INFLUENCE OF FERROMAGNETIC ORDERING ON THE BANDWIDTH AND MOBILITY OF THE SMALL POLARON

By S. Klama

Ferromagnetics Laboratory, Institute of Physics of the Polish Academy of Sciences, Poznań*

(Received December 8, 1969)

The influence of exchange interactions on the bandwidth and mobility of a small polaron is discussed in a simple cubic lattice for high temperatures ($T \gg T_t = \frac{1}{2}\theta \operatorname{arsh}^{-1}\gamma'$, where θ is the Einstein temperature and γ' is the carrier-lattice interaction parameter). A system of localized magnetic moments is treated in the constant coupling approximation. Different temperature dependences (for $S > \frac{1}{2}$) of the polaron's subbandwidths for the two directions of its spin are obtained, as well as the possibility of a steep increase in mobility and a change in activation energy on transition into the paramagnetic region.

1. Introduction

In recent years a number of theoretical and experimental papers (for a review see [11a]) have been devoted to problems of transport in semiconductor metal oxides. Particular attention was paid to the examination of electrical and optical properties of nickel oxide, a typical representative of a large group of antiferromagnetic oxides of transition metals with small current carrier mobility ($\mu < 1$ cm^2 V^{-1} s^{-1}). In explaining the experimental data, two models are used: the band model [1–4] and the hopping model [11, 12, 13, 17, 19], but often neglecting the exchange interactions in the crystal, despite the fact that the same electrons are responsible for the electrical and the magnetic phenomena in these compounds (where the ionic bond plays an important role). The hopping mechanism has been proposed by Verwey [5] to explain the electric conductivity in these compounds, relating in to the occurrence in the lattice of cations with distinct valences (conductivity by cations) and moreover assuming perfect localization of carriers, so that the displacement of a carrier from one site to another can be treated as thermally activated diffusion process.

Little attention has hitherto been paid to the influence of exchange interactions on the electric conductivity of these compounds. Appel [11], in his discussion of hopping conductivity, indicates that antiferromagnetic ordering in a crystal modifies the expression for the mobility by a factor $(1-M^2(T)/M^2(0))$, where $M(T)/M(0)$ stands for the relative sublattice magnetization. Within the framework of semiphenomenological theory, Turov and Irkhin [6] considered the influence of a magnetic ordering on the carrier's energy spectrum in a crystal

* Address: Zakład Ferromagnetyków, Instytut Fizyki PAN, Poznań, Fredry 10, Polska.

(without carrier-lattice interaction) and come to the conclusion that exchange interaction gives rise to a splitting of the conductivity band into two subbands and, consequently, a change in activation energy to be expected to occur in the Curie (or Néel) point. A similar result has been obtained by Bulayevsky and Khomsky [3] when considering the energy spectra of current carriers in antiferromagnetic semiconductors (only transfers *via* anion were allowed). They showed that due to Pauli's principle, the electron and hole bands are considerably narrowed below the transition point, whereas above it they undergo a widening (decrease in energy gap). The influence of exchange couplings on the conductivity in ferromagnetic semiconductors has been discussed by Haas [7, 9], who showed that in the case of ferromagnetic ordering the carrier mobility has a minimum in the neighbourhood of the Curie point and increases above this temperature, presumably corresponding to the resistance maximum measured by Molnar and Methfessel [9] in gadolinium-admixtured europium selenides ($Eu_{1-x}\,Gd_x\,Se$).

In the present paper, the influence of a ferromagnetic ordering on a polaron's bandwidth and mobility is discussed. The same formalism is simultaneously applied for discussing the interaction of a carrier (in the *s*-state) with the lattice vibrations as well as with magnetic moments localized at sites of the simple cubic lattice, these interactions being dealt with in the effective field approximation.

2. *Hamiltonian and wave function*

Let us consider an extra electron (or hole) in an ideal ionic lattice localized at the j-th site in a state described by a wave function of the atomic (or Wannier) type.

Let us further assume that the motion of the electron (or hole) in the lattice is so slow that it produces a stable polarization by distorting the lattice in its nearest neighbourhood. The polarization now reacts on the carrier, lowering its energy. The quasi-particle arising by this dynamic interaction of the electron and lattice is termed a polaron. We restrict our considerations to the case when the extent of lattice distortion induced by extra carrier is smaller than the lattice constant a (small polaron).

In absence of external fields, the Hamiltonian of the system can be written in the following form:

$$\mathcal{H} = \mathcal{H}_p + \mathcal{H}_{\text{int}}, \tag{2.1}$$

where $\mathcal{H}_p$ describes the unperturbed system and consists of the terms:

$$\mathcal{H}_p = \mathcal{H}_0 + \mathcal{H}_L + \mathcal{H}_I + \mathcal{H}_H + \mathcal{H}_{\text{eph}}, \tag{2.2}$$

where

$$\mathcal{H}_0 = \frac{\boldsymbol{p}^2}{2m} + U(\boldsymbol{r} - \boldsymbol{R}_j) \tag{2.3}$$

is the sum of the operators of kinetic energy of the carrier and its potential energy in the field of the j-th ion. The second term of Eq. (2.2):

$$\mathcal{H}_L = \frac{1}{2} \sum_{\boldsymbol{q}} (P_{\boldsymbol{q}}^2 + \omega_{\boldsymbol{q}}^2 Q_{\boldsymbol{q}}^2) \tag{2.4}$$

describes the lattice vibrations (in the harmonic approximation), and $\boldsymbol{q}$ is the phonon wave vector. The next term of (2.2):

$$\mathscr{H}_I = -2I \sum_{\text{n. n.}} S_i \langle S_k \rangle \tag{2.5}$$

is the operator describing the system of magnetic moments localized at lattice sites in the effective field approximation. In Eq. (2.5), summation extends over nearest neighbours; I is the exchange integral; S_i — the spin operator of a spin localized at the i-th site. The interaction of localized spins is treated in the effective field approximation; thus, Eq. (2.5) can be rewritten in the form

$$\mathscr{H}_I = -z\lambda \sum_i S_i^z, \tag{2.5a}$$

where z stands for the coordination number, and $\lambda = I \langle S_k^z \rangle$. $\mathscr{H}_H$ is the exchange interaction energy between the carrier's spin and a spin localized at a site, which is now occupied by the carrier. In our further considerations this site will be termed the carrier's *own* site. To simplify the calculations we neglect contributions to the energy $\mathscr{H}_H$ from the transversal components of the spin operators and we preserve only the Ising part of the interaction. Thus, the fourth term in Eq. (2.2) takes the form:

$$\mathscr{H}_H = -As^z S_j^z, \tag{2.6}$$

where A is Hund's integral; s^z and S_j^z stand for operators of the z — components of the carrier's spin and the spin localized at the j-th site, respectively. The last term in Eq. (2.2) describes the interaction between the carrier and lattice in the linear approximation with respect to the phonon coordinates $Q_{\boldsymbol{q}}$[12]; it takes the form;

$$\mathscr{H}_{\text{eph}} = -\sqrt{\frac{2}{\mathscr{N}}} \sum_{\boldsymbol{q}} \gamma Q_{\boldsymbol{q}} \sin\left(\boldsymbol{q} \cdot R_j + \frac{\pi}{4}\right), \tag{2.7}$$

where $\mathscr{N}$ — number of unit calls in the system, and γ is the interaction parameter.

The Hamiltonian describing the perturbation consists of two terms:

$$\mathscr{H}_{\text{int}} = \mathscr{H}_1 + \mathscr{H}_{s-d}, \tag{2.8}$$

where

$$\mathscr{H}_1 = \sum_{l(\neq j)} U(\boldsymbol{r} - \boldsymbol{R}_l) \tag{2.8a}$$

is the periodical lattice potential resulting from all ions expcet the carrier's own ion, and

$$\mathscr{H}_{s-d} = -\sum_{\delta} J_{j+\delta}\, \mathbf{s}\, \mathbf{S}_{j+\delta}. \tag{2.9}$$

The expression (2.9) represents the interaction of the carrier localized at the j-th site with the localized magnetic moments of neighbours belonging to the first coordination sphere, $J_{j+\delta}$ is an exchange integral of the s-d type. It should be kept in mind that $A > |J_{i+\delta}|$.

The wave function of the unperturbed system can be written as the product of the following functions:

a) the wave function of the carrier localized at site $\boldsymbol{R}_j$

$$|j\rangle \equiv \varphi(\boldsymbol{r} - \boldsymbol{R}_j) \tag{2.10}$$

b) the eigenfunction of the z-component of the carrier spin operator

$$|\sigma> \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\sigma = \pm 1) \tag{2.11}$$

c) the function describing the system of localized magnetic moments

$$|\{n_l\}> \equiv |n_1, \ldots, n_N> = \prod_l |n_l>, \tag{2.12}$$

where n_l is the eigenvalue of the operator of the z-component of the spin localized at the l-th site,

d) the unperturbed phonon wave function $|\{N_q\}>$.

We consider the case of strong coupling between the carrier and the lattice vibrations and therefore have to include the Hamiltonian $\mathscr{H}_{\text{eph}}$ (2.7) into the zeroth approximation Hamiltonian, so that now the oscillator wave function of the crystal $|\{N_q\}>$ has to fulfil the relation [15, 19]:

$$\mathscr{H}_L|\{N_q\}> + <j|\mathscr{H}_{\text{eph}}|j>|\{N_q\}> = E_q|\{N_q\}>,$$

which can be further decomposed into a set of single-particle equations of the form:

$$\left\{\frac{1}{2}(P_q^2+\omega_q^2 Q_q^2) - \gamma\sqrt{\frac{2}{\mathscr{N}}}\left\langle j\left|Q_q \sin\left(\boldsymbol{q}\cdot\boldsymbol{R}_j + \frac{\pi}{4}\right)\right|j\right\rangle\right\} X_{N_q} = \varepsilon_q X_{N_q}. \tag{2.13}$$

By way of the simple canonical transformation $Q'_q = Q_q - Q_q^j$, we obtain an equation of the oscillator with displaced coordinate in the form:

$$\sum_q \tfrac{1}{2}(P_q^2+\omega_q^2 Q_q'^2)\, X_{N_q} = \sum_q (\varepsilon_q - \varepsilon_b^{(j)}(\boldsymbol{q}))\, X_{N_q}, \tag{2.14}$$

where ε_q stands for the energy eigenvalue determined by Eq. (2.13), and

$$Q_q^{(j)} = \sqrt{\frac{2}{\mathscr{N}}}\, \gamma\omega_q^{-1} \sin\left(\boldsymbol{q}\cdot\boldsymbol{R}_j + \frac{\pi}{4}\right). \tag{2.15}$$

Consequently the interaction of the carrier with the lattice modifies the lattice wave function by changing its argument, making it depend on the site coordinate, and changes the energy of the system by the amount

$$E_b = -\sum_q \varepsilon_b^{(j)}(\boldsymbol{q}) = -\frac{1}{\mathscr{N}}\sum_q \omega_q^{-2} \sin^2\left(\boldsymbol{q}\cdot\boldsymbol{R}_j + \frac{\pi}{4}\right), \tag{2.16}$$

which simultaneously defines lowering of the carrier energy level resulting from interaction with the lattice (formation of the polaron). Finally, the lattice part of the wave function of the system takes the form:

$$|\{N_q^{(j)}\}> = \prod_q X_{N_q}^{(j)}\left\{\sqrt{\frac{\omega_q}{\hbar}}(Q_q - Q_q^{(j)})\right\} = \prod_q X_{N_q}^{(j)}\left\{\sqrt{\frac{\omega_q}{\hbar}}\, Q'_q(\boldsymbol{R}_j)\right\}, \tag{2.17}$$

where

$$X_N(\alpha) = 2^N N!\pi^{1/2})^{-1/2} e^{-\alpha^2/2} H_N(\alpha)$$

and $H_N(\alpha)$ is a Hermite polynomial of order N.

3. *The bandwidth*

To determine the bandwidth, we shall resort to a modified tight binding method [14, 15, 19]. The modification consists in using, instead of the product of the atomic (orbital) wave function $\varphi(\boldsymbol{r}-\boldsymbol{R}_j)$ and the oscillator wave function $X_{N_q}[Q_q]$ (independent of the lattice site coordinate $\boldsymbol{R}_j$), the product of $\varphi(\boldsymbol{r}-\boldsymbol{R}_j)$ and $X^{(j)}_{N_q}[Q'_q(\boldsymbol{R}_j)]$, the latter now depending on the site index due to Eq. (2.17). The wave function of the polaron with wave vector k can be written as follows:

$$\psi_{\boldsymbol{k}} = \sum_i e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i} |i, \sigma, \{n_l\}, \{N^{(j)}_q\}>. \tag{3.1}$$

Solving the Schrödinger equation:

$$\mathscr{H}\psi_{\boldsymbol{k}} = E\psi_{\boldsymbol{k}}, \tag{3.2}$$

and restricting our considerations to the case of the simple cubic lattice we obtain

$$\begin{aligned} E \equiv E(\sigma', \{n'_l\}, \{N^{(j)}_q\}) = E_0(\sigma', \{n'_l\}, \{N^{(j)}_q\}) + \\ + E_1(\sigma', \{n'_l\}, \{N^{(j)}_q\}) + \\ + 2M_{j,j+\delta}(\sigma', \{n'_l\}, \{N^{(j)}_q\}) \sum_{r=x,y,z} \cos k_r a, \end{aligned} \tag{3.3}$$

where $E_0(\sigma', \{n'_l\}, \{N^{(j)}_q\})$ is the energy of the unperturbed system and $E_1(\sigma', \{n'_l\}, \{N^{(j)}_q\})$ the diagonal (with respect to site indices) matrix element of the perturbation operator. We shall further take into consideration only the matrix element $M_{j,j+\delta}$, which determines the bandwidth $\Gamma(\sigma')$ by way of the relation:

$$\Gamma(\sigma') = 2z|\langle M_{j,j+\delta}(\sigma', \{n'_l\}, \{N^{(j)}_q\})\rangle_{\mathrm{Av}}|, \tag{3.4}$$

where averaging extends over the lattice states $\{N_q\}$ and $\{n'_l\}$ at fixed σ'. The matrix element appearing in (3.4) is of the form:

$$M_{j,j+\delta}(\sigma', \{n'_l\}, \{N^{(j)}_q\}) = \mathscr{A}(\sigma', \{n'_l\})\langle N^{(j+\delta)}_q | N^{(j)}_q\rangle, \tag{3.4a}$$

where

$$\begin{aligned} \mathscr{A}(\sigma', \{n'_l\}) = \sum_{\{n_l\},\sigma} \langle j+\delta, \sigma, \{n_l\}|\mathscr{H}_{\mathrm{int}}|\, j, \sigma', \{n'_l\}\rangle \\ |j, \sigma', \{n'_l\}> \equiv |j>|\sigma'>|\{n'_l\}>. \end{aligned} \tag{3.5}$$

Inserting the explicite form of $\mathscr{H}_{\mathrm{int}}$ into Eq. (3.5), we obtain:

$$\begin{aligned} \mathscr{A}(\sigma', \{n'_l\}) = \sum_{\{n_l\}} \sum_{\delta} \sum_{\sigma} \langle j+\delta|\mathscr{H}_1|j\rangle \langle\sigma|\sigma'\rangle \langle\{n_l\}|\{n'_l\}\rangle - \\ - \sum_{\{n_l\}} \sum_{\delta} \sum_{\sigma} \langle j+\delta|J_{j+\delta}|j\rangle \langle\sigma|s^z|\sigma'\rangle \langle\{n_l\}|S^z_{j+\delta}|\{n'_l\}\rangle - \\ - \tfrac{1}{2} \sum_{\{n_l\}} \sum_{\delta} \sum_{\sigma} \langle j+\delta|J_{j+\delta}|j\rangle \{\langle\sigma|s^-|\sigma'\rangle \langle\{n_l\}|S^+_{j+\delta}|\{n'_l\}\rangle + \\ + \langle\sigma|s^+|\sigma'\rangle \langle\{n_l\}|S^-_{j+\delta}|\{n'_l\}\rangle\}. \end{aligned} \tag{3.6}$$

In the transformation (2.9), previous to insertion into Eq. (3.5), the definitions $S^+_j = S^x_j \pm$ $\pm iS^y_j$ and $s^\pm = s^x \pm i\, s^y$ as well as commutation relations for $s^\pm$, $S^\pm$ and s^z, S^z have been

used. We shall average the Eq. (3.6) over states of the system of localized spins with the weight factor

$$f(n_l) = \prod_l e^{F - z\lambda\beta n_l}, \tag{3.7}$$

where

$$F = -\ln \sum_{n=0}^{2S} e^{-z\lambda\beta n};$$

in determining the parameter λ, we use the constant coupling approximation (see Appendix). On averaging we obtain:

$$\langle \mathscr{A}(\sigma', \{n_l'\})\rangle_{\mathrm{Av}} = M - zJ \sum_{\sigma} \langle\sigma|s^z|\sigma'\rangle A_1(S, T) -$$

$$- \frac{1}{2} zJ \sum_{\sigma} \{\langle\sigma|s^-|\sigma'\rangle A_2(S, T) + \langle\sigma|s^+|\sigma'\rangle A_3(S, T)\}, \tag{3.8}$$

where

$$J \equiv \langle j+\delta|J_{j+\delta}|j\rangle, \quad M \equiv \langle j+\delta|\mathscr{H}_1|j\rangle.$$

Assuming the z-axis as the quantization direction, we can calculate the matrix elements of (3.8). They amount to:

$$A_1(S, T) = \sum_{\{n_l\}} \sum_{\{n_l'\}} f(n_l') \langle\{n_l\}|S_k^z|\{n_l'\}\rangle$$

$$= -S \frac{M(T)}{M(0)} = -S + \frac{(S+1)\mathrm{sh}(Sz\lambda\beta) - S\mathrm{sh}((S+1)z\lambda\beta)}{\mathrm{ch}((S+1)z\lambda\beta)\mathrm{ch} - (Sz\lambda\beta)}, \tag{3.9}$$

$$A_2(S, T) = \sum_{\{n_l\}} \sum_{\{n_l'\}} f(n_l') \langle\{n_l\}|S_k^+|\{n_l'\}\rangle$$

$$= (\sum_{n=0}^{2S} e^{-z\lambda\beta n})^{-1} \sum_{n=0}^{2S} e^{-z\lambda\beta(n-1)} [n(2S-n+1)]^{1/2}, \tag{3.10a}$$

$$A_3(S, T) = \sum_{\{n_l\}} \sum_{\{n_l'\}} f(n_l') \langle\{n_l\}|S_k^-|\{n_l'\}\rangle$$

$$= (\sum_{n=0}^{2S} e^{-z\lambda\beta n})^{-1} \sum_{n=0}^{2S} e^{-z\lambda\beta(n+1)} [(2S-n)(n+1)]^{1/2}. \tag{3.10b}$$

After simple calculations, performing summation over σ in Eq. (3.8), we obtain:

$$\langle \mathscr{A}(\sigma', \{n_l'\})\rangle_{Av} = M - \tfrac{1}{2} zJA_1(S, T) [\Delta(\sigma', +1) - \Delta(\sigma', -1)] -$$

$$- \tfrac{1}{2} zJ\{A_2(S, T) [1 - \Delta(\sigma', -1)] + A_3(S, T) [1 - \Delta(\sigma', +1)]\}. \tag{3.11}$$

The values of $A_i(S, T)$ $(i = 1, 2, 3)$ for the cases $S = \frac{1}{2}$, 1 and 2 are presented in Table I and are shown in Fig. 1;

$$\Delta(x, y) = \begin{cases} 1 \text{ for } x + y \\ 0 \text{ for } x \neq y. \end{cases} \tag{3.12}$$

TABLE I

S \ A	$A_1(S, T)$	$A_2(S, T)$	$A_3(S, T)$
$\frac{1}{2}$	$(e^{z\lambda\beta}+1)^{-1} - \frac{1}{2}$	$(e^{-z\lambda\beta}+1)^{-1}$	$(e^{z\lambda\beta}+1)^{-1}$
1	$\frac{1+2\,e^{-z\lambda\beta}}{2\,\mathrm{ch}\,(z\lambda\beta)+1} - 1$	$\frac{\sqrt{2}(1+e^{z\lambda\beta})}{2\,\mathrm{ch}\,(z\lambda\beta)+1}$	$\frac{\sqrt{2}(1+e^{-z\lambda\beta})}{2\,\mathrm{ch}\,(z\lambda\beta)+1}$
2	$\frac{1+2e^{-z\lambda\beta}+3e^{-2z\lambda\beta}+4e^{-3z\lambda\beta}}{2\,\mathrm{ch}(z\lambda\beta)+e^{-2z\lambda\beta}+e^{-3z\lambda\beta}+1} - 2$	$\frac{2(e^{z\lambda\beta}+e^{-2z\lambda\beta})+\sqrt{6}\,(1+e^{-z\lambda\beta})}{2\,\mathrm{ch}\,(z\lambda\beta)+e^{-2z\lambda\beta}+e^{-3z\lambda\beta}+1}$	$\frac{2(1+e^{-3z\lambda\beta})+\sqrt{6}e^{-z\lambda\beta}(1+e^{-z\lambda\beta})}{2\,\mathrm{ch}\,(z\lambda\beta)+e^{-2z\lambda\beta}+e^{-3z\lambda\beta}+1}$

The factor determining the overlapping of the oscillator wave functions, occurring in (3.4a) can be rewritten, according to Holstein [12], as follows:

$$\begin{aligned} \langle N_{\boldsymbol{q}}^{(j+\delta)} | N_{\boldsymbol{q}}^{(j)} \rangle = \prod_{\boldsymbol{q}} \left\{ 1 - \frac{4}{\mathcal{N}} \left(N_{\boldsymbol{q}}^{(j+\delta)} + \frac{1}{2} \right) \gamma_{\delta,\boldsymbol{q}} \cos^2 \left[\frac{1}{2} \boldsymbol{q}(\boldsymbol{R}_{j+\delta} + \boldsymbol{R}_j) + \frac{\pi}{4} \right] \right\} \times \\ \times \Delta(N_{\boldsymbol{q}}^{(j+\delta)}, N_{\boldsymbol{q}}^{(j)}) \pm \left\{ \sqrt{\frac{8}{\mathcal{N}}}\, \varepsilon_\delta \gamma_{\delta,\sigma}^{\frac{1}{2}} \cos \left[\frac{1}{2} \boldsymbol{q}(\boldsymbol{R}_{j+\delta} + \boldsymbol{R}_j) + \frac{\pi}{4} \right] \times \right. \\ \left. \times \left[\frac{1}{2} \left(N_{\boldsymbol{q}}^{(j+\delta)} + \frac{1}{2} \pm \frac{1}{2} \right) \right]^{\frac{1}{2}} \right\} \Delta(N_{\boldsymbol{q}}^{(j+\delta)}, N_{\boldsymbol{q}}^{(j)} \pm 1), \end{aligned} \tag{3.13}$$

where

$$\gamma_{\delta \boldsymbol{q}} = \frac{\gamma^2}{\omega_{\boldsymbol{q}}^2 \hbar \omega_{\boldsymbol{q}}} \sin^2 \frac{1}{2} \boldsymbol{q} \cdot \boldsymbol{R}_\delta, \tag{3.14}$$

$$\varepsilon_\delta = \begin{cases} +1 \text{ for } \boldsymbol{q} \cdot R > 0 \\ -1 \text{ for } \boldsymbol{q} \cdot R < 0, \end{cases}$$

$$R_\delta = R_{j+\delta} - R_j.$$

The expression (3.13) describe only processes without change of the phonon distribution and two-phonon processes. In calculating the bandwidth, we make use of the diagonal matrix element (without changing the phonon distributions in both states) whereas the non-diagonal element is neglected as small, following Holstein [12] (see also [11a]). Therefore in Eq. (3.13) we take into consideration only the first term, which we write in the form:

$$\langle N_{\boldsymbol{q}}^{(j+\delta)} | N_{\boldsymbol{q}}^{(j)} \rangle = \exp \left\{ - \sum_{\boldsymbol{q}} \frac{(1+2N_{\boldsymbol{q}})}{\mathcal{N}} \gamma_{\delta,\boldsymbol{q}} \right\}. \tag{3.15}$$

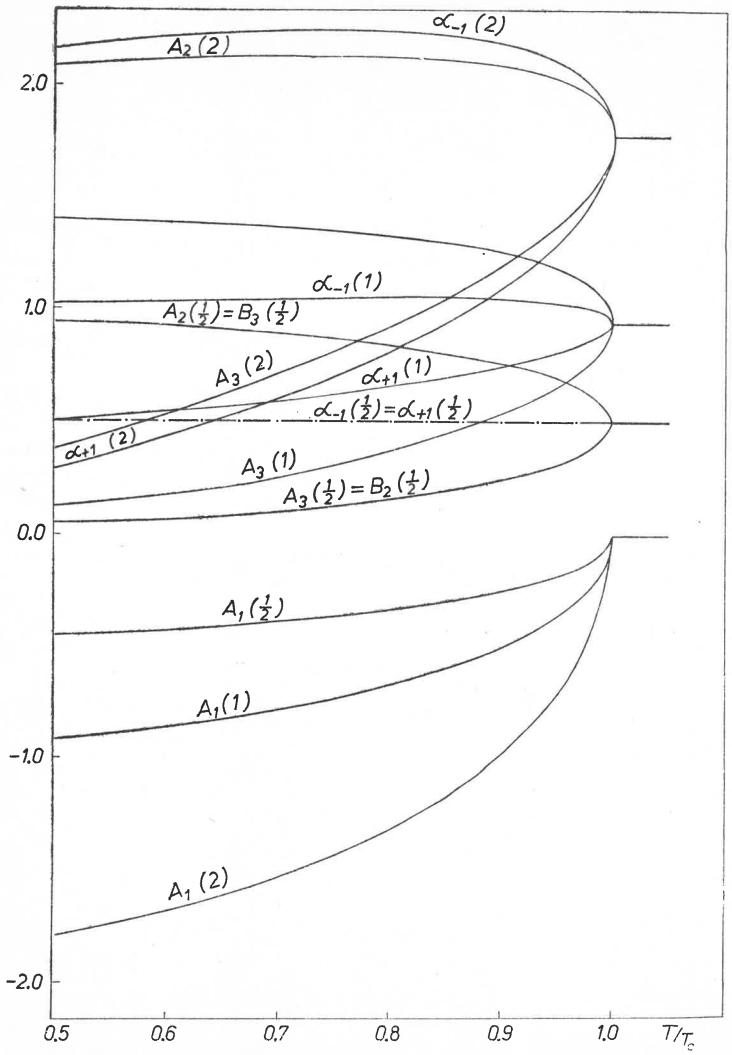

Fig. 1. Temperature-dependence of the parameters $A_i(S)$ and $\alpha_{\sigma'}(S)$ for $S=\frac{1}{2}, 1, 2$ $(i=1, 2, 3)$ and $B_2(\frac{1}{2})$, $B_3(\frac{1}{2})$

The expression (3.15) has to be averaged previous to insertion into (3.4). One obtains:

$$\langle\langle N_{\boldsymbol{q}}^{(j+\delta)}|N_{\boldsymbol{q}}^{(j)}\rangle\rangle_{\mathrm{Av}}=\sum_{\{N_{\boldsymbol{q}}\}}\varrho(N_{\boldsymbol{q}})\langle N_{\boldsymbol{q}}^{(j+\delta)}|N_{\boldsymbol{q}}^{(j)}\rangle=\exp\left\{-\sum_{\boldsymbol{q}}\frac{(1+2\bar{N}_{\boldsymbol{q}})}{\mathcal{N}}\gamma_{\delta,\boldsymbol{q}}\right\},\quad(3.16)$$

where

$$\varrho(N_{\boldsymbol{q}})=\exp\left(-N_{\boldsymbol{q}}\beta\hbar\omega_{\boldsymbol{q}}\right)\left[\sum_{N_{\boldsymbol{q}}}\exp\left(-N_{\boldsymbol{q}}\beta\hbar\omega_{\boldsymbol{q}}\right)\right]^{-1}\quad(3.17)$$

$$\bar{N}_{\boldsymbol{q}}\equiv(e^{\beta\hbar\omega_{\boldsymbol{q}}}-1)^{-1},\qquad\beta\equiv\frac{1}{kT}.$$

Inserting (3.11) and (3.16) into (3.4), we finally obtain the expression for the bandwidth:

$$\Gamma(\sigma') = 2z\left\{M + \frac{1}{2}zJ[A_1(S,T)+A_2(S,T)]\Delta(\sigma',-1) - \right.$$

$$-\frac{1}{2}zJ[A_1(S,T)-A_3(S,T)]\Delta(\sigma',+1)+$$

$$\left.+\frac{1}{2}zJ[A_2(S,T)+A_3(S,T)]\right\}\exp\left\{-\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\operatorname{cth}\frac{\beta\hbar\omega_q}{2}\right\}. \tag{3.18}$$

The temperature-dependence of the pre-exponential factor in (3.18) is determined, according to the carrier spin states, by way of the factors:

$$\alpha_{+1}(S,T) = A_1(S,T)+A_2(S,T), \tag{3.19}$$

$$\alpha_{-1}(S,T) = A_3(S,T)-A_1(S,T).$$

The temperature-dependence of (3.19) is shown in Fig. 1 for $S = 1/2$, 1 and 2. The expression (3.18) can now be rewritten as follows:

$$\Gamma(\sigma') = 2z\left\{M - \frac{1}{2}zJ\alpha_{\sigma'}(S,T)\right\}\exp\left\{-\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\operatorname{cth}\frac{\beta\hbar\omega_q}{2}\right\}. \tag{3.20}$$

Introducing mean values of the quantities dependent on q [17]:

$$\bar{\omega}_q = \omega_0, \quad \bar{\gamma}_{\delta,q} = \bar{\gamma}_q \sin^2\frac{1}{2}\boldsymbol{q}\cdot\boldsymbol{R} \equiv \gamma' \tag{3.21}$$

we obtain, for $z = 6$,

$$\Gamma(\sigma') = 12|[M-3J\alpha_{\sigma'}(S,T)]|\exp\left(-\gamma'\operatorname{cth}\frac{\theta}{2T}\right);\ (\sigma' = \pm 1). \tag{3.22}$$

Exchange interaction in the crystal gives rise to a splitting of the conductivity band (for $T < T_c$) into two subbands for $\sigma' = +1$ and $\sigma' = -1$, respectively. The temperature-dependence of the width for these subbands described by Eq. (3.22) for both values σ' and for the following typical values of the parameters [11, 16, 19]

$$M = 0.5\ \text{eV}, \quad J = 0.2\ \text{eV}, \quad \theta = \frac{\hbar\omega_0}{k} = 900°\text{K}, \quad \gamma' = 8$$

is shown in Fig. 2, for $S = \frac{1}{2}$, 1, 2. For comparison, the temperature-dependence of the polaron bandwidth is also presented, however without the exchange interactions. As shown in Fig. 2, when $S = \frac{1}{2}$, the widths for both subbands are equal to one another and the exchange interactions do not affect the shape of their temperature-dependence. At $S > \frac{1}{2}$, a more important part is played by the exchange interactions, which affect the temperature-dependence of the polaron's subbands, at fixed S, this dependence differs for $\sigma' = +1$ and $\sigma' = -1$ (when $T < T_c$).

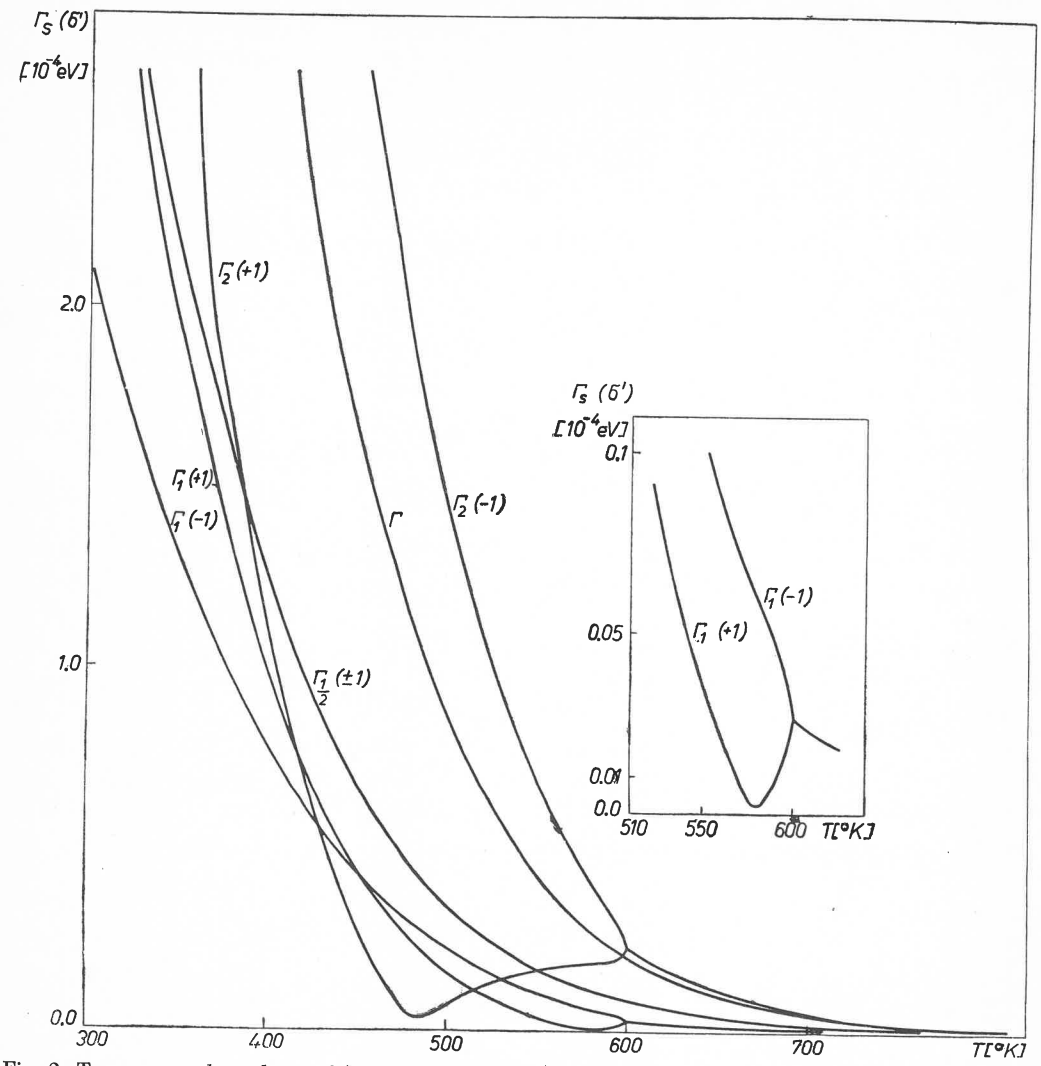

Fig. 2. Temperature-dependence of the widths of the polaron's subbands for $S = \frac{1}{2}, 1, 2$ ($T_c = 600°\mathrm{K}$, $\gamma' = 8$, $J = 0.2$ eV, $M = 0.5$ eV, $\theta = 900°\mathrm{K}$). The curve Γ shows the temperature-dependence of the polaron bandwidth calculated without taking into account exchange interactions

4. *Mobility of polarons*

As seen from Eq. (3.20), the bandwidth depends strongly on temperature *via* the oscillator overlapping integral (3.16). With increasing temperature, the band narrows and above a certain temperature T_t [12, 13] the polaron loses its Bloch character and the band description becomes unadequate for it[1]. The band description loses its validity when the

[1] The temperature T_t is simultaneously the point in which the diagonal, $N_{\boldsymbol{q}}^{(j+\delta)} = N_{\boldsymbol{q}}^{(j)}$, and the nondiagonal, $N_{\boldsymbol{q}}^{(j+\delta)} = N_{\boldsymbol{q}}^{(j)} \pm 1$, transitions exchange their roles. For $T < T_t$, the main part is played by diagonal transitions whereas the nondiagonal ones contributing to polaron scattering between states of the band and can be neglected. When $T > T_t$, the phonon-nondiagonal transitions become most important [12, 13, 11a].

polaron band width becomes smaller than the uncertainty of the polaron state energy *i. e.* $\Gamma(\sigma') \ll \hbar/\tau_j$, where

$$\frac{1}{\tau_j} = \sum_{\delta,\sigma} \sum_{\{n_l\}} \sum_{\{N_q^{(j+\delta)}\}} W(j, \sigma', \{n_l'\}, \{N_q^{(j)}\} \to j+\delta, \sigma, \{n_l\}, \{N_q^{(j+\delta)}\})$$

and $\Gamma(\sigma')$ is determined by Eq. (3.20). Above the temperature T_t the hopping mechanism becomes predominant. The polaron is in principle localized, and its motion becomes diffusional. Electric conductivity is now due to hopping of the carrier from a site j to a site $j+\delta$.

The transition probability per unit time is expressed in the well-known form

$$W(j, \sigma', \{n_l'\}, \{N_q^{(j)}\} \to j+\delta, \sigma, \{n_l\}, \{N_q^{(j+\delta)}\})$$

$$= \frac{2\pi}{\hbar} |\langle j+\delta, \sigma, \{n_l\}, \{N_q^{(j+\delta)}\}| \mathscr{H}_{\text{int}} | j, \sigma', \{n_l'\}, \{N_q^{(j)}\}\rangle|^2 \, \delta(E-E') \tag{4.1}$$

where the matrix element is calculated in the basis of localized wave functions with the factors (2.10), (2.11), (2.12) and (2.17). The argument of the Dirac δ-function has the form:

$$E-E' = \sum_q \hbar\omega_q (N_q - N_q') + \frac{1}{2} A(n_j' - S)\sigma' - \frac{1}{2} A(n_j - S)\sigma + \Delta E. \tag{4.2}$$

The second and third terms of (4.2) express the difference in the carrier's energy levels depending on its spin direction; whereas the last term represents the change in energy of the localized spins system connected with the transition from site j to site $j+\delta$ at well-defined spin direction in the initial and final states, with

$$\Delta E = \begin{cases} -z\lambda & \text{for } n_{j+\delta}' \to n_{j+\delta} + 1 \\ 0 & \text{for } n_{j+\delta}' \to n_{j+\delta} \\ +z\lambda & \text{for } n_{j+\delta}' \to n_{j+\delta} - 1 \end{cases}$$

Denoting

$$\mathscr{B}(\sigma', \sigma, \{n_l'\}, \{n_l\}) \equiv \langle j+\delta, \sigma, \{n_l\}| \mathscr{H}_{\text{int}} | j, \sigma', \{n_l'\}\rangle$$

we find

$$\mathscr{B}(\sigma', \sigma, \{n_l',\} \{n_l\}) = M\Delta(\sigma, \sigma') \prod_f \Delta(n_f', n_f) -$$

$$- \frac{1}{2} J[\Delta(\sigma, -1)\Delta(\sigma', -1) - \Delta(\sigma, -1)\Delta(\sigma', -1)] \sum_\delta (n_{j+\delta}' - S) \prod_f \Delta(n_f', n_f) -$$

$$- \frac{1}{2} J \sum_\delta \{\Delta(\sigma, -1)[1-\Delta(\sigma', -1)][(2S - n_{j+\delta}')(n_{j+\delta}'+1)]^{\frac{1}{2}} \times$$

$$\times \Delta(n_{j+\delta}'+1, n_j) \prod_{f(\neq j+\delta)} \Delta(n_f', n_f) +$$

$$+ \Delta(\sigma, +1)[1-\Delta(\sigma', +1)][(2S - n_{j+\delta}'+1)n_{j+\delta}']^{\frac{1}{2}} \Delta(n_{j+}' - 1, n_j) \prod_{f(\neq j+\delta)} \Delta(n_f', n_f)\}. \tag{4.3}$$

To obtain the total probability of the transition, one has to average the expression (4.1) over the initial states of phonons and localized spins and then to perform a summation over

all final states, obtaining

$$W_T = \sum_{\delta,\sigma} \sum_{\{N_q^{(j)}\}} \sum_{\{N_q^{(j+\delta)}\}} \sum_{\{n_l\}} \sum_{\{n_l'\}} f(n_l')\, \varrho(N_q)\, W(j, \sigma', \{n_l'\}, \{N_q^{(j)}\} \to$$
$$\to j+\delta, \sigma, \{n_l\}, \{N^{(j+\delta)}\}), \tag{4.4}$$

where $f(n_l)$ is determined by Eq. (3.10) and $\varrho(N_q)$ by (3.17). Substituting (3.13) and (4.1) in (4.3) as well as (3.10) and (3.17) in (4.4), and using the integral representation $\delta(x)$ in the form $\delta(x) = \lim_{t\to\infty} \frac{1}{2\pi\hbar} \int_{-t}^{+t} \exp\left(\frac{ixt'}{\hbar}\right) dt'$, we obtain after simple calculations

$$W_T(\sigma') = \frac{zM^2}{\hbar^2}\left[1+\frac{1}{4}z^2\left(\frac{J}{M}\right)^2 B_1(S,T)+z\frac{J}{M}A_1(S,T)\right]\Delta(\sigma',-1)\times$$
$$\times\int dt' \exp\left\{\frac{it'}{\hbar}\left[\frac{1}{2}AA_1(S,T)(\sigma'+1)\right]+\Lambda(\boldsymbol{q},t')\right\}+$$
$$+\frac{zM^2}{\hbar^2}\left[1+\frac{1}{4}z^2\left(\frac{J}{M}\right)^2 B_1(S,T)-z\frac{J}{M}A_1(S,T)\right]\Delta(\sigma',+1)\times$$
$$\times\int dt' \exp\left\{\frac{it'}{\hbar}\left[\frac{1}{2}AA_1(S,T)(\sigma'-1)\right]+\Lambda(\boldsymbol{q},t')\right\}+$$
$$+\frac{z^3}{4\hbar^2}J^2B_3(S,T)[1-\Delta(\sigma',-1)]\times$$
$$\times\int dt' \exp\left\{\frac{it'}{\hbar}\left[\frac{1}{2}AA_1(S,T)(\sigma'+1)+z\lambda\right]+\Lambda(\boldsymbol{q},t')\right\}+$$
$$+\frac{z^3}{4\hbar^2}J^2B_2(S,T)[1-\Delta(\sigma',+1)]\times$$
$$\times\int dt' \exp\left\{\frac{it'}{\hbar}\left[\frac{1}{2}AA_1(S,T)(\sigma'-1)-z\lambda\right]+\Lambda(\boldsymbol{q},t')\right\}, \tag{4.5}$$

where

$$\Lambda(\boldsymbol{q},t') = \sum_{\boldsymbol{q}} \frac{2\gamma_{\delta,\boldsymbol{q}}}{\mathcal{N}}[-(2\bar{N}_{\boldsymbol{q}}+1)+(2\bar{N}_{\boldsymbol{q}}+1)\cos\omega_{\boldsymbol{q}}t'+i\sin\omega_{\boldsymbol{q}}t']$$

and $A_1(S,T)$ is determined by Eq. (3.9), and

$$B_1(S,T) \equiv \sum_{n=0}^{2S} f(n)\,(n-S)^2$$
$$= \Big(\sum_{n=0}^{2S} e^{-z\lambda\beta n}\Big)^{-1} \sum_{n=0}^{2S} e^{-z\lambda\beta n}(n-S)^2, \tag{4.6a}$$
$$B_2(S,T) \equiv \sum_{n=0}^{2S} f(n+1)\,(2S-n)\,(n+1)$$
$$= \Big(\sum_{n=0}^{2S} e^{-z\lambda\beta n}\Big)^{-1} \sum_{n=0}^{2S} e^{-z\beta\lambda(n+1)}\,(2S-n)\,(n+1), \tag{4.6b}$$

$$B_3(S,T) \equiv \sum_{n=0}^{2S} f(n-1)\, n(2S-n+1)$$
$$= \Big(\sum_{n=0}^{2S} e^{-z\beta\lambda n}\Big)^{-1} \sum_{n=0}^{2S} e^{-z\lambda\beta(n-1)} n(2S-n+1). \tag{4.6c}$$

The coefficients $B_i(S, T)$ for $S = \frac{1}{2}$, 1 and 2 are presented in the Table II. Their temperature dependence is shown in Figs 1 and 3.

TABLE II

S \ B	$B_1(S, T)$	$B_2(S, T)$	$B_3(S, T)$
$\frac{1}{2}$	$\frac{1}{4}$	$A_3\left(\frac{1}{2}, T\right)$	$A_2\left(\frac{1}{2}, T\right)$
1	$\frac{2\,\mathrm{ch}\,(z\lambda\beta)}{1+2\,\mathrm{ch}\,(z\lambda\beta)}$	$\sqrt{2}\,A_3(1, T)$	$\sqrt{2}\,A_2(1, T)$
2	$\frac{4(e^{z\lambda\beta}+e^{-3z\lambda\beta})+e^{-2z\lambda\beta}+1}{2\,\mathrm{ch}\,(z\lambda\beta)+e^{-2z\lambda\beta}+e^{-3z\lambda\beta}+1}$	$\frac{4(1+e^{-3z\lambda\beta})+6e^{-z\lambda\beta}(1+e^{-z\lambda\beta})}{2\,\mathrm{ch}\,(z\lambda\beta)+e^{-2z\lambda\beta}+e^{-3z\lambda\beta}+1}$	$\frac{6(1+e^{-z\lambda\beta})+4(e^{z\lambda\beta}+e^{-2z\lambda\beta})}{2\,\mathrm{ch}\,(z\lambda\beta)+e^{-2z\lambda\beta}+e^{-3z\lambda\beta}+1}$

When deriving the expression (4.5), we replaced $(n_j'-S)$ by $\langle n_j'-S\rangle$ as well as (n_j-S) by $\langle n_j-S\rangle$, and assumed that $\langle n_j'-S\rangle = \langle n_j-S\rangle = A_1(S, T)$. This assumption means that the magnetic moment direction of the carrier's own ion is the same before and after the jump and, moreover, is determined by the magnetization only. This assumption ceases to be valid in the near neighbourhood of the Curie point. To derive the integrals of Eq. (4.5), we introduce the transformation [12, 13, 17] $t' \to \frac{i\beta\hbar}{2} + \tau$. The integration contour is now of the form shown in Fig. 4.

The preceding integrals can now be written in the form of a sum of integrals:

$$\int \ldots \to \int_{-t}^{+t} \ldots + \int_{-t}^{t-i\beta\hbar/2} \ldots + \int_{-t-i\delta\hbar/2}^{-t} \ldots \tag{4.7}$$

As proved by Holstein[2] the last two integrals in (4.7) vanish for $t \gg \omega_q^{-1}$; we thus consider only the first right-hand side integral of (4.7). After some simple transformation, Eq. (4.5) can be rewritten in the form:

$$W_T(\sigma') = W_T^d(\sigma') + W_d^{nd}(\sigma'), \tag{4.8}$$

where the first term of the right hand side stands for the probability of the carrier's transition without change of spin direction (spin-diagonal transition); whereas the second term corresponds to a transition with spin flipping. Both terms are of the following forms, respectively:

$$W_T^d(\sigma') = \frac{zM^2}{\hbar^2}\left[1+\frac{1}{4}z^2\left(\frac{J}{M}\right)^2 B_1(S, T)+z\frac{J}{M}A_1(S, T)\right]\Delta(\sigma', -1)\times$$
$$\times\exp\left\{-2\sum_q \frac{\gamma_{\delta,q}}{\mathcal{N}}\,\mathrm{cth}\,\frac{\beta\hbar\omega_q}{2} - \frac{\beta}{2}\left[\frac{1}{2}AA_1(S, T)\,(\sigma'+1)\right]\right\}\times$$

[2] See also the discussion of Klinger [13].

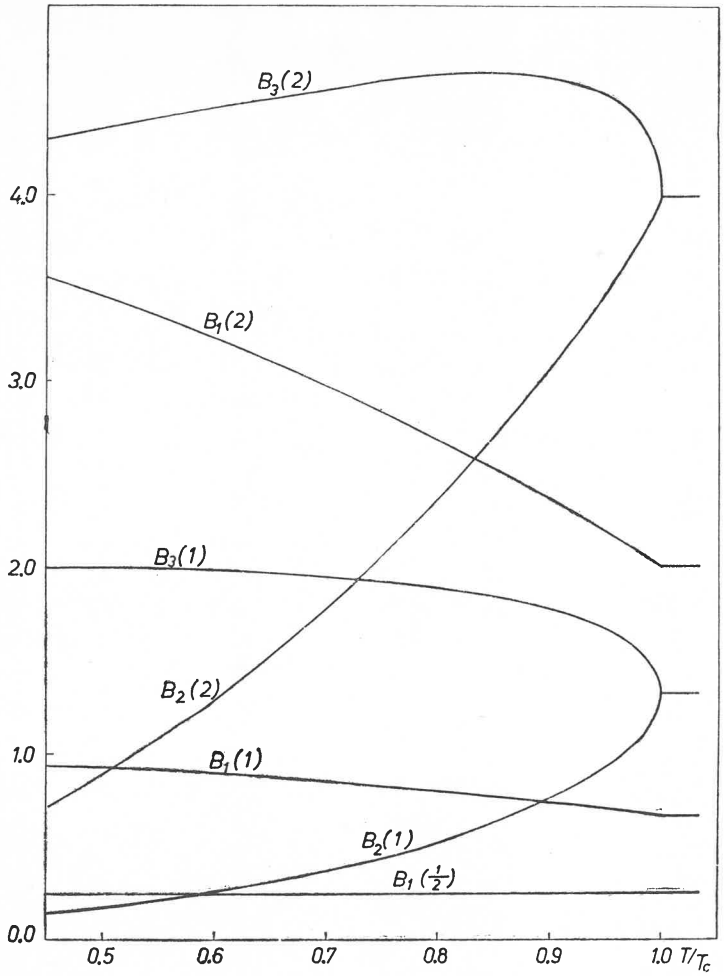

Fig. 3. Temperature-dependence of the parameters $B_i(S)$ for $S = \frac{1}{2}, 1, 2$ $(i = 1, 2, 3)$

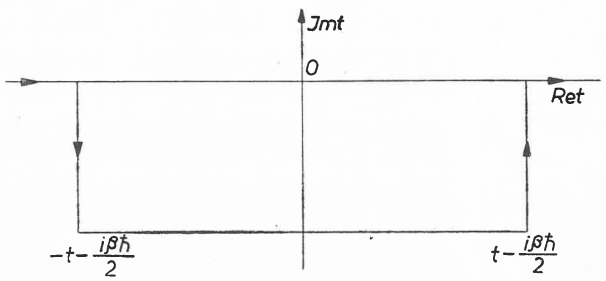

Fig. 4. Contour for integration over the time in Eq. (4.5)

$$\times \int_{-\infty}^{+\infty} d\tau \cos\left\{\left[\frac{1}{2} AA_1(S, T)(\sigma'+1)\right]\frac{\tau}{\hbar}\right\} \exp\left\{2\sum_{q}\frac{\lambda_{\delta,q}}{\mathcal{N}}\frac{\cos\omega_q\tau}{\operatorname{sh}\left(\frac{\beta\hbar\omega_q}{2}\right)}\right\} +$$

$$+\frac{zM^2}{\hbar^2}\left[1+\frac{1}{2}z^2\left(\frac{J}{M}\right)^2 B_1(S, T) - z\frac{J}{M}A_1(S, T)\right]\Delta(\sigma', +1)\times$$

$$\times\exp\left\{-2\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\operatorname{cth}\frac{\beta\hbar\omega_q}{2} - \frac{\beta}{2}\left[\frac{1}{2}AA_1(S, T)(\sigma'-1)\right]\right\}\times$$

$$\times\int_{-\infty}^{+\infty} d\tau \cos\left\{\left[\frac{1}{2}AA_1(S, T)(\sigma'-1)\right]\frac{\tau}{\hbar}\right\}\exp\left\{2\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\frac{\cos\omega_q\tau}{\operatorname{sh}\left(\frac{\beta\hbar\omega_q}{2}\right)}\right\}, \tag{4.9a}$$

$$W_T^{nd}(\sigma') = \frac{z^3J^2}{4\hbar^2}B_3(S, T)[1-\Delta(\sigma', -1)]\exp\left\{-2\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\operatorname{cth}\frac{\beta\hbar\omega_q}{2} -\right.$$

$$\left. -\frac{\beta}{2}\left[\frac{1}{2}AA_1(S, T)(\sigma'+1) - z\lambda\right]\right\}\times$$

$$\times\int_{-\infty}^{+\infty} d\tau \cos\left\{\left[\frac{1}{2}AA_1(S, T)(\sigma'+1) - z\lambda\right]\frac{\tau}{\hbar}\right\}\exp\left\{2\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\frac{\cos\omega_q\tau}{\operatorname{sh}\left(\frac{\beta\hbar\omega_q}{2}\right)}\right\} +$$

$$+\frac{z^3J^2}{4\hbar^2}B_2(S, T)[1-\Delta(\sigma', +1)]\exp\left\{-2\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\operatorname{cth}\frac{\beta\hbar\omega_q}{2} -\right.$$

$$\left. -\frac{\beta}{2}\left[\frac{1}{2}AA_1(S, T)(\sigma'-1) + z\lambda\right]\right\}\times$$

$$\times\int_{-\infty}^{+\infty} d\tau \cos\left\{\left[\frac{1}{2}AA_1(S, T)(\sigma'-1) + z\lambda\right]\frac{\tau}{\hbar}\right\}\exp\left\{2\sum_{q}\frac{\gamma_{\delta,q}}{\mathcal{N}}\frac{\cos\omega_q\tau}{\operatorname{sh}\left(\frac{\beta\hbar\omega_q}{2}\right)}\right\}. \tag{4.9b}$$

Denoting $f(\tau) = \sum_{q}\frac{2\gamma_{\delta q}}{\mathcal{N}}\frac{\cos\omega_q\tau}{\operatorname{sh}\left(\frac{\beta\hbar\omega_q}{2}\right)}$, we can (following Klinger [13][3]) define a temperature T_t for which $f(0) = 1$ and distinguish two cases: $f(0) > 1$ when $T \gg T_t$, and $f(0) < 1$ when $T \ll T_t$. In the present paper, we restrict our considerations to the first case only. The integrals of (4.9) can be derived resorting to the saddle point method, and we get the principal contribution to the integral in the neighbourhood of $\tau = 0$. Simple calculations yield

$$W_T^d(\sigma') = \frac{z\sqrt{\pi}M^2}{\hbar}\sqrt{\frac{\beta}{E(T)}}\left\{\left[1+\frac{1}{4}z^2\left(\frac{J}{M}\right)^2 B_1(S, T) + z\frac{J}{M}A_1(S, T)\right]\times\right.$$

$$\left.\times\Delta(\sigma', -1) + \left[1+\frac{1}{4}z^2\left(\frac{J}{M}\right)^2 B_1(S, T) - z\left(\frac{J}{M}\right)A_1(S, T)\right]\Delta(\sigma', +1)\right\}e^{-\beta\mathcal{E}(T)}, \tag{4.10a}$$

[3] $T_t = \frac{\theta}{2}\,[\operatorname{arsh}\gamma']^{-1}$, $\theta \equiv \frac{\hbar\omega_0}{k}$; for $\gamma' = 10$, $T_t \cong \frac{1}{6}\theta$.

$$W_T^{nd}(\sigma') = \frac{z^3\sqrt{\pi}}{4\hbar} J^2 \sqrt{\frac{\beta}{E(T)}} \left\{ B_3(S, T)\,[1 - \Delta(\sigma', -1] \exp\left[-\frac{\beta}{4}\,(AA_1(S, T)(\sigma' + 1) + \right.\right.$$

$$\left. + 2z\lambda) - \frac{\beta(AA_1(S, T)(\sigma' + 1) + 2z\lambda)^2}{16\,E(T)} \right] +$$

$$+ B_2(S, T)\,[1 - \Delta(\sigma', +1)] \exp\left[-\frac{\beta}{4}\,(AA_1(S, T)(\sigma' - 1) - 2z\lambda) - \right.$$

$$\left.\left. - \frac{\beta(AA_1(S, T)(\sigma' - 1) - 2z\lambda)^2}{16\,E(T)} \right] \right\} e^{-\beta\mathscr{E}(T)}, \tag{4.10b}$$

where

$$\mathscr{E}(T) = \frac{2}{\beta} \sum_{q} \frac{\gamma_{\delta,q}}{\mathcal{N}} \operatorname{th} \frac{\beta\hbar\omega_q}{4},$$

$$E(T) = \beta \sum_{q} \frac{\gamma_{\delta,q}}{\mathcal{N}} \frac{(\hbar\omega_q)^2}{\operatorname{sh}\left(\dfrac{\beta\hbar\omega_q}{2}\right)},$$

for temperature $T > \dfrac{\hbar\omega_0}{2k} \equiv \dfrac{\theta}{2}$, $\mathscr{E}(T) \simeq \dfrac{1}{4} E(T)$.

The polaron mobility can be derived by means of the well-known relation of Einstein

$$\mu(\sigma') = \frac{|e|a^2}{kT} W_T(\sigma') \tag{4.11}$$

which can be rewritten on averaging over the initial states of the carrier spin:

$$\mu_S = \sum_{\sigma'} p(\sigma')\mu(\sigma') = \frac{|e|a^2}{kT} \sum_{\sigma'} p(\sigma') W_T(\sigma'), \tag{4.12}$$

where

$$p(\sigma') = e^{-\sigma' z\lambda\beta} / 2\operatorname{ch}(z\lambda\beta).$$

Substituting (4.10a) and (4.10b) *via* (4.8) in (4.12), we finally come to an expression describing the mobility of a polaron with spin in a crystal exhibiting ferromagnetic ordering as a function of the value of the spin S localized at a site and of the temperature:

$$\mu_S = \mu \left\{ 1 + \frac{1}{4} z^2 (J/M)^2 B_1(S, T) + z(J/M) A_1(S, T) \operatorname{th}(z\lambda\beta) + \right.$$

$$+ \frac{1}{8} z^2 (J/M)^2 \frac{1}{\operatorname{ch}(z\lambda\beta)} \exp\left[-\frac{(AA_1(S, T) + z\lambda)^2}{4(\hbar\omega_0)^2} \frac{1}{\gamma'} \operatorname{sh} \frac{\theta}{2T} \right] \times$$

$$\times \left[B_2(S, T) \exp\left(\frac{1}{2}\,\beta\, AA_1(S, T) + \frac{3}{2}\, z\lambda\beta \right) + \right.$$

$$\left.\left. + B_3(S, T) \exp\left(-\frac{1}{2}\,\beta AA_1(S, T) - \frac{3}{2}\, z\lambda\beta \right) \right] \right\}; (T > T_t), \tag{4.13}$$

where

$$\mu = \frac{|e|a^2}{kT} \frac{z\sqrt{\pi}}{\hbar^2\omega_0} M^2 \sqrt{\frac{1}{\gamma'} \operatorname{sh} \frac{\theta}{2T}} \exp\left(-2\gamma' \operatorname{th} \frac{\theta}{4T} \right) \tag{4.14}$$

is the polaron mobility obtained without taking into account the exchange interactions in the crystal [13]. The temperature-dependence of the mobilities μ_S and μ, given respectively by (4.13) and (4.14), as well as μ_S/μ for $S = 1$ and 2, $T_c = 600°\mathrm{K}$, $\theta = 900°\mathrm{K}$, $\gamma' = 10$,

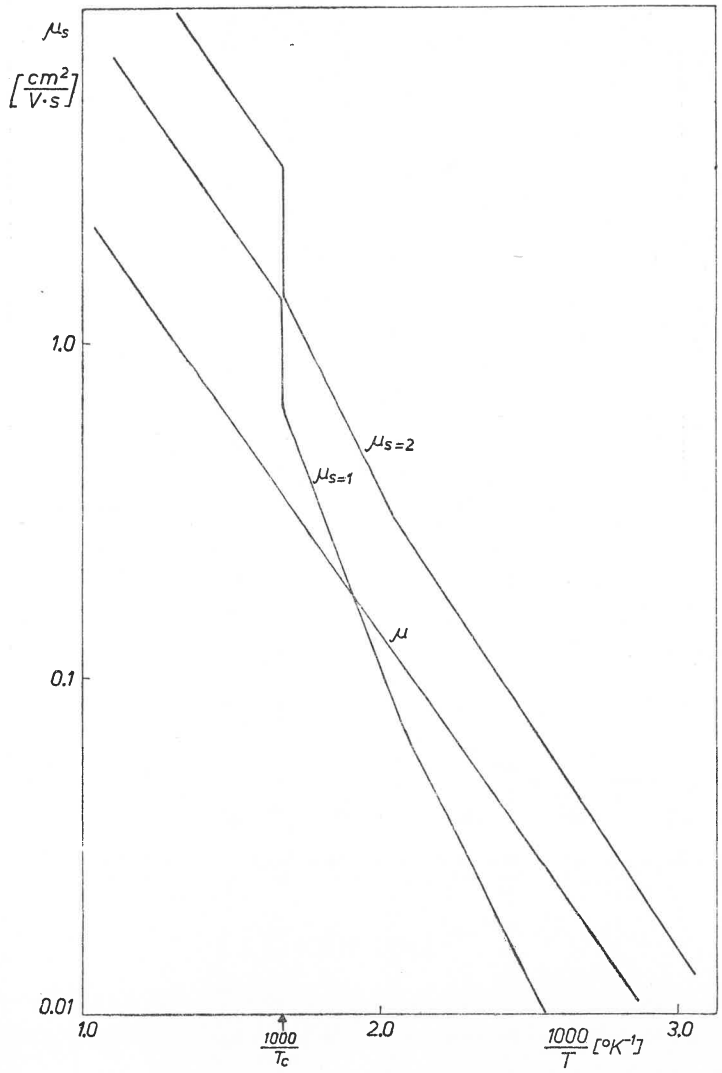

Fig. 5. Mobilities μ_S and μ as functions of $10^3/T$ plotted from Eqs (4.13) and (4.14), respectively (values of parameters are printed after Eq. (4.14))

$A = 10\,\mathrm{eV}$, $J/M = 0.4$, $a = 4\,\text{Å}$, are represented in Figs 5 and 6, respectively. As seen from Fig. 5, in the Curie point a steep increase of the polaron mobility is observed, as well as a change in the activation energy. In the region of magnetic ordering the activation energy is larger than in the paramagnetic phase.

The author is indebted to Dr J. Morkowski for suggesting the investigation and for his unstined help throughout the duration of the work.

The computational work was performed in the computing laboratory of the Institute of Physics of the Polish Academy of Sciences.

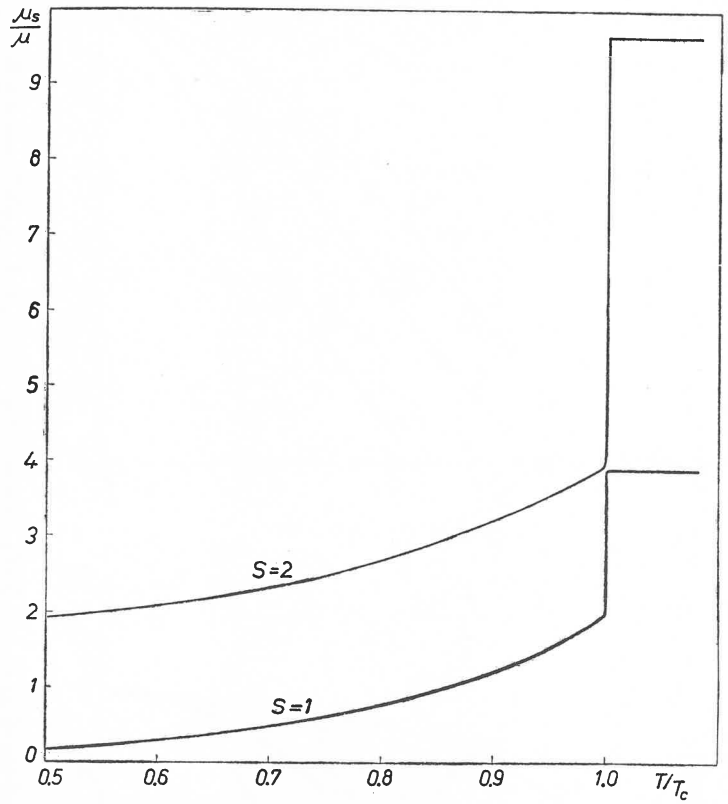

Fig. 6. Relative mobility of the polaron as a function of T/T_c (for $T_c = 600°K$) plotted from Eq. (4.13)

APPENDIX

To determine the temperature-dependences of $A_i(S, T)$ and $B_i(S, T)/(i = 1, 2, 3)$, one has first to obtain the temperature-dependence of λ. From the condition of self-consistence in the constant coupling approximation [8]:

$$2SB_S(Sz\lambda\beta) = Z^{-1} \sum_{n=0}^{2S} \sum_{m=-n}^{+n} m \exp\left[C(S)\frac{T_c}{T} n(n+1)+(z-1)\lambda\beta m\right], \qquad \text{(A.1)}$$

where

$$Z = \sum_{n=0}^{2S} \sum_{m=-n}^{+n} \exp\left[C(S)\frac{T_c}{T} n(n+1)+(z-1)\lambda\beta m\right],$$

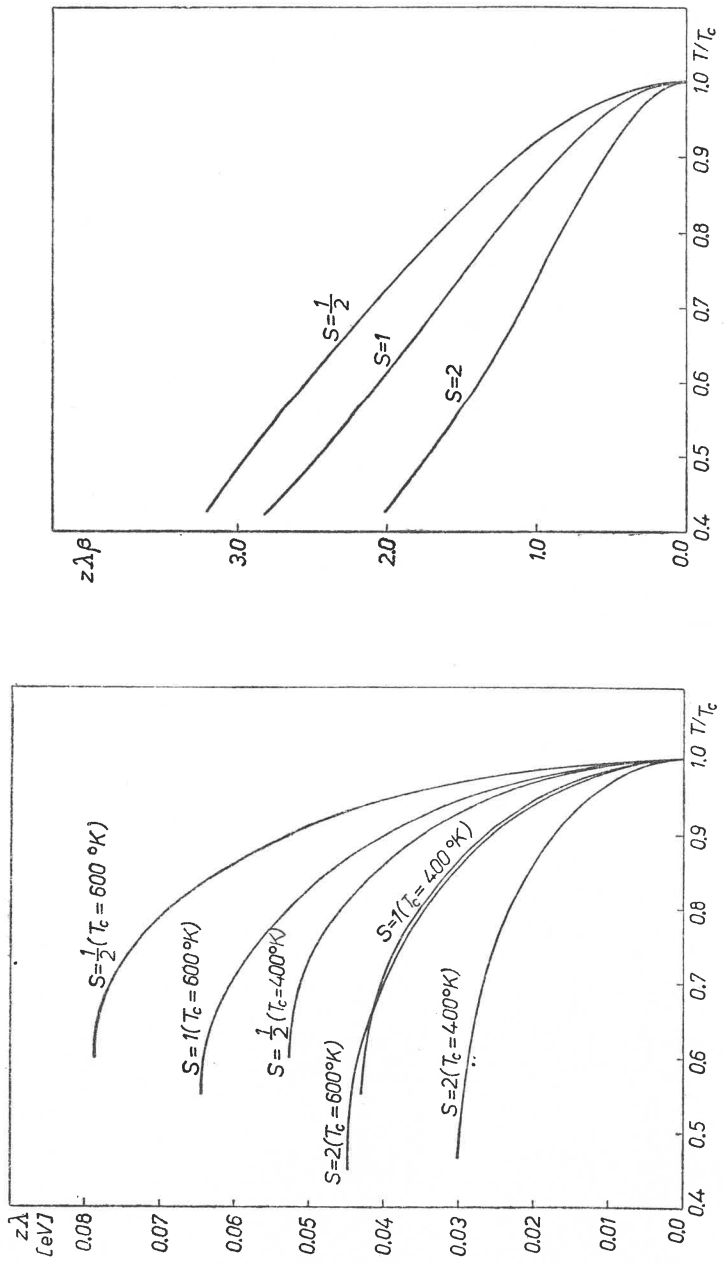

Fig. 7. *a*) Temperature-dependence of the effective field parameter $z\lambda$ for $S = \frac{1}{2}, 1, 2$; $T_c = 400°\mathrm{K}$ and $600°\mathrm{K}$.
b) $z\lambda\beta$ as a function of T/T_c for $S = \frac{1}{2}, 1, 2$

$B_S(x)$ is Brillouin function. The parameter $C(S) \equiv |I|\beta_c$ appearing in Eq. (A.1) can be calculated for all values of the spin S, from the following relation:

$$\sum_{n=0}^{2S} (2n+1) \exp\left[C(S)n(n+1)\right] \left[2zS(S+1) - (z-1)n(n+1)\right] = 0. \tag{A.2}$$

The analytic form of $\lambda(T)$ can be determined only for the special case $S = \frac{1}{2}$ and $z = 6$, where we have:

$$\lambda\beta = \operatorname{arch}\left\{\left[1+\left(1+\left[1+\exp\left(-2C\left(\frac{1}{2}\right)T_c/T\right)\right]^2\right)^{\frac{1}{2}}\right] \times \right.$$
$$\left. \times \left[2\left(1+\exp\left(-2C\left(\frac{1}{2}\right)T_c/T\right)\right)\right]^{-1}\right\}. \tag{A.3}$$

For $S > \frac{1}{2}$, Eqs (A.1) and (A.2) have to be solved numerically. The values of the parameters amount to $C(\frac{1}{2}) = 0.549306$; $C(1) = 0.169505$; $C(3) = 0.086257$; $C(2) = 0.052877$. The temperature-dependence of $z\lambda\beta$ and $z\lambda$ is shown in Figs 7*a* and *b*, respectively.

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