Magnetic Dipole Energy in Hexagonal Crystals

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The magnetic fields at dipole positions in two hexagonal arrays of parallel dipoles are computed by two methods. One of these methods is also used to find the field in hexagonal close packing at a point on the hexagonal axis near a vacated dipole position. The hexagonal close-packed arrangement with axial ratio $c=2\times 6^{\frac{1}{2}}/3$ (as for spheres) is found to be magnetically stable by a small margin when magnetization is along the hexagonal axis. The general expressions for the energy per dipole in homogeneously strained hexagonal arrays are solved and applied to two arrays, one simple hexagonal (H), the other close-packed hexagonal (HC), both with $c=2\times 6^{\frac{1}{2}}/3$. The results are applicable in cases where c differs slightly from this value.

IN previous papers[1] we have considered the magnetic fields in cubic or nearly cubic arrays of parallel dipoles. We here extend the discussion to certain hexagonal arrays. These are of particular interest in view of the magnetic behavior of hexagonal cobalt crystals, in which the sixfold axis ($\mathbf{a}_3$) is the only easy direction of magnetization.

In unstrained arrays the method of Lorentz is at once applicable in the form already presented, but some assumption must be made regarding the relative dimensions of the unit of structure. This unit is a right prism with rhombic base, the internal angles of the rhombus being 120° and 60°. The origin is taken at an obtuse corner of the base, $\mathbf{a}_1$ and $\mathbf{a}_2$ are edges of the base and $\mathbf{a}_3$ is the altitude of the prism. In order to include the atomic arrangement of hexagonal cobalt, which is, within experimental error, that of a close-packing of spheres, without special assumptions at a later stage we choose the ratio $a_3/a_1=2\times 6^{\frac{1}{2}}/3$. With this particular choice we can if desired use a rectangular system of coordinate axes in fixing dipole positions, and can express their coordinates in this system as an integral multiple r_i'' of a pseudo-cubic parameter $a_0''=a_1 2^{\frac{1}{2}}/6$. These rectangular axes, $\mathbf{a}_i''$, are equally inclined to $\mathbf{a}_3$ and lie in planes perpendicular to $\mathbf{a}_1$, $\mathbf{a}_2$, and $-(\mathbf{a}_1+\mathbf{a}_2)$. The last of these vectors is an auxiliary axis in the basal plane, which is used in designating planes by Miller-Bravais indices.

With respect to the rectangular axes just mentioned the selection rule for the points of a simple hexagonal lattice (H), for which $N=1$, is as follows:

$$r_i''=3n_i+4;\quad \sum_i r_i''=12n\geqq 0, \tag{1}$$

$$r_i''=3n_i-4;\quad \sum_i r_i''=12n<0. \tag{2}$$

The additional points for hexagonal close-packing (HC), $N=2$, which does not constitute a single space-lattice, are obtained by adding to these all points for which

$$r_i''=3n_i+4;\quad \sum_i r_i''=6n>0, \tag{3}$$

$$r_i''=3n_i-4;\quad \sum_i r_i''=6n<0. \tag{4}$$

The easy direction of magnetization, here most naturally assumed for the direction of $\mathbf{p}$, has pseudo-cubic indices [111].

It is no longer necessary, as in cubic arrays, that the local field vanish at a dipole position, so we proceed to calculate $\sum'\delta h_i''$ for the origin as well as for a nearby point on the principal axis. Table I shows how much the sums fluctuate as the limiting sphere increases. It is not possible, from these computations, to fix even the sign of the limiting value with any certainty though the difference between nearby points converges well enough. It is clear therefore that the method of Ewald[1] must here be relied upon. Its application requires the construction of new formulae based on those furnished by Kornfeld[2] for the general

[1] L. W. McKeehan, Phys. Rev. [2] **43**, 913–923, 924–930, 1025–1029 (1933).

[2] H. Kornfeld, Zeits. f. Physik **22**, 27–43 (1924).

TABLE I. *Hexagonal close-packing (HC).*

For $c=2\times 6^{\frac{1}{2}}/3$ $\quad p_1=p_2=0,\ p_3=1$

$3r^2$	$\Sigma' N$	$\Sigma'\delta h_i$ at 0,0,0	$\Sigma'\delta h_i$ at 0,0,$(0.055\times 6^{\frac{1}{2}})$	Difference
3	12	0	0.34558	0.34558
6	18	0	0.20080	.20080
8	20	1.49997	1.76311	.26314
9	38	−1.64273	−1.39386	.24887
11	50	1.65571	1.89742	.24171
12	56	0.43097	0.69745	.26648
15	68	− .62066	−0.35761	.26305
17	80	− .02249	0.21703	.22952
18	86	− .46694	−0.22709	.23985
19	92	.66547	0.92123	.25576
20	104	.89315	1.13313	.23998
21	128	− .92070	−0.66652	.25418
22	134	− .20305	.05456	.25761
25	146	.74187	.99822	.25633
27	158	.09674	.35744	.26070
29	182	− .12809	.12305	.25114
30	194	− .62384	− .37074	.25310
31	206	− .18614	.06287	.24901
32	208	.00136	.25229	.25093
33	220	− .43811	− .18543	.25268
34	226	− .28705	− .03627	.25078
35	250	.41545	.66946	.25401
36	256	.17975	.43536	.25561
37	268	.38762	.63992	.25230
39	292	− .38420	− .12792	.25628
41	298	− .12405		
43	304	− .07787		
44	328	.17586		
45	340	− .11647		
46	352	− .05971		
	Limit	0.00225		

case, and we must abandon pseudo-cubic axes $\mathbf{a}_i''$ in favor of hexagonal axes $\mathbf{a}_i$.

It follows from symmetry that for $\mathbf{p}$ along $\mathbf{a}_3$ any resultant local field also lies along $\mathbf{a}_3$. It will therefore be sufficient to compute the magnetic potential energy per dipole, from which we can easily derive the magnitude of the local field. We will, however, leave $\mathbf{p}$ unrestricted for the present. As usual we may eliminate the dimensions of the particular lattice in question by putting $a_1=a_2=1$, $a_3=c$. Dipole positions are defined by vectors $\mathbf{r}$ and the selection rule for (H) would then be

$$r_1=n_1;\quad r_2=n_2;\quad r_3c=n_3c. \tag{5}$$

We use r_3c for the component along $\mathbf{a}_3$ so as to keep all r_i integral. When we try to construct the reciprocal or $\mathbf{q}$ lattice, however, we find its fundamental vectors have very inconvenient forms. It is easier in finding them to make temporary use of an orthorhombic system of axes for both $\mathbf{r}$ and $\mathbf{q}$. We put

$$\mathbf{a}_1'''=\mathbf{a}_1,\quad \mathbf{a}_2'''=-\tfrac{1}{2}\mathbf{a}_1+(3^{\frac{1}{2}}/2)\mathbf{a}_2,\quad \mathbf{a}_3'''=\mathbf{a}_3, \tag{6}$$

and the selection rule for orthorhombic components in (H) is

$$r_1'''=r_1-r_2/2,\quad r_2'''=r_2\,3^{\frac{1}{2}}/2,\quad r_3'''c=r_3c, \tag{7}$$

where r_1, r_2, r_3c are the corresponding hexagonal components. In the reciprocal lattice the points are selected by

$$q_1'''=q_1,\quad q_2'''=(q_1+2q_2)/3^{\frac{1}{2}},\quad q_3'''/c=q_3/c, \tag{8}$$

where $\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3/c$ are the fundamental hexagonal vectors in the reciprocal lattice. In r_1''' and r_2''' the integer r_2 must be the same, in q_1''' and q_2''', q_1 must be the same. Otherwise $r_1r_2r_3$, $q_1q_2q_3$ are unrestricted integers, except that $q_1=q_2=q_3=0$ is excluded.

The expressions for r^2 and q^2 are now easily seen to be

$$r^2=(r_1^2-r_1r_2+r_2^2)+r_3^2c^2, \tag{9}$$

$$q^2=(4/3)(q_1^2+q_1q_2+q_2^2)+q_3^2/c^2, \tag{10}$$

and we will have no further use for the orthorhombic axes. For abbreviation in our final equations we will put

$$r_{12}^2=(r_1^2-r_1r_2+r_2^2), \tag{11}$$

$$q_{12}^2=(4/3)(q_1^2+q_1q_2+q_2^2). \tag{12}$$

The energy factor per dipole becomes

$$u=u_0+u_3p_3^2 \tag{13}$$

and the coefficients u_0, u_3 are each composed of several convergent summations

$$u_0=u_{00}+u_{0r0}+u_{0r2}+u_{0q2}, \tag{14}$$

$$u_3=u_{3r2}+u_{3q2}, \tag{15}$$

wherein

$$u_{00}=-4\epsilon^3/3\,\pi^{\frac{1}{2}}, \tag{16}$$

$$u_{0r0}=\epsilon^3\textstyle\sum' n_r g_1(\epsilon r), \tag{17}$$

$$u_{0r2}=-(\epsilon^5/2)\textstyle\sum' n_r r_{12}^2 g_2(\epsilon r), \tag{18}$$

$$u_{3r2}=-c^2\epsilon^3\textstyle\sum' n_r r_3^2 g_2(\epsilon r)-u_{0r2}, \tag{19}$$

$$u_{0q2}=\pi\,2^{\frac{1}{2}}\textstyle\sum' n_q q_{12}^2 q^{-2}\exp(-\pi^2q^2/\epsilon^2), \tag{20}$$

$$u_{3q2}=(2\pi\,2^{\frac{1}{2}}/c^2)\textstyle\sum' n_q q_3^2 q^{-2}\times\exp(-\pi^2q^2/\epsilon^2)-u_{0q2}. \tag{21}$$

The factors n_r and n_q are the number of points with a given form $r_1r_2r_3$ and $q_1q_2q_3$, respectively. The possible values are 2, 6, 12 or 24 depending upon the form according to the following scheme:

$$\begin{aligned} n_r = \ & 2 \text{ if } \{r_1=r_2=0;\ r_3\neq 0\},\\ & 6 \text{ if } \{r_1=0;\ r_2\neq 0;\ r_3=0\} \quad \text{or if} \quad \{r_1=r_2\neq 0;\ r_3=0\},\\ & 12 \text{ if } \{r_1=0;\ r_2\neq 0;\ r_3\neq 0\} \quad \text{or if} \quad \{r_1=r_2\neq 0;\ r_3\neq 0\},\\ & 24 \text{ if } \{r_1\neq 0;\ r_2\neq 0;\ r_1\neq r_2;\ r_3\neq 0\}. \end{aligned}$$

The same conditions hold if we substitute n_q for n_r and $q_1q_2q_3$ for $r_1r_2r_3$.

In (*HC*) Eqs. (16), (17), (18), (19) retain their form but we get an additional set of terms in each summation due to a change in the selection rule for r_i which may now take fractional values. The complete selection rule is:

$$r_i=n \quad \text{and} \quad r_1=n_1+\tfrac{2}{3};\quad r_2=n_2+\tfrac{1}{3};\quad r_3=n_3+\tfrac{1}{2}.$$

It is now possible for n_r to take the value 3, this occurring if $r_2=r_1/2\neq n$; $r_3=0$. An additional case for $n_r=6$ is obtained if $r_2=r_1/2\neq n$; $r_3\neq 0$.

Eqs. (20) and (21) take new forms

$$u_{0q2}=\pi N 2^{\frac{1}{3}}\sum{}'f n_q q_{12}{}^2 q^{-2}\exp(-\pi^2q^2/\epsilon^2), \tag{22}$$

$$u_{3q2}=(2\pi N 2^{\frac{1}{3}}/c^2)\sum{}'f n_q q_3{}^2 q^{-2}\exp(-\pi^2q^2/\epsilon^2), \tag{23}$$

where f depends upon the form $q_1q_2q_3$ as shown below.

$4q_1+2q_2+3q_3$	f
$6n$	1
$6n\pm 1$	3/4
$6n\pm 2$	1/4
$6n+3$	0.

It will be noticed that, as usual, the number of terms in series depending on q is reduced by making the dipole array more complex.

TABLE II. *Coefficients for Eq.* (13) *in unstrained arrays with* $c=2\times 6^{\frac{1}{2}}/3$.

Array	N	u_0	u_3	$2\pi N\,2^{\frac{1}{3}}/3$	$u_0+2\pi N\,2^{\frac{1}{3}}/3$
(*H*)	1	−5.51483	7.65872	2.96192	−2.55291
(*HC*)	2	−5.92046	−0.01014	5.92384	0.00338

The computations, carried out for two choices of ϵ, *viz.*, $\epsilon=3^{\frac{1}{2}}$ and $\epsilon=2$, give the results presented in Table II. Besides u_0 and u_3 this table gives the correction $2\pi N\,2^{\frac{1}{3}}/3$ which compensates the effect of remote dipoles in the infinite array and the part of the energy due to the local field, $u_0+2\pi N\,2^{\frac{1}{3}}/3$ which does not depend upon the direction of **p**. For $p_3=1$, the case treated by the method of Lorentz, we get, for (*HC*), $u=0.00338-0.01014=-0.00676$ showing that the assumed direction of magnetization is stable, but only by a small amount. The fluctuations to be expected in a real crystal would completely mask so small a stabilizing field. In (*H*) on the other hand this direction for **p** gives a high maximum for u, corresponding to great instability.

Vibrations restricted to the hexagonal axis should help to stabilize **p** along the observed easy direction of magnetization, as is seen by considering the positive field factor values in the last column of Table I.

There seems to be only one statement in the literature of this subject in regard to dipole fields in hexagonal arrays. This appears in a note (in German) by Akulov[3] appended to a longer paper[4] (in Russian). The statement is that the Lorentz formula for the field $(4\pi I/3)$ at a dipole also holds for hexagonal close packing with an accuracy of one part in a thousand. Neither the note nor the longer paper contains any evidence for the statement which is, however, almost exactly correct, since the maximum deviation from the Lorentz energy factor, 5.92384, is 0.00676, or 0.1141 percent.

The energy per dipole in homogeneously strained hexagonal arrays (*H*) and (*HC*) has also been computed. The necessary formulae are derived in the usual way from those given by Kornfeld,[2] which are applicable to any crystal system.

The magnetic energy per dipole due to straining is

[3] N. S. Akulov, *Problèmes modernes de l'électromagnétisme. Recueil consacré au dixième anniversaire du laboratoire de magnetisme de Moscou*, p. 44, 1931.

[4] N. S. Akulov, reference 3, pp. 37–43.

$$u=\sum_{ij} H_{ij}A_{ij}, \tag{24}$$

where A_{ij} are the tensor components of the strain. For convenience we impose the condition $j\geqq i$. The coefficients H_{ij} are then as follows:

$$H_{11}=H_{110}+H_{1111}p_1^2+H_{1133}p_3^2, \tag{25}$$

$$H_{12}=H_{1212}p_1p_2, \tag{26}$$

$$H_{13}=H_{1313}p_1p_3, \tag{27}$$

$$H_{33}=H_{330}+H_{3333}p_3^2. \tag{28}$$

Not all of these coefficients are independent, for

$$H_{1111}=H_{1212}=2H_{110}. \tag{29}$$

In equations for H_{22}, H_{23}, analogous to (25), (27) appear the following coefficients, related as indicated to those just defined:

$$H_{220}=H_{110};\quad H_{2222}=H_{1111};\quad H_{2233}=H_{1133};$$
$$H_{2323}=H_{1313}. \tag{30}$$

Each H_{ii0}, H_{iijj} and H_{ijij} consists of several convergent summations according to the equations:

$$H_{110}=-H_{1r}+H_{12r}-H_{1q}+H_{12q}, \tag{31}$$

$$H_{1133}=-H_{12r}+H_{13r}+H_{1q}-H_{3q}-H_{12q}+H_{13q}, \tag{32}$$

$$H_{1313}=-H_{1r}-H_{3r}+2H_{13r}-H_{1q}-H_{3q}+2H_{13q}, \tag{33}$$

$$H_{330}=-H_{3r}+H_{13r}-H_{1q}+H_{13q}, \tag{34}$$

$$H_{3333}=-2H_{3r}-H_{13r}+H_{33r}-3H_{3q}-H_{13q}+H_{33q}, \tag{35}$$

the component summations in which are:

$$H_{1r}=(\epsilon^5/2)\sum{}'n_r r_{12}^2 g_2(\epsilon r), \tag{36}$$

$$H_{3r}=c^2\epsilon^5\sum{}'n_r r_3^2 g_2(\epsilon r), \tag{37}$$

$$H_{12r}=(\epsilon^7/8)\sum{}'n_r r_{12}^4 g_3(\epsilon r), \tag{38}$$

$$H_{13r}=(c^2\epsilon^7/2)\sum{}'n_r r_{12}^2 r_3^2 g_3(\epsilon r), \tag{39}$$

$$H_{33r}=c^4\epsilon^7\sum{}'n_r r_3^4 g_3(\epsilon r), \tag{40}$$

$$H_{1q}=\pi N\,2^{\frac{1}{2}}\sum{}'f n_q q_{12}^2 q^{-2}\exp(-\pi^2q^2/\epsilon^2), \tag{41}$$

$$H_{3q}=(2\pi N\,2^{\frac{1}{2}}/c^2)\sum{}'f n_q q_3^2 q^{-2}\exp(-\pi^2q^2/\epsilon^2), \tag{42}$$

$$H_{12q}=\pi N\,2^{\frac{1}{2}}\sum{}'f n_q q_{12}^4 q^{-4}\{(\pi^2q^2/\epsilon^2)+1\}\exp(-\pi^2q^2/\epsilon^2), \tag{43}$$

$$H_{13q}=(4\pi N\,2^{\frac{1}{2}}/c^2)\sum{}'f n_q q_{12}^2 q_3^2 q^{-4}\{(\pi^2q^2/\epsilon^2)+1\}\exp(-\pi^2q^2/\epsilon^2), \tag{44}$$

$$H_{33q}=(8\pi N\,2^{\frac{1}{2}}/c^4)\sum{}'f n_q q_3^4 q^{-4}\{(\pi^2q^2/\epsilon^2)+1\}\exp(-\pi^2q^2/\epsilon^2). \tag{45}$$

The factor f in Eqs. (41) to (45) inclusive is 1 for (*H*) and has values 1, 3/4, 1/4, or 0 for (*HC*) according to the tabulation following Eqs. (22) and (23). The results of computation for $\epsilon=3$ and $\epsilon=2$ are given in Table III, all the values in which agreed to less than half a unit in the fifth decimal place for the two values of ϵ.

It is obvious that the results here presented may be applied to unstrained arrays (*H*) and (*HC*) in which $c\sim 2\times 6^{\frac{1}{2}}/3$ for any such array may be derived from the case here treated by regard-

TABLE III. *Homogeneously strained hexagonal arrays.*

Coefficient—Eqs. (25)–(28)	(*H*)	(*HC*)
H_{110}	4.14282	3.86345
H_{1111}	8.28564	7.72690
H_{1133}	−11.82832	−1.54571
H_{1212}	8.28564	7.72690
H_{1313}	− 7.71230	4.62534
H_{330}	− 0.02679	2.30760
H_{3333}	8.96613	10.84874

ing the crystal as strained, with $A_{33}=3c/2\times 6^{\frac{1}{2}}-1$ as the only strain component different from zero. If A_{33}, so computed, is small enough to justify the assumption that effects of strain are linear this does not invalidate Eq. (24) by which we must find the correction term for Eq. (13). As already mentioned, c for cobalt has so nearly the theoretical value for close-packed spheres that the artifice is unnecessary in this case of greatest interest.