The $z$ components (parallel with the particle track) are

$$E_{tz} = \frac{\partial}{\partial z}\left\{ +\Phi(r) - \frac{Z_1 e}{\gamma} \frac{\exp[-\Omega(\rho^2+\gamma^2 z^2)^{\frac{1}{2}}/V]}{(\rho^2+\gamma^2 z^2)} \right\}$$

$$- Z_1 e \frac{\Omega^2}{V^2} \frac{z}{|z|} \int_{\gamma|z|}^{\infty} dx \frac{\exp[-\Omega(\rho^2+x^2)^{\frac{1}{2}}/V]}{(\rho^2+x^2)^{\frac{1}{2}}},$$

$$+ (E_{tz})_{\text{Čerenkov}} \quad \text{(A-7)}$$

$$E_{lz} = -\frac{\partial}{\partial z}\Phi(r). \quad \text{(A-8)}$$

The additional term in the expression for $E_t$ corresponds to the existence of the Čerenkov wake behind the particle ($z<0$). Assuming for simplicity that only one of the resonances at $\omega=\omega_1$ is important in the expression for dielectric constant, we find that

$$(\mathbf{E}_t)_{\text{Čerenkov}} = \frac{2Z_1 e \omega_1^3}{\Omega(\Omega^2+\omega_1^2)} \boldsymbol{\nabla}(\omega_1 z^2/\Omega^2 - \rho^2)^{-\frac{1}{2}}$$

$$\text{if} \quad \omega_1 z/\Omega < -\rho, \quad \text{(A-9)}$$

and

$$(\mathbf{E}_t)_{\text{Čerenkov}} = 0 \quad \text{if} \quad \omega_1 z/\Omega > -\rho. \quad \text{(A-10)}$$

These expressions are approximately valid as long as the field point is located sufficiently far from the surface of the cone $z=-\Omega\rho/\omega_1$. The apparent singularity on this cone does not exist but arises from the approximation to the more exact expression for $(\mathbf{E}_t)_{\text{Čerenkov}}$. It is to be noted that the angle of opening of the cone in the expression for $E_t$ is

$$\vartheta = \tan^{-1}(\omega_1/\Omega). \quad \text{(A-11)}$$

The third term in (A-7) for $E_{tz}$, i.e.,

$$(E_{tz})_3 = Z_1 e \frac{\Omega^2}{V^2} \frac{z}{|z|} \int_{\gamma|z|}^{\infty} dx \frac{\exp[-\Omega(\rho^2+x^2)^{\frac{1}{2}}/V]}{(\rho^2+x^2)^{\frac{1}{2}}} \quad \text{(A-12)}$$

is of some interest and does not appear to have been noted before. This portion of the field is independent of the resonant frequency $\omega_1$, but goes to zero for very low medium density. Exactly the same term arises in the transverse field expressions for a particle passing through a plasma.[7] This term is antisymmetric in the $z$ coordinate and possesses a discontinuity at $z=0$. It arises from the Lorentz-contracted field of the line polarization charge which exists behind the incident particle.

[7] J. Neufeld and R. H. Ritchie, Phys. Rev. **98**, 1632 (1955).

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# Dipolar Sums in the Primitive Cubic Lattices

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Dipole-wave sums, important in many magnetic and electric problems involving dipole-dipole interactions, are defined, and numerical values are given at sets of independent points in **k**-space equivalent to a 512-fold sampling of the first Brillouin zone of each of the three primitive cubic lattices. Strong size, shape, and position dependence of these sums is shown to occur in a pathological region about the origin in **k**-space. The dipole-wave sums are shown to be related to dipole-field factors at points within the unit cell. The dipolar anisotropy energy in the antiferromagnet MnO is discussed as an illustration of the use of dipole-wave sums.

## I. INTRODUCTION

WE introduce the lattice sums

$$S_n(\mathbf{k}) = \rho^{-1} \sum_l{}' |\mathbf{r}_l|^{-n} \exp(i\mathbf{k}\cdot\mathbf{r}_l); \quad \text{(1a)}$$

$$S_n{}^{ij}(\mathbf{k}) = \rho^{-1} \sum_l{}' r_l{}^i r_l{}^j |\mathbf{r}_l|^{-n} \exp(i\mathbf{k}\cdot\mathbf{r}_l). \quad \text{(1b)}$$

Here $i, j = x, y, z$; the primed sum is to be taken over all lattice vectors $\mathbf{r}_l$ except $\mathbf{r}_l = 0$; and $\rho$ is the number of lattice points per unit volume.

Specifically, we shall be interested in $S_3(\mathbf{k})$ and $S_5{}^{ij}(\mathbf{k})$, which we shall call *dipole-wave sums*. Our interest in these sums arises from their importance in

many magnetic problems involving dipole-dipole interactions. In particular, we have made extensive use of dipole-wave sums in the quantum-mechanical problem of dipolar ferromagnetism.[1] Furthermore, these sums find use in the calculation of dipole-field factors (see Secs. VI, VII, and VIII) and of exciton energies.[2] They are important in the considerations of lattice stability of polar crystals that arise, for example, in connection with ferroelectrics and antiferroelectrics.

[1] M. H. Cohen and F. Keffer, Phys. Rev. **94**, 1412 (1954), and following paper [Phys. Rev. **99**, 1135 (1955)].
[2] W. R. Heller and A. Marcus, Phys. Rev. **84**, 809 (1951).

TABLE I. The choice of the unit of distance $a$ for each lattice is made clear by the specification of the primitive lattice vectors in the table.

| Direct lattice type | Direct lattice vectors | | | Reciprocal lattice vectors | | | $\rho a^3$ | $\tau a^2$ |
|---|---|---|---|---|---|---|---|---|
| | $\mathbf{r}_1/a$ | $\mathbf{r}_2/a$ | $\mathbf{r}_3/a$ | $\mathbf{b}_1 a$ | $\mathbf{b}_2 a$ | $\mathbf{b}_3 a$ | | |
| Simple cubic (sc) | 1,0,0 | 0,1,0 | 0,0,1 | 1,0,0 | 0,1,0 | 0,0,1 | 1 | $\frac{1}{2}$ |
| Face-centered cubic (fcc) | 0,1,1 | 1,0,1 | 1,1,0 | $\bar{\frac{1}{2}},\frac{1}{2},\frac{1}{2}$ | $\frac{1}{2},\bar{\frac{1}{2}},\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},\bar{\frac{1}{2}}$ | $\frac{1}{2}$ | $\frac{1}{4}$ |
| Body-centered cubic (bcc) | $\bar{1},1,1$ | $1,\bar{1},1$ | $1,1,\bar{1}$ | $0,\frac{1}{2},\frac{1}{2}$ | $\frac{1}{2},0,\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},0$ | $\frac{1}{4}$ | $\frac{1}{4}$ |

## II. METHOD OF OBTAINING DIPOLE-WAVE SUMS

### A. Calculation of $S_n(\mathbf{k})$

Our notation conforms, in the main, to that introduced by Born and his students.[3-5] Some slight changes have been made, however, to suit our special purposes.

The most generally useful method of evaluating slowly convergent lattice sums is due to Ewald.[6] This method uses generalized theta functions and their transformation formula, and is most elegantly expounded by Born and Bradburn.[5] In particular, these authors show that for an infinite lattice [see their Eq. (4.7)]:

$$S_n(\mathbf{k}) = \rho^{-1}[(\pi\tau)^{\frac{1}{2}n}/\Gamma(\tfrac{1}{2}n)][S_A + S_B - (2/n)], \quad (2)$$

with

$$S_A = \sum_l{}'[\exp(i\mathbf{k}\cdot\mathbf{r}_l)\varphi_{\frac{1}{2}n-1}(\tau r_l{}^2\pi)],$$
$$S_B = \rho\tau^{-\frac{3}{2}}\sum_l\varphi_{\frac{1}{2}-\frac{1}{2}n}[(2\pi\mathbf{b}_l - \mathbf{k})^2/4\pi\tau].$$

In this expression $S_A$ is summed over the direct lattice, $\mathbf{r}_l$; $S_B$ is summed over the reciprocal lattice, $\mathbf{b}_l$. The sum $S_n(\mathbf{k})$ is independent of the choice of Ewald's parameter $\tau$, the idea being to choose this parameter for equally rapid convergence in the sums over the direct and the reciprocal lattices. The $\varphi$ functions (introduced by Misra[3]) are defined by

$$\varphi_m(x) = \int_1^\infty \beta^m e^{-\beta x} d\beta. \quad (3a)$$

These functions satisfy the recurrence formula

$$\varphi_m(x) = \varphi_0(x) + (m/x)\varphi_{m-1}(x); \quad (3b)$$

and, in particular,

$$\varphi_0(x) = e^{-x}/x,$$
$$\varphi_{-1}(x) = -\mathrm{Ei}(-x),$$
$$\varphi_{-\frac{1}{2}}(x) = (\pi/x)^{\frac{1}{2}}[1 - \Phi(x^{\frac{1}{2}})].$$

Here $\mathrm{Ei}(-x)$ is the exponential integral, and $\Phi(x)$ is Gauss' error function.

Table I shows a set of lattice vectors and other parameters for the three primitive cubic lattices, expressed in terms of convenient units of distance.

[3] R. D. Misra, Proc. Cambridge Phil. Soc. **36**, 173 (1940).
[4] M. Born and M. Bradburn, Proc. Cambridge Phil. Soc. **39**, 104 (1943).
[5] M. Bradburn, Proc. Cambridge Phil. Soc. **39**, 113 (1943).
[6] P. P. Ewald, Ann. Physik **64**, 253 (1921).

### B. Calculation of $S_5{}^{ij}(\mathbf{k})$

We note that

$$S_n{}^{ij}(\mathbf{k}) = \frac{\partial}{\partial k^i}\frac{\partial}{\partial k^j}S_n(\mathbf{k}). \quad (4)$$

Using $S_5(\mathbf{k})$ as given by Eq. (2), we readily obtain $S_5{}^{ij}(\mathbf{k})$ from Eq. (4). In taking derivatives we observe that

$$\frac{\partial}{\partial x}\varphi_m(x) = -\varphi_{m+1}(x).$$

The result is

$$S_5{}^{ij}(\mathbf{k}) = \rho^{-1}[(\pi\tau)^{5/2}/\Gamma(5/2)][S_C + S_D + \delta^{ij}S_E], \quad (5)$$

with

$$S_C = \sum_l{}'[r_l{}^i r_l{}^j \exp(i\mathbf{k}\cdot\mathbf{r}_l)\varphi_{\frac{3}{2}}(\tau r_l{}^2\pi)],$$
$$S_D = -(\rho/4\pi^2\tau^{7/2})\sum_l[(2\pi b_l{}^i - k^i)(2\pi b_l{}^j - k^j)$$
$$\times \varphi_0\{(2\pi\mathbf{b}_l - \mathbf{k})^2/4\pi\tau\}],$$
$$S_E = (\rho/2\pi\tau^{5/2})\sum_l\varphi_{-1}\{(2\pi\mathbf{b}_l - \mathbf{k})^2/4\pi\tau\}.$$

## III. SELECTING A SAMPLE OF k-SPACE

The dipole-wave sums will be of use in numerical integrations (summations) over $\mathbf{k}$-space; hence the values of $\mathbf{k}$ for which sums are calculated must be chosen with care.

Since the sums are taken over all direct lattice points, their values will repeat in the various Brillouin zones (BZ) of $\mathbf{k}$-space. Thus, we need consider only the first zone. Furthermore, within this zone there will be considerable repetition of values due to cubic symmetry.

The choice of the $\mathbf{k}$ sampling is detailed below for the three cubic lattices.

### A. Simple Cubic

If we define integers $q^i (i = x, y, z)$ by the relation

$$8k^i = (2\pi/a)q^i, \quad (\text{sc}) \quad (6)$$

we go from boundary to boundary of the first BZ on allowing $q^i$ to vary from $-4$ to $+4$. Our sampling of $\mathbf{k}$-space thus consists of the 512 number triples $(q^x, q^y, q^z)$, properly weighted at surfaces, edges, and corners of the BZ as discussed in Sec. IV. We need not evaluate 512 different sums, however, because of the following types of relationships imposed by cubic symmetry:

(1) Reflections, such as

$$S_3(l,m,n) = S_3(-l,m,n),$$
$$S_5{}^{xy}(l,m,n) = -S_5{}^{xy}(-l,m,n), \quad (7)$$
$$S_5{}^{xx}(l,m,n) = S_5{}^{xx}(-l,m,n).$$

(2) Permutations, such as

$$S_3(l,m,n) = S_3(m,l,n),$$
$$S_5{}^{xy}(l,m,n) = S_5{}^{yx}(m,l,n). \quad (8)$$

Thus we need evaluate sums for only the 35 points given by

$$4 \geq q^x \geq q^y \geq q^z \geq 0. \quad \text{(sc)} \quad (9)$$

### B. Face-Centered Cubic

Here we define integers $q^i$ by the relation

$$16k^i = (2\pi/a)q^i, \quad \text{(fcc)} \quad (10)$$

with $q^i$ varying from $-8$ to $+8$.

Again the symmetry relationships of Eqs. (7) and (8) reduce the number of points we need consider.

The first BZ is now to be pictured in the reciprocal bcc lattice. If we stretch this reciprocal lattice by the scale factor $2\pi$, the first BZ is then a Wigner-Seitz unit cell of a bcc. In order to stay inside this zone we must further restrict ourselves to points such that $q^x + q^y + q^z \leq 12$. This may also be seen from consideration of inversion symmetry and the fact that in our bcc the point $(8+l, 8+m, 8+n)$ is equivalent to $(l,m,n)$.

Furthermore, since the reciprocal lattice is a bcc we must sample it with a bcc-like array of points; this restricts us to $q^x, q^y, q^z$ all odd or all even.

Thus we need evaluate sums for only the 30 points given by

$$8 \geq q^x \geq q^y \geq q^z \geq 0,$$
$$q^x + q^y + q^z \leq 12, \quad \text{(fcc)} \quad (11)$$
$$q^x, q^y, q^z \text{ all odd or all even.}$$

The equivalence of the boundary points (8,2,2) and (6,6,0) further reduces us to 29 points.

### C. Body-Centered Cubic

This is somewhat similar to the fcc. We define integers $q^i$ by

$$16k^i = (2\pi/a)q^i. \quad \text{(bcc)} \quad (12)$$

The first BZ is now a Wigner-Seitz unit cell of an fcc lattice. We fill this with an fcc-like array of points, and need evaluate sums for only the 29 points given by

$$8 \geq q^x \geq q^y \geq q^z \geq 0,$$
$$q^x + q^y \leq 8, \quad \text{(bcc)} \quad (13)$$
$$q^x + q^y + q^z \text{ even.}$$

### IV. NUMERICAL INTEGRATION IN k-SPACE

In applications of our work, sums like

$$\sum_{k'} f(k') = N\bar{f} \quad (14)$$

occur.[1] The summation is carried out over the $N$ values of $k'$ inside the first BZ which satisfy appropriate boundary conditions. Since $f(k')$ is known only at certain points $k$, the actual average, $\bar{f}$, must be replaced by an approximate average, $\langle f \rangle$, obtained by numerical integration.

The $k$'s chosen in III reproduce the reciprocal lattice (times $2\pi$) on a scale 8 times smaller. Each $k$ may, therefore, be thought to lie at the center of a cell geometrically similar to, but 512 times smaller than, the first BZ. We then replace the average value of $f$ in a small cell by the value of $f$ at the center in performing the numerical integration. Cells at faces, edges, and corners of the first BZ do not lie entirely within it and must be assigned fractional weights, $W_k$. Thus,

$$\langle f \rangle = (512)^{-1} \sum_k f(k) W_k. \quad (15)$$

The summation in (15) should, of course, be performed first over those $k$'s for which $f(k)$ is the same, in particular for $k$'s connected by $2\pi$ times a reciprocal lattice vector.

A list of face, edge, and corner points and their weights is given in Table II. All points related by a permutation or reflection have the same weight.

### V. BEHAVIOR NEAR k = 0

It turns out that the sums $S_3(k)$ and $S_5{}^{ij}(k)$ for both finite and infinite lattices are rapidly varying functions of $k$ in the vicinity of the point $k = 0$. We study the small $k$ behavior in this section because of its importance in specific applications, e.g., in ferromagnetic resonance, and in obtaining representative values for numerical integrations.

### A. Infinite Lattice

To avoid divergences we form the combination

$$D^{ij}(k) = 3S_5{}^{ij}(k) - S_3(k)\delta^{ij}. \quad (16)$$

We note that $D^{ij}(0)$ is the conventional dipole-field factor for lattice points. Direct evaluation yields

$$D^{ij}(0) = 0. \quad (17)$$

On the other hand, an expression for $D^{ij}(k)$ valid in the limit of small $k$ may be obtained by manipulation of Eqs. (2) and (5),

$$D^{ij}(k) = 4\pi^2 \rho^{-1} \tau^{5/2} \{S_C + S_D + (2\pi\tau)^{-1}(\tfrac{2}{3} - S_A)\delta^{ij}\};$$

$$\lim_{k \to 0} S_A(k) = \sum' \varphi_{\frac{1}{2}}(\pi r_l^2 \tau);$$

$$\lim_{k \to 0} S_C(k) = \tfrac{1}{3}\delta^{ij} \sum' r_l^2 \varphi_{\frac{3}{2}}(\pi r_l^2 \tau);$$

$$\lim_{k \to 0} S_D(k) = -\tfrac{1}{3}\rho\delta^{ij}\tau^{-7/2} \sum' b_l^2 \varphi_0(\pi b_l^2 \tau)$$

$$- (\rho/4\pi^2\tau^{7/2})k^i k^j \varphi_0(k^2/4\pi\tau).$$

Putting these together, using the recurrence formula (3b) for the $\varphi$'s, and using Poisson's summation for-

mula,[7] one obtains

$$\lim_{\mathbf{k}\to 0} D^{ij}(\mathbf{k}) = \rho(4\pi/3)[\delta^{ij} - 3(k^i k^j/k^2)]. \quad (18)$$

Equation (18) is structure-independent and in fact could have been obtained by replacing the sum by an integral and surrounding the origin by a sphere of exclusion.[8] Comparing Eq. (17) and Eq. (18) we see that $D^{ij}(\mathbf{k})$ is only piecewise continuous at $\mathbf{k}=0$ and that the average of $D^{ij}(\mathbf{k})$ in the neighborhood of $\mathbf{k}=0$ is equal to $D^{ij}(0)$.

Now the original definition of $D^{ij}(\mathbf{k})$,

$$D^{ij}(\mathbf{k}) = \rho^{-1} \sum_l{}'(3r_l^i r_l^j - r_l^2 \delta^{ij}) r_l^{-5} \exp(i\mathbf{k}\cdot\mathbf{r}_l), \quad (19)$$

is in fact the explicit Fourier series for $D^{ij}(\mathbf{k})$ which is periodic in $\mathbf{k}$. We might therefore expect that a study of the convergence of Eq. (19) near $\mathbf{k}=0$ would throw some light on its piecewise continuity. Accordingly we turn to a discussion of $D^{ij}(\mathbf{k})$ in finite lattices.

## B. Pathological Behavior Near $k=0$ in Finite Lattices

In finite lattices the $D^{ij}(\mathbf{k})$ are not as directly useful at very small $\mathbf{k}$ as are other dipolar sums more directly related to the geometry of the sample. For example, for a long thin cylinder the plane-wave factor in the sum can be replaced by a cylindrical wave. Nevertheless, certain difficulties in the behavior of dipole-wave sums near small $\mathbf{k}$ occur for all types of waves. To illustrate these difficulties we now calculate $D^{ij}(\mathbf{k})$ for a finite lattice of given shape, chosen spherical for convenience. The finite sum is related to the infinite sum by

$$\sum_V = \sum_\infty - \sum_{\infty-V}. \quad (20)$$

The sum $\sum_{\infty-V}$ may be converted into an integral for small $\mathbf{k}$ and large volume $V$. Hence for a sphere of radius $R$, taking the origin of the sum in the center of the sphere,

$$D^{ij}(\mathbf{k}) = \frac{4\pi}{3}\left(\delta^{ij} - \frac{3k^i k^j}{k^2}\right)$$
$$- \int_R^\infty \frac{3r^i r^j - r^2}{r^5}\exp(i\mathbf{k}\cdot\mathbf{r})d^3r. \quad (21)$$

The integral is easily evaluated and leads to

$$D^{ij}(\mathbf{k}) = \frac{4\pi}{3}\left(\delta^{ij} - \frac{3k^i k^j}{k^2}\right)\left[1 - \frac{3j_1(kR)}{kR}\right], \quad (22)$$

which goes to zero as $k \to 0$. Thus, as it must, the discontinuity disappears for the finite lattice. It becomes instead a rapid variation of $D^{ij}(\mathbf{k})$ near $\mathbf{k}=0$, a fact

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[7] In our particular case this is the theta-function transformation

$$\tau^{\frac{3}{2}}\sum_l \exp(-\pi r_l^2 \tau) = \rho \sum_l \exp(-\pi b_l^2/\tau).$$

See reference 5 or 6.

[8] See T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).

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TABLE II. Weights of face, edge, and corner points.

| sc | | fcc | | bcc | |
|---|---|---|---|---|---|
| $q$ | $W_q$ | $q$ | $W_q$ | $q$ | $W_q$ |
| $4q_y q_z$ | $\frac{1}{2}$ | 444 | $\frac{1}{2}$ | 440 | $\frac{1}{2}$ |
| $44q_z$ | $\frac{1}{4}$ | 642 | $\frac{1}{2}$ | 442 | $\frac{1}{2}$ |
| 444 | $\frac{1}{8}$ | 800 | $\frac{1}{2}$ | 530 | $\frac{1}{2}$ |
| | | 820 | $\frac{1}{2}$ | 532 | $\frac{1}{2}$ |
| | | 660 | $\frac{1}{2}$ | 620 | $\frac{1}{2}$ |
| | | 822 | $\frac{1}{3}$ | 710 | $\frac{1}{2}$ |
| | | 840 | $\frac{1}{4}$ | 622 | $\frac{1}{3}$ |
| | | | | 444 | $\frac{1}{4}$ |
| | | | | 800 | $\frac{1}{6}$ |

which must be recognized in physical applications of the $D^{ij}(\mathbf{k})$.

One sees from Eq. (22) that the finite sum differs from the infinite sum only for $\mathbf{k}$'s such that $kR \leq 10$. Since the separation $\Delta\mathbf{k}$ between $\mathbf{k}$'s in the numerical integration is such that $\Delta ka \sim 1$, where $a=$ lattice constant, this difference between the finite and the infinite sums is appreciable only over an extremely small region of the cell about $\mathbf{k}=0$. We shall call this region the *pathological region*.

Further, the value for the finite lattice, $D^{ij}(0)=0$ for a sphere, represents very poorly the region about $\mathbf{k}=0$ in the numerical integration, a consequence of the rapid variation of $D^{ij}(\mathbf{k})$ near $\mathbf{k}=0$. A more representative value would be obtained by using Eq. (18) alone or together with the next terms in an expansion in powers of $\mathbf{k}$ of $D^{ij}(\mathbf{k})$ for an *infinite* lattice and averaging over a sphere approximating the $\mathbf{k}=0$ cell. An accurate value is not important since there are 512 cells in the numerical integration, with inaccuracy only at $\mathbf{k}=0$.

The difference between the infinite and finite sums, $G^{ij}(\mathbf{k})$, is proportional to $j_1(kR)/kR$. Let $\epsilon$ be a small positive number. Then if Eq. (19) is uniformly convergent for all $\mathbf{k}$, it is possible to find a value of $R$ such that for all radii greater than $R$, $|G^{ij}(\mathbf{k})| < \epsilon$ for all $\mathbf{k}$. But if we include the point $\mathbf{k}=0$ in the region of variability of $\mathbf{k}$, then for $k \ll 1/R$, $|G^{ij}(k)| \sim 1$ for radii $\gg R$. Thus the Fourier series (19) for $D^{ij}(\mathbf{k})$ in an infinite lattice is not uniformly convergent near $\mathbf{k}=0$. Hence $D^{ij}(\mathbf{k})$ cannot be a uniformly continuous function of $\mathbf{k}$. Since the Fourier series exists, the function must be piecewise continuous, a conclusion in accord with the results of the previous section.

Let us repeat for emphasis that the above considerations hold in detail only when the origin of the sum is at the center of the sphere. A similar treatment of the case when the origin of the sum lies at an arbitrary point within the sphere yields the result that the dipole-wave sums show a strong *position dependence* when $kR \leq 10$.

The dipole-wave sums rapidly become independent of origin as $kR$ increases beyond 10. In the special case of $k=0$ the dipole-wave sums are completely independent of origin (except for origins in the layer immediately next the surface).

TABLE III. Structure-dependent terms.

|  | fcc | bcc |
|---|---|---|
| $\alpha$ | 4.004 | 4.124 |
| $\beta$ | 1.237 | 0.849 |
| $\gamma^{xxxx}$ | −4.288 | −3.487 |
| $\gamma^{xxyy}$ | −1.710 | −1.591 |

Although all considerations have been made explicitly for a sphere, similar results have been obtained for an infinite cylinder and for an infinite flat plate. We expect, therefore, that such behavior occurs for all shapes.

To sum up, we find that $D^{ij}(\mathbf{k})$ is not a uniformly convergent series and has an associated discontinuity at $\mathbf{k}=0$ in the function it represents for an infinite lattice. A strong size, shape, and position dependence of the finite sum occurs for a very small region near $\mathbf{k}=0$. Finally, the *infinite* sum, appropriately weighted, may always be used in numerical integration over all $\mathbf{k}$-space, even for finite lattices.

## C. Infinite Lattice, Structure Dependent Terms

In Sec. IV $\mathbf{k}$-space was divided into 512 cells for purposes of numerical integration, and the value of the dipole-wave sum at the center of each cell was used to approximate its average value over the cell. In Sec. V.B it was shown that finite-lattice behavior extends over a negligible region of the cell surrounding the origin, and it becomes necessary to consider the infinite lattice behavior in the central cell in more detail in order to find representative values for numerical integration. To do this we carry the expansion of the infinite sums further than in Sec. VA by including terms of order $k^2$. The terms of order $k^2$ to be added to Eq. (18) are

$$k^2 a^2\left[\alpha\frac{k^i k^j}{k^2}+\beta\delta^{ij}+\gamma^{ijmn}\frac{k^m k^n}{k^2}\right], \qquad (18')$$

where

$\alpha = \tau^{-1}\{1+\tfrac{1}{3}\sum_l'\varphi_0(\pi b_l^2/\tau)[1+(4\pi b_l^2/\tau)]\}$ ;

$\beta = (\pi\tau^{\frac{3}{2}}/3\rho)\sum_l' r_l^2\varphi_{\frac{1}{2}}(\pi\tau r_l^2)$
$\qquad + (1/3\tau)\sum_l'\varphi_0(\pi b_l^2/\tau)[1+(\pi b_l^2/\tau)]$ ;

$\gamma^{ijmn} = -(2\pi^2\tau^{5/2}/\rho)\sum_l' r_l^i r_l^j r_l^m r_l^n \varphi_{\frac{3}{2}}(\pi\tau r_l^2)$
$\qquad - (4/\tau)\sum_l'\varphi_0(\pi b_l^2/\tau)b_l^i b_l^j b_l^m b_l^n$
$\qquad\qquad \times[b_l^{-4}+(\pi^2/2\tau^2)+(\pi/\tau b_l^2)]$.

We have evaluated $\alpha, \beta$, and the independent non-zero values of $\gamma^{ijmn}$ for the fcc and bcc. These are given in Table III.

## VI. TABULATIONS AND CHECKS

The calculated values of $S_3(\mathbf{k})$ and $S_5^{ij}(\mathbf{k})$ for our samplings of $\mathbf{k}$-space are given in Tables IV, V, and VI. The representative integers $q^i$ are defined in Eqs. (6), (10), and (12).

TABLE IV. Simple cube.

| $q^x q^y q^z$ | $S_3$ | $S_5{}^{xx}$ | $S_5{}^{yy}$ | $S_5{}^{zz}$ | $S_5{}^{xy}$ | $S_5{}^{xz}$ | $S_5{}^{yz}$ |
|---|---|---|---|---|---|---|---|
| 100 | 12.465 | 1.298 | 5.584 | 5.584 | 0 | 0 | 0 |
| 110 | 8.391 | 2.067 | 2.067 | 4.257 | −1.838 | 0 | 0 |
| 111 | 6.111 | 2.037 | 2.037 | 2.037 | −1.151 | −1.151 | −1.151 |
| 200 | 4.678 | −1.452 | 3.065 | 3.065 | 0 | 0 | 0 |
| 210 | 3.514 | −0.962 | 1.771 | 2.706 | −1.178 | 0 | 0 |
| 211 | 2.597 | −0.671 | 1.634 | 1.634 | −0.920 | −0.920 | −0.485 |
| 220 | 1.315 | −0.363 | −0.363 | 2.042 | −1.153 | 0 | 0 |
| 221 | 0.772 | −0.276 | −0.276 | 1.325 | −0.960 | −0.514 | −0.514 |
| 222 | −0.405 | −0.135 | −0.135 | −0.135 | −0.602 | −0.602 | −0.602 |
| 300 | 1.247 | −2.750 | 1.998 | 1.998 | 0 | 0 | 0 |
| 310 | 0.745 | −2.428 | 1.317 | 1.857 | −0.528 | 0 | 0 |
| 311 | 0.303 | −2.170 | 1.236 | 1.236 | −0.446 | −0.446 | −0.220 |
| 320 | −0.363 | −1.799 | −0.114 | 1.551 | −0.613 | 0 | 0 |
| 321 | −0.688 | −1.649 | −0.093 | 1.055 | −0.530 | −0.289 | −0.274 |
| 323 | −1.434 | −1.328 | −0.053 | −0.053 | −0.361 | −0.361 | −0.351 |
| 330 | −1.354 | −1.318 | −1.318 | 1.283 | −0.363 | 0 | 0 |
| 331 | −1.587 | −1.237 | −1.237 | 0.888 | −0.320 | −0.172 | −0.172 |
| 332 | −2.135 | −1.055 | −1.055 | −0.025 | −0.227 | −0.226 | −0.226 |
| 333 | −2.664 | −0.888 | −0.888 | −0.888 | −0.149 | −0.149 | −0.149 |
| 400 | 0.222 | −3.155 | 1.689 | 1.689 | 0 | 0 | 0 |
| 410 | −0.134 | −2.879 | 1.150 | 1.595 | 0 | 0 | 0 |
| 411 | −0.461 | −2.642 | 1.091 | 1.091 | 0 | 0 | −0.153 |
| 420 | −0.959 | −2.282 | −0.057 | 1.380 | 0 | 0 | 0 |
| 421 | −1.218 | −2.123 | −0.048 | 0.954 | 0 | 0 | −0.201 |
| 422 | −1.827 | −1.766 | −0.030 | −0.030 | 0 | 0 | −0.268 |
| 430 | −1.737 | −1.767 | −1.150 | 1.181 | 0 | 0 | 0 |
| 431 | −1.937 | −1.669 | −1.091 | 0.823 | 0 | 0 | −0.133 |
| 432 | −2.413 | −1.443 | −0.953 | −0.016 | 0 | 0 | −0.179 |
| 433 | −2.878 | −1.232 | −0.823 | −0.823 | 0 | 0 | −0.121 |
| 440 | −2.046 | −1.574 | −1.574 | 1.102 | 0 | 0 | 0 |
| 441 | −2.224 | −1.498 | −1.498 | 0.771 | 0 | 0 | 0 |
| 442 | −2.649 | −1.319 | −1.319 | −0.011 | 0 | 0 | 0 |
| 443 | −3.067 | −1.148 | −1.148 | −0.771 | 0 | 0 | 0 |
| 444 | −3.239 | −1.080 | −1.080 | −1.080 | 0 | 0 | 0 |

TABLE V. Face-centered cube.

| $q^x q^y q^z$ | $S_3$ | $S_5^{xx}$ | $S_5^{yy}$ | $S_5^{zz}$ | $S_5^{xy}$ | $S_5^{xz}$ | $S_5^{yz}$ |
|---|---|---|---|---|---|---|---|
| 111 | 11.093 | 3.698 | 3.698 | 3.698 | −1.368 | −1.368 | −1.368 |
| 200 | 9.398 | 0.527 | 4.435 | 4.435 | 0 | 0 | 0 |
| 220 | 5.513 | 1.244 | 1.244 | 3.025 | −1.958 | 0 | 0 |
| 222 | 3.447 | 1.149 | 1.149 | 1.149 | −1.300 | −1.300 | −1.300 |
| 311 | 3.851 | −0.384 | 2.118 | 2.118 | −1.043 | −1.043 | −0.373 |
| 331 | 1.355 | 0.087 | 0.087 | 1.182 | −1.662 | −0.619 | −0.619 |
| 333 | 0.157 | 0.052 | 0.052 | 0.052 | −1.233 | −1.233 | −1.233 |
| 400 | 2.029 | −1.463 | 1.746 | 1.746 | 0 | 0 | 0 |
| 420 | 1.101 | −0.979 | 0.818 | 1.262 | −1.357 | 0 | 0 |
| 422 | 0.462 | −0.697 | 0.579 | 0.579 | −1.147 | −1.147 | −0.712 |
| 440 | −0.512 | −0.394 | −0.394 | 0.276 | −1.422 | 0 | 0 |
| 442 | −0.662 | −0.330 | −0.330 | −0.003 | −1.311 | −0.876 | −0.876 |
| 444 | −0.810 | −0.270 | −0.270 | −0.270 | −1.205 | −1.205 | −1.205 |
| 511 | −0.060 | −1.595 | 0.767 | 0.767 | −0.562 | −0.562 | −0.182 |
| 531 | −0.755 | −0.981 | 0.052 | 0.174 | −1.161 | −0.459 | −0.414 |
| 533 | −0.940 | −0.592 | −0.174 | −0.174 | −1.040 | −1.040 | −0.996 |
| 551 | −1.432 | −0.395 | −0.395 | −0.642 | −0.980 | −0.402 | −0.402 |
| 600 | −0.978 | −1.979 | 0.501 | 0.501 | 0 | 0 | 0 |
| 620 | −1.192 | −1.605 | 0.226 | 0.188 | −0.661 | 0 | 0 |
| 622 | −1.284 | −1.282 | −0.001 | −0.001 | −0.619 | −0.619 | −0.540 |
| 640 | −1.581 | −0.846 | −0.162 | −0.572 | −0.815 | 0 | 0 |
| 642 | −1.375 | −0.595 | −0.186 | −0.595 | −0.804 | −0.578 | −0.804 |
| 660 | −1.815 | −0.227 | −0.227 | −1.359 | −0.516 | 0 | 0 |
| 711 | −1.661 | −1.850 | 0.095 | 0.095 | −0.181 | −0.181 | −0.146 |
| 731 | −1.744 | −1.224 | −0.095 | −0.425 | −0.405 | −0.167 | −0.370 |
| 800 | −1.824 | −2.052 | 0.114 | 0.114 | 0 | 0 | 0 |
| 820 | −1.871 | −1.698 | −0.0002 | −0.172 | 0 | 0 | 0 |
| 840 | −1.918 | −0.902 | −0.114 | −0.902 | 0 | 0 | 0 |

We believe the accuracy of these tables to be within rounding-off error of the figures as given. Several interesting checks have been made, the most important of which is provided by the relation

$$S_3(\mathbf{k}) = S_5^{xx}(\mathbf{k}) + S_5^{yy}(\mathbf{k}) + S_5^{zz}(\mathbf{k}). \qquad (23)$$

The left and right sides of this relation were calculated independently and checked against each other only after all the numbers were tabulated. In this way the number of significant figures was established. To within rounding-off error of the numbers as given, no violations of Eq. (23) were found.

It is important to know how representative is our sampling of k-space. To study this we have formed

TABLE VI. Body-centered cube.

| $q^x q^y q^z$ | $S_3$ | $S_5^{xx}$ | $S_5^{yy}$ | $S_5^{zz}$ | $S_5^{xy}$ | $S_5^{xz}$ | $S_5^{yz}$ |
|---|---|---|---|---|---|---|---|
| 110 | 10.760 | 2.925 | 2.925 | 4.190 | −2.048 | 0 | 0 |
| 200 | 6.768 | −0.231 | 3.500 | 3.500 | 0 | 0 | 0 |
| 211 | 4.598 | 0.356 | 2.121 | 2.121 | −1.295 | −1.295 | −0.622 |
| 220 | 3.163 | 0.481 | 0.481 | 2.201 | −1.935 | 0 | 0 |
| 222 | 1.350 | 0.451 | 0.451 | 0.451 | −1.126 | −1.126 | −1.126 |
| 310 | 2.090 | −1.045 | 1.390 | 1.745 | −1.137 | 0 | 0 |
| 321 | 0.736 | −0.605 | 0.325 | 1.016 | −1.541 | −0.697 | −0.386 |
| 330 | −0.078 | −0.510 | −0.510 | 0.941 | −1.819 | 0 | 0 |
| 332 | −0.674 | −0.409 | −0.409 | 0.145 | −1.222 | −0.594 | −0.594 |
| 400 | −0.111 | −1.577 | 0.844 | 0.844 | 0 | 0 | 0 |
| 411 | −0.230 | −1.321 | 0.545 | 0.545 | −0.755 | −0.755 | −0.076 |
| 420 | −0.480 | −1.141 | −0.028 | 0.690 | −1.411 | 0 | 0 |
| 422 | −0.913 | −0.883 | −0.015 | −0.015 | −0.950 | −0.950 | −0.134 |
| 431 | −0.969 | −0.834 | −0.545 | 0.412 | −1.548 | −0.286 | −0.066 |
| 433 | −1.439 | −0.616 | −0.411 | −0.411 | −0.612 | −0.612 | −0.060 |
| 440 | −1.023 | −0.787 | −0.787 | 0.551 | −1.770 | 0 | 0 |
| 442 | −1.325 | −0.659 | −0.659 | −0.006 | −1.218 | 0 | 0 |
| 444 | −1.619 | −0.540 | −0.540 | −0.540 | 0 | 0 | 0 |
| 510 | −1.344 | −1.383 | −0.073 | 0.112 | −0.609 | 0 | 0 |
| 521 | −1.424 | −1.043 | −0.418 | 0.038 | −1.010 | −0.408 | +0.113 |
| 530 | −1.276 | −0.808 | −0.808 | 0.341 | −1.456 | 0 | 0 |
| 532 | −1.461 | −0.645 | −0.645 | −0.170 | −0.995 | −0.367 | +0.367 |
| 600 | −2.090 | −1.221 | −0.435 | −0.434 | 0 | 0 | 0 |
| 611 | −2.001 | −1.029 | −0.487 | −0.487 | −0.375 | −0.375 | +0.137 |
| 620 | −1.848 | −0.844 | −0.844 | −0.159 | −0.782 | 0 | 0 |
| 622 | −1.755 | −0.585 | −0.585 | −0.585 | −0.523 | −0.523 | +0.523 |
| 710 | −2.369 | −0.858 | −0.858 | −0.654 | −0.210 | 0 | 0 |
| 800 | −2.572 | −0.857 | −0.857 | −0.857 | 0 | 0 | 0 |

TABLE VII. Lattice-point field factors of Luttinger and Tisza sc arrays.

| Array | LT field factor | sc Dipole-wave sum | Value from Table IV |
|---|---|---|---|
| $Z_1$ | 0 | $D^{zz}(0,0,0)$ | $0^a$ |
| $Z_2$ | $-9.687$ | $D^{zz}(0,0,4)=D^{xx}(4,0,0)$ | $-9.687$ |
| $Z_3$ | $4.844$ | $D^{zz}(4,0,0)$ | $4.845^b$ |
| $Z_4$ | $4.844$ | $D^{zz}(0,4,0)=D^{zz}(4,0,0)$ | $4.845$ |
| $Z_5$ | $5.351$ | $D^{zz}(4,4,0)$ | $5.352^c$ |
| $Z_6$ | $-2.676$ | $D^{zz}(0,4,4)=D^{xx}(4,4,0)$ | $-2.676$ |
| $Z_7$ | $-2.676$ | $D^{zz}(4,0,4)=D^{xx}(4,4,0)$ | $-2.676$ |
| $Z_8$ | 0 | $D^{zz}(4,4,4)$ | 0 |

a For a sphere.
b Since $D^{zz}(4,0,0)=D^{yy}(4,0,0)$ and $\Sigma_i D^{ii}(4,0,0)=0$, $D^{xx}(4,0,0)=-2D^{zz}(4,0,0)$. Therefore, the LT value is probably correct. Our error could have occurred in multiplying the rounding-off in $S^{zz}$ by 3.
c Similarly, $D^{zz}(4,4,0)=-2D^{xx}(4,4,0)$. Therefore our value is probably correct.

sums over the $N$ values of $\mathbf{k'}$ inside the first BZ of the type

$$N^{-1}\sum_{\mathbf{k'}}[S_5^{ij}(\mathbf{k'})]^2=\rho^{-2}\sum_l'[r_l^i r_l^i|r_l|^{-5}]^2. \quad (24)$$

The right-hand side converges so rapidly it may be directly summed. The left-hand side, then, may be approximated from our tables. The agreement with the direct sums for six such approximate sums was found to hold to three significant figures—results of truly surprising accuracy. Further details on such sampling checks will be presented in a following paper.[1]

An interesting feature of the dipole-wave sums is that, for example, the sc value of $3S_5^{zz}(0,0,4)-S_3(0,0,4)$ $=D^{zz}(0,0,4)$ is the $z$-component of the dipole-field factor at a lattice point of the Luttinger-Tisza[9] (LT) dipolar array $Z_2$. This array, which has alternate $xy$ planes of dipoles pointing in the $+z$ and $-z$ directions, is one of the 8 basic arrays considered by LT. The lattice-point field factors for the other 7 arrays may also be obtained from appropriate dipole-wave sums. Table VII compares our values with those given by LT. Similar checks may be made for a few of the fcc and bcc arrays, but the results will not be given here. The agreement is excellent. In Sec. VII we show how it is possible to obtain from the dipole-wave sums the dipole-field factors at positions other than lattice points.

## VII. DIPOLE-FIELD FACTORS FOR SITES WITHIN THE UNIT CELL

Consider the sum

$$D^{ij}(\mathbf{r}_m/\nu)=\sum_{\mathbf{k}}D^{ij}(\mathbf{k})W_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}_m). \quad (25)$$

One can show by inserting Eq. (19) into Eq. (25) and inverting the order of summation that $D^{ij}(\mathbf{r}_m/\nu)$ is the dipole-field factor at the point $\mathbf{r}_m/\nu$ within the unit cell. That is,

$$\rho D^{ij}(\mathbf{r}_m/\nu)=$$
$$\sum_l \frac{3(r_l^i-r_m^i\nu^{-1})(r_l^j-r_m^j\nu^{-1})-(r_l-r_m\nu^{-1})^2\delta^{ij}}{|r_l-r_m\nu^{-1}|^5}. \quad (26)$$

Here $\mathbf{r}_m$ is an appropriately selected lattice vector, and $\nu$ is the ratio of the separation between two points of the reciprocal lattice and the corresponding points in the sampling of $\mathbf{k}$-space. For our choice of points, $\nu=8$. Eq. (25) may be inverted to express dipole-wave sums in terms of dipole-field factors.

Thus the values of dipole-wave sums tabulated in this paper can be used to obtain dipole-field factors at 512 points inside the unit cell of each of the three primitive cubic lattices.

## VIII. DIPOLAR ANISOTROPY IN ANTIFERROMAGNETIC MnO

Recently Kaplan[10] has calculated the dipolar anisotropy energy in the antiferromagnet MnO by use of dipole-field factors at various sites within an fcc lattice. We show here how this energy may be obtained in a very simple way by use of the dipole-wave sums.

Consider the fcc sum $D^{ij}(4,4,4)$. The exponential factor of this sum is just $\pm1$ at the various lattice points of an fcc, and in particular reproduces an antiferromagnetic array such that all values $+1$ fall on alternate (111) planes, and the values $-1$ on the in-between planes. Just such an array is observed in MnO by neutron diffraction experiments.[11] The dipolar energy in such an array of $N$ spins is given by

$$E=-\tfrac{1}{2}N(g\beta s)^2 D^{ZZ}(4,4,4). \quad (27)$$

Here $D^{ZZ}(4,4,4)$ is the dipole-wave sum with respect to the spin direction. If this latter has direction cosines $\alpha, \beta, \gamma$ with respect to the cube axes, we have in terms of our tabulated dipole-wave sums:

$$E=-\tfrac{1}{2}N(g\beta s)^2(\alpha^2 D^{xx}+\beta^2 D^{yy}+\gamma^2 D^{zz}$$
$$+2\alpha\beta D^{xy}+2\alpha\gamma D^{xz}+2\beta\gamma D^{yz}), \quad (28)$$

where all the $D^{ij}$ have the argument $(4,4,4)$. From Table V we find

$$D^{ij}(4,4,4)=-3.615(1-\delta^{ij}),$$

and thus

$$E=3.615N(g\beta s)^2(\alpha\beta+\alpha\gamma+\beta\gamma). \quad (29)$$

Kaplan obtains the same result, his numerical constant being $(57.41/16)=3.588$.

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