increased $\Delta\omega_E$, since $m_\parallel$ is the resultant effective mass of the electrons and holes, and is therefore determined by the smallest of these masses. Thus the most favorable case for observing this effect is one in which the effective mass is small and the forbidden zone is not too wide (of the order of 1 — 2 ev), so that the relative value of the shift $\Delta\omega_E/\omega_0$ is not too small. The origin of this effect is analogous to the self-ionization which causes widening in the lines of atomic spectra. This case was considered by Lanczos, in whose work[4] it is shown that spectral lines which are separated from the series limit by a frequency $\Delta\omega$ widen and merge into a comlex spectrum when the applied field satisfies the condition $\Delta\omega_E \sim \Delta\omega$. The basic qualitative difference between the two cases is that in crystals this shift has nothing at all to do with the existence of any discrete lines corresponding to bound states of electrons or holes, much less to any broadening of such lines. Furthermore, the cases most suitable for the observation of the effect are those in which such states are completely absent, i.e., when the field E is so strong that $\hbar\Delta\omega_E$ is greater than the binding energy, and consequently bound states are practically non-existent. Under the opposite conditions,[5] the picture is similar to the one put forward by Lanczos.

Obviously there will be an analogous shift of the lower threshold which corresponds to absorption with the formation of phonons.

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[1] V. W. Houston, Phys. Rev. **57**, 184 (1940).

[2] G. Dresselhaus, Phys. Rev. **105**, 135 (1957).

[3] L. V. Keldysh, J. Exptl. Theoret. Phys. (U.S.S.R.) **33**, 994 (1957), Soviet Phys. JETP **6**, 763 (1958).

[4] C. Lanczos, Z. Physik **62**, 518 (1930).

[5] E. F. Gross, Progress Phys. Sciences **63**, 575 (1957).

Translated by D. C. West
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DEPENDENCE OF THE HYPERFINE STRUCTURE OF F CENTERS ON THE ORIENTATION OF A CRYSTAL IN AN EXTERNAL MAGNETIC FIELD

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The spin Hamiltonian for the interaction between an F-center electron and the angular momenta of the first and second coordinational spheres surrounding the nuclei have been obtained by using the continual and orbital models of F centers in KCl-type lattices. The dependence of the frequency of spin-nuclear transitions on the orientation of the crystal in an external static magnetic field is considered. Comparison of theory with experiment leads to a satisfactory agreement between the angular dependences and (to order of magnitude) of the spin-Hamiltonian coefficient. The square of the F-center wave function in the potassium and chlorine sites of the lattice have been determined by comparison with experiment.

1. The spin-electron resonance of F center in an ionic crystal was considered in Refs. 1 to 3. The most general form of the spin Hamiltonian was obtained in Ref. 4 for the interaction between the localized electron in the crystal and the momenta of the surrounding nuclei. The same reference gives also the spin Hamiltonian of the F center with allowance for the interaction between the electron of the F center and the nuclei of the first coordinational sphere. It was emphasized in Refs. 2 to 4 that the spin Hamiltonian has an anisotropy which, as indicated, should cause the parameters of the

spin-resonance absorption band to depend on the orientation of the crystal in an external static magnetic field.

In a recently published article, Feher[5] was able to resolve the lines due to a change in orientation of the spins of the individual nuclei surrounding the F center upon absorption of radio waves. It has been indicated in the same reference that it is possible to explain the experimental results by using the following spin Hamiltonian for the interaction between the electron and one of the nuclei surrounding the F center:

$$\mathscr{H}_k = A(\mathbf{I}_k\mathbf{S}) + BI_{zk}S_z + Q'\left[I_{zk}^2 - \frac{1}{3}I_k(I_k+1)\right]. \qquad (1)$$

Here S and I_k are the respective spins of the electron of the F center and of the nucleus in the k-th site; A and B are phenomenological coefficients of the hyperfine interaction, and Q' is the coefficient of quadrupole interaction. The coefficients in (1) were determined by Feher from comparison of the frequencies obtained from (1) with the experimental values.

If the quadrupole interaction is disregarded, the Hamiltonian (1) is contained, as a particular case, in the general spin Hamiltonian obtained in Ref. 4. What is important, however, is the fact that in Refs. 2 to 4 it was possible to calculate the coefficients of the spin Hamiltonian theoretically. Using the results of these works, we shall derive below a general form for the spin Hamiltonian of the hyperfine interaction between the F-center electron and the magnetic momenta of the nuclei of the first and second coordinational spheres. An investigation of the anisotropy of the spin-Hamiltonian coefficients leads to good agreement with the results of Feher's experiments.

2. The general form of the spin Hamiltonian of the interaction of a localized electron in a crystal with the magnetic moment of the k-th nucleus of the lattice is of the form[4]:

$$\mathscr{H}_k = 4\pi\frac{\mu\mu_k}{SI_k}\,|\psi(\rho_k=0)|^2(\mathbf{I}_k\mathbf{S}) + \sum_{p,q}A_{pqk}I_{pk}S_q, \qquad (2)$$

where ψ is the electron wave function, while μ and μ_k are the Bohr magneton and the magnetic moment of the nucleus in the k-th site respectively; p and q represent the rectangular coordinate axis and assume values from 1 to 3;

$$A_{pqk} = \frac{\mu\mu_k}{SI_k}\int\frac{x_{qk}}{\rho_k^3}\frac{\partial|\psi|^2}{\partial x_{pk}}\,dV. \qquad (3)$$

Here x_{qk} is the q-th component of the radius vector $\boldsymbol{\rho}_k$ drawn to the point from the k-th lattice site.

We shall henceforth take into account the most important interaction, that with the nuclei of the first and second coordinational spheres. We shall choose the rectangular system of coordinates (x_{1k}, x_{2k}, x_{3k}) in such a manner that its center is in the k-th site, and the x_{3k} axis is directed along the radius vector $\mathbf{R}_k$ drawn from the F center to the k-th site.

The form of the ψ function depends on the model of the F center. In the case of the continual model (method of effective mass[6] and strong-coupling approximation) we have

$$\psi = \varphi(r)\sum_k c_k\psi_k(\rho_k),$$

where $\varphi(r)$ is the smoothed wave function, spherically symmetrical about the lattice defect, and $\psi_k(\rho_k)$ are the atomary 4s-functions of K and Cl^-. If we make allowance in ψ for the contribution of the ions of the first and second coordinational spheres, and also of the contribution of the central ion Cl^- (the last component), we have

$$\psi = \varphi(r)\left[c_1\sum_{i=1}^{6}\psi_i(\rho_i) + c_2\sum_{i=7}^{18}\psi_i(\rho_i) + c_3\psi_0(r)\right].$$

In the orbital model of the F center[7] we have

$$\psi = c_1\sum_{i=1}^{6}\psi_i(\rho_i) + c_2\sum_{i=7}^{18}\psi_i(\rho_i),$$

where, as in the preceding case, the first sum contains the wave functions of the alkali atoms of the first coordinational sphere, and the second sum contains the corresponding functions of Cl^{--} (Ref. 8). We note that the functions ψ are even with respect to x_{1k} and x_{2k} in both models.

Let us consider first the hyperfine interaction between the F-center electron and one of the nuclei of the first coordinational sphere. In this case the axes of the local system of coordinates are directed along the principal crystallographic axes, and the coordinates x_{1k} and x_{2k} enter in an identical manner in $|\psi|^2$ and ρ_k. A consequence of the evenness of $|\psi|^2$ and ρ_k with respect to x_{1k} and x_{2k} is the vanishing of all coefficients A_{pqk} with $p \neq q$. Next, since x_{1k} and x_{2k} enter into $|\psi|^2$ and ρ_k in an identical manner, $A_{11} = A_{22}$. The non-vanishing coefficients are $A_{11} = A_{22}$ and A_{33}.

From (2) and (3) we have

$$\begin{aligned}\mathscr{H}_k = 4\pi\frac{\mu\mu_k}{SI_k}|\psi(\rho_k=0)|^2(\mathbf{I}_k\mathbf{S}) + A_{11}(I_{x_{1k}}S_{x_{1k}} + I_{x_{2k}}S_{x_{2k}})\\ + A_{33}I_{x_{3k}}S_{x_{3k}} = A(\mathbf{I}_k\mathbf{S}) + B(\mathbf{I}_k\mathbf{R}_k)(\mathbf{S}\mathbf{R}_k),\end{aligned} \qquad (4)$$

where

$$A = \frac{\mu\mu_k}{SI_k}\left[4\pi|\psi(\rho_k=0)|^2 + \int\frac{x_{1k}}{\rho_k^3}\frac{\partial|\psi|^2}{\partial x_{1k}}\,dV\right],$$

$$B = \frac{\mu\mu_k}{R_k^2 SI_k}\int\left(x_{3k}\frac{\partial|\psi|^2}{\partial x_{3k}} - x_{1k}\frac{\partial|\psi|^2}{\partial x_{1k}}\right)\frac{1}{\rho_k^3}dV. \tag{5}$$

We note that when A and B are calculated, for example with the aid of the continual model, use is made of integrand components containing two-center functions of the type $\varphi^2(r)\psi_i^2(\rho_i)$ (Refs. 3, 4) and the like.

Let us examine the spin Hamiltonian of the hyperfine interaction between the F-center electron with the chlorine nucleus of the second coordinational sphere. The x_{3k} axis of the local system of coordinates will now be oriented along one of the twelve (110) directions, the x_{2k} axis along another similar direction, and the x_{1k} axis will be directed along one of the (100) crystallographic axes. In this case all the coefficients A_{ppk} are different. The coefficients A_{pqk} with $p \neq q$ vanish as before (the evenness of the ψ functions with respect to x_{1k} and x_{2k}). Thus, if k denotes the number of the chlorine nucleus of the second coordination sphere

$$\mathcal{H}_k = 4\pi\frac{\mu\mu_k}{SI_k}|\psi(\rho_k = 0)|^2(\mathbf{I}_k\mathbf{S}) + A_{11}I_{x_{1k}}S_{x_{1k}} + A_{22}I_{x_{2k}}S_{x_{2k}}$$
$$+ A_{33}I_{x_{3k}}S_{x_{3k}} = A'(\mathbf{I}_k\mathbf{S}) + B'(\mathbf{I}_k\mathbf{R}_k)(\mathbf{S}\mathbf{R}_k) + CI_{x_{1k}}S_{x_{1k}}. \tag{6}$$

Here

$$A' = \frac{\mu\mu_k}{SI_k}\left[4\pi|\psi(\rho_k = 0)|^2 + \int\frac{x_{2k}}{\rho_k^3}\frac{\partial|\psi|^2}{\partial x_{2k}}dV\right]$$

$$B' = \frac{\mu\mu_k}{R_k^2 SI_k}\int\left(x_{3k}\frac{\partial|\psi|^2}{\partial x_{3k}} - x_{2k}\frac{\partial|\psi|^2}{\partial x_{2k}}\right)\frac{1}{\rho_k^3}dV,$$

$$C = \frac{\mu\mu_k}{SI_k}\int\left(x_{1k}\frac{\partial|\psi|^2}{\partial x_{1k}} - x_{2k}\frac{\partial|\psi|^2}{\partial x_{2k}}\right)\frac{1}{\rho_k^3}dV. \tag{6a}$$

It is useful to bear in mind the following relation between the coefficients A_{11}, A_{22}, and A_{33}:

$$A_{11} + A_{22} + A_{33}$$
$$= \frac{\mu\mu_k}{SI_k}\int\left(x_{1k}\frac{\partial|\psi|^2}{\partial x_{1k}} + x_{2k}\frac{\partial|\psi|^2}{\partial x_{2k}} + x_{3k}\frac{\partial|\psi|^2}{\partial x_{3k}}\right)\frac{1}{\rho_k^3}dV \tag{7}$$
$$= -\frac{\mu\mu_k}{SI_k}\int \operatorname{grad}\frac{1}{\rho_k}\operatorname{grad}|\psi|^2 dV = -\frac{\mu\mu_k}{SI_k}4\pi|\psi(\rho_k = 0)|^2.$$

If $A_{11} = A_{22}$, a connection is obtained between the coefficients A and BR of Ref. 4. In the general case, however, it follows from (7) that

$$B'R_k^2 = -3\left(A' - \frac{\mu\mu_k}{SI_k}\frac{8\pi}{3}|\psi(\rho_k = 0)|^2\right) - C. \tag{8}$$

In addition, it can be shown that

$$A = \frac{\mu\mu_k}{SI_k}\frac{8\pi}{3}|\psi(\rho_k = 0)|^2 - b.$$

Introducing the notation

$$a = \frac{\mu\mu_k}{SI_k}\frac{8\pi}{3}|\psi(\rho_k = 0)|^2 \tag{9}$$

and taking (8) and (9) into account, we get

$$A' = a - b,$$
$$B'R_k^2 = 3b - C. \tag{10}$$

If C = 0, then (5) and (6) lead to formula (1). Thus, in the case of nuclei of alkaline ions, the Hamiltonian (1) is correctly chosen, and in the case of interaction with the chlorine nuclei, the Hamiltonian (1) of Feher's work must be supplemented with a term $CI_{x_{1k}}S_{x_{1k}}$.

3. Feher observed transitions in which $\Delta S_H = 0$ and $\Delta I_H = \pm 1$ (S_H and I_H are the spin projections on the external static magnetic field H). The frequencies of these transitions are $h\nu = g_n\beta_n H + E_{S_H, I_H} - E_{S_H, I_{H_1}}$, where g_n, β_n are the nuclear g factor and Bohr magneton and E_{S_H, I_H} is the energy of the hyperfine interaction.

Assuming the field H to be in a plane perpendicular to the (001) direction and to make an angle θ with the (100) direction, we obtain for the transition frequencies the expressions given in Tables I and II.

TABLE I

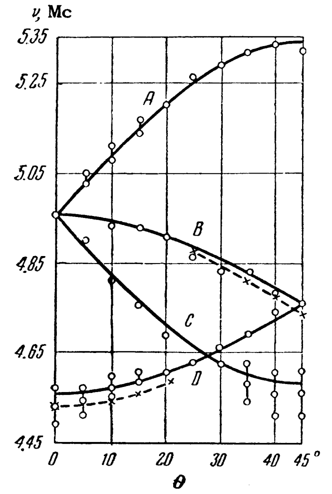
Directions along which the metal ions are located	Transition frequency	No. of ions
(001)	$h\nu = g_n\beta_n H + {}^1/_2 A$	2
(010)	$h\nu = g_n\beta_n H + {}^1/_2 A +$ $+ {}^1/_2 BR^2_K \sin^2\theta$	2
(100)	$h\nu = g_n\beta_n H + {}^1/_2 A +$ $+ {}^1/_2 BR^2_K \cos^2\theta$	2

The angular variations of the frequencies agree with experiment (diagram). Thus, it is seen that when $\theta = 0$ the frequencies ν'_{001}, ν''_{001}, and ν_{010} coincide, and when θ varies from 0 to 45° the frequency ν''_{001} increases and the other two decrease. Further, the frequency ν_{100} is less than the frequency ν_{010} at $\theta = 0$. As θ increases, ν_{100} increases and becomes equal to ν_{010} at $\theta = 45°$.

4. We shall compare quantitatively the angular dependences of Table II with Feher's experimental data. For this purpose it is necessary to determine three parameters. Two of these (A' and $B'R_{Cl}^2$) enter in all four $\nu = \nu(\theta)$ curves, while one parameter, C, is contained in only two curves (ν_{010} and ν_{100}). It is possible to determine A' and $B'R_{Cl}^2$ from the experimental points of one curve,

TABLE II

Direction, perpendicular to the plane in which the chlorine ions are located	Transition frequency	No. of ions	Designations of ions in Ref. 5
(001)	$h\nu'_{001} = g_n\beta_n H + {}^1/_2\ A' + {}^1/_4 B'R^2_{\text{Cl}}(1 - \sin 2\theta)$	2	*C*
(010)	$h\nu''_{001} = g_n\beta_n H + {}^1/_2\ A' + {}^1/_4 B'\ R^2_{\text{Cl}}(1 + \sin 2\theta)$	2	*A*
	$h\nu_{010} = g_n\beta_n H + {}^1/_2\ (A' + C) + {}^1/_4\ (B'R^2_{\text{Cl}} - 2C)\cos^2\theta$	4	*B*
(100)	$h\nu_{100} = g_n\beta_n H + {}^1/_2\ (A' + C) + {}^1/_4\ (B'R^2_{\text{Cl}} - 2C)\sin^2\theta$	4	*D*



while C can be calculated from the experimental data of another curve (all three parameters cannot be determined from one experimental curve). Inserting the values of the parameters thus obtained into the two other functions $\nu = \nu(\theta)$, we can make an independent quantitative comparison with experiment. We have determined the parameters $g_n\beta_n H + A'/2$ and $B'R^2_{\text{Cl}}$ from the experimental points (Ref. 5) of the ν''_{001} curve, and have evaluated C from the points of ν_{100}.

It must be noted that the spread in the experimental data makes it impossible to obtain a sufficiently accurate value of C (diagram).

The above method was used to find the following values for Cl^{35} ($H \approx 3{,}000$ oersteds)

$$A'/h \approx 6.66\,\text{Mc};\quad B'R^2_{\text{Cl}}/h \approx 1.52\,\text{Mc};$$
$$C/h \approx -0.04 \div -0.1\,\text{Mc}. \tag{11}$$

Using (10), we get

$$a/h \approx 7.1\,\text{Mc};\qquad b/h \approx 0.5\,\text{Mc}. \tag{11a}$$

a and b of (11a) coincide approximately with the analogous values obtained by Feher (judging from the values of Ref. 5, the field H was somewhat greater than 3,000 oersteds).

Expression (9) makes it possible to find the value of the wave function of the F center in the sites of the first and second coordination spheres. Denoting by $\psi^2_{\text{F}}(\text{K})$ and $\psi^2_{\text{F}}(\text{Cl})$ the squares of the F-center wave functions in the sites indicated, we get

$$\psi^2_F(\text{K}) \approx 0.70 \cdot 10^{24}\,\text{cm}^{-3};\quad \psi^2_F(\text{Cl}) \approx 0.11 \cdot 10^{24}\,\text{cm}^{-3};$$
$$\psi^2_F(\text{K})/\psi^2_F(\text{Cl}) \approx 6.4 \tag{12}$$

We determined $\psi^2_{\text{F}}(\text{K})$ using the experimental value a/h = 21.6 Mc (Ref. 5) for K^{39}, while $\psi^2_{\text{F}}(\text{Cl})$ was determined from (11a).

Using the orbital model of the F center, and restricting ourselves to the first coordination sphere, we can determine $\psi^2_{\text{K}}(0)$ (the square of the wave function of the 4s state of potassium in the potassium site) in an approximation that does not take into account the overlapping of the functions:

$$\psi^2_K(0) \approx 6\psi^2_F(\text{K}) = 4.2 \cdot 10^{24}\text{cm}^{-3}.$$

Reference 3 contains a method for calculating the coefficients of the spin Hamiltonian (5) in the continual F-center model. According to Ref. 3, and also according to Ref. 9, $A'/A \approx 0.2$, whereas experiment yields $A'/A \approx 0.32$ (A′ and A are the Hamiltonian coefficients for Cl^{35} and K^{39} respectively). A continual-model computation gives lower values of A′/A. This is readily understood since the smoothed F-center wave function $\varphi(r)$ diminishes very rapidly in KCl (small state radii), making the macroscopic approximation inaccurate. For the same reason, the absolute values of A, A′, and BR^2 from (5) and (6a), calculated in the continual model (Refs. 3, 9), agree with experiment only in order of magnitude.

It is interesting to calculate the coefficients of the spin Hamiltonian in the orbital model, where better agreement with experiment can be expected.

Experiment[5] leads to the following value of the ratio $A/BR^2 \approx 7$ for the coefficients of the isotropic and anisotropic terms for K. Calculations using a smoothed F-center wave function of the form $\varphi = (2\beta/\pi)^{3/2}e^{-\beta r^2}$ leads to $A/BR^2 \approx 5$. Better agreement can be obtained between theory and experiment by using a more accurate approximation for the smoothed wave function.[10]

$$\varphi = \frac{\alpha^{3/2}}{\sqrt{7\pi}}(1 + \alpha r)\,e^{-\alpha r}.$$

Let us note, finally, that the frequencies of the spin-nuclear transitions for Cl^{37} are less than the corresponding frequencies for Cl^{35} by approximately a factor of 1.2, which corresponds, within experimental error, to the ratio $\mu_{Cl^{35}}/\mu_{Cl^{37}}$. This should be, according to (5) and (6a).

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[1] Kip, Kittel, Levy, and Portis, Phys. Rev. **91**, 1066 (1953).

[2] M. F. Deigen and L. A. Shul' man Оптика и спектроскопия (Optics and Spectroscopy) **3**, 21 (1957).

[3] M. F. Deigen, J. Exptl. Theoret. Phys. (U.S.S.R.) **33**, 773 (1957), Soviet Phys. JETP **6**, 594 (1958).

[4] V. Ia. Zevin, Оптика и спектроскопия (Optics and Spectroscopy) **3**, 660 (1957).

[5] G. Feher, Phys. Rev. **105**, 1122 (1957).

[6] S. I. Pekar, J. Exptl. Theoret. Phys. (U.S.S.R.) **16**, 933 (1946).

[7] T. Muto, Progr. Theoret. Phys. **4**, 243 (1949); T. Inui and J. Uemura, Progr. Theoret. Phys. **5**, 252, 395 (1950).

[8] K. B. Tolpygo and O. F. Tomasevich, Укр. физ. журн. (Ukrainian Physics J.) **3**, No. 1 (1958).

[9] L. A. Shul' man, Оптика и спектроскопия (Optics and Spectroscopy) (in press).

[10] S. I. Pekar, Исследования по электронной теории кристаллов (Investigations on the Electron Theory of Crystals), GTTI, 1951.

Translated by J. G. Adashko
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POLARIZATION IN HIGH-ENERGY ELASTIC SCATTERING

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A study is made of polarization phenomena in elastic scattering at high energies. It is shown that nuclear beams with considerable polarization can be obtained by small-angle elastic scattering. The applicability of the "black nucleus" and "gray absorbing nucleus" approximations to high-energy p — p scattering is discussed.

1. The present paper contains a discussion of the problem of polarization phenomena at high energies. We determine what peculiarities appear in the polarization phenomena in the approximation in which "diffraction" expressions appear for the scattering cross-sections averaged over the spins, and what sort of information can be obtained from the results of experiments on the polarization at high energies, at which the elastic scattering is to a large extent determined by the presence of inelastic processes.

We consider first the scattering of particles with spin $\frac{1}{2}$ by spinless particles [the case $(0, \frac{1}{2})$].

In most of the published works,* after introducing the effective potential, one makes various assumptions about the radial variation of the potentials, and discusses the results of comparison with the experimental data from the point of view of determining the parameters of the effective potential

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*There are many papers in which polarization phenomena in scattering by nuclei are discussed by the use of the concepts of the optical model. We mention the papers of Riesenfeld and Watson[1] and of Brown,[2] which provide references to other papers. The writer takes occasion to thank Dr. Brown for sending him a number of unpublished notes.