Letters to the Editor

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F-Center Wave Functions and Electronic *g*-Values in KCl Crystals*

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RECENTLY Hutchison and Noble[1] have observed electronic spin resonance in a KCl crystal colored with excess K. The resonance is believed to be associated with *F*-centers, but one cannot without confirmatory experiments exclude the possibility of contributions from other types of centers.[2] They observed the splitting factor $g=1.995\pm0.001$, which differs from the free electron $g=2.0023$ by $\Delta g=-0.007\pm0.001$. This shift, although small, has significant implications for the angular dependence of the ground state of the *F*-center electron. We show below that it is not possible to account for the order of magnitude of the shift using the standard theoretical model[3] of an *S*-electron in a central field. The shift Δg may, however, be explained approximately if the ground state has predominantly *G*-character, or if we use a molecular orbital wave function representing the excess electron as shared among the cations which bound the vacancy. The two models are closely related, but the molecular orbital viewpoint is perhaps more attractive on general grounds.

The spin-orbit interaction to the first order of perturbation theory gives $\Delta g=0$ if the ground state has *S*-character. The nonspherical components of the potential energy arise in large part from the charges of the six K^+ ions adjacent to the vacancy; these components mix the ground state with functions having $L=4$ and higher. Writing the additions as $\psi_G{}^M$, an improved ground-state function may be written

$$\psi'=\psi_S'+b(\psi_G{}^4+\psi_G{}^{-4}), \tag{1}$$

and the lowest excited state of interest here is expected to have the form

$$\psi''=\psi_S''+c(\psi_G{}^4-\psi_G{}^{-4}). \tag{2}$$

We neglect $\psi_G{}^0$ and terms with $L>4$. Both ψ' and ψ'' have $\Delta g=0$.

The spin-orbit interaction $\lambda\mathbf{L}\cdot\mathbf{S}$ will mix some ψ'' in ψ'. If for simplicity we set $b=c$, then for the perturbed ground state

$$\Delta g\cong-\frac{64b^2}{(1+2b^2)^2}\cdot\frac{\lambda}{\Delta}, \tag{3}$$

where Δ is the energy separation between the two states considered. We may safely assume that Δ is of the order of 1 ev, but it is more difficult to estimate λ. If we suppose that the $\psi_G{}^4$ function is chiefly concentrated about a circle passing through four of the K^+ ions surrounding the vacancy, we estimate $\lambda\approx10^{-17}$ erg, where the effective potential is taken as e^2/r with r measured from the center. Then $\lambda/\Delta\approx10^{-5}$, and in the limit $b\gg1$ we have $\Delta g\approx-2\times10^{-4}$. For $b=0.1$, $\Delta g\approx-6\times10^{-8}$, which is much too small.

We must thus suppose that there is a strong mixture of *G*-function in the ground state; there is no other possibility of accounting for the observed Δg value. The difference between the calculated maximum $\Delta g\approx-2\times10^{-4}$ and the observed $\Delta g\approx-7\times10^{-3}$ may not be significant in view of the considerable uncertainties surrounding the estimate of λ made above. The estimate using Eq. (7) below is closer, however.

It thus appears that we might use a *G*-function as a starting approximation rather than an *S*-function. The lowest energy *G*-function[4] in the cubic potential of the six K^+ ions is nondegenerate and transforms as $x^4+y^4+z^4$, as does also the molecular orbital,

$$\Psi=\sum_{i=1}^{6}\psi_i, \tag{4}$$

proposed by Muto,[5] and Inui and Uemura,[6] for the *F*-center ground state. Here ψ_i is the wave function of the valence electron when on the ith of the six neighboring K^+ ions.

On the molecular orbital model the important spin-orbit effects arise through the electrostatic polarization of the K atoms by the vacancy. The ground state of the valence electron on the K atom is normally pure $4s$, but the unsymmetrical electrical field associated with the vacancy will polarize the K atom, thus mixing a large amount of $4p$ function into the ground state. The polarized ground-state function for the atom on the positive x side of the vacancy is

$$\psi_1=\psi_S-(\epsilon/\sqrt{2})(\psi_P{}^1-\psi_P{}^{-1}). \tag{5}$$

The axis of quantization is taken along the $z$axis. The other ψ_i will be composed of similar mixtures of $4s$ and $4p$ functions, taken in such a way as to possess electric dipole moments in the direction of the vacancy. Spin-orbit interaction with the other $4p$ states will partially lift the quenching of the angular momenta of the atoms in the $x-y$ plane. In the presence of spin-orbit interaction $\lambda\mathbf{L}\cdot\mathbf{S}$, we have to first order

$$\psi_1=\psi_S-\frac{\epsilon}{\sqrt{2}}\psi_P{}^1\left(1+\frac{\lambda}{2\Delta}\right)+\frac{\epsilon}{\sqrt{2}}\psi_P{}^{-1}\left(1-\frac{\lambda}{2\Delta}\right). \tag{6}$$

The change in the g-factor for the *F*-center will then be

$$\Delta g=-\frac{4}{3}\frac{\lambda}{\Delta}\cdot\frac{\epsilon^2}{1+\epsilon^2}. \tag{7}$$

From the $4p$ doublet splitting of the K atom we obtain $\lambda=38$ cm^{-1}. For Δ we use the $4s-4p$ separation, which is close to the *F*-band energy. With hydrogenic wave functions we estimate $\epsilon=0.9$, which is consistent with an estimate on the basis of polarizability of a K atom. We find $\Delta g=-1.7\times10^{-3}$, of the correct order of magnitude, but somewhat too small. It would be raised somewhat by considering higher states.

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[1] C. A. Hutchison, Jr., and G. A. Noble, Phys. Rev. **87**, 1125 (1952); for earlier work see C. A. Hutchison, Jr., Phys. Rev. **75**, 1769 (1949); M. Tinkham and A. F. Kip, Phys. Rev. **83**, 657 (1951).
[2] *V*-centers may probably be excluded, as they might be expected to have a g larger than the free electron value; because of the strong spin-orbit interaction in a chlorine atom, we estimate $\Delta g\approx0.1$ for a *V*-center in KCl.
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[4] H. A. Bethe, Ann. Physik **3**, 133 (1929); see p. 166.
[5] T. Muto, Prog. Theoret. Phys. **4**, 243 (1949).
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A Suggested Scheme for Meson Production

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A MASS of facts[1–8] is rapidly accumulating concerning the existence of two classes of particles, the first with masses intermediate between the π-meson and the proton, and the second with masses greater than the proton. Unsystematized, these facts tend to present a confusing appearance to a casual inspection. The purpose of this note is to suggest a classification of all observed particles, based on the properties of first-order wave equations, and the existence, already suggested from several quarters,[9] of isobaric excited states of the nucleon, and to propose a model for the structure of the nucleon.