Magnetic Quadrupole Field and Energy in Cubic and Hexagonal Crystals

L. W. McKEEHAN, *Sloane Physics Laboratory, Yale University*

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In crystalline arrays of equal and co-directed ideal bar magnets or circular Amperian current loops the magnetic field at certain important points and the magnetic potential energy of the array depend, if the linear dimensions of the magnetic elements are small in comparison with the shortest distance between elements, upon a series of terms, the first of which would be due to a similar array of dipoles. The second term, which, by analogy, has been styled the quadrupole term, depends upon a sum, over all points of the array except the origin, of the fourth-order zonal harmonic of a certain angle, divided by the fifth power of the radius to the point. This sum is evaluated by a precise method for several cubic and hexagonal arrays, and the results are compared with such published values as are available.

Introduction

NUMEROUS investigators have attempted to explain the existence of easy directions of magnetization in ferromagnetic crystals by the interaction of magnetic elements more complicated than dipoles. Ewing's theories of 1890[1] and 1922[2] are of this type, though the necessary crystalline symmetry of the model appears by implication rather than explicitly. In them Ewing sought to confer particular stability upon co-directed bar magnets (with point poles) or upon Amperian currents in parallel planes, by magnetic forces alone. He did not do much quantitative work with this model because it appeared, by approximate methods, that even in a single row of elements the magnetic potential energy minimum for the saturated state was not deep enough to explain the observed stability with respect to heat or other disorganizing agents, nor shallow enough to allow the observed easy transition from one direction of saturation to another under the control of magnetic forces. In other words the molecular field is not wholly, nor even principally, magnetic.

Ewing limited his analysis to the effect of adjacent bar magnets so that his theory is essentially that of a one-dimensional crystal. The two-dimensional crystal, for adjacent magnets only, has been treated by Honda and Okubo[3] who calculated the equilibrium orientation of a centrally pivoted bar magnet under the simultaneous action of an applied magnetic field and the magnetic fields of eight similar bar magnets centrally pivoted in a plane containing the applied field, at the adjacent points of a square net, and constrained to be parallel to the magnet under investigation. In the absence of an applied field this model is magnetically stable for magnetization parallel to the edges of the square meshes of the net. In both of these studies the extension to three dimensions was qualitative.

Peddie attacked the three-dimensional crystal by direct summation of the magnetic fields of near-by elements at the center and at either pole of one of the equal and co-directed bar magnets. In his first paper[4] the magnet centers occupied the points of a face-centered cubic lattice (F). In a second note[5] he computed similar constants for the simple cubic lattice (S), and still later[6] extended the analysis to other than cubic lattices, but did not compute the constants for these more complicated cases. This theoretical work has been

[1] J. A. Ewing, Rep. Brit. Ass. 740–741 (1890); Proc. Roy. Soc. **A48**, 342–358 (1890); Phil. Mag. [5] **30**, 205–222 (1890).

[2] J. A. Ewing, Proc. Roy. Soc. (Edinburgh) **42**, 97–128 (1922); Proc. Roy. Soc. **A100**, 449–460 (1922); Phil. Mag. [6] **43**, 493–503 (1922).

[3] K. Honda, J. Okubo, Sci. Rep. Tohoku Imp. Univ. **5**, 153–214 (1916); **6**, 183–196 (1917); Phys. Rev. **10**, 705–742 (1917).

[4] W. Peddie, Proc. Roy. Soc. (Edinburgh) **25**, 1025–1059 (1905).

[5] W. Peddie, Proc. Roy. Soc. (Edinburgh) **28**, 643–651 (1908).

[6] W. Peddie, Proc. Roy. Soc. (Edinburgh) **32**, 216–246 (1912).

reviewed and extended by Forrest[7] who extracted from Peddie's tables the essential constants for the body-centered cubic lattice (I) and for the diamond arrangement (D). Forrest also made some computations for a few noncubic lattices. The body-centered cubic case has also been investigated by Mahajani,[8] who, however, chose equal circular current loops rather than equal bar magnets as the magnetic elements in the model crystal. Finally, Akulov[9] has computed the mutual magnetic energy of what may be called cubic lattices, (S) and (I), of magnetic quadrupoles, as dependent upon their direction of magnetization.

Whether field components or magnetic potential energies are computed the mathematical difficulty lies in the evaluation of series of the form

$$\sum_n F_n \sum_r{}' (a_0 r)^{-n-1} P_n(\cos\{\mathbf{p},\mathbf{r}\}), \qquad (1)$$

where $a_0\mathbf{r}$ is the vector from the lattice point chosen as origin to any other, $\mathbf{p}$ is a unit vector in the direction of all the magnetic axes, $\{\mathbf{p},\mathbf{r}\}$ is the angle between $\mathbf{p}$ and $\mathbf{r}$, and P_n (cos θ) is the surface zonal harmonic of order n. The parameter a_0 is that lattice parameter in terms of which all vectors $\mathbf{r}$ must be expressed. The coefficients F_n depend upon the quantity sought and upon the nature of the magnetic element which is chosen. The presence of zonal harmonics indicates that we have already restricted ourselves to magnetic elements with full axial symmetry. The absence of magnetic charges makes $F_0=0$ and if the lattice has reflection planes through its lattice points perpendicular to $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$, the sums with respect to r are all zero unless n is even. Finally, if the lattice is cubic the sum with respect to r is zero for $n=2$ so that the first term differing from zero is $F_4\sum_r{}'(a_0r)^{-5}P_4$ (cos $\{\mathbf{p},\mathbf{r}\}$).

For ideal bar magnets of moment P and of length a smaller than the shortest distance between lattice points Peddie[6] gives expressions for the magnetic field components at the center and at the poles of each magnet due to all the rest of the array. In our notation[10] the component parallel to $\mathbf{p}$ takes the following forms:

At a magnet center

$$\mathbf{H}_0\cdot\mathbf{p} = P\sum_{n=2}^{n=\infty} n\, 2^{-n} a^{n-2} \sum_r{}' (a_0r)^{-n-1} P_n(\cos\{\mathbf{p},\mathbf{r}\}). \qquad (2)$$

At a magnet pole

$$\mathbf{H}_a\cdot\mathbf{p} = P\sum_{n=2}^{n=\infty} n\, a^{n-2} \sum_r{}' (a_0r)^{-n-1} P_n(\cos\{\mathbf{p},\mathbf{r}\}). \qquad (3)$$

In both these series n is restricted to even integers.

Mahajani[8] derives the magnetic potential energy per magnet, obtaining, in our notation,

$$U = -P^2 \sum_{n=2}^{n=\infty} a^{n-2} \sum_r{}' (a_0r)^{-n-1} P_n(\cos\{\mathbf{p},\mathbf{r}\}) \qquad (4)$$

subject to the same restriction (n even).

Mahajani also treats the case of circular Amperian current loops of radius b and magnetic moment P, obtaining the first two terms in U, which are:

$$U_2 = -P^2 \sum_r{}' (a_0r)^{-3} P_2(\cos\{\mathbf{p},\mathbf{r}\}), \qquad (5)$$

$$U_4 = +3P^2 b^2 \sum_r{}' (a_0r)^{-5} P_4(\cos\{\mathbf{p},\mathbf{r}\}). \qquad (6)$$

The term U_4 is equivalent to Akulov's "quadrupole" energy per elementary magnet if we put his "quadrupole moment" equal to Pb. It would seem rather better to call Pa the quadrupole moment for the ideal bar magnet, in which case the quadrupole moment for the circular current loop has the imaginary value $Pb(-1)^{\frac{1}{2}}$ but the concept of quadrupoles is so nonphysical at best that we prefer to call $(\mathbf{H}\cdot\mathbf{p})_4$ and U_4 the quadrupole field and the quadrupole energy without closer analysis of what this may imply.

The dimensionless sum

$$S_2 = \sum_r{}' r^{-3} P_2(\cos\{\mathbf{p},\mathbf{r}\}) \qquad (7)$$

has already been considered in some detail in papers[10] on dipole fields and dipole energies. The corresponding sum

$$S_4 = \sum_r{}' r^{-5} P_4(\cos\{\mathbf{p},\mathbf{r}\}) \qquad (8)$$

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[7] J. Forrest, Phil. Mag. [6] **50**, 1009–1018 (1925); Trans. Roy. Soc. (Edinburgh) **54**, 601–701 (1926); Phil. Mag. [7] **3**, 464–476 (1927).

[8] G. S. Mahajani, Proc. Camb. Phil. Soc. **23**, 136–143 (1926); Phil. Trans. **A228**, 63–114 (1929).

[9] N. S. Akulov, Zeits. f. Physik **57**, 249–256 (1929).

[10] L. W. McKeehan, Phys. Rev. **43**, 913, 924, 1022, 1025 (1933).

now engages our attention. We substitute

$$P_4(\cos\theta)=(1/8)(35\cos^4\theta-30\cos^2\theta+3), \quad (9)$$

put

$$\cos\{\mathbf{p},\mathbf{r}\}=r^{-1}\sum_i p_i r_i \quad (10)$$

and then make use of any symmetry of the lattice to simplify the formulae for computation. The sum S_4 is absolutely convergent but converges so slowly as r increases that it turns out to be better here, as it was in computing S_2, to use the method of Ewald rather than that of Lorentz.

Cubic Arrays

In cubic arrays Eq. (8) reduces to

$$S_4=(7R_c/8)\{5(p_1^4+p_2^4+p_3^4)-3\}, \quad (11)$$

where the single coefficient R_c may be written

$$R_c=R_{11}-3R_{23}, \quad (12)$$

with

$$R_{11}=\sum_r{}' r_1^4 r^{-9}, \quad (13)$$

$$R_{23}=\sum_r{}' r_2^2 r_3^2 r^{-9}. \quad (14)$$

A convenient auxiliary sum is

$$R_0=\sum_r{}' r^{-5}, \quad (15)$$

because

$$3R_{11}+6R_{23}-R_0=0. \quad (16)$$

Since

$$p_1^4+p_2^4+p_3^4=1-2(p_2^2p_3^2+p_3^2p_1^2+p_1^2p_2^2), \quad (17)$$

an alternative form of Eq. (11) is

$$S_4=(7R_c/4)\{1-5(p_2^2p_3^2+p_3^2p_1^2+p_1^2p_2^2)\}. \quad (18)$$

Peddie[6] and Forrest[7] obtain by direct summation a quantity $(G-D)$, which in our notation is $-R_c/2$, $-R_c/16$ or $-R_c/512$ according to the unit of length they chose, a_0 for (S), $a_0/2$ for (I) and (F), $a_0/4$ for (D). The limiting value of r in each of these summations is 10 of their units. The tables given by Forrest[7] (pp. 676–679) contain several mistakes, and a recomputation shows that some of these also appear in Peddie's tables upon which they are based. Table I shows the changes that are necessary, and the values of R_c derived from the corrected values of $(G-D)$.

Mahajani[8] obtains for (I), the only array he considers, lower and upper limits for a quantity $(3Q-P)$, which in our notation is $-R_c/32$, by an ingenious artifice. He notes that a related

Table I.

Array	$(G-D)$* Forrest	$(G-D)$* Corrected	R_c
(S)	-3.8461	-3.55204	1.7760
(I)	0.0628	0.11101	-1.7761
(F)	0.26622	0.26896	-4.3034
(D)	0.11928	0.11946	-61.164

* Peddie's notation.

coefficient, $B_5=3^{\frac{5}{2}}R_0$, has already been computed to the necessary degree of precision by Jones and Ingham.[11] If we designate by a subscript the value of r with which we terminate any summation, understanding the subscript ∞ for the convergence limit, we may write Mahajani's inequalities:

$$(R_{11}-R_{23})>(R_{11}-R_{23})_r, \quad (19)$$

$$(R_{11}-R_{23})<(R_{11}-R_{23}-R_0)_r+(R_0). \quad (20)$$

From (16), (19) and (20) we then find

$$(R_c)<(5/3)(R_{11}-R_{23}-R_0)_r+(13/9)(R_0), \quad (21)$$

$$(R_c)>(5/3)(R_{11}-R_{23})_r-(2/9)(R_0). \quad (22)$$

In checking Mahajani's computations it appeared that the limiting value $r=5^{\frac{1}{2}}$ which he proposed to use was not consistently adhered to in (21) and (22), and that his results were further vitiated by an inaccurate decimal equivalent for $3^{\frac{1}{2}}$, used in deriving R_0 from B_5. After making the necessary corrections the computations were extended to $r=10^{\frac{1}{2}}$, reducing the range of uncertainty in R_c to about half its value for $r=5^{\frac{1}{2}}$. Furthermore, values of R_c have been found for (S) and (F) as well as for (I), using additional data from Jones and Ingham.[11] The results are presented in Table II.

Akulov[9] computed two coefficients, A_0' and A' for (S), A_0'' and A'' for (I). In our notation $A_0=(21/2)NR_c$ and $A=-(105/4)NR_c$. Akulov did not notice that the constant term in (18) is exactly 1/5 the coefficient of $(p_2^2p_3^2+p_3^2p_1^2+p_1^2p_2^2)$. (He gives the ratio as 0.200/2 but his own figures in the same paragraph support the correct value.) His method has been carried through much more precisely for (S), (I) and

[11] J. E. Jones and A. E. Ingham, Proc. Roy. Soc. **A107**, 636–653 (1925). The method used is essentially that of Ewald.

TABLE II.

Array	Up to $r=5^{\frac{1}{2}}$ $(3Q-P)$*		R_c
	Mahajani	Corrected	
(*I*)	>0.032	>0.043481	<-1.3914
	<0.064	<0.059864	>-1.9156

Array	Up to $r=10^{\frac{1}{2}}$ $(3Q-P)$*	R_c
(*S*)	>-0.058576	$<\ 1.8744$
	<-0.054445	$>\ 1.7423$
(*I*)	$>\ 0.049674$	<-1.5896
	$<\ 0.057608$	>-1.8434
(*F*)	$>\ 0.122294$	<-3.9134
	$<\ 0.138719$	>-4.4390

* Mahajani's notation.

(*F*). In each case the results have been checked by computation with two different values of the arbitrary parameter ϵ, *viz.*, $\epsilon=2$ and $\epsilon=3$. The formulae for computation may be put in the following form, analogous to that used in dipole computations.[10]

$$S_4=(Q_4+R_4+R_3+R_2+R_0)+(Q_4'+Q_4''+R_4'+R_4'')\times(p_2^2p_3^2+p_3^2p_1^2+p_1^2p_2^2), \quad (23)$$

$$Q_4=\frac{4\pi^3N}{3}\sum{}'fn_q(q_1^4+q_2^4+q_3^4)q^{-2}\times\exp\left(\frac{-\pi^2q^2}{\epsilon^2}\right), \quad (24)$$

$$R_4=(\epsilon^9/12)\sum{}'n_r(r_1^4+r_2^4+r_3^4)g_4(\epsilon r), \quad (25)$$

$$R_3=-(\epsilon^7/2)\sum{}'n_rr^2g_3(\epsilon r), \quad (26)$$

$$R_2=(3\epsilon^5/4)\sum{}'n_rg_2(\epsilon r), \quad (27)$$

$$R_0=-6\epsilon^5/5\pi^{\frac{1}{2}}, \quad (28)$$

$$Q_4'=-2Q_4, \quad (29)$$

$$Q_4''=4\pi^3N\sum{}'fn_qq^2\exp(-\pi^2q^2/\epsilon^2)-3Q_4, \quad (30)$$

$$R_4'=-2R_4, \quad (31)$$

$$R_4''=(\epsilon^9/4)\sum{}'n_rr^4g_4(\epsilon r)-3R_4. \quad (32)$$

From these, by comparison with (18), we get

$$R_c=(4/7)(Q_4+R_4+R_3+R_2+R_0)=-(4/35)(Q_4'+Q_4''+R_4'+R_4''). \quad (33)$$

Table III gives results for R_c, those newly computed being correct to five decimal places.

TABLE III.

Array	Akulov	R_c	McKeehan R_c
(*S*)	$A_0'=+18.65$	1.7757	1.77613
	$A'=-46.635$	1.7766	
(*I*)	$A_0''=-37.295$	-1.7760	-1.77562
	$A''=+93.24$	-1.7760	
(*F*)			-4.11336

HEXAGONAL ARRAYS

In hexagonal arrays Eq. (8) reduces to

$$S_4=R_hP_4(\cos\{\mathbf{p},\mathbf{a}_3\}) \quad (34)$$

or

$$S_4=(R_h/8)(35p_3^4-30p_3^2+3). \quad (35)$$

Making the same substitutions as in our previous paper on hexagonal arrays[12] we find

$$R_h=Q_{4h}+R_{4h}+R_{3h}+R_{2h}+R_{0h}=Q_{4h}'+R_{4h}'+R_{3h}'=Q_{4h}''+R_{4h}'', \quad (36)$$

in which

$$Q_{4h}=\frac{64\pi^3N3^{\frac{1}{2}}}{81c}\sum{}'fn_qq_{12}^4q^{-2}\exp\left(\frac{-\pi^2q^2}{\epsilon^2}\right); \quad (37)$$

$$R_{4h}=(3\epsilon^9/32)\sum{}'n_rr_{12}^4g_4(\epsilon r); \quad (38)$$

$$R_{3h}=-(\epsilon^7/3)\sum{}'n_rr_{12}^2g_3(\epsilon r); \quad (39)$$

$$R_{2h}=(\epsilon^5/3)\sum{}'n_rg_2(\epsilon r); \quad (40)$$

$$R_{0h}=-8\epsilon^5/15\pi^{\frac{1}{2}}; \quad (41)$$

$$Q_{4h}'=\frac{128\pi^3N3^{\frac{1}{2}}}{27c^3}\sum{}'fn_qq_{12}^2q_3^2q^{-2}\times\exp\left(\frac{-\pi^2q^2}{\epsilon^2}\right)-2Q_{4h}; \quad (42)$$

$$R_{4h}'=\frac{3\epsilon^9c^2}{4}\sum{}'n_rr_{12}^2r_3^2g_4(\epsilon r)-2R_{4h}; \quad (43)$$

$$R_{3h}'=-\frac{2\epsilon^7c^2}{3}\sum{}'n_rr_3^2-R_{3h}; \quad (44)$$

$$Q_{4h}''=\frac{32\pi^3N3^{\frac{1}{2}}}{27c^5}\sum{}'fn_qq_3^4q^{-2}\times\exp(-\pi^2q^2/\epsilon^2)-Q_{4h}'-Q_{4h}; \quad (45)$$

[12] L. W. McKeehan, Phys. Rev. **43**, 1025 (1933).

$$R_{4h}''=(\epsilon^9c^4/4)\sum{}'n_r r_3{}^4 g_4(\epsilon r)-R_{4h}'-R_{4h}. \qquad (46)$$

From these equations we obtain for the simple hexagonal lattice with axial ratio $c=\frac{2}{3}6^{\frac{1}{2}}$, $R_h=2.54563$, and for hexagonal close-packing with the same axial ratio $R_h=0.90174$. Each of these results has been computed in several ways. No previous numerical results are available for comparison. Peddie[6] gives formulae for his method of computation, but since he uses orthorhombic axes the extremely simple form of Eq. (34) does not appear in his equations, and neither he nor Forrest attempts to evaluate any of their numerous coefficients.