

Magnetic Scattering of Neutrons from Rare Earth Ions

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The differential cross section for the magnetic scattering of thermal neutrons by paramagnetic rare earth ions is derived theoretically assuming that the ions have Russell Saunders coupling and are in the Hund ground state. Satisfactory agreement with the measured cross sections of Er_2O_3 and Nd_2O_3 is obtained using hydrogenic radial wave function with $Z-S \approx 23$ and 20 for Er^{+++} and Nd^{+++} , respectively.

THEORETICAL treatments of the magnetic scattering of slow neutrons by atomic electrons have been given by Bloch,¹ Schwinger,² and Halpern and Johnson.³

The very thorough-going paper of Halpern and Johnson was primarily concerned with scattering from the iron group atoms for which susceptibility measurements⁴ and slow neutron scattering data⁵ indicate that the orbital currents are nearly completely quenched by the crystalline fields.

The magnetic properties of the solid salts and oxides of the rare earths, on the other hand, clearly indicate that for these ions there is little quenching by the crystalline fields; in the preceding paper Koehler and Wollan obtain a magnetic contribution to the forward scattering from Er_2O_3 and Nd_2O_3 which is, within a few percent, equal to that which one would expect to obtain from the free rare earth ions in their ground state.

Our main purposes here are to derive a theoretical expression for the magnetic scattering of paramagnetic rare earth ions and to analyze the experimental data for Er_2O_3 and Nd_2O_3 presented in the preceding paper on this basis. In Sec. I general formulas analogous to those of Halpern and Johnson,³ but including the effects of orbital currents, are obtained. In Sec. II the techniques for doing the integrals and sums over angular and spin variables which are involved in these calculations are discussed, the assumption being made that the magnetic electron shell is coupled according to the Russell-Saunders scheme with the Hund value for ground state. Finally, in Sec. III the results of Secs. I and II are applied to the experiments of Koehler and Wollan with Er_2O_3 and Nd_2O_3 , and satisfactory agreement is obtained.

SECTION I. GENERAL FORMULAS

The term in the Hamiltonian which describes the interaction of the neutron with the atomic electrons is taken to be

$$H_{\text{int}} = - (e/c) \sum_i \alpha_i \cdot \mathbf{A}_N(\mathbf{r}_i - \mathbf{r}_N), \quad (1)$$

¹ F. Bloch, Phys. Rev. **50**, 259 (1936).

² J. Schwinger, Phys. Rev. **51**, 544 (1937).

³ O. Halpern and M. Johnson, Phys. Rev. **55**, 898 (1939).

⁴ J. H. Van Vleck, *Electric and Magnetic Susceptibilities* (Oxford University Press, London, 1932), Chap. IX.

⁵ Shull, Strauser, and Wollan, Phys. Rev. **83**, 333 (1951).

where α_i is the Dirac velocity operator for the i th electron and $\mathbf{A}_N(\mathbf{r}) = g_N \mathbf{S}_N \times \mathbf{r} r^{-3}$, and \mathbf{S}_N and g_N are, respectively, the spin operator and the Landé g factor for the neutron ($g_N = -1.9e/M_N c$).

If a neutron of momentum $\hbar \mathbf{p}_0$ is incident on an atom, then the scattered wave will be (in the Born approximation):

$$\Psi_S = \sum_f \frac{2iMg_N e}{\hbar^2 c} (\chi_f \psi_f | \mathbf{S}_N \cdot \mathbf{k} k^{-2} \times \sum_i \alpha_i e^{i\mathbf{k} \cdot \mathbf{r}_i} | \chi_0 \psi_0) \times \frac{e^{i\mathbf{p}_f \cdot \mathbf{r}_N}}{r_N} \chi_f \psi_f, \quad (2)$$

where ψ is an energy eigenfunction of the atom; χ is the spin state of the neutron, $\mathbf{k} = \mathbf{p}_0 - \mathbf{p}_f$; M is the mass of the neutron; and subscripts 0 and f serve to distinguish the quantities before and after the collision. The sum is over all possible states of the atom consistent with energy conservation. Energy conservation is given by $\hbar^2(2M)^{-1}(\mathbf{p}_0^2 - \mathbf{p}_f^2) = E_f - E_0$, where E is the energy of the atom.

Schwinger,² using a method similar to that used below, has shown that for very small k (forward direction, elastic scattering),

$$i(e/c) (\psi_f | k^{-2} \mathbf{k} \times \sum_i \alpha_i e^{i\mathbf{k} \cdot \mathbf{r}_i} | \psi_0) = (e/2mc) (\psi_f | k^{-1} \mathbf{k} \times \sum_i (\mathbf{L}_i + 2\mathbf{S}_i) | \psi_0) = k^{-1} \mathbf{k} \times \mathbf{M}, \quad (3)$$

where \mathbf{M} is the atomic magnetic moment.

Upon making the Pauli non-relativistic approximation, one obtains:

$$i\mathbf{J}_{f0}(\mathbf{k}) \equiv i(e/c) (\psi_f | \sum_i \alpha_i e^{i\mathbf{k} \cdot \mathbf{r}_i} | \psi_0) = i(e/c) \sum_i \int d^3r_i \{ (\hbar/2im) [\bar{\psi}_f \nabla \psi_0 - (\nabla \bar{\psi}_f) \psi_0] - (1/m) \nabla \times \bar{\psi}_f \mathbf{S}_i \psi_0 \} e^{i\mathbf{k} \cdot \mathbf{r}_i} = (ie/2mc) (\psi_f | \sum_i \mathbf{p}_i e^{i\mathbf{k} \cdot \mathbf{r}_i} + e^{i\mathbf{k} \cdot \mathbf{r}_i} \mathbf{p}_i + 2i\mathbf{k} \times \mathbf{S}_i e^{i\mathbf{k} \cdot \mathbf{r}_i} | \psi_0). \quad (4)$$

Halpern and Johnson³ have used the relations (2) and (4) to discuss the scattering from atoms for which the term in (4) which represents the orbital currents, $(\psi_f | \sum_i \mathbf{p}_i e^{i\mathbf{k} \cdot \mathbf{r}_i} + e^{i\mathbf{k} \cdot \mathbf{r}_i} \mathbf{p}_i | \psi_0)$, is zero.

It is convenient to transform the orbital current term in (4) as follows:

$$\begin{aligned} (\hbar/mi)[\mathbf{p}(\mathbf{k}\cdot\mathbf{r})^n+(\mathbf{k}\cdot\mathbf{r})^n\mathbf{p}] &= 2[H, \mathbf{r}(\mathbf{k}\cdot\mathbf{r})^n] \\ &- (\hbar/i)(n/m)[(\mathbf{p}\cdot\mathbf{k})(\mathbf{k}\cdot\mathbf{r})^{n-1}\mathbf{r}+(\mathbf{k}\cdot\mathbf{r})^{n-1}\mathbf{r}(\mathbf{p}\cdot\mathbf{k})] \\ &= 2(n+1)^{-1}[H, \mathbf{r}(\mathbf{k}\cdot\mathbf{r})^n]- (\hbar/im)(n/n+1)\mathbf{k} \\ &\quad \times [\mathbf{L}(\mathbf{k}\cdot\mathbf{r})^{n-1}+(\mathbf{k}\cdot\mathbf{r})^{n-1}\mathbf{L}], \quad (5) \end{aligned}$$

$$\begin{aligned} [\mathbf{p}e^{i\mathbf{k}\cdot\mathbf{r}}+e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}] &= (2mi/\hbar)[H, \mathbf{r}(i\mathbf{k}\cdot\mathbf{r})^{-1}(e^{i\mathbf{k}\cdot\mathbf{r}}-1)] \\ &- i\mathbf{k}\times[\frac{1}{2}\mathbf{L}f(\mathbf{k}\cdot\mathbf{r})+f(\mathbf{k}\cdot\mathbf{r})\frac{1}{2}\mathbf{L}], \quad (6) \end{aligned}$$

where

$$f(\mathbf{k}\cdot\mathbf{r}) = 2 \sum \frac{(i\mathbf{k}\cdot\mathbf{r})^n}{(n+2)n!} = \frac{2}{(i\mathbf{k}\cdot\mathbf{r})^2} \int_0^{i\mathbf{k}\cdot\mathbf{r}} xe^x dx,$$

m is the electron mass, and H is the Hamiltonian for the atomic electrons. Substituting (6) into (4), one now obtains

$$\begin{aligned} i\mathbf{J}_{f_0}(\mathbf{k}) &= (e/2mc)(\psi_f|\mathbf{k}\times\sum_i\{\frac{1}{2}\mathbf{L}_i f(\mathbf{k}\cdot\mathbf{r}_i) \\ &\quad +f(\mathbf{k}\cdot\mathbf{r}_i)\frac{1}{2}\mathbf{L}_i+2\mathbf{S}_i e^{i\mathbf{k}\cdot\mathbf{r}_i}\} \\ &\quad -2m(E_f-E_0)\hbar^{-1}\sum_i\mathbf{r}_i(i\mathbf{k}\cdot\mathbf{r}_i)^{-1}(e^{i\mathbf{k}\cdot\mathbf{r}_i}-1)|\psi_0). \quad (7) \end{aligned}$$

The second sum is zero if $E_f=E_0$ and indeed is always negligible for slow neutron ($E\approx 0.1$ eV) scattering.⁶ With the neglect of the small term, (7) becomes⁷

$$i\mathbf{J}_{f_0}(\mathbf{k}) = +\mathbf{k}\times(e/2mc)(\psi_f|\sum_i\frac{1}{2}\mathbf{L}_i f(\mathbf{k}\cdot\mathbf{r}_i) +f(\mathbf{k}\cdot\mathbf{r}_i)\frac{1}{2}\mathbf{L}_i+2\mathbf{S}_i e^{i\mathbf{k}\cdot\mathbf{r}_i}|\psi_0). \quad (7')$$

Substituting (7') into (2), one obtains

$$\begin{aligned} \Psi_S &= \left(\frac{M e g_N}{2m c \hbar^2}\right) \sum_f (\chi_f \psi_f | S_{N+} P_- \\ &\quad + S_{N-P+} | \chi_0 \psi_0) \chi_f \psi_f \frac{e^{i\mathbf{p}_f \cdot \mathbf{r}_N}}{r_N}, \quad (2') \end{aligned}$$

where

$$\mathbf{P} = \sum_i [\frac{1}{2}(\mathbf{L}_i f(\mathbf{k}\cdot\mathbf{r}_i) + f(\mathbf{k}\cdot\mathbf{r}_i)\mathbf{L}_i) + 2\mathbf{S}_i e^{i\mathbf{k}\cdot\mathbf{r}_i}],$$

and P_{\pm} , $S_{N\pm}$ are defined with respect to the direction of $\mathbf{k}=\mathbf{p}_0-\mathbf{p}_f$; namely, if \mathbf{k} is taken to define the Z direction, $A_{\pm}=A_x\pm iA_y$, where \mathbf{A} is any vector. (2') expresses the fact that the component of $\mathbf{S}_N+\sum_i(\mathbf{L}_i+\mathbf{S}_i)$ in the \mathbf{k} direction is a collision invariant. If one writes $S_{N+}P_-+S_{N-P+}$ in the form $2\mathbf{S}_N\cdot[\mathbf{P}-k^{-2}\mathbf{k}$

⁶ A rough estimation of its relative magnitude may be made as follows: $\mathbf{k}\times\mathbf{L}\sim\hbar^{-1}|\Delta p_N||p_e|\tilde{r}_e$, where $|\Delta p_N|$ is the change in the magnitude of the neutron's momentum as the result of the scattering process, $|p_e|$ is the average momentum of the electron, \tilde{r}_e is the electron's radius;

$$2m\hbar^{-1}(E_f-E_0)\mathbf{r}_e\sim m(\hbar M)^{-1}|\Delta p_N|^2\tilde{r}_e.$$

Therefore,

$$|2m\hbar^{-1}(E_f-E_0)\mathbf{r}_e| \div |\mathbf{k}\times\mathbf{L}| \sim (m/M)\cdot(|\Delta p_N|/|p_e|)\sim 10^{-2} \text{ or } 10^{-3},$$

since $|\Delta p_N|\sim p_N$ and $(\hbar/p_N)\sim 1\text{\AA}$ and $(\hbar/|p_e|)$ is $O(1\text{\AA})$.

⁷ In the appendix it is shown that

$$(e/2mc)\int\psi_f^*\frac{1}{2}[\mathbf{L}f(\mathbf{k}\cdot\mathbf{r})+f(\mathbf{k}\cdot\mathbf{r})\mathbf{L}]\psi_0 d\mathbf{r} = \int\mathbf{M}_{f_0}^L e^{i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r},$$

where $\mathbf{M}_{f_0}^L(\mathbf{r})$ is the "equivalent magnetic dipole density" of the orbital currents.

$\times(\mathbf{P}\cdot\mathbf{k})]$ in (2'), then (2') becomes identical with Eq. (4.1) of Halpern and Johnson except for the inclusion in \mathbf{P} of the orbital currents.

From (2') one has for the differential scattering cross section (if one assumes unpolarized incident neutrons)

$$\frac{d\sigma}{d\Omega} = \left(\frac{M e g_N}{2m c \hbar}\right)^2 \sum_f \frac{p_f}{2p_0} [|\langle\psi_f|P_-|\psi_0\rangle|^2 + |\langle\psi_f|P_+|\psi_0\rangle|^2]. \quad (8)$$

Equation (8) refers to the scattering from a single ion initially in a state ψ_0 ; but in substances in which the effect of exchange forces acting between the magnetic shells of adjacent ions are negligible, there will be no correlation in the sense of the currents in adjacent ions and hence no net coherence in the magnetic scattering from such a substance. Now whereas gadolinium is known to become ferromagnetic at $T=16^\circ\text{C}$ and there* is an indication of the possible onset of long-range magnetic order in metallic erbium at $T=70^\circ\text{K}$, the susceptibilities⁴ and neutron scattering cross sections of the rare earth salts and oxides are well accounted for on the assumption of little or no ordering of neighboring magnetic moments except possibly at very low temperatures. Thus Koehler and Wollan detected no magnetic coherent scattering from Er_2O_3 and Nd_2O_3 down to $T=20^\circ\text{K}$. The assumption is then made that for these substances the influence of its neighbors on a given ion is representable by an effective electrostatic "crystalline field." The magnetic scattering from such a substance is then given by summing (8) over the statistically determined initial states ψ_0 of its magnetic ions.

SECTION II. THE EVALUATION OF $\langle\psi_f|P_{\pm}|\psi_0\rangle$ FOR THE GROUND STATES OF THE RARE EARTHS, IN PARTICULAR FOR Er^{+++} AND Nd^{+++}

Russell-Saunders coupling with Hund's rule is supposed to apply to the ground state of the rare earths. The wave function for n electrons in the $4f$ shell is taken to be of the form

$$\psi_M = \phi_{4f, n}(r_1, \dots, r_N) \Theta_{l, L, S, J, M}, \quad (9)$$

where ϕ is a symmetrical function of the radial coordinates of the n electrons, Θ a function of the angle and spin variables of the electrons which is an eigenfunction of L_i^2 , with eigenvalues $L_i^2=l(l+1)\hbar^2=12\hbar^2$, $\mathbf{L}^2=(\sum\mathbf{L}_i)^2$, $\mathbf{S}^2=(\sum\mathbf{S}_i)^2$, $\mathbf{J}^2=(\sum\mathbf{L}_i+\mathbf{S}_i)^2$, and some component of \mathbf{J} with eigenvalue M . S has its maximum value possible, L its maximum consistent with this S , and $J=||L|-|S||$, if the shell is less than half filled, $J=||L|+|S||$, if the shell is more than half filled. We shall assume that the crystalline field may lift the M degeneracy and possibly mix states of different M 's but does not cause an appreciable admixture of different J states.⁸ In dealing with atoms containing more than half-filled shells we shall perform calculations for the

⁸ Since the next J state lies some 2000–3000°K above the ground state for Er or Nd, this assumption should be valid.

magnetically equivalent model consisting of the closed-shell deficiency number of electrons. Thus Er^{+++} , which has a deficiency of three electrons from a closed 4f shell, is replaced by an atom containing three 4f electrons with, of course, the same L, S, J as Er^{+++} .

The elements $\langle \psi_J | P_{\pm} | \psi_0 \rangle$ where the ψ 's are of the form (9) may now be brought to a form containing known coefficients and radial integrals only by straightforward application of the Wigner-Eckart⁹ theorem and the concept of tensor operators as developed by Wigner⁹ and Racah.¹⁰ According to Racah the irreducible tensor of rank k , $T_q^{(k)}$ transforms under rotations the same as the spherical harmonics $Y_{k,q} = P_k^q(\theta)e^{iq\varphi}$, and so satisfies

$$\begin{aligned} [J_{\pm}, T_q^k] &= [k(k+1) - q(q\pm 1)]^{\frac{1}{2}} T_{q\pm 1}^k, \\ [J_z, T_q^k] &= q T_q^k. \end{aligned} \quad (10)$$

The Wigner-Eckart theorem states

$$\begin{aligned} \langle \alpha' J' M' | T_q^k | \alpha J M \rangle \\ = (-1)^M G(\alpha' J'; T^k; \alpha J) (J J' M' - M | J J' k q), \end{aligned} \quad (11)$$

where G does not depend on M, M' , or q , and a general expression from which the vector addition coefficient $(j_1 j_2 m_1 m_2 | j_1 j_2 j m)$ may be determined is given by Wigner⁹ and Racah.¹⁰ For our purposes it is convenient to introduce the special tensor $T_q^k \equiv \mathcal{Y}_{k,q}(\mathbf{J})$ such that

$$\langle J' M' | \mathcal{Y}_{k,q} | J M \rangle = (-1)^M \delta_{J J'} (J J' M' - M | J J k q). \quad (12)$$

Defining $\mathcal{O}_k(M_J)$ by

$$\langle J M | \mathcal{Y}_{k,0} | J M \rangle \equiv \langle J M | \mathcal{O}_k(J_z) | J M \rangle = \mathcal{O}_k(M_J), \quad (13')$$

we have^{10,11}

$$\begin{aligned} \mathcal{O}_k(M_J) &= \left[\binom{2k}{k} \binom{2J+1+k}{2k+1} \right]^{-\frac{1}{2}} \\ &\times \sum_{\nu=0}^k (-1)^{\nu} \binom{k+\nu}{k} \binom{2J-\nu}{k-\nu} \binom{J-M}{\nu}. \end{aligned} \quad (13)$$

From (10) we have

$$\mathcal{Y}_{k,q^+}(\mathbf{J}) = (-1)^q \mathcal{Y}_{k,-q}(\mathbf{J}), \quad (14)$$

and from (12),

$$\begin{aligned} \sum_{M M'} \langle J M | \mathcal{Y}_{k',q^+}(\mathbf{J}) | J' M' \rangle \langle J' M' | \mathcal{Y}_{k,q}(\mathbf{J}) | J M \rangle \\ = \sum_M \langle J M | \mathcal{Y}_{k',q^+}(J) \mathcal{Y}_{k,q}(J) | J M \rangle = \delta_{kk'} \delta_{qq'}. \end{aligned} \quad (15)$$

⁹ E. Wigner, *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspectren* (J. W. Edwards, Ann Arbor, 1944).

¹⁰ G. Racah, *Phys. Rev.* **62**, 438 (1942).

¹¹ The expression for the orthogonal-with-respect-to-summing polynomials $\mathcal{O}_k(M)$ is also given by C. Jordan, *Calculus of Finite Differences* (Chelsea Publishing Company, New York, 1950). Note that the polynomial $P_k(M_j)$ is defined for $M_j > J$ although of course it then hasn't the significance of a vector addition coefficient.

One further result which is needed is

$$\begin{aligned} J_+ \mathcal{O}_k(J_z) + \mathcal{O}_k(J_z) J_+ &= \alpha_{k,k-1}(J) \mathcal{Y}_{k-1,+1}(J) \\ &+ \alpha_{k,k+1}(J) \mathcal{Y}_{k+1,+1}(J). \end{aligned} \quad (16)$$

Taking account of Eqs. (10) and (13), we have

$$\begin{aligned} \mathcal{O}_k(M) + \mathcal{O}_k(M+1) &= [k(k-1)]^{-\frac{1}{2}} \\ &\times \alpha_{k,k-1} [\mathcal{O}_{k-1}(M) - \mathcal{O}_{k-1}(M+1)] + [(k+1)(k+2)]^{-\frac{1}{2}} \\ &\times \alpha_{k,k+1} [\mathcal{O}_{k+1}(M) - \mathcal{O}_{k+1}(M+1)]. \end{aligned} \quad (17)$$

From (15) one may deduce

$$\mathcal{O}_n(M+1) = \mathcal{O}_n(M) + \sum_{r=0}^{n-1} C_{nr} \mathcal{O}_r(M), \quad (18)$$

where

$$C_{nr}(J) = \mathcal{O}_n(J+1) \mathcal{O}_r(J) + (-1)^{r+n+1} \mathcal{O}_n(J) \mathcal{O}_r(J+1),$$

and $\mathcal{O}_n(M)$ is the polynomial of order n in M given by the right side of (13). Substituting (18) in (17) one obtains

$$\begin{aligned} [(k+1)(k+2)]^{-\frac{1}{2}} C_{k+1,r} \alpha_{k,k+1} + [k(k+1)]^{-\frac{1}{2}} C_{k-1,r} \alpha_{k,k-1} \\ + C_{k,r} + 2\delta_{kr} = 0. \end{aligned} \quad (19)$$

Putting in (19) $r=k$ and $r=k-1$ successively one obtains

$$\begin{aligned} \alpha_{k,k+1}(J) &= -2[(k+1)(k+2)]^{\frac{1}{2}} / C_{k+1,k}(J) \\ \alpha_{k,k-1}(J) &= ([k(k+1)]^{\frac{1}{2}} / C_{k-1,k-2}(J)) \\ &\cdot [(2C_{k+1,k-2}(J) / C_{k+1,k}(J)) - C_{k,k-2}]. \end{aligned} \quad (20)$$

Since according to (13) the polynomial

$$\mathcal{O}_k(M) \sim \sum_{\nu=0}^k (-1)^{\nu} \binom{k+\nu}{k} \binom{2J-\nu}{k-\nu} \binom{J-M}{\nu}$$

is zero if $k > 2J$, $|M| \leq J$, care must be used in interpreting (20) for $k=2J$.

From (2') we have

$$\begin{aligned} P_{\pm} &= \sum_n \frac{1}{2} L_{n\pm} f(\mathbf{k} \cdot \mathbf{r}_n) + \frac{1}{2} f(\mathbf{k} \cdot \mathbf{r}_n) L_{n\pm} + 2S_{n\pm} e^{i\mathbf{k} \cdot \mathbf{r}_n} \\ &= \sum_n \sum_{\nu=0}^{\infty} i^{\nu} (2\nu+1) \{ f_{\nu}(kr_n) \frac{1}{2} [L_{n\pm} P_{\nu}(\theta_n) + P_{\nu}(\theta_n) L_{n\pm}] \\ &\quad + 2g_{\nu}(kr_n) S_{n\pm} P_{\nu}(\theta_n) \}, \end{aligned} \quad (21)$$

where

$$f_{\nu}(x) = 2x^{-2} \int_0^x y g_{\nu}(y) dy,$$

$$g_{\nu}(x) = (\pi/2)^{\frac{1}{2}} x^{-\frac{1}{2}} J_{\nu+\frac{1}{2}}(x),$$

the subscript n refers to the n th electron, and θ is measured from the \mathbf{k} direction. Now from Eqs. (10)-

TABLE I. $G(\alpha', J'; T^v; \alpha, J)$ defined by Eq. (11) and evaluated for special cases by use of Eqs. (26) and (27) and reference 8.

ν	$G(L=6, J; \mathcal{Y}_\nu(L); 6, J)$			$G(l_1=l_2=l_3=3, L=6; \mathcal{Y}_\nu(L_n); 3, 3, 3, 6)$
	$G(l=3; Y_\nu(\theta, \phi; l=3)$	$J=9/2$	$J=15/2$	
0	2.645	0.877	1.108	1.365
1		0.857	1.093	0.849
2	-0.6105	0.818	1.065	0.147
3		0.758	1.011	-0.296
4	2.127	0.683	0.952	-0.226
5		0.590	0.8805	0.260
6	-0.1869	0.487	0.794	0.593
7		0.374	0.688	

(21) we have

$$\int \phi_{4f, n}^* \Theta^*_{i_1 \dots i_n; L; S; J; M} P_{\pm} \phi_{4f, n} \Theta_{i_1 \dots i_n; L; S; J; M} d^3n x$$

$$= \pm (JM' \left| \sum_{\nu=0}^l (-1)^\nu \{ F_{2\nu}^L(k) [\mathcal{G}_{2\nu, 2\nu-1}^L(\mathbf{J}) \right.$$

$$+ \mathcal{G}_{2\nu, 2\nu+1}^L(\mathbf{J})] + 2F_{2\nu}^S(k) [\mathcal{G}_{2\nu, 2\nu-1}^S(\mathbf{J})$$

$$\left. \times \mathcal{Y}_{2\nu-1, \pm 1}(\mathbf{J}) + \mathcal{G}_{2\nu, 2\nu+1}^S(\mathbf{J}) \mathcal{Y}_{2\nu+1, \pm 1}(\mathbf{J}) \} \right| JM), \quad (22)$$

where

$$F_{\nu}^S(k) = \int \phi_{4f, n} \phi_{4f, n} g_{\nu}(kr_i) d^3n x, \quad (23)$$

$$F_{\nu}^L(k) = \int \phi_{4f, n}^* \phi_{4f, n} f_{\nu}(kr_i) d^3n x,$$

where r_i is the radial coordinate of any of the n electrons, and where from (11) and (16) we have

$$\mathcal{G}_{\nu, \nu \pm 1}^L = \frac{2\nu+1}{2} G(l; \mathcal{Y}_\nu(\theta, \phi); l) \alpha_{\nu, \nu \pm 1}(l)$$

$$\times G(l_1 \dots l_n, L; \sum_n \mathcal{Y}_{\nu \pm 1}(\mathbf{L}_n); l_1 \dots l_n; \mathbf{L})$$

$$\times G(L, S, J; \mathcal{Y}_{\nu \pm 1}(L); L, S, J), \quad (24)$$

$$\mathcal{G}_{\nu, \nu \pm 1}^S = (2\nu+1) G(l; Y_\nu(\theta, \phi); l)$$

$$\times G(l_1 \dots l_n, L; \mathcal{Y}_\nu(\mathbf{L}_n); l_1 \dots l_n, \mathbf{L})$$

$$\times [\alpha_{\nu, \nu \pm 1}(J) G(L, S, J; \mathcal{Y}_\nu(\mathbf{L}); L, S, J)$$

$$- \alpha_{\nu, \nu \pm 1}(L) G(L, S, J; \mathcal{Y}_{\nu \pm 1}(\mathbf{L}); L, S, J)]. \quad (25)$$

Racah has shown that

$$G(l; Y_n(\theta, \phi); l) = (-1)^{n/2} \frac{(2l+1)}{(2n+1)^{\frac{1}{2}}} \frac{n!}{(\frac{1}{2}n!)^2}$$

$$\times \frac{(l+\frac{1}{2}n)!}{(l-\frac{1}{2}n)!} \left(\frac{(2l-n)!}{(2l+n+1)!} \right)^{\frac{1}{2}} \quad n = \text{even} \quad (26)$$

$$= 0 \quad (n = \text{odd}).$$

$G(L, S, J; \mathcal{Y}_n(\mathbf{L}); L, S, J)$ is (except for a multiplying factor) the Racah function W whose values have been

tabulated by Biedenharn,¹² and in virtue of the simple Hund's scheme for the coupling of the individual L_n 's to give $L[L=L+(l-1)+\dots+(l-n+1)]$,

$$G(l_1 \dots l_n, L; \mathcal{Y}_\nu(\mathbf{L}_n); l_1 \dots l_n, L)$$

$$= [\mathcal{O}_\nu(l) + \mathcal{O}_\nu(l-1) + \dots + \mathcal{O}_\nu(l-n+1)] / n \mathcal{O}_\nu(L). \quad (27)$$

In the next section the \mathcal{G} 's are evaluated for Nd and Er.

In (22) the $\mathcal{Y}_{\nu, q}$'s are defined with respect to axes whose z direction is along $\mathbf{k} = \mathbf{p}_0 - \mathbf{p}_f$. If we call this axis S_0 and an axis rotated by Euler angles (α, β, γ) with respect to S_0, S , then we have

$$\mathcal{Y}_{\nu, q}(S_0) = \sum_{q'=-\nu}^{\nu} \mathcal{D}_{q, q'}(\alpha, \beta, \gamma) \mathcal{Y}_{\nu, q'}(S), \quad (28)$$

where the $\mathcal{D}^\nu(\alpha, \beta, \gamma)$'s are the irreducible representations of the three-dimensional rotation group.

From the unitarity of the \mathcal{D} matrix and the orthogonality of the \mathcal{Y} 's it may be deduced that

$$\langle \mathcal{D}_{q, q'}(\alpha, \beta, \gamma) \mathcal{D}_{q'', q'''}(\alpha, \beta, \gamma) \rangle_{av}$$

$$= \delta_{\nu\nu'} \delta_{qq'} \delta_{q''q'''} / (2\nu+1), \quad (29)$$

where in (29) the average is made over all possible orientations of the rotated frame.

If the sample under consideration is a powdered crystal sample with perfectly randomly oriented microcrystals, then in virtue of (29), (28), and (22), (8) becomes

$$\frac{d\sigma}{d\Omega} = \left(\frac{M e g_N}{2m\hbar} \right)^2 \sum_{\nu=0}^l \sum_{\psi_f} \frac{p_f}{p_o} [\mathcal{G}_{2\nu, 2\nu+1}^L F_{2\nu}^L(k)$$

$$- \mathcal{G}_{2\nu+2, 2\nu+1}^L F_{2\nu+2}^L(k) + 2 \mathcal{G}_{2\nu, 2\nu+1}^S F_{2\nu}^S(k)$$

$$- 2 \mathcal{G}_{2\nu+2, 2\nu+1}^S F_{2\nu+2}^S(k)]^2 (4\nu+3)^{-1}$$

$$\times \sum_{q=(2\nu+1)}^{2\nu+1} | \langle \psi_f | \mathcal{Y}_{2\nu+1, q} | \psi_o \rangle |^2, \quad (30)$$

where it is to be noted that in (30), k , for a given scattering angle, satisfies

$$k^2 = k_o^2 p_f / p_o + (p_f - p_o)^2$$

$$\doteq k_o^2 \left(1 - \frac{E_f - E_o}{2E_{N_o}} \right) + \frac{2M(E_f - E_o)}{\hbar^2} \frac{E_f - E_o}{4E_{N_o}}.$$

If we assume that $(E_f - E_o)/E_{N_o}$ is sufficiently small,

TABLE II. $\alpha_{k, k \pm 1}(J)$ defined by Eq. (16) and evaluated by use of Eqs. (18) and (20).

n	$\alpha_{n, n+1}(J)$				$\alpha_{n, n-1}(J)$			
	$J=3$	$9/2$	6	$15/2$	$J=3$	$9/2$	6	$15/2$
0	5.656	8.150	10.59	13.03	0	0	0	0
2	3.70	5.598	7.409	9.190	-2.450	-3.590	-4.694	-5.810
4	2.870	4.738	6.611	8.363	-2.941	-4.029	-5.407	-6.744
6	0	3.831	5.867	7.745	-1.645	-3.620	-5.258	-6.830

¹² L. C. Biedenharn, Oak Ridge National Laboratory Report ORNL-1098 (unpublished).

TABLE III. $\mathcal{G}_{\nu, \nu \pm 1}^{L, S}(l, L, J)$ defined by Eqs. (24) and (25) and evaluated for $l=3, L=6, J=9/2$ (Nd) by use of Tables I and II.

ν	$\mathcal{G}_{2\nu, 2\nu+1}^L(9/2)$	$\mathcal{G}_{2\nu+2, 2\nu+1}^L(9/2)$	$\mathcal{G}_{2\nu, 2\nu+1}^S(9/2)$	$\mathcal{G}_{2\nu+2, 2\nu+1}^S(9/2)$
0	16.3	8.3	-7.0	-0.488
1	-3.81	-18.9	-0.465	5.83
2	12.6	0.92	2.87	-1.93
3	0	0	0.473	0

 TABLE IV. $\mathcal{G}_{\nu, \nu \pm 1}^{L, S}(l, L, J)$ defined by Eqs. (24) and (25) and evaluated for $l=3, L=6, J=15/2$ (Er) by use of Tables I and II.

ν	$\mathcal{G}_{2\nu, 2\nu+1}^L(15/2)$	$\mathcal{G}_{2\nu+2, 2\nu+1}^L(15/2)$	$\mathcal{G}_{2\nu, 2\nu+1}^S(15/2)$	$\mathcal{G}_{2\nu+2, 2\nu+1}^S(15/2)$
0	20.9	10.4	10.4	0.475
1	-5.08	25.2	1.03	-4.14
2	18.8	1.37	-9.3	1.14
3	0	0	3.04	0

then (30) may be approximated by expanding the expression in square brackets and (p_f/p_0) in powers of $(E_f - E_0/E_{N0})$, neglecting powers higher than the first; if at the same time we multiply by the statistical weight $g(E_0) = (e^{-E_0/kT}/\sum E_0 e^{-E_0/kT})$ and sum over the initial states ψ_0 , we obtain

$$\frac{d\sigma}{d\Omega} = \left(\frac{M e g_N}{2 m c \hbar} \right)^2 \left\{ \sum_{\nu=0}^l \left[\frac{B_\nu^2(k_0)}{2J+1} + \Delta_\nu \right] \right\}, \quad (31)$$

where

$$B_\nu^2(k) = \left[\mathcal{G}_{2\nu, 2\nu+1}^L F_{2\nu}^L(k) - \mathcal{G}_{2\nu+2, 2\nu+1}^L F_{2\nu+2}^L(k) + 2 \mathcal{G}_{2\nu, 2\nu+1}^S F_{2\nu}^S(k) + 2 \mathcal{G}_{2\nu+2, 2\nu+1}^S F_{2\nu+2}^S(k) \right]^2,$$

and the crystalline effects are contained in

$$\begin{aligned} \Delta_\nu = \sum_{\psi_f, \psi_0} \frac{E_f - E_0}{2E_{N0}} & \left\{ \left(B_\nu^2(k_0) + k_0^2 \frac{\partial B_\nu^2}{\partial k^2} \right) [g(E_f) - g(E_0)] \right. \\ & \left. + \frac{2M(E_f - E_0)}{\hbar^2} \frac{\partial B_\nu^2}{\partial k^2} [g(E_f) + g(E_0)] \right\} \\ & \times \frac{1}{2(4\nu+3)} \sum_{q=-(2\nu+1)}^{2\nu+1} |\langle \psi_f | Y_{2\nu+1, q}(\mathbf{J}) | \psi_0 \rangle|^2. \quad (32) \end{aligned}$$

In the next section the possibility of (32)'s explaining the possible small decrease of cross section from the free ion value for Er^{+++} is discussed.

SECTION III. CROSS SECTIONS FOR Er^{+++} AND Nd^{+++}

In Tables I and II we give the G^S 's¹³ and α^S 's¹⁴ for $\text{Er}(l_i=3, L=6, S=3/2, J=15/2)$ and $\text{Nd}(l_i=3, L=6, S=3/2, J=9/2)$, and in Tables III and IV the values of the \mathcal{G} 's¹⁵ are given for these two cases. The figures given in Tables III and IV are not all significant; each entry should be taken to have a probable error of about 1 percent or less. The assumption has been made in deriving Eq. (31) for the powdered crystal

¹³ Equations (11), (26), and (27).

¹⁴ Equations (16)-(20).

¹⁵ Equations (24) and (25).

cross section that the ground state is an eigenstate of J , that the effect of neighboring ions on a given ion can be approximated by an electrostatic field, and finally that the splitting energies due to the crystalline field is small compared to the energy of the incident neutron.

If we neglect the terms Δ_ν and substitute from Tables III and IV into (31), then we have an expression for the cross section involving the radial integrals $F_\nu(k)$'s. If we assume that charge distribution may be approximated fairly well by hydrogen-like $4f$ wave functions, $\varphi(r) \sim r^3 e^{-r/2a}$, then the integrals defining the $F_\nu(k)$'s [Eq. (23)] may be done analytically and are functions of ka .

In Table V we give values of $F_\nu^{L, S}(ka)$ for a range of parameters ka . In Tables VI and VII we give the $B_\nu^2(ka)$ for Er^{+++} and Nd^{+++} . It is seen from Tables VI and VII that the differential cross section may be approximated to within 5 percent accuracy by just the first term, B_0^2 , in the moment expansion given by Eq. (31) for $ka < 0.4$. Since for the measurements reported on in the previous paper the values of ka for which significant accuracy could be obtained were $ka = 8\pi a_0 \sin\theta/2(Z-S)^{-1}\lambda^{-1} = 0.4$, we may keep only the term B_0^2 in (31).

$$\begin{aligned} \frac{d\sigma}{d\Omega} \doteq & \left(\frac{M e g_N}{2 m c} \right)^2 (2J+1)^{-1} \left[\mathcal{G}_{0, 1}^L F_0^L(ka) + \mathcal{G}_{2, 1}^L F_2^L(ka) \right. \\ & \left. + \mathcal{G}_{0, 1}^S F_0^S(ka) + \mathcal{G}_{2, 1}^S F_2^S(ka) \right]^2, \quad ka < 0.4. \quad (33) \end{aligned}$$

Substituting $g_N = -1.91e/Mc$, $e^2/mc^2 = 2.81 \cdot 10^{-13}$ cm,

 TABLE V. $F_\nu^{L, S}$ defined by Eq. (23) and evaluated for the case $\phi^* \phi \sim r^6 \exp(-r/a)$.

$k^2 a^2$	F_0^L	F_2^L	F_4^L	F_6^L	F_0^S	F_2^S	F_4^S	F_6^S
0	1.00	0	0	0	1.00	0	0	0
0.01	0.928	0.030	0	0	0.862	0.058	0	0
0.05	0.696	0.119	0.011	0.001	0.452	0.189	0.021	0.001
0.10	0.496	0.181	0.036	0.009	0.172	0.241	0.057	0.007
0.15	0.362	0.211	0.063	0.022	0.034	0.233	0.089	0.018
0.25	0.208	0.222	0.112	0.061	-0.055	0.166	0.123	0.042
0.35	0.132	0.209	0.146	0.104	-0.058	0.101	0.126	0.062
0.5	0.0782	0.179	0.174	0.158	-0.084	0.040	0.105	0.078

TABLE VI. B_ν^2 defined by Eq. (31) and evaluated for Er with assumptions given in Sec. III by use of Tables IV and V.

k^2a^2	B_0^2	B_1^2	B_2^2	B_3^2	ΣB_ν^2
0	978	0	0	0	978
0.05	319	0	0	0	319
0.10	103	0.2	0	0	103
0.15	31.7	1.2	0.1	0	32.9
0.25	1.92	5.61	0.7	0	8.2
0.35	0.03	10.6	1.9	0	12.5
0.50	0.35	15.8	4.0	0	20.2

we get

$$\frac{d\sigma_{Er}}{d\Omega} = \frac{7.2 \times 10^{-26}}{16} \text{ cm}^2 [20.9F_0^L(ka) - 10.4F_2^L(ka) + 10.45F_0^S(ka) - 0.47F_2^S(ka)]^2, \quad (34)$$

$$\frac{d\sigma_{Nd}}{d\Omega} = \frac{7.2 \times 10^{-26}}{10} \text{ cm}^2 [16.3F_0^L(ka) - 8.3F_2^L(ka) - 7.0F_0^S(ka) + 0.49F_2^S(ka)]^2, \quad (35)$$

for the free ion cross section for $ka < 0.4$ for Er^{+++} and Nd^{+++} , respectively. We plot $F_{0,2}^L, F_{0,2}^S$ in Fig. 1. According to Eq. (21)

$$\begin{aligned} g_0(x) &= \sin x/x, \\ g_2(x) &= \left[\left(-1 + \frac{3}{x^2} \right) \frac{\sin x}{x} - \frac{3 \cos x}{x^2} \right], \\ f_0(x) &= \frac{2}{x^2} (1 - \cos x), \\ f_2(x) &= \frac{2}{x^2} \left(2 + \cos x - \frac{3 \sin x}{x} \right), \end{aligned} \quad (36)$$

and so we get for the F 's, assuming hydrogenic $4f$ wave functions,

$$\begin{aligned} F_0^S(ka) &= (8ka)^{-1} \frac{\sin 8 \tan^{-1} ka}{(1+a^2k^2)^4}, \\ F_2^S(ka) &= (8ka)^{-1} \left[-\frac{\sin 8 \tan^{-1} ka}{(1+a^2k^2)^4} + \frac{1}{14} (ka)^{-1} \right. \\ &\quad \times \left. \frac{\sin 6 \tan^{-1} ka}{(1+a^2k^2)^3} - \frac{3}{7} (ka)^{-1} \frac{\cos 7 \tan^{-1} ka}{(1+a^2k^2)^{7/2}} \right], \\ F_0^L(ka) &= \frac{1}{28} (ka)^{-2} \left[1 - \frac{\cos 7 \tan^{-1} ka}{(1+a^2k^2)^{7/2}} \right], \\ F_2^L(ka) &= \frac{1}{28} (ka)^{-2} \left[2 + \frac{\cos 7 \tan^{-1} ka}{(1+k^2a^2)^{7/2}} \right. \\ &\quad \left. - \frac{1}{2} (ka)^{-1} \frac{\sin 6 \tan^{-1} ka}{(1+a^2k^2)^3} \right]. \end{aligned} \quad (37)$$

Noting that the term F_2^S makes a negligibly small contribution to (34) and (35) over the region considered and that $\mathcal{G}_{0,1}^L$ and $\mathcal{G}_{0,1}^S$ are in fact $\mathbf{L} \cdot \mathbf{J} [J(J+1)]^{-1} \times [\frac{2}{3}J(J+1)(2J+1)]^{\frac{1}{2}}$ and $2\mathbf{S} \cdot \mathbf{J} [J(J+1)]^{-1} [\frac{2}{3}J(J+1)(2J+1)]^{\frac{1}{2}}$, respectively, Eqs. (34) and (35) may be well approximated by

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= 7.2 \times 10^{-26} \frac{2(\mathbf{L} \cdot \mathbf{J})^2}{3J(J+1)} \left[F_0^L(ka) + \frac{2\mathbf{S} \cdot \mathbf{J}}{\mathbf{L} \cdot \mathbf{J}} F_0^S(ka) \right. \\ &\quad \left. - 0.50F_2^L(ka) \right]^2 \text{ cm}^2 \\ &= 1.96 \times 10^{-24} [F_0^L(ka) + \frac{1}{2}F_0^S(ka) - 0.50F_2^L(ka)]^2 \text{ cm}^2, \text{ for } \text{Er}^{+++} \\ &= 1.94 \times 10^{-24} [F_0^L(ka) - 0.427F_0^S(ka) - 0.50F_2^L(ka)]^2 \text{ cm}^2 \text{ for } \text{Nd}^{+++}. \end{aligned} \quad (38)$$

In Fig. 2 a comparison of (38) with the experimental cross section obtained by Koehler and Wollan is presented; the abscissa is $\sin(\frac{1}{2}\theta)/\lambda = (8\pi a_0)^{-1}(Z-S)ka$, the best fits being obtained with $Z-S=23$ and 20 for Er and Nd, respectively. As explained in the previous paper, there is an uncertainty in the magnitude of the nuclear incoherent scattering which causes an uncertainty in the base line from which the magnetic scattering is to be measured; Koehler and Wollan estimate this to be of the order of ± 6 percent of the forward magnetic scattering for Er. This is indicated in the figure by three curves derived from the experimental points having a constant difference. Curve (a) gives the free ion cross section in the forward direction which is consistent with their estimated base-line uncertainty; curve (c) is the reasonable lower bound, and curve (b) is the median of (a) and (c). The magnetic cross section for Nd as shown in Fig. 2 is small; the base line was chosen so as to give the free ion cross section in the forward direction, and it is seen that the theoretical curve fits quite well.

The free ion theoretical curve is seen to give a reasonably good fit to curve (a) for Er. On the other hand, if curve (b) represents more nearly the actual magnetic scattering, then the difference of the theoretical curve and (b) may be attributed to crystalline field splittings of the type envisaged in the last section. Considering only the term $\nu=0$ in (31), the effect of the crystalline fields will then be to add to the cross section

TABLE VII. B_ν^2 defined by Eq. (31) and evaluated for Nd with assumptions given in Sec. III by use of Tables III and V.

k^2a^2	B_0^2	B_1^2	B_2^2	B_3^2	ΣB_ν^2
0	87.2	0	0	0	87.2
0.05	53.6	0.2	0.04	0	53.8
0.10	30.4	0.2	0.4	0	31.0
0.15	16.4	0.06	1.1	0	17.6
0.25	4.1	0.2	3.2	0	7.5
0.35	0.6	1.4	5.0	0	7.0
0.50	0	3.9	6.3	0	10.2

a term

$$\delta\sigma(k^2) = \sum_{\psi_f, \psi_0} \frac{E_f - E_0}{2E_{N_0}} \left\{ \left[\sigma_0(k^2) + k^2 \frac{d\sigma_0}{dk^2} \right] [g(E_f) - g(E_0)] + \frac{2M(E_f - E_0)}{\hbar^2} \frac{d\sigma_0}{dk^2} [g(E_f) + g(E_0)] \right\} \times \frac{2J+1}{6} \sum_{-1}^1 |\langle \psi_f | Y_{1,q} | \psi_0 \rangle|^2, \quad (39)$$

where $\sigma_0(k^2)$ is given by Eq. (34) and k^2 refers to the elastically scattered k at the given angle.

As may be seen from an inspection of the curve for σ_0 , over most of the region with which we are concerned $k^2(d\sigma_0/dk^2) < \sigma_0(k^2)$; and, therefore, the expression (39) for $\delta\sigma$ is negative definite. From (39) $\delta\sigma/\sigma_0 \approx (E_f - E_0)/E_{N_0}$; and, since crystalline field splittings of the order of 100 cm^{-1} ^{16,17} are expected here, it is not at all improbable that the cross section in the forward direction is actually as small as indicated by curve (b) or (c).

However, it should be pointed out that, if there is a decrease in cross section from the free ion value resulting from the above mechanism, then because of the change of the population factors $g(E, T)$ a considerable change would be generally expected in $\delta\sigma(k^2)$ in going from room temperature to 20°K ; whereas, in fact, according to Koehler and Wollan's experiment only a change of a few percent which is attributed to the change in the nuclear diffuse scattering is observed. Experiments using higher energy neutrons are being considered to obtain additional information concerning this point.

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APPENDIX

An alternative derivation of (7') from (4) which brings out the physical interpretation of the form (7) proceeds as follows:

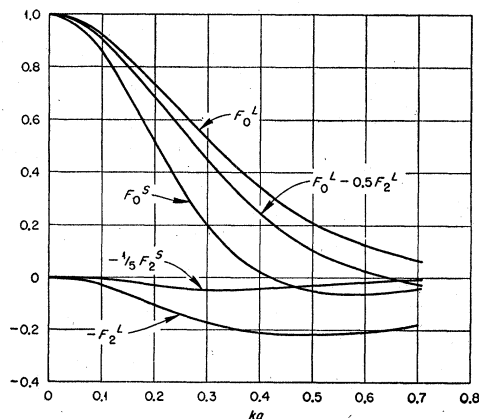


FIG. 1. $F_{0,2}^{L,S}$ defined by Eq. (23) for case $\phi^* \phi \sim r^0 \exp(-r/a)$.

¹⁶ F. A. Spedding, J. Chem. Phys. 5, 316 (1937).

¹⁷ B. Bleaney, Physica 17, 175 (1951).

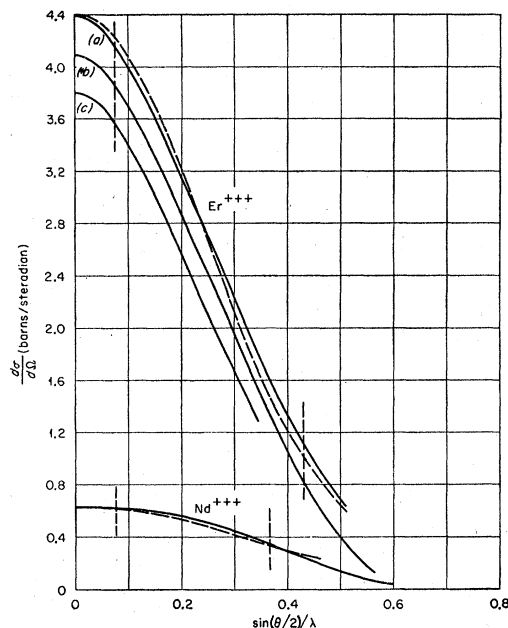


FIG. 2. The solid curves represent the measured values and the dashed curves the theoretical free ion values assuming hydrogenic radial wave function with $Z-S$ 23 and 20 for Er^{+++} and Nd^{+++} , respectively. The three curves (a), (b), and (c) for Er^{+++} represent the experimental base line uncertainty as explained in the text. The vertical dashed lines represent the regions outside of which the experimental values are uncertain.

Let ψ_0, ψ_f refer to states with the same energy; then for

$$\mathbf{j}_L = (e\hbar/2mci) [\psi_f^* \nabla \psi_0 - (\nabla \psi_f^*) \psi_0],$$

we have

$$\nabla \cdot \mathbf{j}_L = 0.$$

Therefore an \mathbf{M}_L may be defined so that

$$\mathbf{j}_L = \nabla \times \mathbf{M}_L.$$

Therefore the term in (4)

$$\int d^3r e^{ik \cdot r} \mathbf{j}_L = -i\mathbf{k} \times \int \mathbf{M}_L e^{ik \cdot r} d^3r.$$

We may take for \mathbf{M}_L ,

$$\mathbf{M}_L = r^{-2} \mathbf{r} \times \int_r^\infty \rho \mathbf{j}_L(r^{-1} \mathbf{r} \rho) d\rho;$$

then, integrating by parts,

$$\begin{aligned} \int \mathbf{M}_L e^{ik \cdot r} d^3r &= \int \frac{1}{2} \mathbf{r} \times \mathbf{j}_L f(k \cdot r) d^3r \\ &= (e/2mc) \int \psi_f^* \frac{1}{2} [\mathbf{L} f(k \cdot r) + f(k \cdot r) \mathbf{L}] \psi_0 d^3r \\ \therefore \int \mathbf{j}_L e^{ik \cdot r} d^3r \\ &= -i\mathbf{k} \times (e/2mc) \int \psi_f^* \frac{1}{2} [\mathbf{L} f(k \cdot r) + f(k \cdot r) \mathbf{L}] \psi_0 d^3r, \end{aligned}$$

in agreement with Eqs. (6) and (7').