Magnetic Dipole Fields in Unstrained Cubic Crystals

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

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Magnetic field components in certain cubic arrays of equal parallel dipoles are computed by two methods for points on the boundary of a dipole domain and for points near a vacated dipole position. The results may be of use in theories of ferromagnetism. Characteristic constants for a nonpolar cubic array of dipoles, previously computed by Bouman, are recomputed more precisely.

THE present state of ferromagnetic theory is somewhat chaotic, but a few definite conclusions have been reached and a direction for further advances may be indicated. The high stability of saturated magnetization in crystal domains containing many atoms each is inexplicable by magnetic forces but so-called exchange forces are of the right order of magnitude to account for it. These exchange forces have been estimated from electrostatic energy associated with states in which one electron in each atom of every adjacent pair has its spin-axis parallel to that of the similar disposable electron in the other member of the pair. The argument is quasi-classical in its postulation of Coulomb electric forces between the electrons in question. It is important to notice that the energy of electrostatic forces between each magnetically disposable electron and the other electrons of the atom are supposed not to be affected by the choice of direction of the electron spin-axis. The exchange interaction may thus be thought of as depending only upon the spatial distribution of the disposable electrons and the electrostatic interaction between them. It is not yet clear how easy directions for magnetization are determined. They may be due to interactions between disposable and other electrons in the same atom, but there seems to be little evidence for a control of the orientation of completed electron-shells by crystal symmetry and such completed shells may be statistically of spherical symmetry, so as to have no resultant magnetic effect. It seems worth while, at least, to consider the hitherto deliberately neglected magnetic interaction between the disposable electrons. This is of the right order of magnitude to allow control of the direction of saturation by weak magnetic forces, and must appear in some form in the completed theory. The complete solution can be outlined as soon as we know the time-average distribution functions for the magnetic field intensity and for the occurrence of the "ferromagnetic" electrons within each atomic domain. This paper makes an attack upon the first of these distribution functions. It seems more likely to be of value because it is already known that the changes in local magnetic fields which can be produced by strain are of the right sort to account almost quantitatively for the corresponding changes in ferromagnetic behavior, and for magnetostriction.

We propose to calculate the magnetic field intensity at selected points in certain cubic arrays of equal magnetic dipoles. The four easiest cases are presented by the simple cubic lattice (S), the body-centered cubic lattice (I), the face-centered cubic lattice (F), and the array characteristic of diamond (D). The last of these is a case of (F) having two dipoles specially placed with reference to each lattice point. The magnetic field intensity $\mathbf{H}$ at any point is proportional to Pa_0^{-3} where P is the magnetic moment of each dipole and a_0 is the edge of the unit cube. For greater generality we will compute a field factor $\mathbf{h}$, independent of P and a_0 and therefore related to $\mathbf{H}$ by the equation

$$\mathbf{H}=\mathbf{h}Pa_0^{-3}. \tag{1}$$

We must therefore replace each vector moment $\mathbf{P}$ by a parallel unit vector $\mathbf{p}$ and each vector translation $\mathbf{V}$ by a parallel vector $\mathbf{v}=\mathbf{V}a_0^{-1}$.

We select any dipole as an origin of rectangular

coordinates parallel to the cubic axes. Then the position of any other dipole is fixed by a vector $\mathbf{r}$ to it from the origin. The different arrays are distinguished in Table I by selection rules for the components r_i, where the subscript i is successively 1, 2 and 3 for each dipole. If two or three components are to be referred to we use subscripts i and j, or i, j and k. An arbitrary integer, positive, negative, or zero is indicated by n_i or by n, and N is the number of dipoles per unit cube.

TABLE I. *Characterization of dipole arrays.*

N is the number of dipoles per unit cube.

Name Selection Rule	Symbol	N
Simple cubic $r_i=n_i$.	(S)	1
Body-centered cubic $r_i=n_i$, and $r_i=n_i+\frac{1}{2}$.	(I)	2
Face-centered cubic $r_i=n_i$ or $n_i+\frac{1}{2}$; $\Sigma_i r_i=n$.	(F)	4
Diamond cubic $r_i=n_i$ or $n_i+\frac{1}{2}$; $\Sigma_i r_i=n$, and $r_i=n_i+\frac{1}{4}$ or $n_i+\frac{3}{4}$; $\Sigma_i r_i=n+\frac{3}{4}$.	(D)	8

We will first suppose that all dipoles are parallel so that $\mathbf{p}$ is the same for all. The magnetic moment per unit volume,

$$\mathbf{I}=N\mathbf{P}a_0^{-3}, \tag{2}$$

corresponds to magnetic saturation. If, in calculating $\mathbf{H}$ we find a term depending on $\mathbf{I}$, the field factor $\mathbf{h}$ will depend in the same way upon $N\mathbf{p}$.

We let s_i be the three coordinates of a point, not occupied by a dipole ($\mathbf{s}\neq\mathbf{r}$), at which the h_i are desired, and put $\mathbf{r}-\mathbf{s}=\mathbf{t}$. The increment of h_i due to the dipole defined by $\mathbf{r}$ is

$$\delta h_i=(3t_i^2t^{-5}-t^{-3})p_i+3t_it_jp_j+3t_it_kp_k, \tag{3}$$

or, for abbreviation,

$$\delta h_i=\delta h_{ii}p_i+\delta h_{ij}p_j+\delta h_{ik}p_k. \tag{4}$$

In a finite crystal h_i in general depends upon the crystal boundary so that we must either sum δh_i for all the dipoles in a specimen, which is inconvenient, or resort to an artifice. One such artifice, that of Lorentz,[1] substitutes for the dipoles beyond a convenient sphere of radius $t_{\lim}$ a continuum with uniform magnetization $N\mathbf{p}$.

[1] H. A. Lorentz, *Theory of Electrons*, pp. 303–306 (1909).

The correction term to the result of summing δh_i up to $t_{\lim}$ is then calculable for some shapes of specimen. For a spherical crystal the correction term vanishes. For an infinite crystal it is $4\pi N\mathbf{p}/3$. We accordingly write for an infinite crystal

$$\mathbf{h}=4\pi N\mathbf{p}/3+\lim\Sigma\delta\mathbf{h}, \tag{5}$$

or in scalar form

$$h_i=4\pi Np_i/3+\lim\Sigma\delta h_i, \tag{6}$$

that is,

$$h_i=\{4\pi N/3+\lim\Sigma\delta h_{ii}\}p_i+\lim\Sigma\delta h_{ij}p_j+\lim\Sigma\delta h_{ik}p_k. \tag{7}$$

The approximation to the final value is slow, but this final value may be predicted with fair certainty after a manageable number of terms have been computed. It saves time and improves precision to choose a symmetrical direction for $\mathbf{s}$, for then the number of terms separately to be computed becomes much less than the number of dipoles included. The field distribution in each dipole domain is the same and $\mathbf{s}$ therefore has a limit, depending upon its direction, beyond which it is unnecessary to increase its magnitude. In general $s_{\lim}\gtrless 3^{\frac{1}{2}}/2$.

Fig. 1 shows one unit cube in each array (that lying between the origin and the dipole at $r_1=r_2=-1$, $r_3=1$) with the positions of its N dipoles indicated by small circles and with one dipole domain outlined about the origin. Corners and other important points on the boundary of each such domain are marked, on the prolongation through them of lines from the origin, with their coordinates: $s_1s_2s_3$.

If a line be drawn from the origin to any point on the boundary of the atomic domain it is easy to see from considerations of symmetry that a given h_i varies from a maximum to a minimum, or *vice versa*, as we traverse the line. A general survey of the field is therefore most easily made by selecting points on the boundary of an atomic domain. Since the field intensities at $\mathbf{s}$ and at $-\mathbf{s}$ are always equal (and parallel) it is necessary to consider only one-half of the atomic domain in selecting such points.

Table II presents h_i for selected points of the sort marked in Fig. 1, for a series of values for $t_{\lim}$, and for two simple directions for $\mathbf{p}$, in arrays (S), (I) and (F). Each line in part C of this table

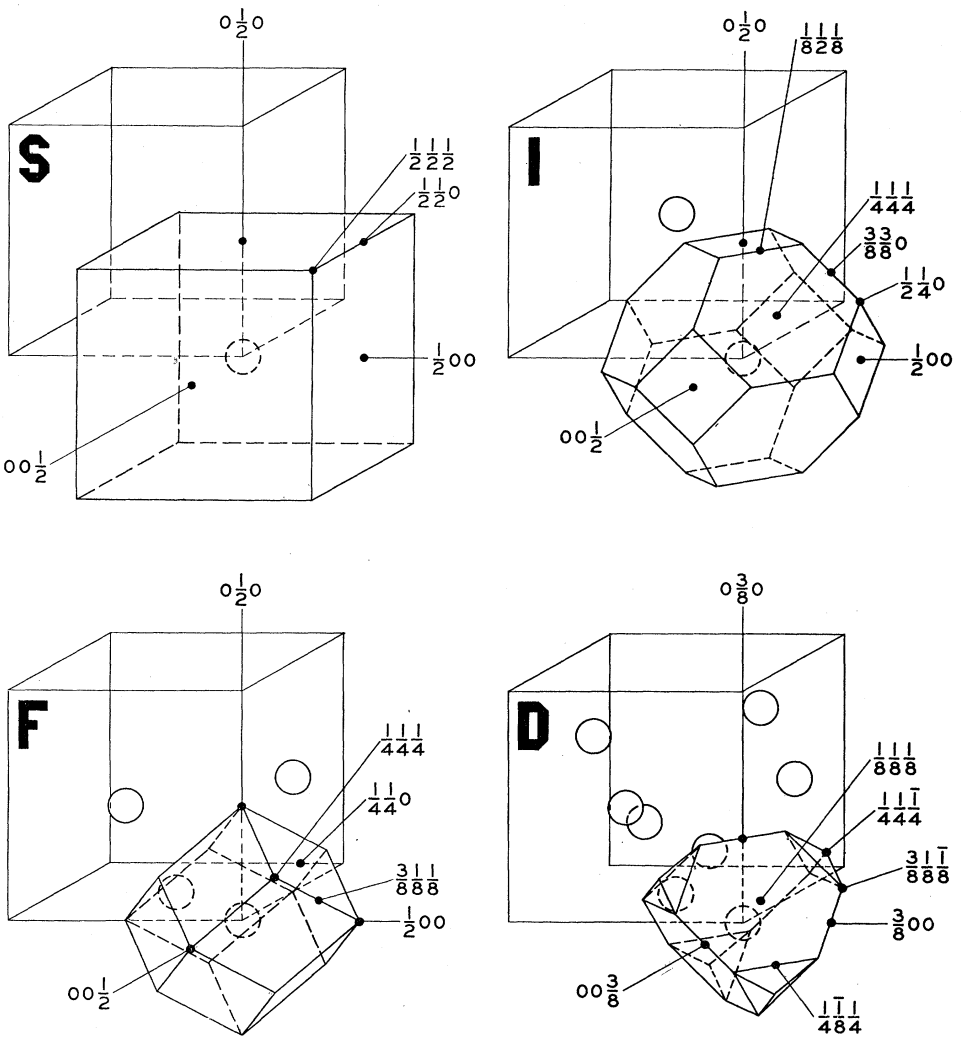

FIG. 1. Dipole domains in cubic arrays: (*S*) Simple cubic, (*I*) Body-centered cubic, (*F*) Face-centered cubic, (*D*) Diamond cubic. Coordinates $s_1 s_2 s_3$ are given in terms of the edge of the unit cube. Circles show the positions of the dipoles associated with the unit cube which is outlined.

corresponds to including an additional group of dipoles all with the same t. Since t is generally an irreducible surd t^2 is preferred as the argument. The number of dipoles, $\sum N$, included at each stage of the summation, is also recorded. It will be noted that $\sum N \sim 4\pi N t^3/3$. The term $4\pi N p_i/3$ is put last, in part A, which summarizes the results, for two reasons. In the first place it tends to smooth out those variations of the local field with which we are chiefly concerned. In the second place it is logically last because it arises from the extension of the array to infinity.

The last column in Table IIA contains values of h_i computed by a second artifice, due to Ewald,[2] applied to the present problem by Kornfeld[3] and justified in detail by Bouman.[4] We write, in analogy with (4)

$$h_i = h_{ii} p_i + h_{ij} p_j + h_{ik} p_k. \tag{8}$$

Each coefficient (h_{ii}, h_{ij}, h_{ik}) is composed of three

[2] P. P. Ewald, Ann. d. Physik [4] **64**, 253–287 (1921).
[3] H. Kornfeld, Zeits. f. Physik **22**, 27–43 (1924).
[4] J. Bouman, Archives Néerlandaises [3A] **13**, 1–28 (1931).

TABLE II, PART A. *Values of h_i for points on the boundary of a dipole domain.* Column 1: Type of array; (*S*), (*I*), or (*F*). Column 2: Components of dipole moment; $p_1p_2p_3$. Column 3: Coordinates of point; $s_1s_2s_3$. Column 4: Column number in part C where a series of values of $M\Sigma\delta h_i$ are given. A dash indicates that all values of $\Sigma\delta h_i$ are zero. Column 5: M. Column 6: Last $\Sigma\delta h_i$ here computed. Column 7: $4\pi Np_i/3$. Column 8: h_i (method of Lorentz). Column 9: h_i (method of Ewald). In columns 4 to 9 inclusive there are three entries for each entry in column 3, corresponding, in that order, to $i=1, 2, 3$.

1	2	3	4	5	6	7	8	9
(*S*)	1 0 0	1/2 1/2 1/2	–	–	0	4.18879	4.18879	4.18879
			–	–	0	0	0	0
			–	–	0	0	0	0
		1/2 1/2 0	1	2	4.39297	4.18879	8.58196	8.52266
			–	–	0	0	0	0
			–	–	0	0	0	0
		0 1/2 1/2	1	−1	− 8.78595	4.18879	− 4.59716	− 4.47894
			–	–	0	0	0	0
			–	–	0	0	0	0
		1/2 0 0	3	1	30.95208	4.18879	35.14087	34.27084
			–	–	0	0	0	0
			–	–	0	0	0	0
		0 1/2 0	3	−2	−15.47604	4.18879	−11.28725	−10.85223
			–	–	0	0	0	0
			–	–	0	0	0	0
	1/3 1/3 1/3	1/2 1/2 1/2	–	–	0	2.41840	2.41840	2.41840
			–	–	0	2.41840	2.41840	2.41840
			–	–	0	2.41840	2.41840	2.41840
		1/2 1/2 0	2	2	2.53628	2.41840	4.95468	4.92056
			2	2	2.53628	2.41840	4.95468	4.92056
			2	−1	− 5.07257	2.41840	− 2.65417	− 2.58592
		1/2 0 0	4	1	17.87019	2.41840	20.28859	19.78628
			4	−2	− 8.93510	2.41840	− 6.51670	− 6.26553
			4	−2	− 8.93510	2.41840	− 6.51670	− 6.26553
(*I*)	1 0 0	1/2 1/4 0	5	2	3.01186	8.37758	11.38944	11.41394
			–	–	0	0	0	0
			–	–	0	0	0	0
		1/4 1/2 0	5	−1	− 6.02371	8.37758	2.35387	2.30489
			–	–	0	0	0	0
			–	–	0	0	0	0
		1/2 1/8 1/8	7	1	10.02019	8.37758	18.39777	18.33361
			–	–	0	0	0	0
			–	–	0	0	0	0
		1/8 1/2 1/8	7	−2	− 5.01010	8.37758	3.36748	3.39958
			–	–	0	0	0	0
			8	1	7.21119	0	7.21119	7.14688
		1/2 0 0	12	1	21.42572	8.37758	29.80330	29.79189
			–	–	0	0	0	0
			–	–	0	0	0	0
		0 1/2 0	12	−2	−10.71286	8.37758	− 2.33528	− 2.32958
			–	–	0	0	0	0
			–	–	0	0	0	0
		3/8 3/8 0	7	−2	− 5.01010	8.37758	3.36748	3.39958
			8	1	7.21119	0	7.21119	7.14688
			–	–	0	0	0	0
		0 3/8 3/8	7	1	10.02019	8.37758	18.39777	18.33661
			–	–	0	0	0	0
			–	–	0	0	0	0
		1/4 1/4 1/4	–	–	0	8.37758	8.37758	8.37758
			14	1	21.43140	0	21.43140	21.24094
			14	1	21.43140	0	21.43140	21.24094
	1/3 1/3 1/3	1/2 1/4 0	6	2	1.73890	4.83680	6.57570	6.58984
			6	−1	− 3.47779	4.83680	1.35901	1.33072
			6	2	1.73890	4.83680	6.57570	6.58984
		1/2 1/8 1/8	9	1	5.78516	4.83680	10.62196	10.58491
			10	1	1.27080	4.83680	6.10760	6.08899
			10	1	1.27080	4.83680	6.10760	6.08899
(*I*)	1/3 1/3 1/3	1/2 1/8 $\bar{1}$/8	9	1	5.78516	4.83680	10.62196	10.58491
			11	−1	− 7.26900	4.83680	− 2.43210	− 2.13651
			11	−1	− 7.26900	4.83680	− 2.43210	− 2.13651
		1/2 0 0	13	1	12.37015	4.83680	17.20695	17.20036
			13	−2	− 6.18507	4.83680	− 1.34827	− 1.34497
			13	−2	− 6.18507	4.83680	− 1.34827	− 1.34497
		3/8 3/8 0	10	1	1.27080	4.83680	6.10760	6.08899
			10	1	1.27080	4.83680	6.10760	6.08899
			9	1	5.78516	4.83680	10.62196	10.58491
		3/8 $\bar{3}$/8 0	11	−1	− 7.26900	4.83680	− 2.43210	− 2.13651
			11	−1	− 7.26900	4.83680	− 2.43210	− 2.13651
			9	1	5.78516	4.83680	10.62196	10.58491
		1/4 1/4 1/4	15	1	24.74685	4.83680	29.58365	29.36734
			15	1	24.74685	4.83680	29.58365	29.36734
			15	1	24.74685	4.83680	29.58365	29.36734
		1/4 1/4 $\bar{1}$/4	–	–	0	4.83680	4.83680	4.83680
			–	–	0	4.83680	4.83680	4.83680
			15	−1	−24.74685	4.83680	−19.91005	−19.69013
(*F*)	1 0 0	1/2 0 0	–	–	0	16.75516	16.75516	16.75516
			–	–	0	0	0	0
			–	–	0	0	0	0
		3/8 1/8 1/8	–	–	0	16.75516	16.75516	16.75516
			16	1	13.35659	0	13.35659	13.49447
			16	1	13.35659	0	13.35659	13.49447
		1/8 3/8 1/8	–	–	0	16.75516	16.75516	16.75516
			16	1	13.35659	0	13.35659	13.49447
			16	−1	−13.35659	0	−13.35659	−13.49447
		1/4 1/4 1/4	–	–	0	16.75516	16.75516	16.75516
			–	–	0	0	0	0
			–	–	0	0	0	0
		1/4 1/4 0	18	2	17.57189	16.75516	34.32705	34.09064
			19	1	57.41342	0	57.41342	57.84236
			–	–	0	0	0	0
		0 1/4 1/4	18	−1	−35.14379	16.75516	−18.38863	−17.91578
			–	–	0	0	0	0
			–	–	0	0	0	0
	1/3 1/3 1/3	1/2 0 0	–	–	0	9.67360	9.67360	9.67360
			–	–	0	9.67360	9.67360	9.67360
			–	–	0	9.67360	9.67360	9.67360
		3/8 1/8 1/8	17	1	15.42286	9.67360	25.09646	25.25567
			–	–	0	9.67360	9.67360	9.67360
			–	–	0	9.67360	9.67360	9.67260
		3/8 1/8 $\bar{1}$/8	–	–	0	9.67360	9.67360	9.67360
			17	1	15.42286	9.67360	25.09646	25.25567
			–	–	0	9.67360	9.67360	9.67360
		3/8 $\bar{1}$/8 $\bar{1}$/8	17	−1	−15.42286	9.67360	− 5.74926	− 5.90849
			17	−1	−15.42286	9.67360	− 5.74926	− 5.90849
			17	−1	−15.42286	9.67360	− 5.74926	− 5.90849
		1/4 1/4 1/4	–	–	0	9.67360	9.67360	9.67360
			–	–	0	9.67360	9.67360	9.67360
			–	–	0	9.67360	9.67360	9.67360
		1/4 1/4 0	20	1	43.32741	9.67360	53.00101	53.07754
			20	1	43.32741	9.67360	53.00101	53.07754
			21	−1	−20.29027	9.67360	−10.61667	−10.34368
		1/4 $\bar{1}$/4 0	22	−1	−23.00252	9.67360	−13.32892	−13.71306
			22	−1	−23.00252	9.67360	−13.32892	−13.71306
			21	−1	−20.29027	9.67360	−10.61667	−10.34368

TABLE II, PART B. Columns 1, 2, 3: Same as in Table II, part A. Column 4: Coordinates of point, $s_1's_2's_3'$, not appearing in part A. Column 5: $h_1'h_2'h_3'$ in terms of $h_1h_2h_3$ as given in columns 8 and 9 of part A for $s_1s_2s_3$ as given in column 3. For ease in reading only the order of $h_1h_2h_3$ is given. Thus 3 1 2 means that $h_1' = h_3$, $h_2' = h_1$, $h_3' = h_2$.

1	2	3	4	5
(S)	1 0 0	1/2 1/2 1/2	1/2 1/2 $\bar{1}$/2	1 2 3
			1/2 $\bar{1}$/2 1/2	1 2 3
			1/2 $\bar{1}$/2 $\bar{1}$/2	1 2 3
		1/2 1/2 0	1/2 0 1/2	1 2 3
			1/2 0 $\bar{1}$/2	1 2 3
			1/2 $\bar{1}$/2 0	1 2 3
		0 1/2 1/2	0 1/2 $\bar{1}$/2	1 2 3
		0 1/2 0	0 0 1/2	1 2 3
	1/3½ 1/3½ 1/3½	1/2 1/2 1/2	1/2 1/2 $\bar{1}$/2	1 2 3
			1/2 $\bar{1}$/2 1/2	1 2 3
			1/2 $\bar{1}$/2 $\bar{1}$/2	1 2 3
		1/2 1/2 0	1/2 0 1/2	2 3 1
			1/2 0 $\bar{1}$/2	2 3 1
			1/2 $\bar{1}$/2 0	1 2 3
			0 1/2 1/2	3 1 2
			0 1/2 $\bar{1}$/2	3 1 2
		1/2 0 0	0 1/2 0	3 1 2
			0 0 1/2	2 3 1
(I)	1 0 0	1/2 1/4 0	1/2 0 1/4	1 2 3
			1/2 0 $\bar{1}$/4	1 2 3
			1/2 $\bar{1}$/4 0	1 2 3
			0 1/2 1/4	1 2 3
			0 1/2 $\bar{1}$/4	1 2 3
			0 1/4 1/2	1 2 3
			0 1/4 $\bar{1}$/2	1 2 3
		1/4 1/2 0	1/4 0 1/2	1 2 3
			1/4 0 $\bar{1}$/2	1 2 3
			1/4 $\bar{1}$/2 0	1 2 3
		1/2 1/8 1/8	1/2 1/8 $\bar{1}$/8	1 2 3
			1/2 $\bar{1}$/8 1/8	1 2 3
			1/2 $\bar{1}$/8 $\bar{1}$/8	1 2 3
		1/8 1/2 1/8	1/8 1/2 $\bar{1}$/8	1 2 3
			1/8 1/8 1/2	1 2 3
			1/8 $\bar{1}$/8 $\bar{1}$/2	1 2 3
			1 8 $\bar{1}$/8 1/2	1 2 3
			1/8 $\bar{1}$/8 $\bar{1}$/2	1 2 3
			1/8 $\bar{1}$/2 1/8	1 2 3
			1/8 $\bar{1}$/2 $\bar{1}$/8	1 2 3
		0 1/2 0	0 0 1/2	1 2 3
		3/8 3/8 0	3/8 0 3/8	1 3 2
			3 8 0 $\bar{3}$/8	1 3 2
			3/8 $\bar{3}$/8 0	1 2 3
		0 3/8 3/8	0 3/8 $\bar{3}$/8	1 2 3
		1/4 1/4 1/4	1/4 1/4 $\bar{1}$/4	1 2 3
			1/4 $\bar{1}$/4 1/4	1 2 3
			1/4 $\bar{1}$/4 $\bar{1}$/4	1 2 3
	1/3½ 1/3½ 1/3½	1/2 1/4 0	1/2 0 1/4	3 1 2
			1/2 0 $\bar{1}$/4	3 1 2
			1/2 $\bar{1}$/4 0	1 2 3
			1/4 1/2 0	2 3 1
			1/4 0 1/2	2 3 1
			1/4 0 $\bar{1}$/2	2 3 1
			1/4 $\bar{1}$/2 0	2 3 1
		1/2 1/8 1/8	1/2 1/8 $\bar{1}$/8	1 2 3

1	2	3	4	5
(I)	1/3½ 1/3½ 1/3½	1/2 1/8 1/8	1/8 1/2 1/8	3 1 2
			1/8 1/8 1/2	2 3 1
			1/8 1/8 $\bar{1}$/2	2 3 1
			1/8 $\bar{1}$/2 1/8	3 1 2
		1/2 1/8 $\bar{1}$/8	1/2 1/8 1/8	1 2 3
			1/8 1/2 $\bar{1}$/8	3 1 2
			1/8 $\bar{1}$/8 1/2	2 3 1
			1/8 $\bar{1}$/8 $\bar{1}$/2	2 3 1
			1/8 $\bar{1}$/2 1/8	3 1 2
		1/2 0 0	0 1/2 0	3 1 2
			0 0 1/2	2 3 1
		3/8 3/8 0	3/8 0 3/8	2 3 1
			0 3/8 $\bar{3}$/8	3 1 2
		3/8 $\bar{3}$/8 0	3/8 0 $\bar{3}$/8	2 3 1
			0 $\bar{3}$/8 3/8	3 1 2
		1/4 1/4 $\bar{1}$/4	1/4 1/4 1/4	2 3 1
			1/4 1/4 $\bar{1}$/4	3 1 2
(F)	1 0 0	1/2 0 0	0 1/2 0	1 2 3
			0 0 1/2	1 2 3
		3/8 1/8 1/8	3/8 1/8 1/8	1 2 3
			3/8 $\bar{1}$/8 1/8	1 2 3
			3/8 $\bar{1}$/8 $\bar{1}$/8	1 2 3
		1/8 3/8 1/8	1/8 3/8 $\bar{1}$/8	1 2 3
			1/8 1/8 3/8	1 3 2
			1/8 $\bar{1}$/8 $\bar{3}$/8	1 3 2
			1/8 $\bar{1}$/8 3/8	1 3 2
			1/8 $\bar{1}$/8 $\bar{3}$/8	1 3 2
			1/8 $\bar{3}$/8 1/8	1 2 3
			1/8 $\bar{3}$/8 $\bar{1}$/8	1 2 3
		1/4 1/4 1/4	1/4 1/4 $\bar{1}$/4	1 2 3
			1/4 $\bar{1}$/4 1/4	1 2 3
			1/4 $\bar{1}$/4 $\bar{1}$/4	1 2 3
		1/4 1/4 0	1/4 0 1/4	1 3 2
			1/4 0 $\bar{1}$/4	1 3 2
			1/4 $\bar{1}$/4 0	1 2 3
		0 1/4 1/4	0 1/4 $\bar{1}$/4	1 2 3
	1/3½ 1/3½ 1/3½	1/2 0 0	0 1/2 0	1 2 3
			0 0 1/2	1 2 3
		3/8 1/8 1/8	1/8 3/8 1/8	3 1 2
			1/8 1/8 3/8	2 3 1
		3/8 1/8 $\bar{1}$/8	3/8 1/8 1/8	3 1 2
			1/8 3/8 $\bar{1}$/8	2 3 1
			1/8 $\bar{1}$/8 3/8	2 3 1
			1/8 $\bar{1}$/8 $\bar{3}$/8	1 2 3
			1/8 $\bar{3}$/8 1/8	3 1 2
		3/8 $\bar{1}$/8 $\bar{1}$/8	1/8 1/8 $\bar{3}$/8	1 2 3
			1/8 3/8 1/8	1 2 3
		1/4 1/4 1/4	1/4 1/4 $\bar{1}$/4	1 2 3
			1/4 1/4 1/4	1 2 3
			1/4 1/4 $\bar{1}$/4	1 2 3
		1/4 1/4 0	1/4 0 1/4	2 3 1
			0 1/4 1/4	3 1 2
		1/4 $\bar{1}$/4 0	1/4 0 $\bar{1}$/4	2 3 1
			0 1/4 $\bar{1}$/4	3 1 2

TABLE II. PART C. Numbered columns contain values of $M\Sigma\delta h_i$ as required in part A. At the left of each group of numbered columns are two columns headed nl^2 and ΣN which give, respectively, the highest value of nl^2 and the total number of dipoles for each tabular value of $M\Sigma\delta h_i$.

$4l^2$	ΣN	1	2	$4l^2$	ΣN	3	4	$16l^2$	ΣN	5	6	$64l^2$	ΣN	7	8	9	10	11
2	4	11.31371	6.53197	1	2	32.	18.47521	5	4	9.15893	5.28791	18	3	15.64366	12.29145	9.03187	2.58053	11.61240
6	12	6.95906	4.01782	5	10	29.71026	17.15323	13	8	3.27714	1.89206	34	5	10.47852	5.45524	6.04978	.12469	6.17447
10	20	8.98292	5.18629	9	20	29.31520	16.92514	21	16	7.83745	4.52495	50	6	9.03037	7.62747	5.21369	1.79688	7.01056
14	36	9.33199	5.38783	13	28	30.78565	17.77410	29	28	5.46338	3.15428	66	10	7.87767	6.41215	4.61226	1.39593	6.00819
18	48	8.35427	4.82334	17	44	30.57081	17.65006	37	32	6.50861	3.75775	82	12	9.83861	6.86623	5.68032	1.12406	6.80438
22	56	8.63618	4.98610	21	60	29.43073	16.99184	45	48	6.05632	3.49662	98	20	10.78641	6.47849	6.22754	.62659	6.85413
26	80	8.30197	4.79315	25	70	29.72769	17.16329	53	60	6.13143	3.53998	114	24	10.87497	8.11678	6.27866	1.54689	8.03859
30	96	8.76936	5.06299	29	94	30.32121	17.50596	61	72	6.60710	3.81461	130	26	10.18411	8.64289	5.87980	2.05008	8.14291
34	112	8.95926	5.17263	33	110	31.05780	17.93123	69	88	6.45175	3.72492	146	34	9.96147	6.49599	5.75126	.87483	6.83913
38	136	8.82984	5.09791	37	118	30.79649	17.78036	77	104	6.96348	4.02037	178	38	9.21537	6.80122	5.32049	1.26644	6.79996
42	152	8.76266	5.05912	41	150	30.68947	17.71857	85	112	6.11798	3.53222	194	48	9.75842	7.48687	5.63403	1.50553	7.35259
46	168	8.20968	4.73986	45	174	30.88735	17.83282	93	120	6.22847	3.59601	210	52	9.70073	6.95810	5.60072	1.21690	7.03065
50	196	8.49569	4.90499	49	192	30.81309	17.78995	101	148	6.02371	3.47779	226	56	10.25018	7.03012	5.91795	1.09987	7.23084
54	228	8.71074	5.02915	53	216	30.79431	17.77910					242	67	9.77923	7.03517	5.64604	1.23874	7.09781
58	236	8.85563	5.11280	57	232	31.07610	17.94179					258	71	9.65281	7.40869	5.57305	1.49089	7.27697
62	268	8.87254	5.12257	61	256	30.95718	17.87314					274	77	10.32024	7.11947	5.95839	1.13123	7.30266
66	300	8.74233	5.04739	65	288	31.03233	17.91653					290	87	10.45037	7.19884	6.03353	1.13949	7.38605
70	316	8.62369	4.97889	69	320	31.07117	17.93895					306	95	10.58541	7.65646	6.11149	1.36472	7.68924
74	356	8.47424	4.89260	73	336	30.90812	17.84481					322	99	10.28380	7.21066	5.93736	1.19440	7.34478
78	372	8.63146	4.98338	77	368	30.78018	17.77095					338	100	10.20141	7.33425	5.88979	1.28954	7.39235
82	388	8.60203	4.96638	81	402	30.66801	17.70618					354	108	9.79490	6.65152	5.65509	1.01271	6.88084
86	428	8.67855	5.01056	85	418	30.87938	17.87822					370	114	9.69924	6.68302	5.59986	1.05851	6.87141
90	468	8.65356	4.99613	89	466	30.99243	17.89349					386	124	9.59500	6.97371	5.53967	1.25644	7.00914
94	500	8.75516	5.05479	93	482	30.96481	17.87754					402	132	10.01216	7.03060	5.78053	1.16886	7.16241
98	536	8.72891	5.03964	97	498	31.05045	17.92699					418	136	10.02019	7.21119	5.78516	1.27080	7.26900
102	552	8.66313	5.00166	101	554	31.10164	17.95654											
106	576	8.78595	5.07257	105	586	30.95208	17.87019											

$4l^2$	ΣN	12	13	$16l^2$	ΣN	14	15	$64l^2$	ΣN	16	17	$4l^2$	ΣN	18	19	20	21	22
1	2	32.	18.47521	3	2	24.63361	28.44444	11	3	19.13725	22.09779	2	2	45.25483	67.88225	52.25578	26.12789	26.12789
2	6	20.68629	11.94324	11	8	19.84930	22.92000	27	7	11.02742	12.73337	6	6	27.83624	59.17295	42.19915	16.07126	26.12789
5	14	18.39656	10.62126	19	14	20.58140	23.76535	43	10	13.68777	15.80528	10	10	35.93167	51.88707	40.32959	20.74516	19.58443
6	22	22.75121	13.13542	27	22	22.60885	26.10645	59	19	12.71119	14.67761	14	18	37.32797	58.17043	44.36037	21.55132	22.80906
9	32	22.35615	12.90733	35	34	21.23249	24.51717	75	26	14.25621	16.46165	18	24	33.41706	61.24329	45.00551	19.29335	25.71216
10	40	20.33229	11.73885	43	40	20.56740	23.74919	91	32	15.07286	17.40464	22	28	34.54474	58.19858	43.57317	19.94441	23.62876
13	48	21.80274	12.58782	51	52	21.02221	24.27436	107	41	12.36218	14.27462	26	40	33.20790	57.97577	43.05862	19.17259	23.88603
14	64	21.45366	12.38628	59	70	21.26636	24.55627	123	47	12.74666	14.71858	30	48	35.07746	56.41780	42.69882	20.25198	22.44685
17	80	21.23882	12.26224	67	76	21.79934	25.17171	139	56	13.17147	15.20911	34	56	35.83703	55.73418	42.52341	20.69052	21.83289
18	92	22.21655	12.82673	75	90	21.41309	24.72570	155	68	14.09582	16.27645	38	68	35.31936	58.23626	43.81854	20.39164	23.42690
21	108	21.07647	12.16851	83	108	21.17447	24.45017	171	83	13.74634	15.87291	42	76	35.05064	58.90805	44.12883	20.23650	23.89233
22	116	20.79455	12.00574	91	120	20.97031	24.21442	187	89	13.41871	15.49459	46	84	32.83874	59.22914	43.67569	18.95945	24.71623
25	126	21.09151	12.17719	99	138	20.75373	23.96435	203	101	13.88960	16.03833	50	98	33.98278	58.16474	43.39141	19.61997	23.77145
26	150	21.42572	12.37015	107	156	21.43140	24.74685	219	113	13.48275	15.56854	54	114	34.84296	57.44793	43.22587	20.11659	23.10928
								235	119	13.38477	15.45541	58	118	35.42252	58.07745	43.79125	20.45120	23.30543
								251	140	13.19241	15.23329	62	134	35.49018	56.75802	43.04901	20.49026	22.52413
								267	146	13.35328	15.41904	66	150	34.96933	57.01845	43.04901	20.18955	22.82484
								283	155	13.09677	15.12285	70	158	34.49475	57.58045	43.23648	19.91555	23.28631
								299	179	13.54985	15.64602	74	178	33.89695	57.59675	43.07332	19.57041	23.46829
								315	197	13.79930	15.93406	78	186	34.52585	58.59757	43.83252	19.93351	23.86440
								331	206	13.81086	15.94741	82	194	34.40812	58.82431	43.92961	19.86554	24.02946
								347	221	13.76224	15.89126	86	214	34.71418	58.49958	43.83049	20.04283	23.75363
								363	234	13.61234	15.71818	90	234	34.61424	57.63007	43.29962	19.98454	23.28047
								379	243	13.46239	15.54503	94	250	35.02064	57.73765	43.47905	20.21977	23.22526
								395	267	13.08594	15.11034	98	268	34.91563	57.83863	43.50704	20.15855	23.31387
								411	285	13.30033	15.35790	102	276	34.65251	57.47317	43.22008	20.00663	23.17883
								427	291	13.35659	15.42286	106	288	35.14379	57.41342	43.32741	20.29027	23.00252

convergent sums so that we may put

$$h_{ii}=h_{iit2}+h_{iit0}+h_{ii\,q2}, \tag{9}$$

and similar expressions for h_{ij} and h_{ik}. The sums containing t in the subscript are taken over all points of the infinite array of dipoles. The sums containing q in the subscript are taken over all points of an infinite array reciprocal to the dipole array.

In constructing the q-array from the dipole array we start with the defining equations:

$$\mathbf{r}=\sum r_i\mathbf{a}_i, \tag{10}$$

$$\mathbf{q}=\sum q_i\mathbf{b}_i, \tag{11}$$

$$\mathbf{b}_i=(\mathbf{a}_j\times\mathbf{a}_k)/[\mathbf{a}_i\cdot(\mathbf{a}_j\times\mathbf{a}_k)]. \tag{12}$$

In our cubic arrays the three fundamental translations have the same magnitude ($a_i=1$) and are at right angles so that the reciprocal array is also cubic and the $b_i=1$. We are now ready to consider the separate sums of Eq. (5) and its analogues. These are:

$$h_{iit2}=-\epsilon^5\sum t_i^2 g_2(\epsilon t), \tag{13}$$

$$h_{ijt2}=-\epsilon^5\sum t_i t_j g_2(\epsilon t), \tag{14}$$

$$h_{iit0}=h_{ijt0}=\epsilon^3\sum g_1(\epsilon t), \tag{15}$$

$$h_{ii\,q2}=4\pi\sum{}' q_i^2 q^{-2}\cos\{2\pi(q_1s_1+q_2s_2+q_3s_3)\}\exp(-\pi^2q^2/\epsilon^2), \tag{16}$$

$$h_{ij\,q2}=4\pi\sum{}' q_iq_jq^{-2}\cos\{2\pi(q_1s_1+q_2s_2+q_3s_3)\}\exp(-\pi^2q^2/\epsilon^2). \tag{17}$$

In the primed summations there is no term with $q=0$. The factor ϵ is an arbitrary parameter upon the value of which the h_{ij} do not depend. (The separate sums, such as h_{iit2}, do depend upon ϵ.) Computations for two different ϵ which give the same h_{ij} are almost certainly correct. All values here given have been checked in this way.

The functions g_1 and g_2 are defined according to the scheme:

$$\phi(\alpha)=2\pi^{-\frac{1}{2}}\int_0^\alpha \exp(-\beta^2)d\beta, \tag{18}$$

$$g_0(\alpha)=\alpha^{-1}[1-\phi(\alpha)], \tag{19}$$

$$g_1(\alpha)=\alpha^{-2}[g_0(\alpha)+2\pi^{-\frac{1}{2}}\exp(-\alpha^2)], \tag{20}$$

$$g_2(\alpha)=\alpha^{-2}[3g_1(\alpha)+4\pi^{-\frac{1}{2}}\exp(-\alpha^2)]. \tag{21}$$

Further functions of this series may be thus defined:

$$g_m(\alpha)=\alpha^{-2}[(2m-1)g_{m-1}(\alpha)+2^m\pi^{-\frac{1}{2}}\exp(-\alpha^2)]. \tag{22}$$

The probability integral $\phi(\alpha)$ is usually tabulated to 4 or 5 decimals. Values to 6 or 7 decimals, depending upon the magnitude of the argument, were found more suitable in the present work.

Eqs. (16) and (17) may be used without further modification provided that the dipole array is first divided into its N simple cubic (S) arrays in each of which a different value of s must be used to define the single point where the h_{ij} are wanted. The summation for each s is then over a simple cubic q-lattice. Inspection shows, however, that for many q values the net contribution from the N sums is zero. We therefore prefer to choose one of the N values of s which must all be used in (13), (14) and (15) and to select the values of q_i which contribute to (16) and (17) by a rule analogous to that which selects r_i in the dipole array. Upon thus confining the summation to one s and to the selected q_i we may rewrite (16) and (17) as follows

$$h_{ii\,q2}=4\pi N\sum{}' f q_i^2 q^{-2}\cos\{2\pi(q_1s_1+q_2s_2+q_3s_3)\}\exp(-\pi^2q^2/\epsilon^2), \tag{23}$$

$$h_{ij\,q2}=4\pi N\sum{}' f q_iq_jq^{-2}\cos\{2\pi(q_1s_1+q_2s_2+q_3s_3)\}\exp(-\pi^2q^2/\epsilon^2). \tag{24}$$

The selection rules and the values of the auxiliary factor f are given in Table III.

The choice of ϵ fixes the number of terms dependent on t and q which must be found to attain a given precision. For a value of ϵ near unity the two series are about equally long. It is better to have rather more terms in the q series than in the t series because the functions in the

TABLE III. *Selection rules and values of the auxiliary factor f.*

Symbol	Selection Rule	f
(S)	$q_i=n_i$.	1
(I)	$q_i=n_i$; $\Sigma_i q_i=2n$.	1
(F)	$q_i=2n_i$, and $q_i=2n_i+1$.	1
(D)	$q_i=2n_i$; $\Sigma_i q_i=4n$, and $q_i=2n_i+1$.	1 1/2

former are easier to compute. The values of ϵ here chosen were 2 and 3.

At any dipole position in these infinite cubic arrays the field due to the rest of the dipoles is $4\pi N\mathbf{p}/3$. At near-by points the field due to a complete array is almost exclusively that due to the nearest dipole, and hence has little interest here. It is, however, worth while to inquire in what field a slightly displaced dipole will find itself, the rest of the array remaining undisturbed. We arrive at the desired result by computing h_i at points with small s and subtracting δh_i for the dipole at the origin.

The method of Lorentz is applicable without any special precautions and gives better approximations the smaller the value of s. Results for representative points in (I) and (F) are given in Table IV, which is similar in its general construction to Table II. The principal difference, besides the omission of one dipole, is that r^2 replaces t^2 as the argument in part C. This is now more convenient because t^2 is no longer necessarily a small submultiple of an integer and because groups for the same r, which produce zero field at the origin, produce only small field components at near-by points. Since each value of r gives rise to several values of t the number of terms separately computed is no longer equal to the number of entries in part C of the table. It is therefore reported (as $\sum T$) in a separate column for each group of $\sum\delta h_i$.

The results have again been checked by the method of Ewald, but in this work it was necessary to find $g_1(\epsilon t)$ and $g_2(\epsilon t)$ for the smallest value of the argument—ϵs—to about 10 figures, in order to justify 5 or 6 figures in the results. The terms in Eqs. (13), (14) and (15) which depend upon this argument are almost equal to the corresponding terms in (4) by which the result for a complete array must be corrected. These correction terms must also be computed to about 10 figures, but this presents no particular difficulty. Values of $\phi(\alpha)$ to 9 decimals have been reported by Burgess,[5] who also gives formulae for computing values to any desired precision. The few values here needed were so computed to 10 or more figures as an additional check upon the tabular entries.

A result of some generality may be derived from Table IV. If one dipole in an infinite lattice oscillates through its mean position it may acquire extra magnetic stability for particular directions of its line of motion. This will still be true if a compact group of dipoles oscillates as a whole. This result does not permit any generalization about the stabilizing or disturbing effect of an elastic wave which displaces layers of dipoles in succession. When we consider thermal agitation we do not see in the first place how thermal motions can be limited as to direction. Furthermore we find that if vibrations along all crystallographically equivalent directions are equally probable the average increase in stability is zero. This may be seen for a particular case in Table V.

It does not appear that the observed directions of easy magnetization in real cubic crystals, which are $<100>$ in iron (I) and $<111>$ in nickel (F), could have been predicted from the results here obtained.

A case treated by Bouman[4] falls within the scope of this paper and has been recomputed here although it is not a case of ferromagnetism. The dipole array is composed of two interpenetrating face-centered arrays in each of which separately the vectors $\mathbf{p}$ are so arranged, consistently with full cubic symmetry, that the magnetic moment per unit cube is zero. This makes the results sensibly independent of the crystal boundary. In magnetically stable arrangements $\mathbf{h}$ at each dipole must have the direction of that dipole axis, $\mathbf{p}$. Bouman shows that the h_i depend upon six constants a, b, c, d, e, f (these are A, B, C, D, E, F in his notation multiplied by the volume of a unit cube to make them pure numbers). Since $3a=2b+c=d+2e=3f=4\pi$ we need only compute c and d.

[5] J. Burgess, Trans. Roy. Soc. (Edinburgh) 39, 257–321 (1898).

TABLE IV, Part A. Values of h_i for points near a vacated dipole position. Column 1: Type of array; (I), or (F). Column 2: Components of dipole moment; $p_1p_2p_3$. Column 3: Coordinates of point; $s_1s_2s_3\times(10)^3$. Column 4: Column number in part C where a series of values of $M\Sigma\delta h_i$ are given. A dash indicates that all values of $\Sigma\delta h_i$ are zero. Column 5: M. Column 6: Last $\Sigma\delta h_i$ here computed. Column 7: $4\pi Np_i/3$. Column 8: h_i (method of Lorentz). Column 9: h_i (method of Ewald). In columns 4 to 9 inclusive there are three entries for each entry in column 3, corresponding, in that order, to $i=1, 2, 3$.

1	2	3	4	5	6	7	8	9
(I)	1 0 0	100 0 0	1	−1	−0.35414	8.37758	8.02344	8.0215
			–	–	0	0	0	0
			–	–	0	0	0	0
		0 100 0	1	2	0.17707	8.37758	8.55465	8.5555
			–	–	0	0	0	0
			–	–	0	0	0	0
		70 70 0	3	−2	−0.10066	8.37758	8.27692	8.2768
			4	1	0.16628	0	0.16628	0.1682
			–	–	0	0	0	0
		0 70 70	3	1	0.20131	8.37758	8.57889	8.5792
			–	–	0	0	0	0
			–	–	0	0	0	0
		55 55 55	–	–	0	8.37758	8.37758	8.3776
			8	1	0.12421	0	0.12421	0.1249
			8	1	0.12421	0	0.12421	0.1249
	1/3½ 1/3½ 1/3½	100 0 0	2	−1	−0.20446	4.83680	4.63234	4.6312
			2	2	0.10223	4.83680	4.93903	4.9395
			2	2	0.10223	4.83680	4.93903	4.9395
		70 70 0	5	1	0.03787	4.83680	4.87467	4.8755
			5	1	0.03787	4.83680	4.87467	4.8755
			6	1	0.11623	4.83680	4.95303	4.9532
		70 $\bar{7}0$ 0	7	−1	−0.15409	4.83680	4.68271	4.6816
			7	−1	−0.15409	4.83680	4.68271	4.6816
			6	1	0.11623	4.83680	4.95303	4.9532
		55 55 55	9	1	0.14343	4.83680	4.98023	4.9812
			9	1	0.14343	4.83680	4.98023	4.9812
			9	1	0.14343	4.83680	4.98023	4.9812
		55 55 $\bar{5}\bar{5}$	–	–	0	4.83680	4.83680	4.8368
			–	–	0	4.83680	4.83680	4.8368
			9	−1	−0.14343	4.83680	4.69337	4.6924

1	2	3	4	5	6	7	8	9
(F)	1 0 0	100 0 0	10	−1	−0.98009	16.75516	15.77507	15.7766
			–	–	0	0	0	0
			–	–	0	0	0	0
		0 100 0	10	2	0.49004	16.75516	17.24520	17.2444
			–	–	0	0	0	0
			–	–	0	0	0	0
		70 70 0	12	−2	−0.17342	16.75516	16.58174	16.5824
			13	1	0.52224	0	0.52224	0.5223
			–	–	0	0	0	0
		0 70 70	12	1	0.34685	16.75516	17.10201	17.1006
			–	–	0	0	0	0
			–	–	0	0	0	0
		55 55 55	–	–	0	16.75516	16.75516	16.7552
			17	1	0.21569	0	0.21569	0.2153
			17	1	0.21569	0	0.21569	0.2153
	1/3½ 1/3½ 1/3½	100 0 0	11	−1	−0.56585	9.67360	9.10775	9.1086
			11	2	0.28293	9.67360	9.95653	9.9560
			11	2	0.28293	9.67360	9.95653	9.9560
		70 70 0	14	1	0.20136	9.67360	9.87496	9.8754
			14	1	0.20136	9.67360	9.87496	9.8754
			15	1	0.20025	9.67360	9.87385	9.8730
		70 $\bar{7}0$ 0	16	−1	−0.40162	9.67360	9.27198	9.2723
			16	−1	−0.40162	9.67360	9.27198	9.2723
			15	1	0.20025	9.67360	9.87385	9.8730
		55 55 55	18	1	0.24906	9.67360	9.92266	9.9222
			18	1	0.24906	9.67360	9.92266	9.9222
			18	1	0.24906	9.67360	9.92266	9.9222
		55 55 $\bar{5}\bar{5}$	–	–	0	9.67360	9.67360	9.6736
			–	–	0	9.67360	9.67360	9.6736
			18	−1	−0.24906	9.67360	9.42454	9.4250

TABLE IV, PART B. Columns 1, 2, 3: Same as in part A. Column 4: Coordinates of point, $s_1's_2's_3'\times(10)^3$, not appearing in part A. Column 5: $h_1'h_2'h_3'$ in terms of $h_1h_2h_3$ as given in columns 8 and 9 of part A for $s_1s_2s_3\times(10)^3$ as given in column 3. For ease in reading only the order of $h_1h_2h_3$ is given. Thus 3 1 2 means that $h_1'=h_3$, $h_2'=h_1$, $h_3'=h_2$.

1	2	3	4	5	1	2	3	4	5
(*I*)	1 0 0	0 100 0	0 0 100	1 2 3	(*F*)	1 0 0	0 100 0	0 0 100	1 2 3
		70 70 0	70 0 70	1 3 2			70 70 0	70 0 70	1 3 2
			70 0 $\overline{70}$	1 3 2				70 0 $\overline{70}$	1 3 2
			70 $\overline{70}$ 0	1 2 3				70 $\overline{70}$ 0	1 2 3
		0 70 70	0 70 $\overline{70}$	1 2 3			0 70 70	0 70 $\overline{70}$	1 2 3
		55 55 55	55 55 $\overline{55}$	1 2 3			55 55 55	55 55 $\overline{55}$	1 2 3
			55 $\overline{55}$ 55	1 2 3				55 $\overline{55}$ 55	1 2 3
			55 $\overline{55}$ $\overline{55}$	1 2 3				55 $\overline{55}$ $\overline{55}$	1 2 3
	$1/3^{\frac{1}{2}}$ $1/3^{\frac{1}{2}}$ $1/3^{\frac{1}{2}}$	100 0 0	0 100 0	3 1 2		$1/3^{\frac{1}{2}}$ $1/3^{\frac{1}{2}}$ $1/3^{\frac{1}{2}}$	100 0 0	0 100 0	3 1 2
			0 0 100	2 3 1				0 0 100	2 3 1
		70 70 0	70 0 70	2 3 1			70 70 0	70 0 70	2 3 1
			0 70 70	3 1 2				0 70 70	3 1 2
		70 $\overline{70}$ 0	70 0 $\overline{70}$	2 3 1			70 $\overline{70}$ 0	70 0 $\overline{70}$	2 3 1
			0 70 $\overline{70}$	3 1 2				0 70 $\overline{70}$	3 1 2
		55 55 $\overline{55}$	55 $\overline{55}$ 55	2 3 1			55 55 $\overline{55}$	55 $\overline{55}$ 55	2 3 1
			55 $\overline{55}$ $\overline{55}$	3 1 2				55 $\overline{55}$ $\overline{55}$	3 1 2

TABLE IV. PART C. Numbered columns contain values of $\Sigma\delta h_i$ as required in part A. At the left of each group of numbered columns are three columns headed nr^2, ΣN and ΣT which give, respectively, the highest value of r^2, the total number of dipoles and the total number of terms for each tabular value of $\Sigma\delta h_i$.

$4r^2$	ΣN	ΣT	1	2	ΣT	3	4	5	6	7	ΣT	8	9
3	8	2	0.75154	0.43390	3	0.39302	0.36162	0.09533	0.22691	0.32224	4	0.24255	0.28007
4	14	5	.32912	.19002	6	.18990	.15374	.03394	.10964	.14358	6	.11716	.13529
8	26	8	.36688	.21182	11	.20731	.17256	.03978	.11969	.15947	9	.12792	.14771
11	50	12	.33806	.19518	16	.19325	.15842	.03568	.11157	.14725	15	.11924	.13768
12	58	14	.36190	.20894	19	.20512	.17004	.03896	.11843	.15739	19	.12657	.14615
16	64	17	.34875	.20135	22	.19871	.16359	.03709	.11473	.15181	21	.12261	.14158
19	88	21	.36146	.20869	29	.20490	.16983	.03890	.11830	.15720	27	.12643	.14599
20	112	26	.35547	.20523	35	.20193	.16694	.03807	.11658	.15465	31	.12460	.14387
24	136	30	.36022	.20797	42	.20427	.16926	.03874	.11794	.15667	36	.12604	.14554
27	168	36	.35414	.20446	49	.20131	.16628	.03787	.11623	.15409	44	.12421	.14343

$4r^2$	ΣN	ΣT	10	11	ΣT	12	13	14	15	16	ΣT	17	18
2	12	3	1.26626	0.73108	5	0.48225	0.66362	0.24393	0.27843	0.52236	3	0.29928	0.34558
4	18	6	.84384	.48719	8	.27913	.45574	.18255	.16116	.34370	5	.17389	.20080
6	42	10	.99517	.57456	15	.35516	.52933	.20308	.20505	.40814	10	.22081	.25497
8	54	13	1.03293	.59637	20	.37257	.54815	.20892	.21511	.42403	13	.23157	.26739
10	78	18	.93941	.54237	28	.32678	.50231	.19568	.18867	.38434	17	.20330	.23475
12	86	20	.96325	.55613	31	.33866	.51394	.19896	.19552	.39448	21	.21063	.24321
14	134	26	.99993	.57731	41	.35659	.53192	.20417	.20588	.41004	28	.22170	.25600
16	140	29	.98678	.56972	44	.35018	.52547	.20230	.20217	.40447	30	.21774	.25143
18	176	36	.97251	.56148	53	.34314	.51849	.20030	.19811	.39840	37	.21339	.24641
20	200	41	.96652	.55802	59	.34016	.51560	.19947	.19639	.39586	41	.21156	.24429
22	224	45	.98024	.56594	66	.34693	.52231	.20139	.20030	.40169	47	.21574	.24911
24	248	49	.98499	.56869	73	.34928	.52463	.20205	.20166	.40371	52	.21719	.25079
26	320	58	.98009	.56585	87	.34685	.52224	.20136	.20025	.40162	62	.21569	.24906

The final expansions for c and d in rapidly convergent form (method of Ewald) are

$$c=-8\pi\sum A_{nc}n^{-1}x^n+128\pi\epsilon^3\sum B_{nc}n^{-1}y^n+768\epsilon\sum B_{nc}n^{-2}y^n+768\sum B_{nc}n^{-\frac{5}{2}}[1-\phi(2^{-1}\pi^{\frac{1}{2}}n^{-\frac{1}{2}}\epsilon)]$$
$$-32\epsilon\sum C_{nc}n^{-1}y^n-32\sum C_{nc}n^{-\frac{3}{2}}[1-\phi(2^{-1}\pi^{\frac{1}{2}}n^{-\frac{1}{2}}\epsilon)], \quad (25)$$

$$d=8\pi\sum A_{nd}n^{-1}x^n+8\pi\epsilon^3\sum B_{nd}n^{-1}y^n+48\epsilon\sum B_{nd}n^{-2}y^n+48\sum B_{nd}n^{-\frac{5}{2}}[1-\phi(2^{-1}\pi^{\frac{1}{2}}n^{-\frac{1}{2}}\epsilon)]$$
$$-16\epsilon\sum C_{nd}n^{-1}y^n-16\sum C_{nd}n^{-\frac{3}{2}}[1-\phi(2^{-1}\pi^{\frac{1}{2}}n^{-\frac{1}{2}}\epsilon)]. \quad (26)$$

TABLE V. *Conditions: Array (I).*

$p_1p_2p_3$	$s_1s_2s_3\times(10)^3$	$\Sigma(h_i-4\pi Np_i/3)$*
$\frac{1}{3^{\frac{1}{2}}}\frac{1}{3^{\frac{1}{2}}}\frac{1}{3^{\frac{1}{2}}}$	55 55 55	+0.4332
	$\overline{55}$ 55 55	−0.1444
	55 $\overline{55}$ 55	−0.1444
	55 55 $\overline{55}$	−0.1444
	$\overline{55}$ $\overline{55}$ 55	−0.1444
	$\overline{55}$ 55 $\overline{55}$	−0.1444
	55 $\overline{55}$ $\overline{55}$	−0.1444
	$\overline{55}$ $\overline{55}$ $\overline{55}$	+0.4332
	Mean value	0

* This is here proportional to the excess negative potential energy of a dipole of moment p at the designated point over its negative potential energy when at the origin.

In these expansions $x=\exp(-\pi/\epsilon^2)$, $y=\exp(-\pi\epsilon^2/4)$, ϵ and $\phi(\alpha)$ have already been defined and the coefficients A_{nc}, etc., except as given in Table VI, have the value zero for all values of n.

The results, checked as usual for two values of ϵ ($2^{\frac{1}{2}}$ and $6^{\frac{1}{2}}/2$) are

$$c=-4.47894, \quad d=34.2708,$$

correct to one digit in the last figure in each. Bouman's value for $d/2$ is 17.14 which is correct as far as it goes. His value for $c/2$ is -2.20 which is not so satisfactory, but the change does not vitiate his qualitative conclusions.

TABLE VI. *Coefficients for Bouman's series.*

Note: For values of n not given the coefficient is zero.

n	A_{nc}	A_{nd}	n	B_{nc}	n	B_{nd}	n	C_{nc}	n	C_{nd}
1	1	1	6	1	1	1	2	1	1	1
2	−4	4	14	2	5	4	6	2	5	4
3	4	4	18	4	9	13	10	2	9	5
4	4	−4	22	1	13	36	14	4	13	4
5	−12	−12	26	8	17	40	18	3	17	8
6	8	−8	30	2	21	8	22	2	21	8
8	16	−16	34	4	25	61	26	6	25	5
9	−19	−19	38	11	29	172	30	4	29	12
10	−40	40	42	8	33	104	34	4	33	8
11	44	44	46	18	37	4	38	6	37	4
12	16	−16	50	8	41	144	42	4	41	16
13	20	20	54	12	45	236	46	4	45	12
14	−48	48	62	20	49	121	50	7	49	9
16	16	−16	66	28	53	204	54	8	53	12
17	−56	−56	70	18	57	296	58	2	57	8
18	20	−20	74	40	61	172	62	8	61	12
19	76	76	78	2	65	400	66	8	65	16
20	80	−80	82	16	69	392	70	4	69	16
21	−152	−152	86	29	73	40	74	10	73	8
22	−56	56	90	40	77	272	78	4	77	16
24	96	−96	94	20	81	321	82	4	81	17
25	−3	−3	98	40	85	520	86	10	85	8
					89	888	90	10	89	24
					93	200	94	8	93	8
					97	424	98	9	97	8