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Hyperfine Interactions in *F* Centers*

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A method of calculating the magnetic and quadrupole hyperfine interactions of an electron with neighboring and next nearest neighboring nuclei in the vacancy model of the *F* center and the change in its spectroscopic splitting factor are presented and carried out in the case of KCl. Two wave functions are used for the *F* electron in this calculation, one obtained from a point-charge treatment of the crystal lattice and the other from a square-well approximation of the vacancy. The results are shown to be nearly the same for these two widely different approximations and are found to be in good qualitative agreement and even fair quantitative agreement with experimental data of Feher and Kip *et al.*

I. INTRODUCTION

RECENT magnetic resonance experiments of Lord and Jen[1,2] and of Feher[3] have conclusively shown that the vacancy model of the *F* center is the correct one. Several authors[4] have obtained theoretical wave functions for this model. Among the early workers were Tibbs, Simpson, and Krumhansl and Schwartz, all of whom used a central-field wave function in a potential that was constant within the vacancy but corresponded to that for a point charge in a continuous dielectric medium outside the vacancy. Various degrees of corrections were introduced for polarization effects due to the action of an effective charge at the vacancy and the *F*-center electron. Muto, and Inui and Uememura later made a LCAO calculation where they took account of the detailed nature of the electron distribution on the neighboring ions in estimating the potential field for the *F*-center electron. Kahn and Kittel[5] and others have used this model for an interpretation of some of the early results of electron resonance measurement, particularly the departure of the spectroscopic splitting factor *g* from the free-electron value and the second moments of electron resonance lines. None of these wave functions without modification give very good qualitative agreement with recent experiments of Feher on the hyperfine interaction of the *F*-center electron with the nearest and next nearest neighboring nuclei.

Recently Gourary and Adrian[6] have made a detailed analysis of the vacancy model. They compute the potential about the *F* center, using a point-charge model for the lattice. By a group-theoretical procedure, they separate the various Kubic harmonic components of the potential. They do not assume a continuum model outside the vacancy as was done by most previous authors. They then solve the Schrödinger equation for the *F*-center electron in this potential by a variational procedure. This will be referred to as the type *A* wave function (type III in the notation of Gourary and Adrian). See Fig. 1. They conclude that if overlaps of the *F*-center electron with electrons on neighboring ions is neglected, the ground state has almost one hundred percent *s* character with negligible admixture of *g* character. However, they point out that in calculating the expectation values of various operators describing the interaction of the *F* electron with neighboring nuclei, one must take into account the overlaps between the *F* electron and the orbitals on the ions by a many-electron technique. An alternative way of taking into account the overlap terms is to make the *F*-center orbital orthogonal to the neighboring orbitals by the Schmidt orthogonalization procedure as pointed out by Löwdin.[7] We shall later see that this gives rise to an appreciable fraction of *g* character in the ground state. Gourary and Adrian have subsequently considered polarization and lattice-distortion effects and show them to have small influence on the *F*-electron wave function.

The spherically symmetrical part of the potential used by Gourary and Adrian has a constant negative value in a spherical region, the radius of which is the lattice constant. There might be some objection to the use of a wave function obtained from this potential, since the only real vacancy is the size of the missing Cl⁻

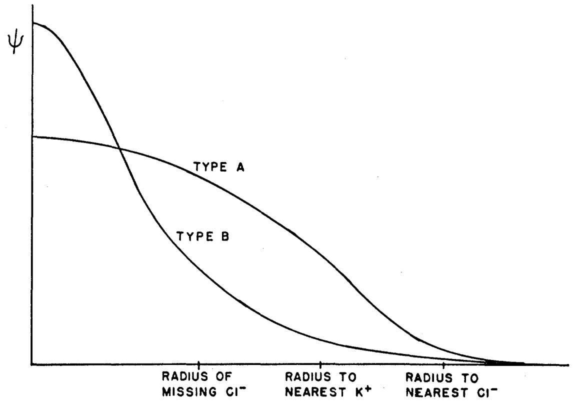

FIG. 1. Graphs of the type *A* and *B* wave functions. The ordinate scale is not the same for the two functions.

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[1] N. W. Lord, Phys. Rev. **105**, 756 (1957).

[2] N. W. Lord and C. K. Jen, Bull. Am. Phys. Soc. Ser. II, **1**, 12 (1956).

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

[4] F. Seitz, Revs. Modern Phys. **26**, 7 (1954), Sec. 23.

[5] A. Kahn and C. Kittel, Phys. Rev. **89**, 315 (1953).

[6] B. S. Gourary and F. J. Adrian, Phys. Rev. **105**, 1180 (1957).

[7] Per-Olov Löwdin, J. Chem. Phys. **18**, 365 (1950).

ion, together with the interstitial space in a unit cell, which has about 50% of the volume of the spherical hole in the potential used by Gourary and Adrian. Thus, for comparison purposes, an arbitrary wave function was chosen which was similar in appearance to the wave function of a particle in a spherical square well the size of the Cl⁻ ion and having the Madelung depth, $\psi_F = e^{-0.6r} - 0.6e^{-r}$, which will be referred to as the type B wave function. (See Fig. 1.) The form of the function was chosen for ease in performing the calculations which are to be described. The calculations based on this wave function are for comparative purposes only and are not to be taken as quantitatively meaningful.

The aim of this paper is to show that there is very good qualitative agreement and, in some cases, a fair quantitative agreement between the various quantities predicted from the type A wave function and the magnetic-resonance data and that the agreement is essentially insensitive to the form of the wave function with which we start.

Feher[3] used the spin Hamiltonian,

$$\mathcal{H} = \sum_\alpha a_\alpha \mathbf{I}_\alpha \cdot \mathbf{S} + \sum_\alpha b_{zz\alpha}(3I_{z\alpha}S_z - \mathbf{I}_\alpha \cdot \mathbf{S}) + \sum_\alpha Q_{zz\alpha}'(3I_{z\alpha}^2 - \mathbf{I}_\alpha^2), \quad (1)$$

to describe the magnetic and electrical hyperfine interaction of the nuclei adjacent to the vacancy, with the F-center electron and the effective positive charge at the vacancy. The z axis is taken in the direction of the applied magnetic field. The form of the anisotropic interactions is taken to be axially symmetric about the line joining the vacancy to nucleus α, so that

$$b_{zz\alpha} = b_\alpha(3\cos^2\theta_H - 1)/2,$$

$$Q_{zz\alpha}' = Q_\alpha'(3\cos^2\theta_H - 1)/2,$$

where θ_H is the angle between the applied magnetic field and the axis of symmetry. From his double-resonance measurements, Feher determined the magnitudes of the hyperfine constants a_α, b_α, and Q_α' for the nearest K^+ and Cl⁻ ions in KCl.

Section II of this paper will deal with the procedure employed in our calculations and a comparison with the experimental data. Section III will include an analysis of the sources of error in the calculations and possible reasons for disagreement with the experimental data. Finally, we shall point out how these calculations suggest improvements which may be made in any subsequent calculation of F-center wave functions.

II. PROCEDURE AND RESULTS

The Hamiltonian describing the magnetic hyperfine interaction between the F electron and a nucleus α is given by[8]

$$\mathcal{H}_\alpha^{\mathrm{hfs}} = \frac{2\beta\mu_\alpha}{I_\alpha}\left[\frac{8\pi}{3}\mathbf{I}_\alpha \cdot \mathbf{S}\delta(r_\alpha) + \frac{3\mathbf{S}\cdot\mathbf{r}_\alpha \mathbf{I}_\alpha\cdot\mathbf{r}_\alpha}{r_\alpha^5} - \frac{\mathbf{S}\cdot\mathbf{I}_\alpha}{r_\alpha^3}\right], \quad (2)$$

where β is the Bohr magneton, μ_α and $\mathbf{I}_\alpha$ are the magnetic moment and spin of nucleus α, $\mathbf{S}$ is the spin momentum of the electron, and $\mathbf{r}_\alpha$ is the position coordinate measured from nucleus α. To get the a and b terms in the spin Hamiltonian of Eq. (1), we must take the expectation value of $\mathcal{H}_\alpha^{\mathrm{hfs}}$ over the F-electron wave function ψ_F. It is easily shown that

$$a_\alpha = \frac{16\pi\beta\mu}{3I_\alpha}\langle\psi|\delta(r_\alpha)|\psi\rangle, \quad (3)$$

$$b_\alpha = \frac{\beta\mu_\alpha}{I_\alpha}\left\langle\psi\left|\frac{3\cos^2\theta_\alpha - 1}{r_\alpha^3}\right|\psi\right\rangle, \quad (4)$$

where θ_α is the angle between the radius vector of the electron from the nucleus α and the line joining α to the vacancy.

The wave functions we shall use for the F electron are of the form

$$\psi_F = \frac{\varphi_F - \sum_{\alpha,i}\langle\alpha_i|F\rangle\psi_{\alpha i}}{[1 - \sum_{\alpha,i}\langle\alpha_i|F\rangle^2]^{\frac{1}{2}}}, \quad (5)$$

where φ_F refers to the F-electron wave function (type A or B) before it is made orthogonal to the orbitals of the neighboring ions, and $\psi_{\alpha i}$ refers to electron i on ion α. This orthogonalization procedure[7] can be shown to be equivalent to taking an antisymmetrized determinantal wave function of all the relevant electrons since the operators we are considering are all one-electron operators. More rigorously, the F-electron wave function should have been made orthogonal to both the neighboring K⁺ and Cl⁻ ions before the variational calculation was carried out by including in the Hamiltonian the effects of the detailed potentials and exchange.

If we consider that the orbitals of one ion do not overlap those of other ions appreciably, we get, in cps,

$$\begin{aligned} a_\alpha/h = \frac{16\pi\beta\mu_\alpha}{3I_\alpha N^2 h}[&\langle F|\delta(r_\alpha)|F\rangle - 2\langle\alpha_{3S}|F\rangle\langle F|\delta(r_\alpha)|\alpha_{3S}\rangle \\ &+ \langle\alpha_{3S}|F\rangle^2\langle\alpha_{3S}|\delta(r_\alpha)|\alpha_{3S}\rangle \\ &+ 2\langle\alpha_{3S}|F\rangle\langle\alpha_{2S}|F\rangle\langle\alpha_{3S}|\delta(r_\alpha)|\alpha_{2S}\rangle \\ &+ \text{similar terms in } \alpha_{1S} \text{ and } \alpha_{2S}], \end{aligned} \quad (6)$$

$$\begin{aligned} b_\alpha/h = \frac{2\beta\mu_\alpha}{I_\alpha N^2 h}[&\langle F|g_\alpha|F\rangle - 2\langle\alpha_{3p}|F\rangle\langle F|g_\alpha|\alpha_{3p}\rangle \\ &+ \langle\alpha_{3p}|F\rangle^2\langle\alpha_{3p}|g_\alpha|\alpha_{3p}\rangle \\ &+ 2\langle\alpha_{3p}|F\rangle\langle\alpha_{2p}|F\rangle\langle\alpha_{3p}|g_\alpha|\alpha_{2p}\rangle \\ &+ \text{similar terms in } \alpha_{2p}], \end{aligned} \quad (7)$$

where g_α stands for the operator $(3\cos^2\theta_\alpha - 1)/r_\alpha^3$ and N represents the normalization factor of Eq. (5). It is clear that to obtain a_α and b_α one must evaluate the various one- and two-center integrals in the brackets of

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[8] See for example, H. A. Bethe, in *Handbuch der Physik* (Springer-Verlag, Berlin, 1933), Vol. 24, Part 1, p. 385.

Eqs. (6) and (7). It happens in this problem that the first two terms in the brackets of Eqs. (6) and (7) are qualitatively insignificant. For example, in the case of a_K these contribute respectively 0.06 and -2.3 Mc/sec, compared to a total of 34 Mc/sec. In the calculations using the type B wave function, the first two terms were omitted. It will be noted that the terms which make the greatest contribution were introduced as a result of the Löwdin orthogonalization procedure which we have used. Results of the magnetic hyperfine calculations are shown in Table I.

To obtain the quadrupole coupling constants for the K^{39} and Cl^{35} nuclei, it is necessary to calculate the electric field gradients at the positions of these nuclei. The field gradient at the nucleus arises from the combined action of the effective positive charge at the vacancy and the F electron. The calculation of this field gradient is somewhat complicated by the fact that the vacancy charge and the F electron act not only directly on the nucleus but indirectly through the quadrupole deformation of the electron shells of the ion containing the nucleus. This leads to shielding factors of the type considered by Sternheimer[9] and Bersohn.[10] The field gradient due to the vacancy is given by $(2e/R_\alpha^3)(1-\gamma_\infty)$ where γ_∞ is the shielding factor and has been found by Wikner[11] to be -13.5 for K^+ and -49.2 for Cl^- (i.e., there is antishielding in both cases). The field gradient due to the F electron acting directly on the nucleus would be

$$-(e/N^2)[\langle F|g_\alpha|F\rangle-2\langle F|\alpha_{3p}\rangle\langle F|g_\alpha|\alpha_{3p}\rangle +\langle F|\alpha_{3p}\rangle^2\langle\alpha_{3p}|g_\alpha|\alpha_{3p}\rangle+\text{similar terms in }\alpha_{2p}], \quad (8)$$

where we have not taken into account the effects of the antishielding. Only the first field-gradient term in Eq. (8) is subject to appreciable antishielding because the principal contributions to the others occur from the region within the ionic radius of ion α. The term $\langle F|g_\alpha|F\rangle$ has to be multiplied by a suitable factor $(1-\gamma_F)$. We expect γ_F to be somewhat smaller in magnitude than γ_∞, as the F electron is not entirely external to the ion α. We shall assume that γ_F is equal to γ_∞ reduced by the fraction of $\langle F|g_\alpha|F\rangle$ which is external to ion α (considered as a sphere of radius equal to the ionic radius). Thus we have, in cps,

$$Q_{zz\alpha}'/h=\frac{3e^2Q_\alpha}{4I(2I-1)h}\left\{\frac{2}{R_\alpha^3}(1-\gamma_\infty)-\frac{1}{N^2}[\langle F|g_\alpha|F\rangle(1-\gamma_F) +\text{unshielded }\langle g_\alpha\rangle\text{ terms}]\right\}. \quad (9)$$

TABLE I. Magnetic hyperfine interactions.

		K^+	Cl^-
a/h, Mc/sec	Type A	34	10.4
	Type B	38	9.7
	Experimental	21.6	7.0
b/h, Mc/sec	Type A	0.99	0.13
	Type B	0.81	0.30
	Experimental	0.95	0.50

TABLE II. Quadrupole hyperfine interactions.

		K^+	Cl^-
Q_{zz}'/h, Mc/sec	Type A	-0.23	$+0.053$
	Type B	-0.42	$+0.15$
	Experimental	±0.2	⋯
Q_{xx}'/h, Mc/sec	Type A	$+0.11$	-0.026
	Type B	$+0.21$	-0.075
	Experimental	∓0.1	±0.032
Q_{yy}'/h, Mc/sec	Type A	-0.11	-0.026
	Type B	-0.21	-0.075
	Experimental	∓0.1	±0.045

It is seen from Eq. (9) that essentially the same integrals are needed in the evaluation of Q' as in the case of b. Results of the nuclear quadrupole-interaction calculations are presented in Table II.

The procedure employed in evaluating the various integrals involved in Eqs. (6), (7), and (9) will now be described. The value of $\langle F|g_\alpha|F\rangle$ can be obtained in a straightforward manner by expressing $\cos\theta_\alpha$ and r_α in terms of polar coordinates about the vacancy. The cross integrals $\langle F|\alpha\rangle$ and $\langle F|g_\alpha|\alpha\rangle$, however, present some difficulty. The classical method of expanding ψ_F in terms of spherical harmonics about α cannot be used as it leads to elliptic integrals. Rather than approximate the functional form of the spherical harmonic expansion, it was found simpler to approximate the functional form of $\langle F|\alpha\rangle$ and $\langle F|g_\alpha|\alpha\rangle$ directly. This was accomplished by making a Taylor expansion,

$$\psi_F(r,0,0)=\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\partial^n\psi_F}{\partial r^n}\bigg|_{R_\alpha}r_\alpha^n, \quad (10)$$

about α, where $\theta_\alpha=0$ is chosen as before along the line $F-\alpha$, and R_α is the distance from the vacancy to α. Then $\psi_F(r_\alpha,\theta_\alpha,\varphi)$ can be obtained in the neighborhood of α by replacing r_α with

$$\delta=R_\alpha\left[\left(1+\frac{r_\alpha^2}{R_\alpha^2}-\frac{2r_\alpha}{R_\alpha}\cos\theta_\alpha\right)^{\frac{1}{2}}-1\right],$$

which is approximated by $r_\alpha[\cos\theta_\alpha-(r_\alpha/2R_\alpha)\sin^2\theta_\alpha]$. The geometrical significance of δ will be apparent from Fig. 2. Thus, with

$$\psi_F(r_\alpha,\theta_\alpha,\varphi)=\sum_{n=0}^{\infty}\frac{1}{n!}\frac{\partial^n\psi_F}{\partial r^n}\bigg|_{R_\alpha} \times r_\alpha^n\left(\cos\theta_\alpha-\frac{r_n}{2R_\alpha}\sin^2\theta_\alpha\right)^n \quad (11)$$

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[9] R. M. Sternheimer, Phys. Rev. **95**, 736 (1954).

[10] T. P. Das and R. Bersohn, Phys. Rev. **102**, 733 (1956).

[11] E. G. Wikner and T. P. Das, Phys. Rev. **109**, 360 (1958).

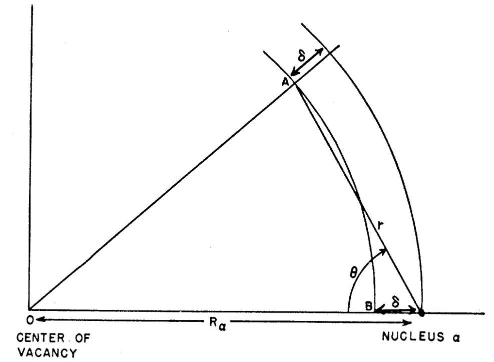

FIG. 2. Geometry of the Taylor expansion of ψ_F. Since ψ_F is spherically symmetric about 0, it has the same value at B as at A. Thus $\psi(r,\theta)=\psi(\delta,0)$.

expressed in powers of r_α, $\cos\theta_\alpha$, and $\sin\theta_\alpha$, the required integrations are straightforward. The first three or four terms of this series were found sufficient to provide satisfactory convergence.

Since ψ_F is a rapidly changing function within the ionic radius of the nearest K$^+$ neighbors, one cannot use for ψ_K the Slater functions which are usually employed in molecular calculations, since they represent only the peripheral regions of the ions satisfactorily. We therefore used Löwdin's[12] analytic approximations of the SCF functions in our calculations. At the nearest Cl$^-$ sites, ψ_F changes slowly, so less accurate wave functions may be used for ψ_{Cl}.

The shift in the spectroscopic splitting factor g was computed by a second-order perturbation calculation using the perturbing Hamiltonian[13]

$$\mathcal{H}=-\frac{e\hbar}{2mc}\mathbf{H}\cdot\mathbf{L}+\sum_\alpha\frac{e\hbar^2}{2m^2c^2}\frac{1}{r_\alpha}\frac{\partial u}{\partial r_\alpha}\mathbf{L}\cdot\mathbf{S}, \tag{12}$$

where the zero-order Hamiltonian for the electron is $P^2/2m+eU$. By assuming an average excitation energy E_F (the F-band energy), one can compute the energy change due to the perturbation by standard matrix multiplication. The part of this second-order energy which is linear in H and M_S may be expressed as $\Delta g\beta HM_S$, where M_S is taken along H. This gives

$$\Delta g=-\frac{e\hbar^2}{m^2c^2E_F}\sum_\alpha\left\langle\psi_F\left|\frac{1}{r_\alpha}\frac{\partial U}{\partial r_\alpha}L_{z\alpha}{}^2\right|\psi_F\right\rangle. \tag{13}$$

We may write this approximately as[14]

$$\Delta g\cong\frac{2}{E_FN^2}\sum_{\alpha,i}\langle F|\alpha_i\rangle^2\left[\frac{e\hbar^2}{2mc^2}\left\langle\alpha_i\left|\frac{1}{r_\alpha}\frac{dU}{dr_\alpha}L_{z\alpha}{}^2\right|\alpha_i\right\rangle\right]. \tag{14}$$

These matrix elements are essentially $\lambda_\alpha\langle\alpha_i|L_z{}^2|\alpha_i\rangle$, where λ_α is the spin-orbit coupling constant for electron i on ion α. For λ_α we have used 2162 cm^{-1} and 881 cm^{-1}, respectively, for $3p$ K^{++} and $3p$ Cl as obtained from optical data.[15] The evaluation of these matrix elements is invariant with respect to orientation of the magnetic field. Thus the [100] orientation may be used, where it will be seen that $\langle\alpha_{3p}|L_z{}^2|\alpha_{3p}\rangle$ is zero for two of the nearest neighbor K$^+$ and unity for the other four. For the nearest Cl$^-$ it is $\frac{1}{2}$ for eight of them and unity for the other four. The various values of Δg are presented in Table III.

III. DISCUSSION

It will be noted from Table I that there is good qualitative agreement between the experimental values and the values calculated from both type A and type B wave functions. The results for both types of wave function agree surprisingly well in view of the large difference in their functional form. It is therefore seen that the results do not depend in an accidental way upon the detailed nature of the particular wave function used.

As has been mentioned, the a interaction depends primarily upon the term involving the density of ionic orbitals at the nucleus. These values, which were obtained from Hartree and Hartree[16,17] SCF calculations, do not necessarily give the most accurate measure of the electron densities at the nuclei.

An important point to note in connection with the b_{Cl} interaction is that Feher observed it to be axially symmetric about the line joining the vacancy and the Cl$^-$ ion. Had there been contributions to b_{Cl} from the electronic wave functions of the neighboring K$^+$ ions which we admixed with ψ_F, the observed axial symmetry would not have been found.

For the same reasons, we expect that this model of the F center would lead to an axially symmetric quadrupole interaction. This is observed to be the case for the K$^+$ interaction, and the qualitative agreement between Q_{zz}' as observed by Feher and our values is satisfactory. For Cl$^-$ the value of Q_{zz}' was not definitely determined by Feher. If we assume that $Q_{xx}'=Q_{yy}'=-\frac{1}{2}Q_{zz}'$, we obtain values of Q_{xx}' and Q_{yy}' which are essentially in agreement with experiment. Both calculations for Q' depend upon the difference between two comparable

TABLE III. Shift in the spectroscopic splitting factor.

Type A	-0.0071
Type B	-0.0072
Experimental	-0.007

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[12] P. Löwdin and K. Appel, Phys. Rev. **103**, 1746 (1956).

[13] F. J. Adrian, Phys. Rev. **107**, 488 (1957).

[14] Here we have neglected the terms $\langle\psi_F|L_z{}^2|\psi_F\rangle$ and $\langle\psi_F|L_z{}^2|\psi_\alpha\rangle$ for the same reasons as advanced in the case of the magnetic hyperfine constants.

[15] C. E. Moore, *Atomic Energy Levels*, National Bureau of Standards Circular No. 467 (U. S. Government Printing Office, Washington, D. C., 1949).

[16] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A156**, 45 (1936).

[17] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A166**, 450 (1938).

numbers and thus suffer somewhat in accuracy. However, it must be noted that if one does not consider the antishielding effects of the electron in detail, the calculated values of the quadrupole hyperfine constants will be grossly in error. For example, if the Sternheimer factor is applied only to the resultant field gradient at the nucleus due to the vacancy charge and the electron, one obtains $Q_{zz}'/h \cong 5$ Mc/sec for K^+, which is too large by a factor of 25.

It is possible that the observed asymmetry in Q' arises from an anisotropic distortion of the lattice in the region of the Cl ions which has not been taken into account in this idealized vacancy model. Another possibility is that the contributions to the field gradient at Cl ions from the regions of overlap with its nearest neighbor ions may be appreciable compared to the various terms in Eq. (9). Since the Cl ion is only on a two-fold symmetry axis passing through the vacancy, the contributions from the overlap regions could possibly lead to an asymmetry in the field gradient.

The numerical agreement of Δg with the experimental value[18] is not to be taken seriously in view of the approximations involved, but it does in fact strongly support the present approach to the problem. The procedure we have used is not rigorous in that there is no way to take into account terms containing the quantities $\langle \alpha_i | (1/r_\alpha)(dU/dr_\alpha) L_{z\alpha}^2 | \alpha_j \rangle$. A better method of calculating Δg has been given by Adrian,[13] but this requires the use of experimental magnetic hyperfine data. The procedure given here has the advantage that it can be used in cases where magnetic hyperfine data are not available.

We have found that both type A and type B wave functions, after normalization, contain about 64% s character when expanded about the vacancy. The remaining 36% is almost all of g character. This is essentially in agreement with the amount of g character which Seitz[19] estimated earlier.

The result of these calculations definitely shows the applicability of the Löwdin orthogonalization process to the calculation of the hyperfine constant of F centers. It would be desirable to repeat this calculation (perhaps in a more rigorous manner) for a wave function obtained in the same manner as the type A wave function, using, however, a potential which would take into account the detailed ionic potentials of the nearest and next nearest neighbors and also the effects of exchange. The net energy term arising from an inclusion of detailed ionic potentials and exchange is positive and, for a given ion, roughly proportional to $\psi_F^2(\alpha)$ at the nucleus. Thus, inclusion of this energy term in the variational calculation will tend to reduce $\psi_F^2(\alpha)$, improving the agreement between the calculated and experimental values for the isotropic magnetic hyperfine interaction a. However, these approximate wave functions, as orthogonalized, are a definite improvement over previous treatments in that they show at least qualitative agreement with all the currently observed magnetic resonance and quadrupole interaction data in KCl.

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

[19] See reference 4, Sec. 22.