz plane, and case (B) in which the current flows also in the y direction but the field is in the xz plane [see Fig. 2(a) and (b)]. Using the above assumptions, the weighted angular average of (3.14) for both cases are given in the form

$$\begin{aligned}\langle|W|^2\rangle_{\mathrm{av}}&\cong\langle|W_0|^2\rangle_{\mathrm{av}}e^{-\lambda}f_A(\lambda,\phi),\\ f_A(\lambda,\phi)&\equiv\frac{4}{\pi}\int_0^1 d\chi(1-\chi^2)^{1/2}\exp[\lambda\sin^2\phi(1-\chi^2)]\end{aligned} \tag{3.16}$$

for case (A) and

$$\begin{aligned}\langle|W|^2\rangle_{\mathrm{av}}&\cong\langle|W_0|^2\rangle_{\mathrm{av}}e^{-\lambda}f_B(\lambda,\phi),\\ f_B(\lambda,\phi)&\equiv\frac{4}{\pi}\int_0^1 d\chi(1-\chi^2)^{1/2}\exp[\lambda\sin^2\phi\,\chi^2]\end{aligned} \tag{3.17}$$

for case (B), respectively. Here,

$$\langle|W_0|^2\rangle_{\mathrm{av}}\equiv\left(\frac{e^2}{6\kappa a^2}\right)^2\left(\frac{\pi b^2}{16a}\right)^{1/2}R^{3/2}\exp(-2R/a) \tag{3.18}$$

corresponds to the zero-field resonance energy and

$$\lambda\equiv(\epsilon\kappa R^3/16m_t^*c^2)H^2. \tag{3.19}$$

We can now compare the present theory with the empirical formula in the following way.

(1) The order of magnitude of the magnetoresistance. In the case in which the magnetic field is parallel to the valley axis, the magnetoresistance coefficient is

$$\gamma+\delta=4.3\times10^{-2},\quad (T=2.26^\circ\mathrm{K})$$

in the empirical formula (2.4), while the corresponding factor in the theory is

$$\begin{aligned}\epsilon/16&=4.2\times10^{-2}\quad\text{for Sb-doped Ge,}\\ &=3.5\times10^{-2}\quad\text{for As-doped Ge,}\end{aligned}$$

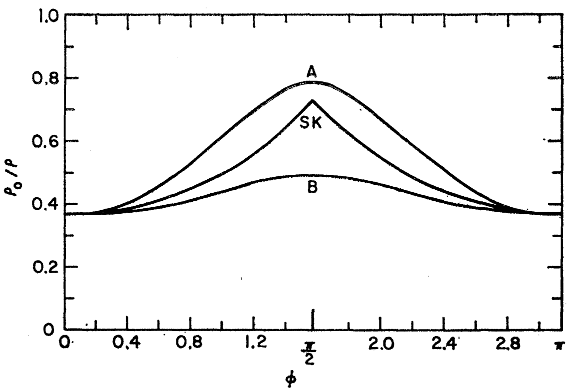

FIG. 3. The anisotropy of the "single valley" magnetoresistance due to the phase-factor effect in the moderately strong field. Curves A and B represent the theoretical values of ρ_0/ρ in the cases (A) and (B), respectively. We tentatively put

$$\epsilon\kappa R^3H^2/16m_t^*c^2=1.$$

The curve SK represents the corresponding empirical formula, where we put $\gamma\kappa R^3H^2/m_t^*c^2=0.32$ and $\delta\kappa R^3H^2/m_t^*c^2=0.68$ by an extrapolation of the experimental values at $T=2.26^\circ$K.

in both cases (A) and (B). The agreement is good if we assume $R=N_D^{-1/3}$. However, as in the case of the shrinking effect, we suppose the theoretical value to be somewhat smaller than the empirical one.

(2) The dependence of the magnetoresistance coefficient on the average donor separation is also in close agreement with experiments.

(3) The anisotropy of the magnetoresistance. We tentatively take the value $\lambda=1$ and plot ρ_0/ρ against ϕ in Fig. 3. We should remark that the empirical formula of SK gives no difference between the cases (A) and (B), while the effect of the phase factor gives a difference which is largest at $\phi=\pi/2$.

In the calculation of the effect of the phase factor we neglect the shrinking of each donor wave function. The latter effect is of the same order of magnitude as the phase-factor effect as is seen from (2.22), (3.16), and (3.17). In our approximation mentioned in Sec. II, the total magnetoresistance is roughly given by the *product* of the contributions from both effects. Owing to our approximation we can safely make the statement that the experiment of SK is qualitatively explained by a combination of the shrinking and the phase-factor effects of donor wave functions. On the experimental side, more direct measurement of the "single valley" anisotropy of the magnetoresistance is desirable, since the empirical formula (2.4) was derived from experiments involving the contributions from the four valleys. Such an experiment is possible with Fritzsche's piezoresistance method.[17]

As pointed out in I, on the other hand, when one considers the anisotropy of the magnetoresistance in a strong magnetic field in n-type germanium, one must take into account the magnetic-field-induced changes

[17] H. Fritzsche, Phys. Rev. **125**, 1552, 1560 (1962).

of the contributions from the four valleys to the ground-state wave function. Such a change in α_p of (2.1) is due to the mixing of the triplet into the singlet states[17] and is caused by two factors, (1) the different magnetic energies of valley minima and (2) the anisotropic g factor of the donor spin.[18] Therefore, a more careful analysis of the anisotropy in (2.4) is required to take these effects into account.

The temperature dependence of the magnetoresistance found by SK cannot be explained by our simple theory. As discussed in I, one might expect that the magnetic field changes the energy splittings between the ground state and the other $1s$-like states and hence the relative electron populations in these states. This, we suppose to be at least one of the causes for the temperature dependence of γ and δ in (2.4).

IV. EXTREMELY STRONG FIELD CASE

This section will be devoted to the calculation of the resonance energy in an extremely strong field case. As discussed in Sec. II, the spatial variation of the donor wave function can be approximated by (2.12), or more generally by

$$F(\mathbf{r})=[(2\pi)^{3/2}a^2b]^{-1/2}\times\exp\{-[(x^2+y^2)/4a^2+z^2/4b^2]\},\quad(4.1)$$

the z axis being in the field direction. The function (4.1) was used by Yafet *et al.*[3] to calculate the energy and the wave function of the hydrogen atom in a strong magnetic field. The effect of the shrinking is involved in a, and to some extent in b. We use here (4.1) for the donor wave functions. Using a procedure similar to that used to get (3.3), we now obtain

$$\begin{aligned}L&\cong-\frac{e^2}{\kappa(2\pi)^{3/2}a^3}\sum_{p=1}^{4}|\alpha_p|^2e^{-i\mathbf{p}\cdot\mathbf{R}}L_1,\\ S&\cong\frac{1}{(2\pi)^{3/2}a^3}\sum_{p=1}^{4}|\alpha_p|^2e^{-i\mathbf{p}\cdot\mathbf{R}}S_1,\end{aligned}\quad(4.2)$$

where

$$\begin{aligned}L_1&=\frac{R_p^2}{4}\int_{-1}^{1}d\nu\int_{1}^{\infty}d\mu\int_0^{2\pi}d\varphi\\&\quad\times\mu\exp[-\beta(\mu^2+\nu^2)-ik\cos\varphi\\&\quad\times(1-\nu^2)^{1/2}(\mu^2-1)^{1/2}],\\ S_1&=\frac{R_p^3}{8}\int_{-1}^{1}d\nu\int_{1}^{\infty}d\mu\int_0^{2\pi}d\varphi\\&\quad\times(\mu^2-\nu^2)\exp[-\beta(\mu^2+\nu^2)-ik\cos\varphi\\&\quad\times(1-\nu^2)^{1/2}(\mu^2-1)^{1/2}].\end{aligned}\quad(4.3)$$

Here, $\beta\equiv R_p^2/8a^2$ in place of (3.5). The evaluation of the integrals can be performed in a way similar to that employed in Sec. III. After integration over φ, one obtains

$$\begin{aligned}L_1&=\pi R_p^2e^{-\beta}\int_0^1 d\nu\, e^{-\beta\nu^2}I_1,\\ S_1&=\frac{\pi}{2}R_p^3e^{-\beta}\left(\int_0^1 d\nu\, e^{-\beta\nu^2}I_2-\int_0^1 d\nu\, \nu^2e^{-\beta\nu^2}I_0\right),\end{aligned}\quad(4.4)$$

where I_n is defined by

$$I_n\equiv\int_0^\infty d\chi(1+\chi^2)^{(n-1)/2}\chi e^{-\beta\chi^2}J_0[k(1-\nu^2)^{1/2}\chi].\quad(4.5)$$

The integral I_n can be evaluated using a Hankel transform,[19]

$$\int_0^\infty d\chi\,\chi e^{-a\chi^2}J_0(b\chi)=(2a)^{-1}\exp(-b^2/4a),\quad(4.6)$$

and making the approximation that I_n is determined by the region $\chi\ll1$, because $\beta\gg1$ in the present case. Then, Eq. (4.4) becomes

$$\begin{aligned}L_1&\cong\frac{\pi R_p^2}{2\beta}e^{-\beta}e^{-k^2/4\beta}\zeta^{-1/2}\frac{\pi^{1/2}}{2}\Phi(\zeta^{1/2}),\\ S_1&\cong\frac{\pi R_p^3}{4\beta}e^{-\beta}e^{-k^2/4\beta}\\&\quad\times\left\{\zeta^{-1/2}\frac{\pi^{1/2}}{2}\Phi(\zeta^{1/2})+\frac{\zeta^{-1}}{2}e^{-\zeta}-\frac{\pi^{1/2}}{4}\zeta^{-3/2}\Phi(\zeta^{1/2})\right\},\end{aligned}\quad(4.7)$$

where $\zeta\equiv\beta-k^2/4\beta$ and $\Phi(x)$ is the error function.

In general, the situation in an extremely strong field in n-type germanium is fairly complicated, since it is no longer permitted to make the approximations that $\alpha\gg1$ and b is nearly independent of the magnetic field. Therefore, we consider the simplest case, that of the transverse "single valley" magnetoresistance in the magnetic field parallel to the valley axis. For the important donor pairs in the plane perpendicular to the axis, we have

$$\begin{aligned}\beta^2&=k^2/4=R^4e^2H^2/64\hbar c^2,\\ \zeta&=0,\end{aligned}\quad(4.8)$$

using (2.12), (3.5), and (3.6). Thus, we obtain

$$|W_p|^2=\frac{1}{18\pi}\left(\frac{e^2}{\kappa a_f}\right)^2\exp\left(-\frac{eR^2H}{4\hbar c}\right)\exp\left(-\frac{eR^2H}{4\hbar c}\right),\quad(4.9)$$

[18] See, for instance, L. M. Roth, Phys. Rev. **118**, 1534 (1960).

[19] See reference 15, p. 30.

where one exponential factor is due to the shrinking and the other due to the phase-factor effect. We can conclude in this case that (1) the shrinking and the phase-factor effects contribute the same order of magnitude to the magnetoresistance even in an extremely strong field, (2) the dependence of the magnetoresistance coefficient on the average donor separation changes from an R^3 dependence in the weak and moderately strong field case to an R^2 dependence, and (3) the dependence of the magnetoresistance on the magnetic field changes from an H^2 to an H dependence.

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Projected Wave-Field Approach to the Many-Electron Problem in Solids*

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The orthogonalized plane wave (O. P. W.) method for treating electrons in solids is generalized to the many-body problem. The core electrons are assumed to be dynamically independent of the valence electrons. Using a field-theoretical approach, a model wave field is introduced whose valence projection is the valence wave field of the physical system. When an appropriate choice is made for the model Hamiltonian, the rapid convergence of the O. P. W. method is incorporated in the many-body perturbation expansion.

An attractive feature of the scheme is that the perturbation expansion can be carried out using zero-order Green's functions appropriate to free electrons. The single-particle self-energy to low order is the sum of the one-body O. P. W. contribution and a screened exchange energy similar to that obtained in the case of the uniform electron gas.

The theory is expected to be most useful for metals and valence crystals for which the single-particle O. P. W. method is known to be appropriate.

I. INTRODUCTION

IN the past few years a great deal of progress has been made in the study of the gas of interacting electrons. We do not want to summarize the results obtained, but we rather refer the reader to some relevant papers on the subject.[1]

Different formalisms have been developed for this problem according to the aspect emphasized. The collective approach of Bohm and Pines is best suited to the study of the plasma oscillations. A perturbation theory was developed by Brueckner, Goldstone, Hubbard, and others for the study of the ground-state correlation energy. An alternative approach to plasma effects has been based on linearization of the Heisenberg equation of motion (Sawada, Fukuda, Brueckner, and Brout; Suhl and Werthamer). This method gives, in principle, also one-particle excitation energies and the ground-state energy.

The powerful Green's function formalism of field theory has been adapted to the many-body problem by Galitski and Migdal[2] and in a more general form by Martin and Schwinger.[3] Klein has shown that within this formalism a one-body model potential can be constructed and made self-consistent to all orders.[4]

In the present paper, we use the Green's function formalism to derive perturbation expressions for valence and conduction states of electrons in a covalent crystal, including correlation effects which are neglected in ordinary band theory. In most recent studies of

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