

Magnetic Interaction and Resultant Anisotropy in Unstrained Ferromagnetic Crystals

L. W. MCKEEHAN

Sloane Physics Laboratory, Yale University, New Haven, Connecticut

(Received May 5, 1937)

The mutual potential energy of two equal and parallel magnets is derived for several especially symmetrical distributions of magnetic moment in each. If R is the distance between magnet centers the first three terms in order of importance depend upon R^{-3} , R^{-5} and R^{-7} . These may be called "dipole," "quadrupole" and "sextupole" terms, respectively. Magnets previously considered as representing the atoms in a ferromagnetic crystal are special cases of one of the general cases here treated. Sextupole terms have not heretofore been included. The distributions of magnetic moment now dealt with permit a closer correspondence between the model magnet in iron, cobalt, and nickel and the probable distribution in these atoms of the electrons responsible for ferromagnetism.

In order to compute ferromagnetic anisotropy—differences in potential energy for differences in direction of magnetization in a crystal—sums of zonal harmonics over the points occupied by atoms are also needed. Such sums

for second and fourth-order harmonics have previously been reported for the crystal structures of interest. Sums of sixth-order harmonics are now given.

Within the space assigned in current pictures of the atom to "ferromagnetic" electrons we find ample room for distributions of magnetic moment, agreeing in total amount with observed saturation values, to account in general for reported anisotropies in iron, cobalt, nickel and their cubic alloys. These distributions seem to depend principally upon the maximum number of codirected electron spins. Reported changes of anisotropy with rise of temperature are such as would result from relative rotations of atomic axes out of exact parallelism.

The effects of magnetostrictive strain, here omitted from consideration, may explain some discrepancies in the sign or magnitude of the sextupole terms. In hexagonal cobalt it must be assumed that the molecular field itself is anisotropic.

I. ELEMENTARY MAGNETS

WE first consider the mutual potential energy, $2U$, of a pair of equal and parallel magnets each of magnetic moment \mathbf{P} and separated by a distance \mathbf{R} . In order to distinguish numerical factors from those involving physical dimensions and units we put $\mathbf{P} = P\mathbf{p}$, where \mathbf{p} is a unit vector, and $\mathbf{R} = a\mathbf{r}$, where \mathbf{r} is a unit vector and a is the length chosen as a unit. (When we deal with crystals a will be the length of one edge of the unit cell.) This makes r a pure number, the values of which depend only upon the symmetry of the crystal.

The simplest possible magnet is a dipole, anything more complicated than this involves some spatial distribution of magnetic moment and may be called a multipole.

Dipole magnets

The mutual potential energy per magnet can be expressed in closed form if the magnets are simple dipoles. It is

$$U_2 = -(P^2/a^3)r^{-3}P_2\{\cos(\mathbf{p}, \mathbf{r})\}. \quad (1)$$

Here $P_2\{u\}$ is the second-order zonal surface harmonic, argument u .

Multipole magnets

For magnets more complicated than simple dipoles the mutual potential energy per magnet must be expanded in series form. One such form is

$$U = -(P^2/a^3) \sum_{n=2}^{n=\infty} r^{-n-1} f_n(\mathbf{p}_a, \mathbf{p}_b, \dots, \mathbf{p}_k, \mathbf{r}), \quad (2)$$

wherein the structure of the multipole fixes the number and the directions of the unit vectors \mathbf{p}_a to \mathbf{p}_k , and the form of the numerical functions f_n . There is no term for $n < 2$ because the magnets are supposed to have no net magnetic charges.

In (2) the magnets are much more generalized than necessary. If we make all the characteristic directions \mathbf{p}_a to \mathbf{p}_k parallel to a single direction \mathbf{p} , and make the structure as symmetrical as possible about a plane perpendicular to \mathbf{p} through its center, the magnet is still complicated enough for practical purposes. It is now what Kornfeld¹ called a zonal multipole and the f_n can be written $F_n P_n\{\cos(\mathbf{p}, \mathbf{r})\}$, F_n being independent of \mathbf{p} and \mathbf{r} , so that (2) becomes

¹ H. Kornfeld, *Zeits. f. Physik* **22**, 27-43 (1924).

$$U_{zm} = -(P^2/a^3)[F_2r^{-3}P_2\{\cos(\mathbf{p}, \mathbf{r})\} \\ + F_4r^{-5}P_4\{\cos(\mathbf{p}, \mathbf{r})\} \\ + F_6r^{-7}P_6\{\cos(\mathbf{p}, \mathbf{r})\} + \dots]. \quad (3)$$

Upon discovering that $F_2=1$ in all cases we recognize the first term as the dipole energy, (1). By analogy it is customary to call the second

term the quadrupole energy, the third term the sextupole energy, and so on. Going still farther some authors proceed to define a "quadrupole moment," "sextupole moment," and so on. The definitions proposed by Kornfeld,¹ and used by Akulov,² correspond to the following rearrangement of (3), the terms in braces being the *squares* of the successive moments.

$$U_{zm} = -\{P^2F_2\}(ar)^{-3}P_2\{\cos(\mathbf{p}, \mathbf{r})\} + 3\left\{-\frac{P^2F_4a^2}{3}\right\}(ar)^{-5}P_4\{\cos(\mathbf{p}, \mathbf{r})\} \\ - 10\left\{\frac{P^2F_6a^4}{10}\right\}(ar)^{-7}P_6\{\cos(\mathbf{p}, \mathbf{r})\} + \dots - (-1)^{\frac{1}{2}n+1}\frac{(n-1)!}{(n/2)!(n/2-1)!} \\ \times \left\{(-1)^{\frac{1}{2}n+1}\frac{(n/2)!(n/2-1)!}{(n-1)!}P^2F_n a^{n-2}\right\}(ar)^{-n-1}P_n\{\cos(\mathbf{p}, \mathbf{r})\} \dots \quad (4)$$

These higher moments are of little or no physical importance, since magnets cannot be constructed which have, let us say, quadrupole moment with no dipole moment. Their definitions also ensure that some of them will be imaginary, e.g., the quadrupole moment of nickel.

Magnetic form factors (F_4, F_6)

In our further analysis we will need F_4 and F_6 for elementary magnets appropriate to atoms of iron, cobalt and nickel. ($F_2=1$ for all models.) The method of deriving the F_n is as follows. Distribute the proposed magnetic moment of one atom, P , consistently with the symmetry already explained, so that the magnetic moment per unit volume is known at all points where it is not zero. Choose a point on the axis of this multipole, well outside its limits. The magnetic field at this point lies along the axis, and can be expressed as a series in ascending negative powers of the distance of the point from the center of the multipole. The potential energy of a dipole with axis parallel to the multipole axis, placed at the point in question, is minus the product of its magnetic moment by the field intensity. The potential energy for nonaxial positions of the dipole is derived from the series thus found by multiplying each term by the appropriate zonal surface harmonic.

Now suppose a second multipole like the first (or of some other type, in case of alloys) and with its axis parallel to that of the first. Place the center of the second multipole on the

axis of the first at such a distance that their magnetic structures do not overlap. The mutual potential energy is found by integrating the expression for the energy per unit magnetic moment, already found as a function of distance and polar angle, over points where the magnetic moment of the second multipole differs from zero. Under the given conditions the series thus obtained converges. Arrange it in ascending negative powers of the single coordinate defining the relative positions of the two structures.

Again extend the result to three dimensions by introducing zonal surface harmonics of appropriate orders. The coefficients of the zonal harmonics in this series are the required F_n .

We are interested in distributions of magnetic moment suggested by, or at least consistent with, spectroscopic data. Slater³ gives tables from which we can conclude that the $3d$ electrons supposed to account for the unbalanced magnetic moment in iron, cobalt, and nickel are concentrated at a distance from the nucleus which can be estimated in each of these elements and which does not vary greatly in this triad. Let us call this distance ρa , expressed as a numerical multiple of the unit length a . We will find the F_n for a few simple structures.

Case 1. Sphere (spherical shell)

It appears without detailed analysis that all distributions of magnetic moment which have

² N. S. Akulov, Zeits. f. Physik 57, 249-256 (1929).

³ J. C. Slater, Phys. Rev. 36, 57-64 (1930).

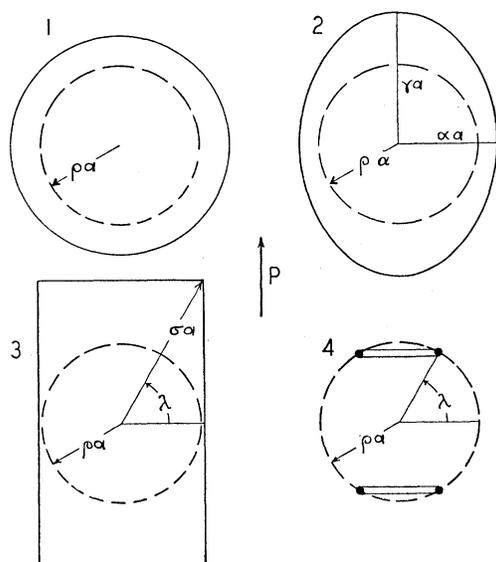


FIG. 1. Cross sections of magnetic elements. (See Table I.)

spherical symmetry, except for the fact that all the elementary volumes have parallel magnetic axes, have $F_n=0$ for $n>2$. Such structures are therefore equivalent to dipoles. This means that our analysis is not really restricted, as it seemed to be, to swarms of point electrons. Spatially extensive electrons, so long as the magnetic moment per unit volume in each is a function only of the radius, give the same results.

Case 2. Spheroid (spheroidal shell)

The next simplest case is that of a uniformly magnetized spheroidal magnet, a spheroid filled with uniform volume distribution of magnetic moment. Symmetry requires the magnetic axis to be the axis of figure. Fig. 1 shows a cross section of such a spheroid, the corresponding ρa being shown as a broken circle within the spheroid of semi-axes αa , αa , γa . Table I gives expressions for F_4 and F_6 in terms of α and γ . It will be noticed that when $\gamma=\alpha$, F_4 and F_6 vanish as they should for a sphere.

Since F_4 and F_6 depend only upon $(\gamma^2-\alpha^2)$, which is the same for all confocal ellipses, it is clear that spheroidal shells and distributions built up by superposing such shells have constant F_4 and F_6 so long as all shells are defined by the same focal points. Notice that prolate spheroids have positive F_4 , oblate spheroids

negative F_4 , but that F_6 can only be positive in either case. The ratio of ρa to γa and αa involves elliptic integrals.

Case 3. Cylinder

A more conventional shape of magnet is a right circular cylinder, uniformly magnetized along its axis, and this is the only model hitherto considered in magnetic interaction studies. Fig. 1 suggests how the length ($\sigma a \sin \lambda$) and radius ($\sigma a \cos \lambda$) of such a cylinder are related to the mean radial distance ρa of its volume elements from its center. The actual relation is very complicated. Table I shows how F_4 and F_6 depend upon the shape and size of the cylinder.

The expressions for F_4 at the limits, $\lambda=0$ and $\lambda=\pi/2$, that is for a circular current loop and for an infinitely thin bar magnet, have been known for many years.

Case 4. Pair of dicircles

None of the structures so far discussed seems suitable for a first approximation to actual atomic magnets. The dependence of ρa upon limiting dimensions of the model structure is highly inconvenient, and unduly increases the labor of computation. There is only one way to avoid this difficulty, by keeping all the magnetic moment on a sphere of radius ρa . Symmetry requires that the simplest general model of this type have its magnetic moment spread uniformly along two parallels of latitude, at $+\lambda$ and $-\lambda$. Each of these circles may be called a dicircle (analogous to dipole). It is easy to see that the limiting cases, $\lambda=0$ and $\lambda=\pi/2$, must give the extreme possible values of F_4 for any distribution not extending beyond ρa . Table I shows that this case, like case 3, permits both positive and negative F_6 .

The restriction to zonal multipoles is not as artificial as it seems, for unless the symmetry of the model atom about the axis of magnetization is equal to or higher than the symmetry of the crystal about the same axis the analysis becomes unmanageable. Since the axis of magnetization is to be unrestricted this means that it must tolerate both four fold and threefold rotations in cubic crystals, that is, it must have complete rotational symmetry. If a physical basis is

TABLE I. *Magnetic form factors, F_4 and F_6 . (See Fig. 1 for definition of symbols.)*

Case 1. Sphere	
$F_4=0; F_6=0.$	
Case 2. Spheroid	
$F_4=12(\gamma^2-\alpha^2)/5; F_6=216(\gamma^2-\alpha^2)^2/35.$	
Case 3. Right circular cylinder	
$F_4=\sigma^2(4-7\cos^2\lambda);$	
$F_6=\sigma^4(128-496\cos^2\lambda+443\cos^4\lambda)/8,$	
$F_4=0$ for $\lambda=\pm 40^\circ-54';$	
$F_6=0$ for $\lambda=\pm 32^\circ-11', \pm 50^\circ-34'.$	
Maxima: $F_4=4\sigma^2; F_6=16\sigma^4, 75\sigma^4/8.$	
Minima: $F_4=-3\sigma^2; F_6=-600\sigma^4/443$ for $\lambda=\pm 41^\circ-34'.$	
Case 4. Pair of dicitrles	
$F_4=6\rho^2(2-3\cos^2\lambda);$	
$F_6=15\rho^4(32-112\cos^2\lambda+89\cos^4\lambda)/4.$	
$F_4=0$ for $\lambda=\pm 35^\circ-16';$	
$F_6=0$ for $\lambda=\pm 25^\circ-07', \pm 48^\circ-32'.$	
Maxima: $F_4=12\rho^2; F_6=120\rho^4, 135\rho^4/4.$	
Minima: $F_4=-6\rho^2;$	
$F_6=-1080\rho^4/89$ for $\lambda=\pm 37^\circ-31'.$	

desired, the model may be thought of as representing the average aspect of a rigid group of electrons with random azimuths in the different atoms of the crystal.

II. FERROMAGNETIC CRYSTALS

Magnetic potential energy density

In an infinite crystal with N zonal multipoles per unit cell of volume V the mean magnetic potential energy density is

$$E=(N/V)\sum' U_{zm}, \quad (5)$$

where the primed summation is to be taken for all pairs of magnets which have one selected magnet in common. (If all the magnets are not alike, or if their environments differ, the selected magnets must include all sorts in proper proportions, and a suitable mean value of E is to be found; see Alloys, below.)

In perfect crystals the indicated summations can be effected to any desired precision. In actual imperfect crystals these ideal values will be more or less departed from. Previous work⁴ has shown that results of computation will be comparable with experiment in crystals where the atoms at small r lie nearly at the points of a perfect lattice with a point at the origin atom, and where there is no systematic deviation from perfect arrangement (no elastic strain).

⁴L. W. McKeehan, Phys. Rev. **43**, 913-923, 924-930, 1022-1024, 1025-1029; **44**, 38-42, 582-584 (1933)

Collecting common factors and using the abbreviation, $S_n=\sum'r^{-n-1}P_n\{\cos(\mathbf{p}, \mathbf{r})\}$, we rewrite (5) in the form

$$E=- (NP^2/Va^3)[F_2S_2+F_4S_4+F_6S_6+\dots]. \quad (6)$$

The volume of the unit cell can be expressed in terms of the parameter a and axial ratios. In cubic crystals the edges of the unit cube being each equal to a , we have $V=a^3$. In hexagonal crystals the edges of the unit prism are a , a and ca , the first two being 120° apart and the third (principal) axis perpendicular to these, so that $V=a^3c\sqrt{3}/2$.

We need S_2 , S_4 and S_6 for body-centered and face-centered cubic lattices and for hexagonal close-packing. It involves no extra work to get these sums for simple cubic and simple hexagonal lattices (primitive lattices) as well.

Lattice sums—dipole terms

In finding S_2 we must specify boundary conditions, because an important part of S_2 (in cubic crystals all of it) depends upon magnets lying outside a large sphere centered at the origin and wholly inside the actual boundary of the specimen. The least special boundary to choose is one at infinity, and this is essentially what we do when we use the rapidly convergent series forms given in Appendix I. Finite boundaries equivalent at the origin to a boundary at infinity are those for which the so-called demagnetizing field is zero. This means that experimental results, corrected for demagnetizing fields, as they usually are, may be compared directly with our calculations, presented in Table II.

 TABLE II. *Coefficients in zonal harmonic lattice sums S_2 , S_4 , and S_6 .*

COEFFICIENT	ATOMIC ARRANGEMENT				
	CUBIC			HEXAGONAL, $c=2\sqrt{6}/3$	
	PRIMITIVE	BODY-CENTERED	FACE-CENTERED	PRIMITIVE	CLOSE-PACKED
S_2	2.09440	4.18879	8.37758		
S_{20}				2.75741	2.96023
S_{22}				-3.82936	0.00507
S_{40}	3.10823	-3.10734	-7.19838	0.95461	0.33815
S_{60}	0.57333	5.44656	-26.63489		
S_{62}				-1.91857	-4.15924
S_{66}				2.66930	2.51851

In cubic crystals S_2 does not depend upon the direction (\mathbf{p}) of the magnetization. The series form (Appendix I) is not needed here, since $S_2 = 2\pi N/3$ in all cases.

In hexagonal crystals

$$S_2 = S_{20} + S_{22}p_3^2. \quad (7)$$

Here p_3 is the component of \mathbf{p} along the hexagonal axis. The series in Appendix I contain a general axial ratio, c , but only a particular value of $c = 2\sqrt{6}/3$ has been used in computing S_{20} and S_{22} for Table II. This is the axial ratio for hexagonal close-packing of spheres. It differs a little from the axial ratio in hexagonal cobalt, $c = 1.624$, but is much more convenient, since many values of r^2 are integers when $c = 2\sqrt{6}/3$. Table II does not show what part of S_{20} depends upon remote magnets. This may be computed directly as $4\pi N\sqrt{3}/9c$. For the two arrangements chosen $N = 1, 4\pi N\sqrt{3}/9c = 1.48096$, and $N = 2, 4\pi N\sqrt{3}/9c = 2.96192$. It will be noticed that in hexagonal close-packing nearby magnets contribute very little to S_{20} .

Lattice sums—quadrupole terms

The sum S_4 converges absolutely, that is, it does not depend appreciably upon remote magnets. In cubic crystals

$$S_4 = S_{40} \{1 - 5(p_2^2 p_3^2 + p_3^2 p_1^2 + p_1^2 p_2^2)\}, \quad (8)$$

wherein p_1, p_2, p_3 are the direction-cosines of \mathbf{p} with respect to the cubic axes.

In hexagonal crystals

$$S_4 = S_{40} \{1 - 10p_3^2 + (35/3)p_3^4\}. \quad (9)$$

This may also be written

$$S_4 = (8S_{40}/3) P_4\{p_3\}. \quad (10)$$

Lattice sums—sextupole terms

Though S_6 converges more rapidly than S_4 its convergence is still so slow that the special forms in Appendix I must be used if precision is desired. In cubic crystals

$$S_6 = S_{60} \{1 - (21/2)(p_2^2 p_3^2 + p_3^2 p_1^2 + p_1^2 p_2^2) + (231/2)p_1^2 p_2^2 p_3^2\}. \quad (11)$$

In hexagonal crystals a rectangular frame of reference is inappropriate, since it conceals the true symmetry of the functions of direction. We

therefore define \mathbf{p} by θ_3 , the angle it makes with the hexagonal axis, and by the azimuth, ϕ , of the plane through \mathbf{p} and the hexagonal axis, measured from the nearest prism face of form $\{100\}$. In terms of these coordinates

$$S_6 = S_{63} P_6\{\cos \theta_3\} + S_{66} \cos 6\phi \sin^6 \theta_3. \quad (12)$$

III. COMPARISON BETWEEN THEORY AND EXPERIMENT

There is already a considerable amount of information about ferromagnetic anisotropy, especially regarding iron, cobalt, nickel and their alloys.⁵ The best way of presenting the experimental findings is to give the values of coefficients appearing in an empirical equation for the magnetic potential energy density as a function of the direction of magnetization. In cubic crystals this is

$$E = K_0 + K_1(p_2^2 p_3^2 + p_3^2 p_1^2 + p_1^2 p_2^2) + K_2 p_1^2 p_2^2 p_3^2. \quad (13)$$

In hexagonal crystals the analogous equation is, to the same degree,

$$E = K_0 + H_1 \cos^2 \theta_3 + H_2 \cos^4 \theta_3 + H_3 \cos^6 \theta_3 + H_4 \cos^6 \phi \sin^6 \theta_3. \quad (14)$$

The way in which K_1 and K_2 , in (13), can be derived from experimental data of various kinds has been described by Bozorth.⁶ No attempt has yet been made to evaluate all the possible coefficients appearing in (14). The constant term in (13) and (14), K_0 , cannot be found by experiment and is of slight interest, anyway, since it is completely negligible in comparison with the potential energy decrease arising from non-magnetic interaction (the molecular field). The forms of (13) and (14) depend only upon crystal-line symmetry, though (13) may be written in various ways by using the identity: $p_1^2 + p_2^2 + p_3^2 = 1$.

Among various ways of fitting model magnets to the experiments the one here chosen is to select an extreme model of plausible type for each of the atoms present, to compute the coefficients in (13) or (14) consistent with these

⁵ For a recent compilation of results see L. W. McKeehan, Phys. Rev. **51**, 136–139 (1937). This should be consulted for the sources of data concerning cubic metals and alloys.

⁶ R. M. Bozorth, Phys. Rev. **50**, 1076–1081 (1936).

model atoms in the actual crystal structure and to compare these computed values with available experimental values. If the computed coefficients are too large we can get a better fit by reducing the dimensions of the model magnet, or by allowing for heat motions and other displacements from ideal arrangements. If the computed coefficients are too small or are of the wrong sign we must admit other causes for anisotropy than those discussed above. One such cause may be given special mention at this point.

Effects of homogeneous strain

It is well known that elastic strains may be large enough to confer extra stability on one of the preferred directions for magnetization in a cubic crystal (directions for minimum E) and may even make magnetization easiest along a direction not preferred in the unstrained crystal.⁷ The lattice sums S_2 , in our notation, become dependent upon the direction of magnetization, \mathbf{p} , even in crystals originally cubic. They depend also upon the strain tensor. The magnetostrain may be considered⁸ as that self-imposed strain which makes the total potential energy—magnetic and elastic—minimal. Our computation of E has ignored these effects upon S_2 and is therefore certain to be inexact. The sums S_4 will also be affected by strain, though less seriously, because the strain does not here upset an exact balance as it does when $S_2=0$ in the unstrained crystal.

The reason for ignoring the effects of strain in this first approximation is that the strain argument gives the wrong sign for the magnetostriction of nickel,⁸ and cannot therefore be as important as was first supposed. The extreme smallness of magnetostrains in comparison with elastic strains known to alter preferred directions for magnetization also means that something else than strain must explain the relatively large differences in E for different directions in well-annealed crystals.

The idea at the bottom of the present analysis, that the shape of the atomic magnet principally accounts for preferred orientations of these magnets in crystals, is not of recent origin.

What is new is the suggestion⁹ that the appropriate shape differs in different atoms, particularly in iron and in nickel.

Theoretical anisotropy

In cubic crystals we find by comparing (6) with (13) that

$$K_0 = -(NP^2/Va^3) \times [F_2S_2 + F_4S_{40} + F_6F_{60} + \dots], \quad (15)$$

$$K_1 = -(NP^2/Va^3) \times [-5F_4S_{40} - (21/2)F_6S_{60} + \dots], \quad (16)$$

$$K_2 = -(NP^2/Va^3)[(231/2)F_6S_{60} + \dots]. \quad (17)$$

In hexagonal crystals we will compare values of E for three important directions: the hexagonal axis, $[001]$; a close-packed line and twofold axis in the basal plane, $[100]$; one of the other set of twofold axes in the basal plane, $[210]$. For these directions we find

$$E_{001} = -(NP^2/Va^3)[F_2S_{20} + F_2S_{22} + (8/3)F_4S_{40} + F_6S_{63} + \dots], \quad (18)$$

$$E_{100} = -(NP^2/Va^3)[F_2S_{20} + F_4S_{40} - (5/16)F_6S_{63} + F_6S_{66} + \dots], \quad (19)$$

$$E_{210} = -(NP^2/Va^3)[F_2S_{20} + F_4S_{40} - (5/16)F_6S_{63} - F_6S_{66} + \dots]. \quad (20)$$

For reasons already given we confine ourselves to dicircle models, case 4 of Fig. 1 and Table I. Data used in computation are collected in Table III.

Pure metals (Table III)

Iron (body-centered cubic).—We put $\lambda=0$ for an equatorial concentration of magnetic moment in iron. That this is necessary was first clearly stated by Mahajani.¹⁰ It is consistent with the large number, four, of disposable spins in iron, since not more than two electrons could occupy the other extreme position, $\lambda=\pi/2$, without interference. We reject the most symmetrical arrangement of four points—in a regular tetrahedron with two of its edges perpendicular to the magnetic axis—because this puts dicircles at $\lambda=\pm 35^\circ-16'$, making $F_4=0$, F_6 negative, so that K_1 becomes negative, contrary to experi-

⁷ R. Becker, *Zeits. f. Physik* **62**, 253–269 (1930); F. Bitter, *Phys. Rev.* **42**, 697–708 (1932).

⁸ N. S. Akulov, *Zeits. f. Physik* **52**, 389–405 (1928).

⁹ R. M. Bozorth, L. W. McKeehan, *Phys. Rev.* **51**, 216 (1937).

¹⁰ G. S. Mahajani, *Proc. Camb. Phil. Soc.* **23**, 136–143 (1926); especially footnote on page 138.

ence. Furthermore, the average number of unbalanced spins per atom lies between two and three so that the existence of four in one atom cannot be typical.

With this assignment of λ we find $K_1=25.46 \times 10^6$ erg. cm^{-3} , $K_2=-167.1 \times 10^6$ erg. cm^{-3} . (Hereafter we suppress the constant factor 10^6 erg. cm^{-3} in E and its parts.) As far as K_1 is concerned a smaller or less extremely equatorial structure would be better, since the experimental value of K_1 at room temperature is only 0.42.

The sign of K_2 is wrong and it is about one thousand times greater than necessary. It remains to be seen whether this discrepancy in sign can be accounted for by magnetostriction. The persistence of relatively high K_2 right up to the temperature (600°C) at which K_1 reaches a very low value is in favor of the dependence of K_2 on some factor which does not change as rapidly with temperature as we expect sextupole magnetic interaction to change.

Nickel (face-centered cubic).—Having selected

TABLE III. Calculated anisotropy of pure metals.

Part 1. Cubic crystals							
ELEMENT		Fe	(Fe)	Co	(Co)	Ni	(Ni)
Magnetic moment per atom*	$P \times 10^{20}$	2.055	2.055	1.5794	1.5794	0.5883	0.5883
Atomic weight	A	55.85	55.84	58.94	58.94	58.69	58.69
Diameter of $3d$ shell**	$2\rho a$	1.53	1.53	1.38	1.38	1.27	1.27
Crystal structure		B.C.C.	F.C.C.	F.C.C.	B.C.C.	F.C.C.	B.C.C.
Number of atoms per cell	N	2	4	4	2	4	2
Lattice parameter***	$a \times 10^8$	2.861	3.646	3.545	2.846	3.517	3.00
Relative radius of $3d$ shell	ρ	0.267	0.210	0.195	0.242	0.181	0.212
Latitude of dicircles	λ	0	0	$\pi/2$	$\pi/2$	$\pi/2$	$\pi/2$
Magnetic form factors							
Quadrupole factor	F_4	-0.4290	-0.2641	0.4546	0.7054	0.3912	0.5376
Sextupole factor	F_6	0.1725	0.0654	0.1722	0.4146	0.1275	0.2409
Anisotropy coefficients							
First (quadrupole part)		10.26	6.84	-8.23	-10.29	-1.03	-0.79
First (sextupole part)		15.20	-13.16	-24.21	22.26	-2.61	1.31
First (total)	K_1	25.46	-6.32	-32.44	11.97	-3.64	0.52
Second (sextupole)	K_2	-167.1	144.7	266.4	-244.9	28.7	-14.4
Part 2. Hexagonal cobalt							
Magnetic moment per atom*	$P \times 10^{20}$			1.5794			
Atomic weight	A			58.94			
Diameter of $3d$ shell**	$2\rho a$			1.38			
Crystal structure				H.C.P.			
Number of atoms per cell	N			2			
Lattice parameter***	a			2.507			
Axial ratio—observed				1.624			
Axial ratio—assumed	$2\sqrt{6}/3$			1.633			
Relative radius of $3d$ shell	ρ			0.275			
Latitude of dicircles	λ			0			$\pi/2$
Magnetic form factors							
Quadrupole factor	F_4			-0.4545			0.9090
Sextupole factor	F_6			0.1937			0.6886
Energy density differences							
$E_{100}-E_{001}$							
Dipole part				0.0072			0.0072
Quadrupole part				0.7279			-0.3640
Sextupole part				-5.5878			-1.5716
Total				-4.8527			-1.9284
$E_{210}-E_{001}$							
Sextupole part				-5.0949			-1.4330
Total				-4.3598			-1.7898
$E_{210}-E_{100}$							
(Sextupole) total				0.4929			0.1386

* Values for Fe and Ni based on M. Fallot, *Dissertation* (Strasbourg, 1935). Magnetic moment per gram-atom, $\sigma_0=221.74$ for Fe, $\sigma_0=60.41$ for Ni; $P=\sigma_0 A/N_0$ with $N_0=6.026 \times 10^{23}$ atoms per gram-atom. Value for Co based on R. I. Allen, F. W. Constant, *Phys. Rev.* **44**, 228-233 (1933). Saturation magnetization $I_{\text{sat}}=1418$, $P=I_{\text{sat}}/Na^3$.

** J. C. Slater, *Phys. Rev.* **36**, 57-64 (1930), column (5), Table I(d), p. 62.

*** Values for stable metals and F.C.C. cobalt from M. C. Neuburger, *Zeits. f. Krist.* **93**, 1-36 (1936).

$\lambda=0$ for iron we put $\lambda=\pi/2$ for nickel, noticing that this is the best of all possible choices for a pair of disposable spins. In this case we have unique data at very low temperatures,¹¹ so that our model should receive its severest test. We compute $K_1=-3.64$; $K_2=28.7$ and can derive from the published curves the following values for comparison at -252.3° : $K_1=-2.8$, $K_2=4.2$. The experimental values are rendered rather uncertain by the fact that saturation was attained only along $[111]$ at the lowest temperature, so that extensive extrapolations were necessary in finding K_1 and K_2 . The agreement is very gratifying.

Cobalt (hexagonal close-packed).—In this crystal structure there is some preference for axial magnetization due merely to dipole terms. But the whole difference in energy in favor of axial magnetization¹² is much too large to be accounted for by dipole terms alone. At -190°C we find $E_{100}-E_{001}=8.81$, $E_{210}-E_{001}=9.44$, and the part due in each of these to dipole interactions is only 0.0072 for the axial ratio $c=2\sqrt{6}/3=1.633$. Shrinking the axial ratio to its experimental value, $c=1.624$, increases the dipole coefficient S_{22} from 0.00507 to 0.03497 and correspondingly raises $E_{100}-E_{001}$ and $E_{210}-E_{001}$ to 0.0500 which is still far too low.¹³ It is therefore necessary to look for higher order terms of proper sign. The first guess, since the number of disposable spins is greater than two, is to put $\lambda=0$. If we consider only the quadrupole terms in addition to dipole terms, we find for $\lambda=0$, $E_{100}-E_{001}=E_{210}-E_{001}=0.735$, which is still inadequate in amount and, moreover, leaves the experimental finding $E_{210}-E_{100}=0.63$ unaccounted for. The last defect is remedied by including the sextupole terms. These yield $E_{210}-E_{100}=0.493$, in reasonable agreement with what seems to be needed. The differences $E_{100}-E_{001}$ and $E_{210}-E_{001}$ change sign, however,

so that the principal problem, to explain the high stability for axial magnetization, is farther from solution than before.

If we try $\lambda=\pi/2$, which is not impossible since the average number of unbalanced spins per atom is here less than two, the sextupole terms account for $E_{210}-E_{100}=0.138$, which is hardly enough. The computed values of $E_{100}-E_{001}$ and $E_{210}-E_{100}$ are again of the wrong sign, though not so negative as for $\lambda=0$. The quadrupole terms now contribute to the anomaly and this is a clue to a possible choice between $\lambda=0$ and $\lambda=\pi/2$, for above 260°C the experiments¹² show that the hexagonal axis is avoided rather than preferred. The relative importance of quadrupole terms, as compared with sextupole terms, should of course be greater at higher temperatures.

We suggest as the best way out that the low temperature preference for the hexagonal axis must have a nonmagnetic origin. This amounts to saying that electrostatic interactions are responsible, or that the molecular field has a maximum along the hexagonal axis at low temperatures, and that this maximum decreases rapidly as the temperature rises so that above 260°C the magnetic interactions, now mainly of quadrupole order, predominate. For the magnetic interactions we therefore propose $\lambda=\pi/2$ as the best first approximation.

Unstable forms

Face-centered cubic cobalt can be preserved at room temperature by quenching from temperatures at which it is the stable form. The metal is ferromagnetic in both modifications and has about the same saturation magnetization.¹⁴ The ferromagnetic anisotropy of the cubic arrangement has not been studied experimentally. We include in Table III predictions of its anisotropy constants at low temperatures (total K_1 , K_2) and at higher temperatures (quadrupole part of K_1). The anisotropy of body-centered cubic nickel and cobalt (neither of these is known to exist) and that of face-centered cubic iron (not known as a pure metal) have also been computed. In these cases it has been necessary to estimate

¹¹ K. Honda, H. Masumoto, Y. Shirakawa, *Sci. Rep. Tohoku Imp. Univ.* **24**, 391–410 (1935).

¹² S. Kaya, *Sci. Rep. Tohoku Imp. Univ.* **17**, 1157–1177 (1928); K. Honda, H. Masumoto, *Sci. Rep. Tohoku Imp. Univ.* **20**, 323–341 (1931); for energy differences based on these experiments see L. W. McKeehan, *Trans. A. I. M. E.* **111**, 11–52 (1934), especially Table 3, p. 47.

¹³ The effect of small changes in c has been discussed in a previous paper, L. W. McKeehan, *Phys. Rev.* **43**, 1025–1029 (1933). In using the formulae there given notice that the present S_2 is $-u/2$ in the earlier notation.

¹⁴ R. I. Allen, F. W. Constant, *Phys. Rev.* **44**, 228–233 (1933).

lattice parameters by extrapolating the parameter-concentration curves of appropriate alloy series, and to assume that the magnetic moment per atom remains the same as in the forms stable at low temperatures. Neither of these procedures is justified. In all these cases the value of λ chosen for the low temperature form has been used throughout.

Alloys (Table IV)

We can now proceed to compute anisotropies in alloys of iron, cobalt, and nickel. We postulate that the magnetic form factors found most suitable for the pure metals are unaltered by mixture. Two types of alloy will be considered. In the solid solution type the distribution of the component atoms over the occupied points is entirely at random. In the perfectly ordered, or superstructure type, the distribution of each component has the full symmetry of the space lattice. This restricts the composition to definite proportions, different in superstructures derived from solid solutions with different space lattices. There is no difficulty, in principle, in dealing with intermediate cases, partial order in compositions consistent with perfect order, or in compositions differing from these, where perfect order is impossible. Such intermediate cases are merely more cumbersome to formulate and compute.

Solid solutions

In Eq. (6) we need to use instead of P^2F_2 , P^2F_4 and P^2F_6 suitable mean values of these quantities. Let the fractions of the nickel, iron, and cobalt be, respectively, f_A , f_B , f_C , and let their magnetic moments per atom be P_A , P_B , P_C . There will be form factors, F_{AA} , F_{6A} and others corresponding to pairs of like atoms, already given in Table III, and new factors, F_{4AB} , F_{6AB} , and others, corresponding to pairs of unlike atoms. With $\lambda_B=0$, $\lambda_A=\lambda_C=\pi/2$ we have the following cross factors:

$$\begin{aligned} F_{4BC} &= -3\rho_B^2 + 6\rho_C^2, \\ F_{4CA} &= 6\rho_C^2 + 6\rho_A^2, \\ F_{4AB} &= 6\rho_A^2 - 3\rho_B^2, \\ F_{6BC} &= (45/8)\rho_B^4 - 45\rho_B^2\rho_C^2 + 40\rho_C^4, \\ F_{6CA} &= 15\rho_C^4 + 90\rho_C^2\rho_A^2 + 15\rho_A^4, \\ F_{6AB} &= 40\rho_A^4 - 45\rho_A^2\rho_B^2 + (45/8)\rho_B^4. \end{aligned}$$

As an example, we have for a ternary solid solution,

$$\begin{aligned} \overline{P^2F_4} &= f_A^2 P_A^2 F_{4A} + 2f_A f_B P_A P_B F_{4AB} \\ &+ 2f_B^2 P_B^2 F_{4B} + 2f_B f_C P_B P_C F_{4BC} \\ &+ f_C^2 P_C^2 F_{4C} + 2f_C f_A P_C P_A F_{4CA}. \end{aligned} \quad (21)$$

Formulae like this have been used to get the values of K_1 and K_2 in Table IV for several series of solid solutions.

Superstructures

In a superstructure alloy the two or more kinds of atom present do not have, even on the average, the same environments, so that in finding the mean energy density we have to include the lattice sums among the variable factors. The only exception to this occurs in cubic structures, the mean environment of each species of atom continuing to possess cubic symmetry so that S_2 still vanishes separately for each species. One formula for a binary alloy will be expanded as an example of what has to be done.

$$\begin{aligned} \overline{P^2F_4S_{40}} &= f_A \bar{S}_{40AA} P_A^2 F_{4A} \\ &+ (f_A \bar{S}_{40AB} + f_B \bar{S}_{40BA}) P_A P_B F_{4AB} \\ &+ f_B \bar{S}_{40BB} P_B^2 F_{4B}. \end{aligned} \quad (22)$$

Here \bar{S}_{4AA} is the mean lattice sum of the fourth order zonal harmonic over those points surrounding an atom of component A which are also occupied by A atoms. This mean is found by considering in turn the various A atoms in the unit cell as origin. Similarly \bar{S}_{40AB} is the mean sum over those points surrounding an A atom which are occupied by B atoms. Notice that \bar{S}_{40BA} is not necessarily the same as \bar{S}_{40AB} .

Binary alloys

Iron-cobalt (body-centered cubic).—In computing K_1 and K_2 for iron-cobalt alloys we have assumed that the lattice parameter a varies linearly with atomic composition,¹⁵ and that the

¹⁵ A. Osawa, Sci. Rep. Tohoku Imp. Univ. **19**, 109–121 (1930). Values of a for iron and for a 50–50 alloy, from unpublished work of F. E. Haworth, agree closely with Osawa's curve of a -vs.-composition.

TABLE IV. *Calculated anisotropy of alloys.*

<i>Part 1. Iron-cobalt—body-centered cubic solid solutions</i>									
Iron atomic percent		100	90	80	70	60	50	40	30
Cobalt atomic percent		0	10	20	30	40	50	60	70
Anisotropy coefficients									
First (quadrupole part)		10.26	7.80	5.43	3.14	0.94	-1.16	-3.18	-5.10
First (sextupole part)		15.20	11.27	8.32	6.89	5.47	5.58	6.75	8.98
First (total)	K_1	25.46	19.07	13.75	9.53	6.41	4.42	3.57	3.88
Second (sextupole)	K_2	-167.1	-123.9	-91.6	-70.2	-60.1	-61.4	-74.2	-98.8
<i>Part 2. Iron-nickel—body-centered cubic solid solutions</i>									
Iron atomic percent		100	90	80					
Nickel atomic percent		0	10	20					
Anisotropy coefficients									
First (quadrupole part)		10.26	7.89	5.87					
First (sextupole part)		15.20	11.34	8.91					
First (total)	K_1	25.46	19.23	14.78					
Second (sextupole)	K_2	-167.1	-124.8	-98.0					
<i>Part 3. Nickel-iron—face-centered cubic solid solutions</i>									
Nickel atomic percent		100	90	80	70	60	50	40	30
Iron atomic percent		0	10	20	30	40	50	60	70
Anisotropy coefficients									
First (quadrupole part)		-1.03	-0.81	-0.43	0.10	0.76	1.54	2.42	3.40
First (sextupole part)		-2.61	-1.71	-1.38	-1.57	-2.21	-3.26	-4.67	-6.40
First (total)	K_1	-3.64	-2.52	-1.81	-1.47	-1.45	-1.72	-2.25	-3.00
Second (sextupole)	K_2	28.7	18.8	15.2	17.2	24.3	35.8	51.4	70.4
<i>Part 4. Nickel-cobalt—face-centered cubic solid solutions</i>									
Nickel atomic percent		100	90	80	70	60	50	40	30
Cobalt atomic percent		0	10	20	30	40	50	60	70
Anisotropy coefficients									
First (quadrupole part)		-1.03	-1.45	-1.95	-2.51	-3.14	-3.83	-4.59	-5.41
First (sextupole part)		-2.61	-3.84	-5.29	-6.69	-8.83	-10.91	-13.19	-15.67
First (total)	K_1	-3.64	-5.29	-7.24	-9.47	-11.97	-14.47	-17.78	-21.08
Second (sextupole)	K_2	28.7	42.2	58.2	76.5	97.2	120.0	145.1	172.4
<i>Part 5. Nickel-iron-cobalt—face-centered cubic solid solutions</i>									
Nickel atomic percent		50	50	50	50	50	50		
Iron atomic percent		50	40	30	20	10	0		
Cobalt atomic percent		0	10	20	30	40	50		
Anisotropy coefficients									
First (quadrupole part)		1.54	0.39	-0.72	-1.80	-2.84	-3.83		
First (sextupole part)		-3.26	-3.60	-3.99	-5.28	-7.56	-10.91		
First (total)	K_1	-1.72	-3.21	-4.71	-7.08	-10.40	-14.74		
Second (sextupole)	K_2	35.8	39.6	43.9	58.0	83.2	120.0		
<i>Part 6. Comparison of solid solutions and superstructure alloys</i>									
Composition			FeCo		Ni ₃ Fe			Ni ₃ Co	
Anisotropy coefficients (solid solution)									
First (quadrupole part)			-1.16		-0.18			-2.22	
First (sextupole part)			5.58		-1.42			-6.10	
First (total)	K_1		4.42		-1.60			-8.32	
Second (sextupole)	K_2		-61.4		15.6			67.0	
Anisotropy coefficients (superstructure)									
First (quadrupole part)			-5.26		-1.62			-1.60	
First (sextupole part)			-4.73		0.28			-5.28	
First (total)	K_1		-9.98		-1.34			-6.88	
Second (sextupole)	K_2		52.0		-3.0			58.1	

atomic moments are unaltered by mixture. The latter assumption is probably wrong, in view of the high magnetizations possible from 30 Co to 50 Co, but the general picture of what happens is not much altered by mistakes in the magnetic moments (P_B and P_C).

The experimental values of K_1 at room temperature agree fairly well in general trend with the computed values of the quadrupole part of K_1 , not at all with total K_1 . We conclude that the relative importance of sextupole terms, which account for positive K_1 at high cobalt contents,

is already greatly diminished at this temperature. The transition point from K_1 positive to K_1 negative cannot be brought to a cobalt content of less than 45 atomic percent even by ignoring sextupole terms entirely, so the quantitative agreement is not wholly satisfactory in this respect. The anomalous sign of observed K_2 in iron is replaced by the expected sign at or near the composition for which K_1 passes through zero. The present theory does not offer any explanation of this.

The formation of the possible superstructure in FeCo should reverse the positive sign of K_1 , and negative sign of K_2 , predicted for very low temperatures in the solid solution. If the quadrupole terms predominate, as we see that they do at room temperature and above, K_1 should merely become more negative, K_2 should still reverse its sign. It would probably be difficult to detect the latter effect because K_2 must be small in comparison with its low temperature limit for either structure.

Iron-nickel (body-centered cubic).—A few points have been computed for body-centered iron-nickel alloys. Nothing is known of their ferromagnetic anisotropy and the assumptions of unaltered moment per atom and of linear change of lattice parameter with increase in nickel content are very rough approximations.

Nickel-iron (face-centered cubic).—Jette and Foote¹⁶ have shown that the lattice parameter varies linearly over a wide range in the nickel rich nickel-iron alloys but not over quite so wide a range as here assumed. As in body-centered iron-cobalt solutions the change in sign of K_1 actually occurs at a composition (24 percent iron) a little too near the starting point to be accounted for, even by ignoring sextupole terms altogether. Except for this the qualitative agreement as to K_1 is reasonably good. The sign of K_2 disagrees with observation. As in all the alloys and pure metals the observed values of K_2 are extremely small in comparison with calculated values. A possible superstructure (not yet observed to occur) at Ni_3Fe has been investigated. The changes in K_1 and K_2 which should result from the formation of the orderly structure are not very striking.

¹⁶ E. R. Jette, F. Foote, Trans. A. I. M. E. 120, 259–276 (1936).

Nickel-cobalt (face-centered cubic).—This series has been reported⁵ to show a positive K_1 , over a narrow range near the nickel end. The calculated K_1 is everywhere negative, and the model does not seem to be flexible enough to accommodate itself to a double change in sign of K_1 . The rapid descent of K_1 as we approach the cobalt end is in agreement with experiment. We prefer to leave the misfit for further study rather than to devise an *ad hoc* hypothesis to explain it. It may be mentioned, however, that if K_1 does have two zero values on this boundary of the ternary diagram it is very surprising that no magnetically soft nickel-cobalt alloys have been developed.

Ternary alloys

Nickel-iron-cobalt (face-centered cubic).—A single cut of the ternary diagram has been made at 50 percent nickel. As expected from the binary alloys, K_1 must be ascribed mainly to quadrupole terms in order to agree qualitatively with the experimental results,⁵ of which several lie on this cut.

IV. CONCLUSION

Most of the minor discrepancies mentioned above could be avoided by using a less extreme type of model, in particular by allowing the dicircle latitude, λ , to have other values than 0 and $\pi/2$. This seemed inadvisable in a first survey of the data, but is actually well justified at temperatures far from absolute zero, for the blurring of exact alignment of magnetic axes can be simulated by allowing λ to vary from either of its limits with rising temperature. It is in favor of our model that moderate departures from either extreme value of λ involve changes in sign of anisotropy coefficients, for this is consistent with the fact that the values of these coefficients fall to very low values long before the Curie point is reached. The quantitative agreement could be bettered in most cases by adjusting the relative radius, ρ , of the sphere on which the dicircles are supposed to lie. It seemed better to carry out the analysis without such refinements. The next logical step would seem to be the inclusion of strain effects, hitherto only considered for dipole magnets at atom centers.

It is a pleasure to acknowledge the part taken

in this development of ferromagnetic theory by Dr. R. M. Bozorth of the Bell Telephone Laboratories, whose acute suggestion of the difference in shape between elementary magnets in nickel and in iron⁹ was the starting point of my

renewed interest in computing magnetic interactions in ferromagnetic crystals, and with whom I have discussed ferromagnetic anisotropy on many occasions, both before and after undertaking the present analysis.

APPENDIX I

Convergent series for zonal harmonic lattice sums

The notation here used is especially convenient for numerical computations.

Taking a lattice point as origin, let the vector distance to any other point be $\mathbf{R} = ar\mathbf{r}$ where a is the length of a convenient edge of the unit cell, r is a numerical multiplier, and \mathbf{r} is a unit vector in the proper direction. In the cubic system a is an edge of the unit cube, in the hexagonal system a is an edge of the rhombus forming the base of the unit prism. Let r_1, r_2, r_3 be numerical factors expressing the coordinates of any point in terms of the three edges of the unit cell, a corresponding to r_1 . In the cubic system,

$$r^2 = r_1^2 + r_2^2 + r_3^2; \text{ and } \overline{r_i^2 r_j^2} = (r_2^2 r_3^2 + r_3^2 r_1^2 + r_1^2 r_2^2)/3.$$

In the hexagonal system,

$$r^2 = r_1^2 - r_1 r_2 + r_2^2 + r_3^2 c^2,$$

where c is the axial ratio, the ratio of the prism height to a . For abbreviation put

$$r_{12}^2 = r_1^2 - r_1 r_2 + r_2^2, \text{ and } l_{12}^6 = r_1^2 r_2^2 (r_1 - r_2)^2.$$

Let n_r be the number of points obtained by permuting $\pm r_1, \pm r_2, \pm r_3$ in ways consistent with the symmetry of the lattice. (In the hexagonal system, for example, $\pm r_3$ does not permute with $\pm r_1$ and $\pm r_2$.)

Let a lattice reciprocal to the \mathbf{R} lattice be defined by its vectors $\mathbf{Q} = a^{-1}q\mathbf{q}$, and by the equations

$$(\mathbf{q}; \mathbf{r}_i) = \begin{cases} 0 & i \neq j. \\ 1 & i = j \end{cases}.$$

Here again q is a numerical multiplier, and \mathbf{q} a unit vector. Let q_1, q_2, q_3 be numerical factors expressing the coordinates of any point in terms of the three edges of the unit cell (but a^{-1} is not in general the edge parallel to q_1). In the cubic system,

$$q^2 = q_1^2 + q_2^2 + q_3^2; \text{ and } q_i^2 q_j^2 = (q_2^2 q_3^2 + q_3^2 q_1^2 + q_1^2 q_2^2)/3.$$

In the hexagonal system

$$q^2 = (4/3)(q_1^2 + q_1 q_2 + q_2^2) + q_3^2 c^{-2}.$$

For abbreviation put

$$q_{12}^2 = (4/3)(q_1^2 + q_1 q_2 + q_2^2),$$

and

$$k_{12}^6 = (64/27)q_1^2 q_2^2 (q_1 + q_2)^2.$$

The selection rules for r_1, r_2, r_3 and for q_1, q_2, q_3 may be stated as follows.

In primitive lattices $r_1, r_2, r_3, q_1, q_2, q_3$ must be integers and f , a factor in q terms for the hexagonal system, is unity. In body-centered lattices, $2r_1, 2r_2, 2r_3, (r_2 + r_3), (r_3 + r_1), (r_1 + r_2), q_1, q_2, q_3, (q_1 + q_2 + q_3)/2$ must be integers. In face-centered lattices, $2r_1, 2r_2, 2r_3, (r_1 + r_2 + r_3), q_1, q_2, q_3, (q_2 + q_3)/2, (q_3 + q_1)/2, (q_1 + q_2)/2$ must be integers. In hexagonal close-packing q_1, q_2, q_3 , and either r_1, r_2, r_3 or $(r_1 - 2/3), (r_2 - 1/3), (r_3 - 1/2)$ must be integers; if $(4q_1 + 2q_2 + 3q_3)/6$ is an integer, $f = 2$; if $(4q_1 + 2q_2 + 3q_3 \pm 1)/6$ is an integer, $f = 3/2$; if $(4q_1 + 2q_2 + 3q_3 \pm 2)/6$ is an integer, $f = 1/2$; and if $(4q_1 + 2q_2 + 3q_3 \pm 3)/6$ is an integer, $f = 0$. In all the summations the origin of coordinates, $r_1 = r_2 = r_3 = 0$, or $q_1 = q_2 = q_3 = 0$, is to be omitted.

A numerical parameter ϵ , which appears in each term of the formulae, may be given any convenient value provided it is the same in all terms. The product $\epsilon r = x$ appears as the argument of a series of numerical factors depending upon the probability integral. These are defined by the equations

$$\begin{aligned} g_0(x) &= x^{-1} \left[1 - \frac{2}{\pi^{\frac{1}{2}}} \int_0^x e^{-a^2} d\alpha \right], \\ g_1(x) &= x^{-2} [g_0(x) + (2/\pi^{\frac{1}{2}})e^{-x^2}], \\ g_2(x) &= x^{-2} [3g_1(x) + (4/\pi^{\frac{1}{2}})e^{-x^2}], \\ g_3(x) &= x^{-2} [5g_2(x) + (8/\pi^{\frac{1}{2}})e^{-x^2}], \\ g_4(x) &= x^{-2} [7g_3(x) + (16/\pi^{\frac{1}{2}})e^{-x^2}], \\ g_5(x) &= x^{-2} [9g_4(x) + (32/\pi^{\frac{1}{2}})e^{-x^2}], \\ g_6(x) &= x^{-2} [11g_5(x) + (64/\pi^{\frac{1}{2}})e^{-x^2}]. \end{aligned} \quad (23)$$

Second-order sums

Cubic—

$$S_2 = (\epsilon^3/6)Sn_r x^2 g_2(x) - (\epsilon^3/2)Sn_r g_1(x) - (2\pi/3)Sn_q \exp(-\pi^2 q^2/\epsilon^2) + 2\epsilon^3/3\pi^{\frac{1}{2}}. \quad (24)$$

Hexagonal—

$$S_{20} = (\epsilon^3/4)Sn_r r_{12}^2 r^{-2} x^2 g_2(x) - (\epsilon^3/2)Sn_r g_1(x) - (2\pi\sqrt{3}/3c)Sfn_q q_{12}^2 q^{-2} \exp(-\pi^2 q^2/\epsilon^2) + 2\epsilon^3/3\pi^{\frac{1}{2}}, \quad (25)$$

$$S_{22} = -(\epsilon^3/4)Sn_r (r_{12}^2 - 2r_3^2 c^2) r^{-2} x^2 g_2(x) + (2\pi\sqrt{3}/3c)Sfn_q (q_{12}^2 - 2q_3^2 c^{-2}) q^{-2} \exp(-\pi^2 q^2/\epsilon^2). \quad (26)$$

Fourth-order sums

Cubic—

$$S_{40} = (\epsilon^5/72)Sn_r (1 - 6\overline{r_i^2 r_j^2} r^{-4}) x^4 g_4(x) - (\epsilon^5/12)Sn_r x^2 g_3(x) + (\epsilon^5/8)Sn_r g_2(x) + (2\pi^2/9)Sn_q (q^4 - 6q_i^2 q_j^2) q^{-2} \times \exp(-\pi^2 q^2/\epsilon^2) - \epsilon^5/5\pi^{\frac{1}{2}}, \quad (27)$$

$$S_{40} = (\epsilon^5/180)Sn_r(1 - 15\overline{r_i^2 r_j^2} r^{-4})x^4 g_4(x) \\ + (4\pi^3/45)Sn_q(q^4 - 15\overline{q_i^2 q_j^2})q^{-2} \exp(-\pi^2 q^2/\epsilon^2). \quad (27a)$$

Hexagonal:—

$$S_{40} = (\epsilon^5/64)Sn_r r_{12}^4 r^{-4} x^4 g_4(x) - (\epsilon^5/8)Sn_r r_{12}^2 r^{-2} x^2 g_3(x) \\ + (\epsilon^5/8)Sn_r g_2(x) + (\pi^3\sqrt{3}/6c)Sfn_q q_{12}^4 q^{-2} \\ \times \exp(-\pi^2 q^2/\epsilon^2) - \epsilon^5/5\pi^{\frac{1}{2}}, \quad (28)$$

$$S_{40} = (\epsilon^5/320)Sn_r(r_{12}^4 - 4r_{12}^2 r_3^2 c^2)r^{-4} x^4 g_4(x) \\ - (\epsilon^5/80)Sn_r(r_{12}^2 - 2r_3^2 c^2)r^{-2} x^2 g_3(x) \\ + (\pi^3\sqrt{3}/30c)Sfn_q(q_{12}^4 - 4q_{12}^2 q_3^2 c^{-2})q^{-2} \\ \times \exp(-\pi^2 q^2/\epsilon^2), \quad (28a)$$

$$S_{40} = (\epsilon^5/2240)Sn_r(3r_{12}^4 - 24r_{12}^2 r_3^2 c^2 + 8r_3^4 c^4)r^{-4} x^4 g_4(x) \\ + (\pi^3\sqrt{3}/210c)Sfn_q(3q_{12}^4 - 24q_{12}^2 q_3^2 c^{-2} \\ + 8q_3^4 c^{-4})q^{-2} \exp(-\pi^2 q^2/\epsilon^2). \quad (28b)$$

There are some errors in formulae corresponding to (28), (28a), (28b), in Phys. Rev. **44**, 38–42 (1933). In particular Eqs. (37), (38), (42), (43), (44), (46) of that paper are incorrect. Numerical results were correctly reported, nevertheless.

Sixth-order sums

Cubic:—

$$S_{60} = (\epsilon^7/2160)Sn_r(1 - 9\overline{r_i^2 r_j^2} r^{-4} + 3r_{12}^2 r_3^2 r_3^2 r^{-6})x^6 g_6(x) \\ - (\epsilon^7/144)Sn_r(1 - 6\overline{r_i^2 r_j^2} r^{-4})x^4 g_5(x) \\ + (\epsilon^7/48)Sn_r x^2 g_4(x) - (\epsilon^7/48)Sn_r g_3(x) \\ - (4\pi^5/135)Sn_q(q^6 - 9\overline{q_i^2 q_j^2} q^2 + 3q_{12}^2 q_3^2 q_3^2)q^{-2} \\ \times \exp(-\pi^2 q^2/\epsilon^2) + \epsilon^7/21\pi^{\frac{1}{2}}. \quad (29)$$

$$S_{60} = (\epsilon^7/14400)Sn_r(2 - 33\overline{r_i^2 r_j^2} r^{-4} + 21r_{12}^2 r_3^2 r_3^2 r^{-6})x^6 g_6(x) \\ - (\epsilon^7/720)Sn_r(1 - 15\overline{r_i^2 r_j^2} r^{-4})x^4 g_5(x)$$

$$- (\pi^5/225)Sn_q(2q^6 - 33\overline{q_i^2 q_j^2} q^2 + 21q_{12}^2 q_3^2 q_3^2)q^{-2} \\ \times \exp(-\pi^2 q^2/\epsilon^2), \quad (29a)$$

$$S_{60} = (\epsilon^7/16800)Sn_r(2 - 63\overline{r_i^2 r_j^2} r^{-4} + 231r_{12}^2 r_3^2 r_3^2 r^{-6})x^6 g_6(x) \\ - (2\pi^5/525)Sn_q(2q^6 - 63\overline{q_i^2 q_j^2} q^2 + 231q_{12}^2 q_3^2 q_3^2)q^{-2} \\ \times \exp(-\pi^2 q^2/\epsilon^2). \quad (29b)$$

Hexagonal:—

$$S_{63} = -(\epsilon^7/720)Sn_r r_{12}^6 r^{-6} x^6 g_6(x) \\ + (\epsilon^7/40)Sn_r r_{12}^4 r^{-4} x^4 g_5(x) \\ - (\epsilon^7/10)Sn_r r_{12}^2 r^{-2} x^2 g_4(x) + (\epsilon^7/15)Sn_r g_3(x) \\ + (8\pi^5\sqrt{3}/135c)Sfn_q q_{12}^6 q^{-2} \exp(-\pi^2 q^2/\epsilon^2) \\ - 16\epsilon^7/105\pi^{\frac{1}{2}}. \quad (30)$$

$$S_{63} = -(\epsilon^7/5040)Sn_r(r_{12}^6 - 6r_{12}^4 r_3^2 c^2)r^{-6} x^6 g_6(x) \\ + (\epsilon^7/420)Sn_r(r_{12}^4 - 4r_{12}^2 r_3^2 c^2)r^{-4} x^4 g_5(x) \\ - (\epsilon^7/210)Sn_r(r_{12}^2 - 2r_3^2 c^2)r^{-2} x^2 g_4(x) \\ + (8\pi^5\sqrt{3}/945c)Sfn_q(q_{12}^6 - 6q_{12}^4 q_3^2 c^{-2})q^{-4} \\ \times \exp(-\pi^2 q^2/\epsilon^2). \quad (30a)$$

$$S_{63} = -(\epsilon^7/15120)Sn_r(r_{12}^6 - 12r_{12}^4 r_3^2 c^2 + 8r_{12}^2 r_3^4 c^4)r^{-6} x^6 g_6(x) \\ + (\epsilon^7/7560)Sn_r(3r_{12}^4 - 24r_{12}^2 r_3^2 c^2 + 8r_3^4 c^4)r^{-4} x^4 g_5(x) \\ + (8\pi^5\sqrt{3}/2835c)Sfn_q(q_{12}^6 - 12q_{12}^4 q_3^2 c^{-2} \\ + 8q_{12}^2 q_3^4 c^{-4})q^{-2} \exp(-\pi^2 q^2/\epsilon^2). \quad (30b)$$

$$S_{63} = -(\epsilon^7/166320)Sn_r(5r_{12}^6 - 90r_{12}^4 r_3^2 c^2 \\ + 120r_{12}^2 r_3^4 c^4 - 16r_3^6 c^6)r^{-6} x^6 g_6(x) \\ + (8\pi^5\sqrt{3}/31185c)Sfn_q(5q_{12}^6 - 90q_{12}^4 q_3^2 c^{-2} \\ + 120q_{12}^2 q_3^4 c^{-4} - 16q_3^6 c^{-6})q^{-2} \exp(-\pi^2 q^2/\epsilon^2). \quad (30c)$$

$$S_{66} = (\epsilon^7/46080)Sn_r(2r_{12}^6 - 27l_{12}^6)r^{-6} x^6 g_6(x) \\ + (\pi^5\sqrt{3}/1080c)Sfn_q(2q_{12}^6 - 27k_{12}^6)q^{-2} \\ \times \exp(-\pi^2 q^2/\epsilon^2). \quad (31)$$

Erratum: The Sign of the Magnetic Moment of the K^{39} Nucleus

H. C. TORREY

Columbia University, New York City

(Phys. Rev. **51**, 501 (1937))

THE title of Fig. 6, p. 506 should read as follows:

“Fig. 6. Asymmetries in deflection patterns of (a) $m = -1$ atoms with negative strong field moments, (b) $m = -1$ atoms with positive strong field moments.”

The description of these curves in the text is correct.