

of the matrix elements determined by the above prescription gives agreement with the 21.7 Mev $N^{14}-N^{14}$ data with $S_L S_{Se} = e^{2i\delta_L}(\delta_L \text{ complex})$ as shown in Fig. 1 and Tables I and II. Of course these results should not be taken too seriously in themselves as uniqueness is not claimed. The further calculations mentioned above should tighten the considerations, and analysis of the mounting heavy ion scattering data at different energies should provide much more rigorous tests for the method of analysis. The above considera-

tions seem to justify the feasibility of this approach which is less extreme than that of the cutoff and optical models and emphasizes the role of the nuclear surface in the phenomena.

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Magnetic Moment of Fe^{57}

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An electron-nuclear double resonance study has been made on the spectrum of neutral iron atoms in silicon. These measurements lead to a value of $+0.0903 \pm 0.0007$ nm for the magnetic moment of Fe^{57} .

A STUDY of the electron spin resonance spectrum of neutral iron atoms in silicon¹ has confirmed that the nuclear spin of Fe^{57} is $\frac{1}{2}$. The present note describes electron-nuclear double resonance measurements² on that spectrum which lead to a value of $+0.0903 \pm 0.0007$ nm for the magnetic moment of Fe^{57} .

The spin Hamiltonian appropriate to $(Fe^{57})^0$ in silicon is

$$\mathcal{H} = g\beta\mathbf{S} \cdot \mathbf{H} + A\mathbf{S} \cdot \mathbf{I} - g_I'\beta_N\mathbf{H} \cdot \mathbf{I}, \quad (1)$$

where the electronic g factor and the hyperfine interaction parameter A are isotropic. The parameter g_I' is an effective nuclear g factor which also is isotropic. As will be discussed later, the electronic g departs from the free electron value (2.0023) and g_I' departs from the nuclear g factor ($\mu/I\beta_N$) if excited electronic states are present which must be taken into account.³ To second order in the hyperfine interaction, the frequency f of the (M, m) to $(M, m-1)$ electron-nuclear double resonance transition is

$$hf = |AM - g_I'\beta_N H| - [M(2m-1) + S(S+1) - M^2]A^2/2h\nu, \quad (2)$$

where M and m are the quantum numbers specifying the orientation of the electron spin S and the nuclear spin I , respectively, and ν is the klystron frequency. Terms higher order in A are negligible for interpretation of the results.

¹ Ludwig, Woodbury, and Carlson, Phys. Rev. Letters 1, 295 (1958).

² G. Feher, Phys. Rev. 114, 1219 (1959); G. Feher, C. S. Fuller, and E. A. Gere, Phys. Rev. 107, 1462 (1957).

³ See, for example, J. M. Baker and B. Bleaney, Proc. Roy. Soc. (London) A245, 156 (1958).

Some resonance parameters⁴ for $(Fe^{57})^0$ in silicon are given in Table I. Since $S=1$ and $I=\frac{1}{2}$, there are three possible electron-nuclear double resonance transitions. An average of several measurements gives the following values: $f=20.943 \pm 0.6925$ Mc/sec for $M=\pm 1$; $f=0.7096$ Mc/sec for $M=0$ ($\nu=14$, 115.4 Mc/sec; $H=4868.6$ gauss). Using all three double resonance frequencies, it is possible to determine from Eq. (2) both the sign and the magnitude of g_I' . Taking $g_I'>0$, one calculates that $g_I'=0.1828 \pm 0.0002$ from the low-frequency transition and $g_I'=0.1824 \pm 0.0009$ from the two high-frequency transitions; the two determinations agree within the experimental error. If, however, g_I' is assumed less than zero, the two determinations differ by 0.009, showing that $g_I'>0$. Thus $g_I'=+0.1828 \pm 0.0002$ for $(Fe^{57})^0$ in silicon.

We believe that the ground-state wave function of $(Fe^{57})^0$ is an orbital singlet. The observations that the resonance lines are sharp at temperatures as high as 78°K and that the electronic g factor is close to the free

TABLE I. Some resonance parameters for several iron spectra in silicon. The hyperfine interaction parameter A is expressed in units of 10^{-4} cm⁻¹. g_I' is an effective nuclear g factor; its sign was determined only for $(Fe^{57})^0$.

Species	S	g	$ A $	g_I'
$(Fe^{57})^0$	1	2.0699	6.984	$+0.1828 \pm 0.0002$
$(Fe^{57})^+$	$\frac{3}{2}$ or $\frac{1}{2}$	3.524	2.985	0.1976 ± 0.0018
$(Fe^{57}Ga^{71})^0$	$\frac{1}{2}$	5.089(∥); 2.530(⊥)	1.438(∥); 4.108(⊥)	0.2071 ± 0.0008

⁴ A more complete discussion of the spectra of iron and other transition metals in silicon has been prepared. H. H. Woodbury and G. W. Ludwig, Phys. Rev. 117, 102 (1960).

electron value support this view. Assuming that one is dealing with an orbital singlet one can use second order perturbation theory, in the manner of Abragam and Pryce,⁵ to calculate the effect of excited electronic states on the electronic g factor. As they show, $g_{ij} = 2.0023\delta_{ij} - 2\lambda\Lambda_{ij}$, where λ is the spin-orbit coupling constant and $\Lambda_{ij} = \sum_{n \neq 0} \langle 0 | L_i | n \rangle \langle n | L_j | 0 \rangle / (E_n - E_0)$. For the case of present interest $\Lambda_{ij} = 0$ for $i \neq j$, $\Lambda_{ii} = \Lambda_{jj} = \Lambda$, and $g = 2.0023 - 2\lambda\Lambda$. Abragam and Pryce omitted (as generally small) the corresponding perturbation of the nuclear g factor. One finds $g_I' = g_I + 2p\Lambda(\beta/\beta_N)$, where $p = 2g_I\beta\beta_N\langle r^{-3} \rangle$. Combining the equations for g and g_I' , the nuclear g factor can be calculated from the effective nuclear g factor and the departure of the electronic g factor from the free electron value:

$$g_I = g_I' - (2.0023 - g)p\beta/\lambda\beta_N. \quad (3)$$

The spectra of several (interstitial) transition metals in silicon are consistent with the hypothesis that in the crystal the $4s$ electrons are transferred to the $3d$ shell, e.g., that the electron configuration of neutral iron is $3d^8$. Using the Lande interval rule, $\lambda \simeq -127 \text{ cm}^{-1}$ for this configuration of the free atom.⁶ To evaluate p , $\langle r^{-3} \rangle$ was calculated from wave functions of Watson⁷ for the $3d^8$ configuration of neutral iron. The value obtained for $\langle r^{-3} \rangle$, 3.9 atomic units, may be compared with the experimental value, 4.3 atomic units, obtained by interpolation from Table 2 of Abragam, Horowitz, and Pryce.⁸ Taking $\langle r^{-3} \rangle$ as 4 atomic units, one finds from Eq. (3) that g_I is 1.2% lower than g_I' , or

⁵ A. Abragam and M. H. L. Pryce, Proc. Roy. Soc. (London) **A205**, 135 (1951).

⁶ C. E. Moore, *Atomic Energy Levels*, National Bureau of Standards Circular No. 467, August 15, 1952 (U. S. Government Printing Office, Washington, D. C. 1952), Vol. 2.

⁷ R. E. Watson, Technical Report No. 12, Solid-State and Molecular Theory Group, Massachusetts Institute of Technology, June 15, 1959 (unpublished).

⁸ A. Abragam, J. Horowitz, and M. H. L. Pryce, Proc. Roy. Soc. (London) **A230**, 169 (1955).

$g_I = +0.1806 \pm 0.0013$, $\mu = +0.0903 \pm 0.0007 \text{ nm}$ for Fe⁵⁷, where an uncertainty of 50% has been assigned to the calculation of the correction term.⁹

Supporting evidence that the above analysis gives an accurate value of g_I for Fe⁵⁷ is furnished by measurements on (Mn⁵⁵)⁻ in silicon,⁴ which is isoelectronic with (Fe⁵⁷)⁰. Analysis of the electron-nuclear double resonance data gives $g_I' = 1.386 \pm 0.002 \text{ nm}$ for (Mn⁵⁵)⁻. Taking $g = 2.0104$, $\lambda = -127 \text{ cm}^{-1}$, $\langle r^{-3} \rangle = 4.0$ atomic units, and using Eq. (3), one finds $g_I = 1.385 \pm 0.002 \text{ nm}$ for Mn⁵⁵, in agreement with the published value.

Electron-nuclear double resonance measurements have also been made on isolated (Fe⁵⁷)⁺ and on neutral (Fe⁵⁷Ga⁷¹) pairs in silicon (see Table I). For (Fe⁵⁷)⁺ two double resonance transitions were observed corresponding to $M = \pm \frac{1}{2}$. These were analyzed using Eq. (2) and lead to $|g_I'| = 0.1976 \pm 0.0018$ for (Fe⁵⁷)⁺. For (Fe⁵⁷Ga⁷¹)⁰ pairs the $M = \pm \frac{1}{2}$ double resonance transitions are readily interpretable only for the magnetic field along the $[111]$ axis of the pair.¹⁰ In this direction $|g_I'| = 0.2071 \pm 0.0008$. In these spectra the electronic g factor is displaced considerably from the free electron value and the ground state may not be an orbital singlet. We have not yet been able to calculate g_I from the measured g_I' for these spectra.

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⁹ Even if the configuration of neutral iron is not $3d^8$, the correction term as calculated in the text probably is in error by less than 50%. For example, for the $3d^6 4s^2$ configuration $\lambda \simeq -100 \text{ cm}^{-1}$ as compared to $\lambda \simeq -127 \text{ cm}^{-1}$ for the $3d^8$ configuration. The assumed value for $\langle r^{-3} \rangle$ is probably correct to within 20%.

¹⁰ See H. H. Woodbury and G. W. Ludwig, following paper.

Magnetic Moment of Au¹⁹⁷

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Chromium-gold and manganese-gold impurity pairs in silicon have been observed by electron spin resonance techniques. Electron-nuclear double resonance studies of the gold hyperfine structure lead to a value of $0.1439 \pm 0.0004 \text{ nm}$ for the magnetic moment of Au¹⁹⁷.

IN the course of a study of chemical impurities in Si by spin resonance techniques, several interesting systems involving Au¹⁹⁷ have been detected. The use of electron-nuclear double resonance has permitted a rather precise determination of the magnetic moment of this nucleus, namely $0.1439 \pm 0.0004 \text{ nm}$.

Spin resonance associated with isolated Au in silicon has not been reported. However, resonant absorption for some of the transition metals has been observed.¹ It has been found that under appropriate conditions

¹ H. H. Woodbury and G. W. Ludwig, Phys. Rev. **117**, 100 (1960).