branch is 374 cm^{-1}.[6] The introduction of the impurity ion may explain the general shift toward lower energy in the doped crystal.

The $SrF_2:Sm^{2+}$ vibronic spectrum also yields a vibrational yield at about 140 cm^{-1}. This may be an acoustic mode but there is insufficient data to make an assignment.

Axe and Sorokin,[8] using the data of Wood and Kaiser, also made an analysis of the vibronic levels in these two crystals. They assumed an XY_8 complex in analogy with the work of Satten *et al.*[9,10] However, Satten's work on the $UC1_6^{=}$ complex showed that the U^{4+} is tightly bound in the complex and interacts mainly with the inner vibrations of this complex. No such complex would be expected in the strongly ionic crystals under consideration here.

[8] J. D. Axe and P. P. Sorokin, Phys. Rev. **130**, 945 (1963).
[9] R. A. Satten, J. Chem. Phys. 29, 658 (1958).
[10] S. A. Pollack and R. A. Satten, J. Chem. Phys. **36**, 804 (1962).

CONCLUSION

It has been shown that a model taking into account vibrations of the entire lattice is able to explain most of the vibronic features observed in $SrF_2:Sm^{2+}$ and $BaF_2:Sm^{2+}$. A model based only on the $k=0$ modes results in fewer transitions than are observed and therefore cannot be correct. An XY_8 complex model is not able to explain as many of the details of the vibronic spectra as simply as does the one presented here, and, in any case, would not be expected to be a reasonable approximation for these crystals.

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Polarization Effects in Slow Neutron Scattering II. Spin-Orbit Scattering and Interference*

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The theory of polarized neutron scattering is extended to include spin-orbit scattering in magnetic substances. The cross section for scattering of a polarized beam includes, in addition to the Schwinger interference term between nuclear and spin-orbit scattering, a polarization-dependent interference term between spin-orbit and magnetic scattering. The latter depends on the real part of the product of magnetic and spin-orbit structure factors, whereas the Schwinger term depends on the imaginary part of the product of the nuclear and spin-orbit structure factors. A calculation shows that this effect should easily be observable in an isotopic mixture of Ni which has no coherent nuclear scattering.

INTRODUCTION

In a recent experiment, Shull[1] has detected the spin-orbit scattering of slow neutrons. This type of scattering was first discussed by Schwinger[2] in connection with the polarization of fast neutron beams. It has since been considered by a number of other authors[3] who have calculated higher order corrections to the Schwinger expression, in the hope of distinguishing these effects from those of the polarizability of the meson cloud of the neutron.

The Schwinger scattering, as measured by Shull, is due to interference between the nuclear and spin-orbit scattering. Because the spin-orbit scattering amplitude is imaginary, this interference term depends on the imaginary part of the nuclear scattering amplitude. In this paper it is shown that in the scattering of neutrons by magnetic substances an interference phenomenon occurs between spin-orbit and magnetic scattering which depends on the real part of the magnetic scattering amplitude. This polarization-dependent term provides an alternate method for the measurement of the spin-orbit scattering amplitude.

The principal interactions of a slow neutron with a solid are the nuclear interaction with the nuclei of the atoms and, in magnetic substances, the interaction of the neutron's magnetic moment with the spin and orbital magnetic moments of the atomic electrons. In addition to these there are a number of others which have, for thermal neutrons, scattering amplitudes of the order of 10^{-3} of the above nuclear and magnetic interactions. These are the magnetic neutron dipole-nuclear dipole interaction, the specific neutron-electron

* Work performed under the auspices of the U. S. Atomic Energy Commission.
[1] C. G. Shull, Phys. Rev. Letters **10**, 297 (1963).
[2] J. Schwinger, Phys. Rev. **73**, 407 (1948).
[3] S. B. Gerasimov, A. I. Lebedev, and V. A. Petrun'kin, Zh. Eksperim. i Teor. Fiz. 43, 1872 (1962) [English transl.: Soviet Phys.—JETP **16**, 1321 (1963)], and other references contained therein.

interaction,[4] and the neutron spin-neutron-orbit interaction. The first of these will produce only incoherent background scattering unless the nuclei are polarized, in which case the effects of the scattering will be the same as those produced by the changes in the coherent nuclear scattering amplitude due to nuclear polarization, so that the probability of observing this directly is small. The second of these, the specific neutron-electron interaction, has been the subject of much experimental and theoretical work.[4] It is a spin-independent interaction so that any interference effects with nuclear scattering will be polarization-independent. In a magnetic material there will be a polarization-dependent interference term between this interaction and the magnetic scattering, but this effect will be of the same form, except for angular dependence, as the nuclear-magnetic interference term, which is generally much larger. Only the third interaction, the spin-orbit scattering, will be considered here. Its physical origin is easily described classically. As the neutron moves through the solid it passes through the electric field of the nuclear and electronic charges. This moving electric field appears in part like a magnetic field which interacts with the neutron magnetic moment and scatters the neutron. We will calculate the scattering due to this field and derive the interference term mentioned above.

SPIN-ORBIT SCATTERING

We will make use of the results and notation of a recent paper[5] on polarization effects in nuclear and magnetic scattering of neutrons. The cross section for elastic scattering in Born approximation is

$$d\sigma/d\Omega'=(m_o/2\pi\hbar^2)^2\,\mathrm{tr}[\langle q|\mathcal{V}^\dagger(\mathbf{k}',\mathbf{k})|q\rangle \times\langle q|\mathcal{V}(\mathbf{k}',\mathbf{k})|q\rangle\rho]. \quad (1)$$

Here ρ is the density matrix for the incident beam, given by Eq. (2) of I, while the operator $\mathcal{V}(\mathbf{k}',\mathbf{k})$ is the Fourier transform of the interaction $V(\mathbf{r})$ between the neutron and the scatterer:

$$\mathcal{V}(\mathbf{k}',\mathbf{k})=\int d\mathbf{r}e^{-i\mathbf{k}'\cdot\mathbf{r}}V(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2)$$

where $\mathbf{k}$ and $\mathbf{k}'$ are, respectively, the initial and final wave vectors of the neutron. The state $|q\rangle$ is the initial state of the scatterer, and the quantum numbers q label the complete electronic and nuclear state of the solid. The final state of the solid is assumed the same as the initial state for the coherent elastic scattering with which we are concerned. The scattering potential $V(\mathbf{r})$ consists of three parts,

$$V(\mathbf{r})=V_N(\mathbf{r})+V_M(\mathbf{r})+V_{so}(\mathbf{r}), \quad (3)$$

where $V_N(\mathbf{r})$ is the potential due to the nuclear interaction, $V_M(\mathbf{r})$ is that due to the magnetic interaction with atomic electrons, and $V_{so}(\mathbf{r})$ is the spin-orbit interaction. The cross section including polarization-dependent terms due to the first two interactions was derived in I and is given by Eq. (15) of I, so that we will consider only those terms in the cross section which involve $V_{so}(\mathbf{r})$, either by itself or in cross terms with $V_N(\mathbf{r})$ or $V_M(\mathbf{r})$.

The interaction $V_{so}(\mathbf{r})$ is given by

$$V_{so}(\mathbf{r})=-\boldsymbol{\mu}\cdot\mathbf{B}(\mathbf{r}), \quad (4)$$

where $\boldsymbol{\mu}=2\gamma(e\hbar/2m_oc)\mathbf{s}$ is the magnetic moment, $\mathbf{s}$ is the spin operator, and $\gamma=-1.91$ is the gyromagnetic ratio of the neutron. The magnetic field $\mathbf{B}(\mathbf{r})$ is that due to the motion of the neutron through the electric fields of the solid,

$$\mathbf{B}(\mathbf{r})=(1/c)\mathbf{E}(\mathbf{r})\times\mathbf{v}=(1/m_oc)\mathbf{E}(\mathbf{r})\times\mathbf{p}, \quad (5)$$

where $\mathbf{p}$ is the momentum of the neutron. The electric field $\mathbf{E}(\mathbf{r})$ is in turn expressible in terms of the potential due to the nuclei and the electrons of the solid.

$$\mathbf{E}(\mathbf{r})=-\boldsymbol{\nabla}\left\{\sum_{\mathbf{n}j}\frac{Z_je}{|\mathbf{r}-\mathbf{R}_{\mathbf{n}j}|}-\sum_i\frac{e}{|\mathbf{r}-\mathbf{r}_i|}\right\}, \quad (6)$$

where $\mathbf{R}_{\mathbf{n}j}=\mathbf{n}+\mathbf{d}_j$ is the position of the jth nucleus (with charge Z_j) in the unit cell which is displaced from the origin by the lattice vector $\mathbf{n}$, and $\mathbf{r}_i$ is the position of the ith electron in the solid. Combining (4), (5), and (6), it is easy to calculate the Fourier transform of $V_{so}(\mathbf{r})$,

$$\begin{aligned}\mathcal{V}_{so}(\mathbf{k}',\mathbf{k})&=\int d\mathbf{r}e^{-i\mathbf{k}'\cdot\mathbf{r}}V_{so}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}\\&=4\pi i\gamma\left(\frac{e\hbar}{m_oc}\right)^2\{\sum_{\mathbf{n}j}Z_je^{i\mathbf{K}\cdot\mathbf{R}_{\mathbf{n}j}}-\sum_i e^{i\mathbf{K}\cdot\mathbf{r}_i}\}\\&\qquad\times\frac{(\mathbf{k}'\times\mathbf{k})}{K^2}\cdot\mathbf{s},\end{aligned} \quad (7)$$

where $\mathbf{K}=\mathbf{k}-\mathbf{k}'$.

Before proceeding, there are some comments which should be made concerning Eq. (5). In the case of electronic spin-orbit coupling an additional factor of 2 appears in the denominator of the expression for the magnetic field. This is a kinematic relativistic effect which arises because the rest frame of the accelerated electron is effectively rotated. This rotation of the charged electron produces a magnetic field which is opposite in direction to and one-half the size of the field (5), and it leads to the famous Thomas "factor" of $\frac{1}{2}$ in electronic spin-orbit coupling.[6] The neutron is also subject to this kinematical effect, but, being uncharged, the rotation does not produce a magnetic field, and no additional factors appear in (5). This

[4] D. J. Hughes, J. A. Harvey, M. D. Goldberg, and M. J. Stafne, Phys. Rev. **90**, 497 (1953); L. L. Foldy, Phys. Rev. **87**, 693 (1952).

[5] M. Blume, Phys. Rev. **130**, 1670 (1963), referred to as I.

[6] W. H. Furry, Am. J. Phys. **23**, 517 (1955).

classical argument is confirmed by a reduction of the Dirac equation for the neutron to nonrelativistic form, where the neutron's magnetic moment is introduced as a Pauli term.[7]

The matrix elements of $\mathcal{V}_{so}(\mathbf{k}',\mathbf{k})$ in the state $|q\rangle$ are evaluated in analogy with x-ray scattering by introducing the form factor $f_j^x(\mathbf{K})$ of the jth ion in the unit cell:

$$\langle q|\mathcal{V}_{so}(\mathbf{k}',\mathbf{k})|q\rangle = i\frac{2\pi\hbar^2}{m_o}\frac{2\gamma e^2}{mc^2}\frac{m}{m_o}\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}} \times\sum_j e^{i\mathbf{K}\cdot\mathbf{d}_j}(Z_j-f_j^x(\mathbf{K}))\frac{(\mathbf{k}'\times\mathbf{k})}{K^2}\cdot\mathbf{s}, \quad (8)$$

where $f_j^x(0)=Z_j$. It has been assumed here that the nuclei are rigidly fixed in the solid; this means only that Debye-Waller factors have been neglected. The x-ray form factor, which is the Fourier transform of the charge density, enters because all of the electrons in the atom contribute to the electric field and hence to the scattering. This is in contrast to the ordinary magnetic scattering of neutrons, where only those electrons with unpaired spin or orbital moments contribute to the scattering. The constants in (8) have been written to give a comparison with the ordinary magnetic scattering amplitude, Eq. (6) of I. We see that, besides the difference in form factors and angular factors, the spin-orbit amplitude is smaller by a factor m/m_o (m=electron mass, m_o=neutron mass) than the magnetic amplitude. This means that the spin-orbit scattering of thermal neutrons is observable only under special circumstances. It should also be noted that the spin-orbit amplitude has a factor i; this will be of importance in the interference effects which we shall derive.

To calculate the cross section it is now only necessary to evaluate the traces over neutron spin variables in (1). On substituting (3) and (2) in (1), we have

$$d\sigma/d\Omega' = (m_o/2\pi\hbar^2)^2 \times\mathrm{tr}[\langle q|\mathcal{V}_N^\dagger+\mathcal{V}_M^\dagger|q\rangle\langle q|\mathcal{V}_N+\mathcal{V}_M|q\rangle\rho +2\,\mathrm{Re}(\langle q|\mathcal{V}_N^\dagger+\mathcal{V}_M^\dagger|q\rangle\langle q|\mathcal{V}_{so}|q\rangle)\rho +\langle q|\mathcal{V}_{so}^\dagger|q\rangle\langle q|\mathcal{V}_{so}|q\rangle\rho]. \quad (9)$$

Of the three groups of terms in the trace, the first represents the nuclear and magnetic scattering, the second, interference between spin-orbit scattering and nuclear and magnetic scattering, and the third, pure spin-orbit scattering. The first has been treated in I, and the result, Eq. (I.15), will be denoted by $(d\sigma/d\Omega')_{NM}$. The third term involves the spin-orbit scattering amplitude twice, so that it is much smaller than the other terms present, and we accordingly neglect it. The only terms remaining to be calculated are the nuclear-spin-orbit and magnetic-spin-orbit interference terms. The trace is calculated using (I.6) and (I.9) for the nuclear and magnetic scattering amplitudes, and the properties (I.2) and (I.7) of the density matrix and the Pauli spin matrices. The nuclear spin-orbit interference term becomes

$$\left(\frac{m_o}{2\pi\hbar^2}\right)^2 2\,\mathrm{Re}\,\mathrm{tr}[\langle q|\mathcal{V}_N^\dagger|q\rangle\langle q|\mathcal{V}_{so}|q\rangle\rho]$$

$$=\frac{2\gamma e^2}{mc^2}\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\frac{1}{K^2}(\mathbf{k}\times\mathbf{k}')\cdot\mathbf{P} \times\mathrm{Im}(F_N^*(\mathbf{K})F_{so}(\mathbf{K})), \quad (10)$$

where

$$F_N(\mathbf{K})=\sum_j e^{i\mathbf{K}\cdot\mathbf{d}_j}a_j$$

and

$$F_{so}(\mathbf{K})=\sum_j e^{i\mathbf{K}\cdot\mathbf{d}_j}(Z_j-f_j^x(\mathbf{K}))$$

are, respectively, the nuclear and spin-orbit structure factors, and a_j is the scattering length for the nuclear species at lattice site j. (It is assumed that the nuclei are unpolarized.) The imaginary rather than the real part of the product of these structure factors enters because of the factor i in the spin-orbit scattering amplitude. This is the interference term derived by Schwinger,[2] and it is converted to his notation by writing $\mathbf{k}\times\mathbf{k}'=\hat{n}\,k^2\sin\theta$, where $\hat{n}$ is a unit vector in the direction of $\mathbf{k}\times\mathbf{k}'$ (perpendicular to the plane of scattering) and θ is the scattering angle. Also, $K=2k\sin(\theta/2)$ for elastic scattering, so that (10) becomes

$$\frac{2\gamma e^2}{mc^2}\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\,\tfrac{1}{2}\cot\frac{\theta}{2}\,(\mathbf{P}\cdot\hat{n}) \times\mathrm{Im}(F_N^*(\mathbf{K})F_{so}(\mathbf{K})). \quad (11)$$

For a monatomic substance with a single atom per unit cell, this becomes

$$\frac{\gamma e^2}{mc^2}\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\cot\frac{\theta}{2}\,(\mathbf{P}\cdot\hat{n})(Z-f^x(\mathbf{K}))\,\mathrm{Im}\,a,$$

the expression discussed by Shull in the analysis of his experiments on vanadium. It is this term which produces the left-right asymmetry in the scattering.

The magnetic-spin-orbit interference is somewhat more complicated, since the magnetic scattering amplitude is neutron-spin-dependent, while the nuclear scattering is, for unpolarized target nuclei, spin-independent. To calculate the trace, we write, using Eq. (6) and Eqs. (9)–(11) of I,

$$\langle q|\mathcal{V}_M|q\rangle=\frac{2\pi\hbar^2}{m_o}\frac{2\gamma e^2}{mc^2}\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}\mathbf{F}_M(\mathbf{K})\cdot\mathbf{s}, \quad (12)$$

where

$$\mathbf{F}_M(\mathbf{K})=\sum_j e^{i\mathbf{K}\cdot\mathbf{d}_j}S_jf_j(\mathbf{K})\mathbf{q}_j \quad (13)$$

is the magnetic vector structure factor, and the other quantities are as defined in I. The form factor $f_j(\mathbf{K})$ is here the magnetic form factor. The interference term

[7] L. L. Foldy, Phys. Rev. 83, 688 (1951).

is then

$$2\left(\frac{m_o}{2\pi\hbar^2}\right)^2 \operatorname{Re}\operatorname{tr}[\langle q|\mathcal{V}_M^\dagger|q\rangle\langle q|\mathcal{V}_{so}|q\rangle\rho]$$
$$=2\left(\frac{2\gamma e^2}{mc^2}\right)^2\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\frac{1}{K^2}$$
$$\times\operatorname{Re}\operatorname{tr}[i(\mathbf{s}\cdot\mathbf{F}_M^*(\mathbf{K}))(\mathbf{s}\cdot(\mathbf{k}'\times\mathbf{k}))$$
$$\times F_{so}(\mathbf{K})(\tfrac{1}{2}+\mathbf{P}\cdot\mathbf{s})].$$

Using Eq. (7) of I this becomes

$$2\left(\frac{2\gamma e^2}{mc^2}\right)^2\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\frac{1}{K^2}$$
$$\times\operatorname{Re}[\tfrac{1}{4}i(\mathbf{k}'\times\mathbf{k})\cdot\mathbf{F}_M^*(\mathbf{K})F_{so}(\mathbf{K})$$
$$+\tfrac{1}{4}\mathbf{P}\cdot((\mathbf{k}'\times\mathbf{k})\cdot\mathbf{F}_M^*(\mathbf{K}))F_{so}(\mathbf{K})] \tag{14}$$
$$=2\left(\frac{\gamma e^2}{mc^2}\right)^2\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\frac{1}{K^2}$$
$$\times\{\operatorname{Im}[(\mathbf{k}\times\mathbf{k}')\cdot\mathbf{F}_M^*(\mathbf{K})F_{so}(\mathbf{K})]$$
$$+\operatorname{Re}[\mathbf{P}\cdot(\mathbf{F}_M^*(\mathbf{K})\times(\mathbf{k}\times\mathbf{k}'))F_{so}(\mathbf{K})]\}.$$

The first term in braces is independent of polarization, and depends on the imaginary part of the product of the structure factors. The second term is much more interesting, however, since it depends on the polarization of the neutron beam and on the real part of the product of the structure factors. To illustrate the nature of the latter term we consider a ferromagnet with a single ion in a center of symmetry per unit cell. In this case the polarization-independent term vanishes, since the structure factors are real, and we have for (14)

$$2\left(\frac{\gamma e^2}{mc^2}\right)^2\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\frac{1}{K^2}$$
$$\times Sf(\mathbf{K})(Z-f^x(\mathbf{K}))\mathbf{P}\cdot(\mathbf{q}\times(\mathbf{k}\times\mathbf{k}'))$$
$$=\left(\frac{\gamma e^2}{mc^2}\right)^2\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2 Sf(\mathbf{K})(Z-f^x(\mathbf{K}))$$
$$\times\cot\frac{\theta}{2}\,\mathbf{P}\cdot(\mathbf{q}\times\hat{n}). \tag{15}$$

This effect is most readily observed in a substance with no nuclear coherent scattering and with a relatively small magnetic cross section. An excellent material would be an isotopic mixture of ferromagnetic nickel, chosen so that the coherent nuclear scattering amplitude vanishes. If the polarization vector $\mathbf{P}$ is in the plane of scattering then the flipping ratio R for a given Bragg peak, i.e., the ratio of intensity with positive polarization $[\mathbf{P}\cdot(\mathbf{q}\times\hat{n})>0]$ to that with negative polarization, is approximately

$$R\approx\frac{1+(m/m_o)[(Z-f^x)/Sfq]\cot(\theta/2)}{1-(m/m_o)[(Z-f^x)/Sfq]\cot(\theta/2)}, \tag{16}$$

where we have used the fact that the cross section for magnetic-Bragg scattering from a ferromagnet is[5,8]

$$\left(\frac{d\sigma}{d\Omega'}\right)_M=\left(\frac{\gamma e^2}{mc^2}\right)^2|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2 S^2 f^2(\mathbf{K})q^2. \tag{17}$$

For the Ni (331) reflection with $\lambda\approx 1.0$ Å, $S=0.6$, $f\approx 0.1$, $Z=28$, and $f^x\approx 10$, we find

$$R\approx(1+0.15)/(1-0.15)=1.35,$$

i.e., approximately a thirty percent effect is expected. This is quite sizeable and should be readily observable. A measurement of this sort may in some cases give information on the relative sizes of x-ray and magnetic form factors, or, if these form factors have been determined in other experiments, an accurate measurement of the spin-orbit scattering is possible. If the nuclear coherent scattering amplitude is not exactly zero, however, the effect will be reduced in magnitude and also complicated by the presence of the ordinary nuclear-magnetic interference term, which depends on $\mathbf{P}\cdot\mathbf{q}$. This term can be distinguished from the spin-orbit-magnetic interference by the fact that the latter changes sign on moving the detector from left to right (since this changes the sign of $\hat{n}$), while the former does not. This provides a simple method for separating the two terms experimentally.

In summary we collect all of the terms derived above and write the cross section for elastic scattering:

$$\frac{d\sigma}{d\Omega'}=\left(\frac{d\sigma}{d\Omega'}\right)_{NM}$$
$$+\frac{\gamma e^2}{mc^2}\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\cot\frac{\theta}{2}$$
$$\times(\mathbf{P}\cdot\hat{n})\operatorname{Im}[F_N^*(\mathbf{K})F_{so}(\mathbf{K})]$$
$$+\left(\frac{\gamma e^2}{mc^2}\right)^2\frac{m}{m_o}|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2\cot\frac{\theta}{2}$$
$$\times\{\operatorname{Im}[\mathbf{F}_M^*(\mathbf{K})\cdot\hat{n}F_{so}(\mathbf{K})]$$
$$+\operatorname{Re}[\mathbf{P}\cdot(\mathbf{F}_M^*(\mathbf{K})\times\hat{n})F_{so}(\mathbf{K})]\}. \tag{18}$$

The expressions for the polarization of the scattered beam are easy to derive, as in I, but the experiments are very much more difficult so the results will not be given here.

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[8] O. Halpern and M. H. Johnson, Phys. Rev. 55, 898 (1939).