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THEORY OF PARAMAGNETIC RESONANCE OF F CENTERS IN IONIC CRYSTALS

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A theory is developed for the hyperfine interaction of a localized electron with nuclear magnetic moments, displaced by a certain distance from the center of symmetry of the electron wave function. The hyperfine structure of the electron energy levels has been derived. The calculation is performed with the aid of "smoothed" and detailed F-center wave functions. The result enables one to develop a theory of paramagnetic absorption of radio-frequency waves by F-centers. As examples, the shape and width of the absorption lines in KCl and NaCl crystals has been obtained.

1. INTRODUCTION

THE application of the methods of radio-spectroscopy to the investigation of localized electronic centers in dielectrics and semiconductors has led to a series of important new results.¹⁻⁵ In particular, it must be pointed out, that these experiments made it possible for the first time to learn something quantitative about the distribution of the electronic ψ -function in a crystal;⁴ to observe the very small effect of the g-shift¹ (spin-electron resonance); to determine the effective mass tensor⁵ (cyclotron resonance), etc.

The spin-resonance absorption of radio-frequency waves by F-centers in alkali halide crystals has been subjected to a particularly thorough experimental investigation. It was shown that the half-width of the absorption line in these crystals was several tens of oersteds. The intensity curves have a nearly gaussian shape. Attempts to explain such a large half-width of the absorption line by means of the interaction of the magnetic moments of the electrons in the various F-centers were not successful, since, for the F-center concentrations attained in the experiments ($10^{17} - 10^{18} \text{ cm}^{-3}$), this interaction leads to a narrow absorption line, whose half-width is of the order of a few hundredths of an oersted. Kip, Kittel, Levy, and Portis⁴ proposed that the reason for the widening of the absorption line was the interaction of the electron in the F-center with the magnetic moments of the nuclei of the metal ions which surround the missing halogen ion.

As is well known, two models are currently accepted in the theory of F-centers, i.e., the "continuum model" and the "molecular orbital."^{7,8} Application of the orbital model, according to which the wave function of the electron has the form of a linear combination of the wave functions of the atoms surrounding the vacancy, led to the correct order of magnitude for the half-width of the absorption line. In contrast to this, estimates of the half-width based on the continuum model resulted in a disagreement between theory and experiment of from three to four orders of magnitude (in Ref. 4, the disagreement was somewhat less because the authors of that work used the somewhat incorrect model of Simpson,⁹ instead of the results of Refs. 6 and 7). Hence, it was concluded that the continuum model was not valid. As we shall

show, this conclusion is unfounded, because two essential points have been missed in Ref. 4, as follows:

1. In the calculations, the results of Fermi¹⁰ for the hyperfine interaction in the s-state of hydrogen were used. The coupling constant in this case is given by the equation:

$$A_H = (16\pi/3I) \mu \mu' \psi^2(0). \quad (\text{A})$$

Here μ and μ' are the magnetic moments of the electron and nucleus respectively; I is the nuclear spin; $\psi(0)$ is the value of the electron's wave function at the point where the proton is situated. Using this expression, Kip et al. substituted for $\psi(0)$ the value of the wave function at the point where the nearest metal ion is found.

However, the Fermi formula is valid only when the center of symmetry of the wave function coincides with the location of the nucleus. In the case of F-centers, the nuclei of the ions are displaced with respect to the center of symmetry of the wave function by the lattice constant. Thus, the wave function does not have spherical symmetry with respect to the ions, and Fermi's formula should not be applied. Therefore, to calculate the spin-resonance broadening correctly, one must construct a theory for the hyperfine interaction between the electron and the magnetic moments of the nuclei displaced by a certain distance from the center of symmetry of the F-center's wave function.

2. The potential for the spin-nuclear interaction is not smooth. Therefore, the calculation of physical effects from such a potential requires that one use detailed functions⁷ rather than the "smoothed" functions used in Ref. 4. This point is indicated in Ref. 11, without, however, any special grounds.

In what follows, we shall develop a theory for the spin-resonance broadening of the electromagnetic emission from F-centers with the help of the observations described above. The continuum model of F-centers and the effective mass method of Pekar^{12,13} are used.

In Sec. 2, the hyperfine interaction between a localized electron in an applied static magnetic field, and the magnetic moments of several nuclei, displaced with respect to the center of symmetry of the electron's wave function, is considered. For this analysis, "smoothed" electron functions are used. In Sec. 3, a similar calculation is performed for detailed wave functions, which permits one to construct a theory for the shape of the paramagnetic resonance absorption line associated with the absorption of radio-frequency waves by F-centers.

2. HYPERFINE INTERACTION OF THE S-ELECTRON WITH THE MAGNETIC MOMENTS OF DISPLACED NUCLEI ("SMOOTHED" F-CENTER FUNCTIONS)

We shall limit ourselves to the Pauli approximation to describe the behavior of the electron, as well as that of the nucleus. In Ref. 14, it is shown that a very general calculation, in which Darwin's relativistic approximation is used to describe the behavior of electrons, leads to the same results.

The energy operator for the interaction between a localized electron and the magnetic moment of the ionic nuclei can be written in the form:

$$\hat{U} = \mu \frac{S}{S} \sum_j H_j, \quad (1)$$

Here H_j is the contribution to the magnetic field from the nucleus of the j -th ion

$$H_j = (\mu_j / I_j) \text{curl curl} (\mathbf{I}_j / \rho_j), \quad (2)$$

where μ_j and I_j are the magnetic moment and the spin of the j -th ion; ρ_j is the distance between the j -th nucleus and the electron. Expanding $1/\rho_j$ into a Fourier series

$$\frac{1}{\rho_j} = \frac{1}{2\pi} \int e^{ik_j \rho_j} \frac{dk_j}{k_j^2} \quad (3)$$

and using (1) and (2), we find

$$\hat{U} = 4\pi \frac{\mu}{S} S \sum_j \delta(\rho_j) \frac{\mu_j}{I_j} \mathbf{I}_j - \frac{1}{2\pi^2} \frac{\mu}{S} \sum_j \frac{\mu_j}{I_j} \int (\mathbf{I}_j \mathbf{k}_j) (\mathbf{S} \mathbf{k}_j) e^{ik_j \rho_j} \frac{dk_j}{k_j^2}. \quad (4)$$

The wave function of the system, Ψ , depends on the rectilinear coordinate, r , of the electron, and on the spin coordinates of the electron, s , and of the nucleus, s_j . In the zero order approximation, when the hyperfine interaction is ignored, Ψ can be written in the form of a product:

$$\Psi(r, s, s_j) = \psi(r) \chi(s) \prod_j \chi'(s_j). \quad (5)$$

Forming the matrix of the operator of Eq. (4) with the rectilinear part of the wave function (5), we obtain the operator for the hyperfine interaction, \hat{W} , depending only on the spins of the electron and of the nuclei

$$\hat{W} = 4\pi \frac{\mu}{S} S \sum_j \frac{\mu_j}{I_j} \mathbf{I}_j \psi^2(R_j) - \frac{1}{2\pi^2} \frac{\mu}{S} \sum_j \frac{\mu_j}{I_j} \int (\mathbf{I}_j \mathbf{k}_j) (\mathbf{S} \mathbf{k}_j) e^{-i\mathbf{k}_j \mathbf{R}_j} \frac{\alpha \mathbf{k}_j}{k_j^2} \cdot \int e^{i\mathbf{k}_j \mathbf{r}} \psi^2(r) d\tau. \quad (6)$$

Here R_j is the distance from the center of symmetry of the wave function to the j -th nucleus.

The second term in (6) can be put in the form

$$\frac{1}{2\pi^2} \frac{\mu}{S} \sum_j \frac{\mu_j}{I_j} \sum_{m,n} I_{jn} S_m \frac{\partial^2}{\partial R_{jm} \partial R_{jn}} F(R_j).$$

The indices m and n signify the components x , y and z . Using as the form of the F-center wave function the expression

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

we obtain

$$F(R_j) = \frac{2\pi^2}{R_j} \left[1 - e^{-2\alpha R_j} \left(1 + \frac{19}{14} \alpha R_j + \frac{5}{7} \alpha^2 R_j^2 + \frac{1}{7} \alpha^3 R_j^3 \right) \right]. \quad (8)$$

In crystals in which the radius of the F-center wave function is not much greater than the lattice constant, one can sum over j in (6) by limiting oneself to the first coordination sphere. In a lattice like NaCl this means summation over six metallic ions, which are closest to the vacancy, all located at the same distance R from the center of the vacancy. In this case \hat{W} simplifies to

$$\hat{W} = AS \sum_{j=1}^6 \mathbf{I}_j + BS \sum_{j=1}^6 R_j (\mathbf{I}_j \mathbf{R}_j), \quad (9)$$

$$A = \frac{\mu\mu'}{SIR^3} \left[-1 + e^{-q} \left(1 + q + \frac{q^2}{2} + \frac{3}{14} q^3 + \frac{5}{56} q^4 + \frac{1}{56} q^5 \right) \right], \quad (10)$$

$$BR^2 = \frac{3\mu\mu'}{SIR^3} \left[1 - e^{-q} \left(1 + q + \frac{q^2}{2} + \frac{q^3}{6} + \frac{q^4}{24} + \frac{q^5}{168} \right) \right],$$

$$q = 2\alpha R.$$

If the z axis coincides with the direction of an applied static magnetic field, \hat{W} can be transformed into the form

$$\hat{W} = \hat{S}_z \sum_{j=1}^6 \Delta_j (\hat{I}_{jx} \cos \alpha_j + \hat{I}_{jy} \cos \beta_j + \hat{I}_{jz} \cos \gamma_j), \quad (11)$$

$$\Delta_j = \sqrt{A^2 + B(2A + BR^2)R_{jz}^2}, \quad \cos \alpha_j = \frac{BR_{jz}R_{jx}}{\Delta_j}, \quad \cos \beta_j = \frac{BR_{jz}R_{jy}}{\Delta_j}, \quad \cos \gamma_j = \frac{A + BR_{jz}^2}{\Delta_j} \quad (12)$$

or

$$\hat{W} = \hat{S}_z \sum_{j=1}^6 \Delta_j \hat{I}_{jn_j}, \quad (13)$$

where n_j are orthogonalized direction cosines defined by (12).

If we form the matrix of the operator \hat{W} with the spin part of the same function (5), we determine the terms of the hyperfine structure

$$W = S_z \sum_{j=1}^6 \Delta_j I_j, \quad (14)$$

where S_z has the same meaning as the spin operator of the electron and I_j is equivalent to $I_j n_j$. As seen from (14) and (15), the energy of the hyperfine interaction depends on the orientation of the magnetic field with respect to the crystal axes. To estimate the maximum width of the spin resonance broadening we apply a magnetic field along one of the crystallographic axes of the crystal and

$$W = S_z \left[A \sum_{j=1}^6 I_j + (A + BR^2) \sum_{j=1}^2 I_j \right] \quad (15)$$

The effective magnetic field, corresponding to the maximum value of W_m , is found to be equal to

$$h = W_m/\mu. \quad (16)$$

Numerical calculations show that for alkali-halide crystals the maximum width $\delta = 2h$ is equal to 1–2 Oersted.

Thus, it has already been shown that taking into account the first of the conditions enumerated in Part 1 leads to an increase by a factor from 10 to 20 of the line width as compared to the estimates made in Ref. 4. This increase in width is not, however, sufficient to bring the theory into agreement with the experiments.

3. PARAMAGNETIC RESONANCE OF F-CENTERS (DETAILED FUNCTIONS)

Equation (6) for the operator of the hyperfine interaction also permits one to proceed with a calculation using detailed wave functions. The latter are written in the following way:

$$\psi(r) = \Omega^{1/2} \varphi u, \quad (17)$$

where φ is the smoothed F-center wave function [Eq. (7)], is the normalized Bloch wave function of the electron at the bottom of the conduction band and Ω is the volume of the fundamental cell of the crystal.

In crystals, in which $\varphi^2(r)$ decreases comparatively rapidly as the distance from the vacancy increases (alkali halides have this property), after substituting (17) into (6), the summation over j is sufficiently accurate if it is limited to the ions in the first coordination sphere (the metal ions). No essential difficulty is introduced if one does the calculation while taking into account the ions in subsequent coordination spheres.

Using the tight binding approximation, the Bloch function u can be written as a linear combination of atomic wave functions. For crystals of the type KCl, these will be, obviously, the atomic functions of potassium (ψ_s) and of the chlorine ion (ψ_q)

$$u = C \left[\sum_s \psi_s + C_1 \sum_q \psi_q \right]. \quad (18)$$

Here C is a normalization constant. The constant C_1^2 , from the evaluation conducted in Ref. (4), is less than unity (in KCl it is approximately 1/6). Summation over s and q is extended over all positive and negative lattice points, respectively.

Substitution of (18) and (17) into (6) and neglecting small triple overlap integrals leads to the following result:

$$\begin{aligned} \hat{W} = & \Omega C \frac{\mu}{S} \hat{S} \sum_j \frac{\mu_j}{I_j} \left\{ 4\pi \hat{I}_j \varphi^2(R_j) \left[\sum_s \psi_s^2(R_j) + C_1^2 \sum_q \psi_q^2(R_j) \right] \right. \\ & \left. - \frac{1}{2\pi^2} \int (\mathbf{I}_j \mathbf{k}_j)(\mathbf{S} \mathbf{k}_j) e^{-i\mathbf{k}_j \mathbf{R}_j} \frac{d\mathbf{k}_j}{k_j^2} \int e^{i\mathbf{k}_j \mathbf{r}} \varphi^2(r) \left[\sum_s \psi_s^2 + C_1^2 \sum_q \psi_q^2 \right] d\tau \right\}. \end{aligned} \quad (19)$$

In Eq. (19), in view of the rapid attenuation of $\varphi^2(r)$ the second and fourth terms are considerably smaller than the first and third. This is true also for the case of a central halogen ion, $q = 0$, (an ion, in an uncolored crystal, replaces the vacancy). In fact, one should substitute the value of the wave function at the point $r = R_j$ into the second term (where R_j is the point at which the metal ion is located). Nevertheless, in view of the rapid attenuation of atomic functions (e.g., the ion Cl^{-}) this term, as has been shown by calculation, at a distance equal to the lattice constant, is considerably less than the terms of the first sum. Numerical calculations show, that even in the integral the main contribution is made by the terms which depend on the wave functions of the metal atoms, and the terms containing ψ_q^2 can be neglected.

Taking all this into account, and also normalizing (18), \hat{W} can be rewritten as follows:

$$\hat{W} = \frac{\mu\mu'}{SI} 4\pi\Omega_0 \varphi^2(R) \psi^2(R) \sum_{j=1}^6 S \mathbf{I}_j - \frac{1}{2\pi^2} \frac{\mu\mu'}{SI} \Omega_0 \sum_{j=1}^6 \sum_{s=1}^6 \int \frac{d\mathbf{k}_j}{k_j^2} (\mathbf{I}_j \mathbf{k}_j)(\mathbf{S} \mathbf{k}_j) e^{-i(\mathbf{k}_j \mathbf{R}_j)} \int e^{i\mathbf{k}_j \mathbf{r}} \varphi^2(r) \psi_s^2(r) d\tau. \quad (20)$$

Here Ω_0 is the volume of the elementary cell of the crystal.

To perform approximate numerical calculations, one replaces $\varphi^2(r)$ in Eq. (20), by the functions of Eq. (7), and $\psi_s^2(r)$ is replaced by the Hartree free-atom wave functions for potassium in KCl and sodium in NaCl.

Performing the integration in Eq. (20) is especially convenient, if φ^2 and ψ_s^2 are approximated by sums

of gaussian exponentials:

$$\psi_s^2 = \frac{1}{4\pi} \sum_p a_p e^{-\alpha_p r^2}, \quad \varphi^2 = \frac{\alpha^3}{7\pi} \sum b_x e^{-\beta_x r^2} \quad (21)$$

($\rho = \mathbf{r} - \mathbf{R}$). The error associated with the approximation in the integration interval does not exceed 7%, if the summation in the first sum is restricted to ten terms for KCl and seven terms for NaCl and to three terms for both crystals in the second summation.

Cumbersome, but in principle not difficult calculations, lead to the following expression for \hat{W} :

$$\hat{W} = (a + A_0 + A_1 + A_2) \sum_{j=1}^6 \hat{S}_z \hat{I}_{jz} + (B_0 + B_1 + B_2) \sum_{j=1}^6 \hat{S}_z \hat{R}_{jz} (\mathbf{I}_j \mathbf{R}_j) + \frac{1}{4} B_2 \sum_{j=1}^6 \sum_{s=1}^4 \hat{S}_z \mathbf{R}_{jz} (\mathbf{I}_j \mathbf{R}_s). \quad (22)$$

Here

$$a = 4\pi \frac{\mu\mu'}{ST} \Omega_0 \varphi^2(R) \psi^2(R), \quad (23)$$

$$A = n_i K \sum_{p,x} a_p b_x \exp \left\{ -\frac{\alpha_p \beta_x R^2}{\alpha_p + \beta_x} \right\} \left[\frac{\Phi'(t_i)}{t_i^2} - \frac{\Phi(t_i)}{t_i^3} \right], \quad (24)$$

$i = 0, 1, 2$; $n_0 = n_1 = 1$; $n_2 = 4$ and $\Phi(t)$ are Kramp's functions

$$t_0 = \frac{\beta_x R}{\sqrt{\alpha_p + \beta_x}}; \quad t_1 = \frac{2\alpha_p + \beta_x}{\sqrt{\alpha_p + \beta_x}}, \quad t_2 = R \sqrt{\frac{\alpha_p^2 + (\alpha_p + \beta_x)^2}{\alpha_p + \beta_x}}.$$

$$B_0 R^2 = K \sum_{p,x} a_p b_x \exp \left\{ -\frac{\alpha_p \beta_x R^2}{\alpha_p + \beta_x} \right\} \left[\frac{\Phi''(t_0)}{t_0} - \frac{3\Phi'(t_0)}{t_0^2} + \frac{3\Phi(t_0)}{t_0^3} \right],$$

$$B_1 R^2 = K \sum_{p,x} a_p b_x \exp \left\{ -\frac{\alpha_p \beta_x R^2}{\alpha_p + \beta_x} \right\} \left[\frac{3\Phi(t_1)}{t_1^3} - 2\Phi'(t_1) \left(1 + \frac{3}{2t_1^2} \right) \right], \quad (25)$$

$$B_2 R^2 = 4K \sum_{p,x} (\alpha_p + \beta_x) R^2 a_p b_x \exp \left\{ -\frac{\alpha_p \beta_x R^2}{\alpha_p + \beta_x} \right\} \left[\frac{\Phi''(t_2)}{t_2^3} - \frac{3\Phi'(t_2)}{t_2^4} + \frac{3\Phi(t_2)}{t_2^5} \right]; \quad K = \frac{\mu\mu'}{ST} \frac{\Omega_0 \alpha^3}{28\sqrt{\pi}}.$$

In Eqs. (24) and (25) A_0 and B_0 are the contribution of terms corresponding to $j = s$; A_1 and B_1 are the contributions from the nucleus opposite the j -th ion and finally, A_2 and B_2 are the contributions of nuclei located in a plane perpendicular to \mathbf{R}_j .

The operator (22) resembles the operator (9) and its eigenvalues can be determined, in the same way as in Sec. 2 (the last term in (22) does not complicate the calculation).

As has been shown by numerical calculation, the terms A_1 and $B_1 R^2$ are smaller than a in alkali halide crystals. Furthermore, A_1 and A_2 , B_1 and B_2 are considerably smaller than A_0 and B_0 respectively. Therefore for these crystals Eq. (22) simplifies as follows

$$\hat{W} = (a + A_0) \sum_{j=1}^6 \hat{S}_z \hat{I}_{jz} + B_0 \sum_{j=1}^6 \hat{S}_z \hat{R}_{jz} (\hat{\mathbf{I}}_j \mathbf{R}_j). \quad (26)$$

In complete analogy with Eqs. (11) and (14), the eigenvalues of Eq. (26) can be written in the form

$$W = S_z \sum_{j=1}^6 \Delta_j I_j, \quad (27)$$

$$\Delta_j = \{(a + A_0)^2 + B_0 R_{jz}^2 [2(a + A_0) + B_0 R^2]\}^{1/2}, \quad (28)$$

S_z and I_j have the same meaning as in Eq. (14). Hence, it follows, that the hyperfine interaction energy, and therefore, the half-width of the spin-resonance absorption band, must depend on the magnitude of the angle between an externally applied static magnetic field and the crystallographic axis. The shape of the line, according to Eq. (27), differs slightly from a gaussian, since I_j contains coefficients which are functions of the size of the nucleus. Calculations show that this effect is not large in crystals of high symmetry (lattices like NaCl), but they can be, generally speaking, significant in crystals with other symmetries.

From the above it follows that, in alkali halide crystals, the shape of the paramagnetic absorption line, in agreement with experiment, is nearly gaussian. For these crystals

$$W \approx S_z (a + A_0) \sum_{j=1}^6 I_j. \quad (29)$$

Using Eq. (29) it is readily shown that the effective magnetic field, h_0 , corresponding to the half width of the absorption line turns out to be equal to

$$h_0 \approx 3.37 (a + A_0)/\mu. \quad (30)$$

Equation (30) leads to the following values: h_0 (KCl) = 8 Oersted; h_0 (NaCl) = 13 Oersted. These values are still several times smaller than the corresponding experimental ones. This difference is explained not so much by failure to include additional coordination spheres, as by failure to satisfy the criteria of the macroscopic approximation in KCl and other alkali halide crystals. Because of this, the value of the wave function $\varphi(r)$ turns out to be decreased at the point $r = R$.

If for purposes of evaluation, one proceeds as in Ref. 4 to make use of the value of ψ_S^2 at zero, which value is carried over from radio-frequency spectroscopic data (following this procedure, however, as is well known, causes the value of $\psi_S^2(0)$ to be underestimated with respect to its Hartree value), h_0 turns out to be 15 Oersted. The experimental value of h_0 is 52 Oersted. Similar results are also obtained for NaCl.

Thus, the continuum model of the F-center leads to theoretically values of the half-width of the absorption line which coincide with corresponding experimental values within an order of magnitude.

I wish to express my gratitude to Prof. S. I. Pekar for his interest in this work.

Note added in proof (August 26, 1957). In a recently published paper, Feher discovered experimentally a dependence of the frequency of nuclear-spin transitions of the ions, surrounding an F-center, which has been saturated by the absorption of radio-frequency waves, on the orientation of the crystal in an external magnetic field.

All the qualitative and quantitative properties of the phenomenon are described by the Hamiltonian of Eq. (22). In particular, it is readily shown, that the spin Hamiltonian can be written in the form

$$\hat{W} = A \sum_{j=1}^6 (S I_j) + B \sum_{j=1}^6 (S R_j) (I_j R_j),$$

where the second anisotropic term indeed leads to the reported angular dependence.

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