Internal Field in General Dipole Lattices*

F. W. DE WETTE AND G. E. SCHACHER†
Argonne National Laboratory, Argonne, Illinois
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The calculation of the internal field in dipole lattices necessitates summing the contributions due to all dipoles in the crystal. These dipole sums are conditionally convergent, which means that they depend on the order of summation (i.e., the shape of the crystal). Rapidly converging expressions for these sums are obtained with the method of *planewise summation*, for lattices of arbitrary symmetry and arbitrary dipole orientation. With these expressions one can evaluate the internal field at an arbitrary point of complex dipole lattices. As an example, the internal electric field at the positions of the water molecules is evaluated for potassium ferrocyanide [$K_4Fe(CN)_6 \cdot 3H_2O$].

I. INTRODUCTION

THE internal electric field produced by electric dipoles located at the lattice points in a crystal is of central importance in the theory of dielectric phenomena. An example is the molecular field theory for ferroelectric materials which has had some success in explaining the phase transitions in barium titanate,[1,2] rochelle salt,[3,4] and other materials. Ferroelectricity is mentioned as an example because of the wide attention the field is receiving at the present time, and because of the direct application of the method of this paper to the necessary theoretical calculations.

The problem with which we are concerned is the evaluation of the contribution to the internal (local) field $\mathbf{E}_{\text{int}}$, due to all the dipoles in an arbitrary dipolar lattice. First, however, a remark concerning the customary expression for the internal field $\mathbf{E}_{\text{int}}$ is in order, since there are some ambiguities in the literature on this point. For this purpose it suffices to consider a cubic crystal with equal parallel dipoles $\mathbf{p}$ at the lattice sites. The internal electric field at a lattice position is then usually expressed as

$$\mathbf{E}_{\text{int}}=\mathbf{E}+\gamma\mathbf{P}. \tag{1}$$

Here $\mathbf{P}=N\mathbf{p}$ is the polarization (N is the number of dipoles per unit volume) and γ is the so-called Lorentz factor.[5] For a monatomic cubic lattice, as in this example, $\gamma=4\pi/3$. $\mathbf{E}$ is the macroscopic electric field in the medium, i.e., it is the $\mathbf{E}$ that appears in the Maxwell equations. In expression (1), however, $\mathbf{E}$ is often called the *externally applied field*.[6] This usage derives from the fact that in the customary experimental setup (see Fig. 1) the value of $\mathbf{E}$ is related to the applied voltage V_0 by the relation $E=V_0/d$. When the condenser is connected to the battery, E has this value whether the dielectric material is in the condenser or not. But to call $\mathbf{E}$ the *external field*, or to say that $\mathbf{E}$ results only from the external charges, as is sometimes done, is incorrect, because according to the Maxwell equations, the field $\mathbf{E}$ is due to both the external charges on the condenser plates *and* the polarization charges on the surface of the dielectric. Thus, in the example of Fig. 1, $\mathbf{E}$ is due to the charges $q_{\text{ext}}-q_{\text{pol}}$ while the external field is due to the charges q_{ext} alone. Therefore, in order to avoid confusion, it would be preferable to use the term *electric field* exclusively for $\mathbf{E}$.

A second remark concerns the dependence of the various quantities in (1) on the shape of the crystal[7] (henceforth called "shape dependence"). Although $\mathbf{E}_{\text{int}}$, $\mathbf{E}$, and $\mathbf{P}$ in general are shape-dependent, the Lorentz factor γ does not depend on the shape of the crystal; it depends only on the crystal symmetry. This can easily be seen by recalling the customary procedure for deriving (1) for a homogeneously polarized dielectric

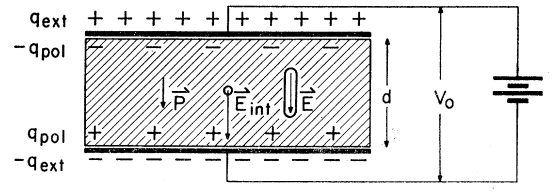

FIG. 1. Field quantities $\mathbf{E}_{\text{int}}$, $\mathbf{E}$, and $\mathbf{P}$, and charges q_{ext} and q_{pol} in a parallel plane condensor (plate distance d) which is connected to a battery of voltage V_0.

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† Present address: Department of Physics, U. S. Naval Postgraduate School, Monterey, California.
[1] A. F. Devonshire, Phil. Mag. **40**, 1040 (1949).
[2] J. C. Slater, Phys. Rev. **78**, 748 (1950).
[3] W. P. Mason, *Piezoelectric Crystals and Their Application to Ultrasonics* (D. Van Nostrand Company, Inc., New York, 1950).
[4] A. F. Devonshire, Phil. Mag. **2**, 1027 (1957).

[5] For a monatomic noncubic crystal a relation equivalent to (1) can in general only be given for the x, y, and z components of the fields separately, i.e.,

$$E_{\text{int},\kappa}=E_\kappa+\Sigma_\nu \gamma_{\kappa,\nu}P_\nu,$$

where κ and ν indicate x, y, z. If the crystal contains a number of different sublattices, then the κ component of the internal field at a site of sublattice i is given by

$$E^{(i)}{}_{\text{int},\kappa}=E_\kappa+\sum_{j(\text{sublattices})}\Sigma_\nu \gamma_{\kappa,\nu}{}^{i,j}P^{(j)}{}_\nu.$$

$P^{(j)}{}_\nu$ is the ν component of the polarization of sublattice j. $\gamma_{\kappa,\nu}$ and $\gamma_{\kappa,\nu}{}^{i,j}$ are generalized Lorentz factors, forming matrices. The remarks in the text about the shape independence of γ equally apply to $\gamma_{\kappa,\nu}$ and $\gamma_{\kappa,\nu}{}^{i,j}$. In the Appendix we express the Lorentz factors in terms of the dipole sums as evaluated in this paper.
[6] See for instance W. Känzig, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 4.
[7] These matters have been discussed earlier by B. R. A. Nijboer and F. W. de Wette, Physica **24**, 422 (1958).

(which we are considering throughout) with polarization $\mathbf{P}$. One has

$$\mathbf{E}_{\text{int}}=\mathbf{E}_{\text{ext}}+\mathbf{E}_{\text{out}}+\mathbf{E}_{\text{sph}}+\mathbf{E}_{\text{in}}, \tag{2}$$

where $\mathbf{E}_{\text{ext}}$ is the electric field arising from the external charges, $\mathbf{E}_{\text{out}}=-L\mathbf{P}$ is the field arising from the polarization charges on the outer surface of the sample (L is the depolarization factor), $\mathbf{E}_{\text{sph}}=(4\pi/3)\mathbf{P}$ is the field due to the polarization charges on the surface of an imaginary sphere around the field point, and $\mathbf{E}_{\text{in}}$ is the field due to all the dipoles inside the sphere. On the other hand, the electric field $\mathbf{E}$ is due to the external charges and the polarization charges on the crystal surface, i.e.,

$$\mathbf{E}=\mathbf{E}_{\text{ext}}+\mathbf{E}_{\text{out}}=\mathbf{E}_{\text{ext}}-L\mathbf{P}. \tag{3}$$

From (1), (2), and (3), it follows immediately that

$$\gamma\mathbf{P}=\mathbf{E}_{\text{sph}}+\mathbf{E}_{\text{in}}. \tag{4}$$

We notice that the explicit shape dependence, which is embodied in the depolarization factor L, is not present in (4), and the left-hand side of (4) is only implicitly shape-dependent through $\mathbf{P}$. In other words, the Lorentz factor γ is shape-independent; it depends only on the crystal symmetry. Another way of seeing this is the following: $\mathbf{E}_{\text{int}}$ is obtained by subtracting from $\mathbf{E}$ the (averaged) field of the reference particle. That is,

$$\mathbf{E}_{\text{int}}-\mathbf{E}=\gamma\mathbf{P} \tag{5}$$

is the field arising from the uncompensated polarization charges on the surface of the little cavity that is created by taking out the reference particle. This difference is clearly a local effect that can depend only on the crystal shape implicitly through the shape dependence of $\mathbf{P}$.

We now return to the purpose of this paper, which is to calculate the total dipole contribution to the internal field $\mathbf{E}_{\text{int}}$ by a direct summation of the contributions of all dipoles. In terms of the quantities in Eq. (2), this means that we will be evaluating $\mathbf{E}_{\text{out}}+\mathbf{E}_{\text{sph}}+\mathbf{E}_{\text{in}}$. Since $\mathbf{E}_{\text{out}}$ contains the depolarization factor L which depends on the crystal shape, it is obvious that this contribution is shape-dependent. Mathematically, this is a result of the fact that the lattice sums which we have to evaluate are conditionally convergent, which means that the value of the infinite sum depends on the order in which the summation is carried out.[8] These sums are of the general form

$$S_j=\sum_\lambda f(x_{\lambda,j},y_{\lambda,j},z_{\lambda,j})r_{\lambda,j}^{-3}, \tag{6}$$

where $x_{\lambda,j}$, $y_{\lambda,j}$, and $z_{\lambda,j}$ are the Cartesian coordinates of the lattice vector $r_{\lambda,j}$ and f is some simple, dimensionless function of its arguments (the notation is explained in Sec. II). A direct consequence of their conditional convergence is that these sums, as they stand, are unsuitable for direct evaluation, except perhaps on a high-speed computer.

The object of all analytical treatments of lattice sums is to transform sums with poor convergence into other sums with rapid convergence. In applying such a treatment to a conditionally convergent sum one has to keep in mind that, although the resultant sums are always absolutely convergent so that the summation order in which they are evaluated in an actual calculation is immaterial, the process of going from the original sum to the rapidly converging one always corresponds to introducing a specific summation order for the original sum. For the dipole sums treated here this means that a "processed" sum corresponds to a particular shape of crystal. This, however, does not limit the applicability of these methods since one can always find the value of the dipole sum corresponding to a different shape of crystal by adding or subtracting the appropriate depolarization fields. As an example, let us consider the case of a slab-shaped crystal, since this is the crystal shape that corresponds to planewise summation, which is used throughout this paper. Suppose the crystal contains parallel dipoles of unit strength and we want to evaluate the component of the electric field in the dipole direction. There exist two extreme orientations of the slab over which the summations can be carried out: (1) the slab is perpendicular to the dipole direction, and (2) the slab is parallel to the dipole direction. In case (1) the value S_1 of the dipole sum contains the depolarization field $-4\pi N$ (N is the number of dipoles per unit volume), whereas the value S_2 calculated according to (2), does not contain this contribution. Hence S_1 and S_2 are related as follows

$$S_2=S_1+4\pi N. \tag{7}$$

Generalization of this example to more complicated cases is straightforward.

In this paper we derive rapidly converging expressions for the internal field in the most general type of dipole lattices. This is done by generalizing a method for the evaluation of dipole sums which was proposed a number of years ago by Nijboer and de Wette.[7,9] The present method can be used to evaluate the internal field at any point of the unit cell of lattices of triclinic symmetry, made up of an arbitrary number of sublattices with dipoles at arbitrary orientations. That is, there is no restriction that all dipoles in the crystal be of the same magnitude or have the same orientation. The results may be reduced to any special case desired with little effort and the number of terms needed for an actual evaluation of the sums is found to be small. The method is quite easy to use and offers advantages over earlier summation recipes.

[8] For a finite sum, corresponding to a finite crystal of given shape, the result of the sum is unambiguous but, of course, shape-dependent. If one goes to the limit of an infinite crystal while maintaining the crystal shape, or in other words, goes over to the infinite sum while maintaining the same summation order, a direct correspondence between the crystal shape and the summation order of the infinite sum is established.

[9] F. W. de Wette, Phys. Rev. **123**, 103 (1961).

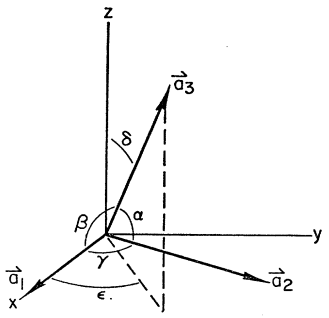

FIG. 2. Choice of the x, y, z directions with respect to the triclinic basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$.

A short discussion of the principles involved in bringing lattice sums into rapidly converging expressions is given in Sec. II. In particular the *method of planewise summation*, which is used throughout this paper, is outlined. In Sec. III this method is applied to dipole lattices of arbitrary structure, in which the dipoles are oriented perpendicular to the planes. The case of general dipole orientations is treated in Sec. IV. Dipole-wave sums are briefly discussed in Sec. V, and in Sec VI we discuss the practical use of the summation formulas presented in Secs. III and IV. As an example the dipole field in potassium ferrocyanide is evaluated in Sec. VII.

II. THE PLANEWISE SUMMATION METHOD

A. Notation

As was mentioned in the introduction, we treat the case of a general dipolar lattice, in which dipoles of varying magnitude and orientation may occupy many nonequivalent sites in the unit cell. Such a composite lattice can always be divided into a number of sublattices, which are simple Bravais lattices, occupied by dipoles of equal magnitude and orientation. The sublattices do not necessarily have the same symmetry as the crystal as a whole nor as each other, and the sublattice unit cell dimensions are not restricted.

The basis vectors for sublattice i will be written as $\mathbf{a}_{1i}$, $\mathbf{a}_{2i}$, and $\mathbf{a}_{3i}$, so that the sublattice translation vector is given by

$$\mathbf{r}_{\lambda i}=\lambda_1\mathbf{a}_{1i}+\lambda_2\mathbf{a}_{2i}+\lambda_3\mathbf{a}_{3i};\quad \lambda_1, \lambda_2, \lambda_3=0, \pm1, \pm2, \text{ etc.} \quad (8)$$

The origin is chosen at the point where one wishes to evaluate the internal electric field. The position of the origin with respect to the origin of the sublattice unit cell is given by

$$-\mathbf{r}_{ji}=-(j_{1i}\mathbf{a}_{1i}+j_{2i}\mathbf{a}_{2i}+j_{3i}\mathbf{a}_{3i});\quad 0\leq j_{1i}, j_{2i}, j_{3i}<1. \quad (9)$$

The total internal field at the origin is found by performing the lattice summation over each sublattice separately, then adding the contributions. In what follows we will treat a sublattice of triclinic symmetry and drop the subscript i, understanding that the calculation is to be performed for each sublattice separately.

The position with respect to the origin of some dipole in the sublattice is given by $\mathbf{r}_{\lambda,j}(r_{\lambda,j},\theta_{\lambda,j},\phi_{\lambda,j})=\mathbf{r}_\lambda+\mathbf{r}_j$. $\theta_{\lambda,j}$ and $\phi_{\lambda,j}$ are the polar angles of $\mathbf{r}_{\lambda,j}$. For an unambiguous choice of the x, y, and z axes refer to Fig. 2: x is chosen parallel to the $\mathbf{a}_1$ triclinic axis while the y axis is chosen so that the x, y plane coincides with the $\mathbf{a}_1$, $\mathbf{a}_2$ plane. z is, of course, perpendicular to the x, y plane, completing the Cartesian coordinate system.

B. Principle of the Summation Method

In order to make the paper self-contained, it is useful to give a brief account of the principle underlying the method of bringing a slowly converging sum into a rapidly converging form.[7,10]

Suppose we wish to evaluate a sum of the type

$$S=\sum_{n=1}^{\infty} f(n), \quad (10)$$

where $f(x)$ goes to zero slowly as $x\to\infty$ and may be infinite for $x=0$. In order to improve the convergence we introduce an auxiliary function $\mathfrak{F}(x)$ which approaches zero rapidly as $x\to\infty$ and which is finite at $x=0$. We may now write

$$S=\sum_{n=1}^{\infty} f(n)\mathfrak{F}(n)+\sum_{n=1}^{\infty} f(n)[1-\mathfrak{F}(n)]. \quad (11)$$

The first sum converges rapidly on account of $\mathfrak{F}$, but the second still has the same rate of convergence as the original sum (10). However, if $f(x)[1-\mathfrak{F}(x)]$ is a slowly varying (smooth) function of x, then its Fourier transform (FT) will be a rapidly converging function in Fourier space. By using the property that the summation of a function over a lattice in real space is equal to the summation of its Fourier transform over the reciprocal lattice (in Fourier space), the second sum in (11) can be converted into a rapidly converging sum over the reciprocal lattice. The necessary condition for rapid convergence, namely that $f(x)[1-\mathfrak{F}(x)]$ be a smooth function at $x=0$ [the smoothness of the function for large values of x is assured by $f(x)$], poses a third condition on $\mathfrak{F}(x)$. In particular, if $f(0)=\infty$, then $1-\mathfrak{F}(x)$ has to approach zero in such a way that the smoothness of $f(x)[1-\mathfrak{F}(x)]$ is assured. The choice of the auxiliary converging function $\mathfrak{F}(x)$ is governed by the conditions listed above, but is not unique for a given $f(x)$.

It is clear from the above that the use of an auxiliary convergence function always leads to two rapidly converging sums, one over the ordinary lattice and the other over the reciprocal lattice. However, if the function $f(x)$ remains finite for $x\to0$, it may not be

[10] See B. R. A. Nijboer and F. W. de Wette, Physica **23**, 309 (1957).

necessary to introduce an auxiliary function. In this case the entire sum (10) may be transformed into Fourier space, and the result is only one rapidly converging series which is over the reciprocal lattice. In the following we will encounter both cases.

We now describe the particular method used in this paper to find rapidly converging expressions for sums of the type given in Eq. (6). Since these sums are conditionally convergent it must be kept in mind, first, that the answers obtained depend on the order in which the summation is carried out in the original sum, and second, that this summation order corresponds to a particular shape of crystal. It turns out that the *planewise summation method*, which corresponds to considering a slab-shaped crystal, has definite computational advantages. We first choose the $\mathbf{a}_3$ direction in some convenient way in the sublattice (remarks concerning this choice are presented below and in the next section). For fixed λ_3 we have a two-dimensional subsum over λ_1 and λ_2. This subsum is brought into a rapidly converging form by transforming it in its entirety into two-dimensional Fourier space. It turns out that the resultant sums can then be summed analytically over λ_3, leaving us in the end with a rapidly converging sum over the two-dimensional reciprocal lattice. The whole method can be schematically indicated as follows:

$$\begin{aligned} S&=\textstyle\sum_{\lambda_1,\lambda_2,\lambda_3} f(\lambda_1,\lambda_2,\lambda_3)\\ &=\textstyle\sum_{\lambda_3}\sum_{\lambda_1,\lambda_2} f(\lambda_1,\lambda_2,\lambda_3)\rightarrow\sum_{\lambda_3}\sum_{\mu_1,\mu_2} g(\mu_1,\mu_2,\lambda_3)\rightarrow\\ &\qquad\textstyle\sum_{\mu_1,\mu_2}\sum_{\lambda_3} g(\mu_1,\mu_2,\lambda_3)\rightarrow\sum_{\mu_1,\mu_2} G(\mu_1,\mu_2)\,, \end{aligned}\tag{12}$$

where $g(\mu_1,\mu_2,\lambda_3)$ is the two-dimensional Fourier transform of $f(\lambda_1,\lambda_2,\lambda_3)$. Since the λ_1, λ_2 summation is treated before the λ_3 summation, the method implies that we first sum the contributions of all dipoles in a plane (λ_3=constant), and next add the contributions of all the planes. However, there exists one case which cannot be treated by this method, namely, when the origin is situated in one of the planes. The summation over this particular plane has to be treated separately, namely, by the first method outlined above using an auxiliary convergence function.

As we pointed out above, the planewise summation method is equivalent to considering a slab-shaped crystal with faces parallel to the $\mathbf{a}_1$, $\mathbf{a}_2$ planes. This means that the total internal field in the origin contains the depolarization field of a flat slab. This field is $-4\pi\mathbf{P}\cdot\mathbf{n}$, where $\mathbf{P}$ is the polarization in the sublattice and $\mathbf{n}$ is the unit vector normal to the surface. In certain cases it may be necessary or advantageous to choose differently oriented sets of $\mathbf{a}_1$, $\mathbf{a}_2$ planes for different sublattices.[11] In that case corrections for the depolarization fields of the different sublattices have to be made so that all correspond to the same crystal shape before they are added together. Similar corrections have to be made if the crystal used in the experimental measurements is not slab-shaped, or is slab-shaped but with the faces in an orientation different from the planes chosen in the summation method. In Eq. (7) we have indicated how the result of the calculations should be corrected to be applicable in such situations.

[11] For instance, if a certain choice of $\mathbf{a}_1$, $\mathbf{a}_2$ planes would cause the origin of one of the sublattices to be in one of these planes, it may be advantageous to make a different choice of $\mathbf{a}_1$, $\mathbf{a}_2$ planes for that particular case, because the treatment for the plane containing the origin is more laborious.

III. SPECIAL CASE: DIPOLES PERPENDICULAR TO PLANES

As a first example we will evaluate the field component in the z direction due to unit dipoles in the z direction in a lattice with triclinic symmetry. This problem is closely related to that of evaluating the z component of the field gradient in a point-ion lattice.[12] The lattice sum to be evaluated is

$$S_{j_1,j_2,j_3}(z,p_z)=\sum_\lambda{}'\frac{2P_2(\cos\theta_{\lambda,j})}{r_{\lambda,j}{}^3}\,,\tag{13}$$

where $\sum_\lambda{}'$ is understood to include sums over λ_1, λ_2, and λ_3. For $j_1=j_2=j_3=0$ the sum must be written with a prime to exclude the dipole at the origin. For convenience we will define the dimensionless lattice vector $\varrho_{\lambda,j}=\mathbf{r}_{\lambda,j}/a_1$, where a_1 is the length of $\mathbf{a}_1$. Then

$$S_{j_1,j_2,j_3}(z,p_z)=\frac{1}{a_1{}^3}\sum_\lambda{}'\frac{2P_2(\cos\theta_{\lambda,j})}{\rho_{\lambda,j}{}^3}\,.\tag{14}$$

In the method of planewise summation the λ_1, λ_2 summation (in the $\mathbf{a}_1$, $\mathbf{a}_2$ planes) is treated before the λ_3 summation is carried out. As we mentioned in the previous section, two cases must be treated separately:

Case 1. The origin lies outside the $\mathbf{a}_1$, $\mathbf{a}_2$ planes ($j_3\neq0$).

Case 2. The origin lies in one of the $\mathbf{a}_1$, $\mathbf{a}_2$ planes ($j_3=0$).

In the second case the plane that contains the origin must be treated separately; the rest of this particular sublattice can be treated as *Case 1*, excluding the term $\lambda_3=0$.

Since the various conditions necessitate treating the sums differently, we will now introduce a notation consistent with the summation conditions. $S_{j_1,j_2,j_3}(\kappa,p_\nu)$ is defined to be the κ component of the field due to unit dipoles in the ν direction, where κ and ν indicate x, y, and z. If $j_3=0$, two summations are performed separately, as we just pointed out: first, a summation over all planes not including the plane $\lambda_3=0$, indicated by $S_{j_1,j_2,0}{}^{\lambda_3}(\kappa,p_\nu)$; and second, over the plane $\lambda_3=0$, indicated by $S_{j_1,j_2,0}{}^{0}(\kappa,p_\nu)$.

A. Case 1: $j_3\neq0$

In Fig. 3 it is shown how the vector $\varrho_{\lambda,j}=\mathbf{r}_{\lambda,j}/a_1$ is decomposed into vectors in the $\mathbf{a}_1$, $\mathbf{a}_2$ plane and a vector

[12] Cf. Ref. 9 and the paper immediately following this one.

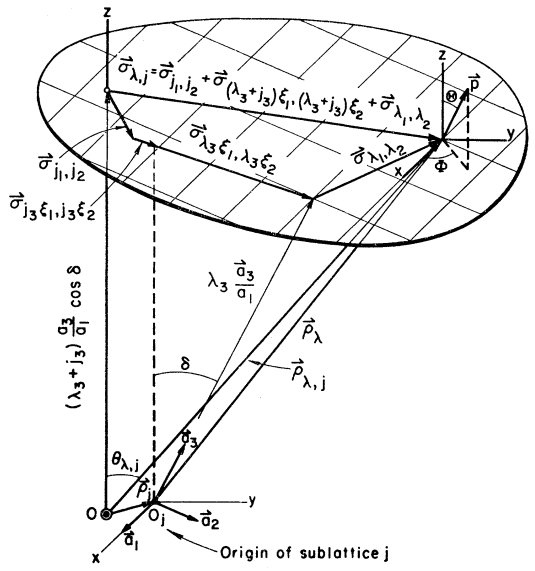

FIG. 3. Decomposition of the lattice vector $\varrho_{\lambda,j}$ in lattices with triclinic symmetry.

perpendicular to this plane. We have $\boldsymbol{\sigma}_{\lambda_1,\lambda_2}=\lambda_1(\mathbf{a}_1/a_1)+\lambda_2(\mathbf{a}_2/a_1)$, and $\boldsymbol{\sigma}_{j_1,j_2}=j_1(\mathbf{a}_1/a_1)+j_2(\mathbf{a}_2/a_1)$. Referring to Fig. 3 we find

$$\boldsymbol{\sigma}_{j_3\xi_1,j_3\xi_2}+\boldsymbol{\sigma}_{\lambda_3\xi_1,\lambda_3\xi_2}=(\lambda_3+j_3)[\xi_1(\mathbf{a}_1/a_1)+\xi_2(\mathbf{a}_2/a_1)], \tag{15}$$

where

$$\xi_1=(a_3/a_1)(\sin\delta)(\cos\epsilon-\sin\epsilon\cot\gamma), \tag{16a}$$

$$\xi_2=(a_3/a_2)(\sin\delta)(\sin\epsilon)/(\sin\gamma). \tag{16b}$$

From the same figure we see that $\cos\theta_{\lambda,j}$ may be written as

$$\cos\theta_{\lambda,j}=(\lambda_3+j_3)(a_3/a_1)(\cos\delta)/\rho_{\lambda,j}. \tag{17}$$

We are now in a position to treat the lattice sum (14). As we mentioned in Sec. II, the λ_1, λ_2 summation can in this case ($j_3\neq 0$) in its entirety be converted into a summation over the two-dimensional reciprocal lattice. The reason that we do not need an auxiliary convergence function is that in each of the planes the summand is well behaved. Using (17) we can write the λ_1, λ_2 summation as a two-dimensional integration

$$S_{j_1,j_2,j_3}(z,p_z)=\frac{1}{a_1{}^3}\sum_{\lambda_3}\int d^2\sigma\{\sum_{\lambda_1,\lambda_2}\delta(\boldsymbol{\sigma}-\boldsymbol{\sigma}_{j_1,j_2}-\boldsymbol{\sigma}_{(\lambda_3+j_3)\xi_1,(\lambda_3+j_3)\xi_2}-\boldsymbol{\sigma}_{\lambda_1,\lambda_2})\}$$
$$\times\frac{2P_2((\lambda_3+j_3)(a_3/a_1)(\cos\delta)/\{\sigma^2+(\lambda_3+j_3)^2(a_3/a_1)^2\cos^2\delta\}^{1/2})}{\{\sigma^2+(\lambda_3+j_3)^2(a_3/a_1)^2\cos^2\delta\}^{3/2}}. \tag{18}$$

We now apply Parseval's formula to the two-dimensional integral. This formula states that if $F(\mathbf{h})$ and $G(\mathbf{h})$ are the (one-, two-, or three-dimensional) Fourier transforms of $f(\boldsymbol{\sigma})$ and $g(\boldsymbol{\sigma})$, respectively, then

$$\int F(\mathbf{h})^*G(\mathbf{h})d\mathbf{h}=\int f(\boldsymbol{\sigma})^*g(\boldsymbol{\sigma})d\boldsymbol{\sigma}. \tag{19}$$

As the functions $f(\boldsymbol{\sigma})$ and $g(\boldsymbol{\sigma})$ we choose $\sum_{\lambda_1,\lambda_2}\delta(\cdots)$ and the remainder of the integrand in (18), respectively. The two-dimensional Fourier transforms (FT_2) of these functions are (see Refs. 10 and 7)

$$[FT_2\{\sum_{\lambda_1,\lambda_2}\delta(\boldsymbol{\sigma}-\boldsymbol{\sigma}_{j_1,j_2}-\boldsymbol{\sigma}_{(\lambda_3+j_3)\xi_1,(\lambda_3+j_3)\xi_2}-\boldsymbol{\sigma}_{\lambda_1,\lambda_2})\}]^*$$
$$=O_a{}^{-1}\sum_{\mu_1,\mu_2}\exp[-2\pi i\{[j_1+(\lambda_3+j_3)\xi_1]\mu_1+[j_2+(\lambda_3+j_3)\xi_2]\mu_2\}]\delta(\mathbf{h}-\mathbf{h}_{\mu_1,\mu_2}), \tag{20}$$

where O_a is the two-dimensional unit cell area (normalized to a_1) in the untransformed two-dimensional lattice, and $\sum_{\mu_1,\mu_2}$ is a summation over the reciprocal two-dimensional lattice. The basis vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ of this reciprocal lattice are related to $\mathbf{a}_1$ and $\mathbf{a}_2$ by

$$(\mathbf{a}_i/a_1)\cdot\mathbf{b}_j=\delta_{ij}. \tag{21}$$

Further, it can be shown that[13] [cf. (I.12) of Ref. 13]

$$FT_2\left\{\frac{2P_2((\lambda_3+j_3)(a_3/a_1)\ (\cos\delta)/\{\sigma^2+(\lambda_3+j_3)^2(a_3/a_1)^2\cos^2\delta\}^{1/2})}{\{\sigma^2+(\lambda_3+j_3)^2(a_3/a_1)^2\cos^2\delta\}^{3/2}}\right\}=4\pi^2h\exp[-2\pi h(a_3/a_1)\ (\cos\delta)|\ (\lambda_3+j_3)|], \tag{22}$$

[13] Space limitations make it impossible to include the derivations of the two-dimensional Fourier transforms of the various functions used in this paper. A multilith copy of appendixes giving these derivations as well as a table of the incomplete gamma functions $\Gamma(\alpha,x)$ for $\alpha=\frac{5}{2}, \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}$, which are used in the numerical evaluation of the lattice sums, may be obtained by writing to the Secretary of the Solid State Science Division, Argonne National Laboratory, Argonne, Illinois, 60440. This material has also been deposited as Document No. 8127 with the ADI Auxiliary Publications Project, Photoduplication Service, Library of Congress, Washington 25, D. C. A copy may be secured by citing the Document number and by remitting $2.50 for photoprints, or $1.75 for 35-mm microfilm. Advance payment is required. Make checks or money orders payable to: Chief, Photoduplication Service, Library of Congress.

where $h=(h_x^2+h_y^2)^{1/2}$. Applying Parseval's formula (19) to (18), using (20) and (22) we find

$$S_{j_1,j_2,j_3}(z,p_z)=4\pi^2 a_1^{-3}O_a^{-1}\sum_{\lambda_3}\sum_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\exp[-2\pi i\{(j_1+j_3\xi_1)\mu_1+(j_2+j_2\xi_2)\mu_2\}-2\pi i\lambda_3(\xi_1\mu_1+\xi_2\mu_2) -2\pi h_{\mu_1,\mu_2}(a_3/a_1)\,(\cos\delta)\,|\,(\lambda_3+j_3)\,|\,]. \quad (23)$$

At this point we have completed the first part of the planewise summation method, namely, the treatment of the two-dimensional sums $\sum_{\lambda_1,\lambda_2}$. Since the series (23) is absolutely convergent in λ_3 as well as in μ_1 and μ_2, the summation order is no longer essential and may be reversed. This gives rise to a geometrical series in λ_3, which can be summed directly to give:

$$S_{j_1,j_2,j_3}(z,p_z)=\frac{4\pi^2}{O_a a_1^3}\sum_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\exp[-2\pi i\{(j_1+j_3\xi_1)\mu_1+(j_2+j_3\xi_2)\mu_2\} \times\left\{\frac{\exp[2\pi i(\xi_1\mu_1+\xi_2\mu_2)-2\pi h_{\mu_1,\mu_2}(a_3/a_1)\,(\cos\delta)\,(1-j_3)]}{1-\exp[2\pi i(\xi_1\mu_1+\xi_2\mu_2)-2\pi h_{\mu_1,\mu_2}(a_3/a_1)\,\cos\delta]}\right. +\left.\frac{\exp[-2\pi h_{\mu_1,\mu_2}(a_3/a_1)\,(\cos\delta)\,j_3]}{1-\exp[-2\pi i(\xi_1\mu_1+\xi_2\mu_2)-2\pi h_{\mu_1,\mu_2}(a_3/a_1)\,\cos\delta]}\right\}. \quad (24)$$

This completes the transformation of Eq. (14) into a rapidly converging expression for the general triclinic case. For lattices of monoclinic or higher symmetry, $\delta=0$, $\xi_1=\xi_2=0$, and Eq. (24) reduces to Eq. (14) of Ref. 9 (where $\alpha=a_3/a_1$). The exponentials involving j_1, j_2, j_3, ξ_1, and ξ_2 usually have the effect of a multiplying constant when terms with the same h_{μ_1,μ_2} are added together. In simple cases they merely determine the signs of such terms. Whenever these exponentials give rise to a complex term, there will always be a complex conjugated term so that their sum is real. This can be most easily checked in (23) by pairwise combining terms for μ_1, μ_2 and $-\mu_1$, $-\mu_2$. This ensures that the total result is real as it must be.

B. Case 2: $j_3=0$

In this case the origin is situated in the plane $\lambda_3=0$. Since the Fourier transform (22) does not exist for $\lambda_3=j_3=0$, the summation over the plane $\lambda_3=0$ has to be treated separately with the aid of an auxiliary convergence function. The contribution due to all other planes [for which (22) is valid] is found by subtracting the term $\lambda_3=0$ from Eq. (23) which, after carrying out the λ_3 summation, gives:

$$S_{j_1,j_2,0}^{\lambda_3}(z,p_z)=\frac{4\pi^2}{O_a a_1^3}\sum_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\exp[-2\pi i(j_1\mu_1+j_2\mu_2)]\left\{\frac{1}{\exp[-2\pi i(\xi_1\mu_1+\xi_2\mu_2)+2\pi h_{\mu_1,\mu_2}(a_3/a_1)\,\cos\delta]-1}\right. +\left.\frac{1}{\exp[+2\pi i(\xi_1\mu_1+\xi_2\mu_2)+2\pi h_{\mu_1,\mu_2}(a_3/a_1)\,\cos\delta]-1}\right\}. \quad (25)$$

The summands in (24) and (25) will be used frequently in what follows, so we will abbreviate these equations as:

$$S_{j_1,j_2,j_3}(z,p_z)=\frac{4\pi^2}{O_a a_1^3}\sum_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\Omega_{j_3}(\mu_1,\mu_2), \quad (24a)$$

$$S_{j_1,j_2,0}^{\lambda_3}(z,p_z)=\frac{4\pi^2}{O_a a_1^3}\sum_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\Omega_0(\mu_1,\mu_2), \quad (25a)$$

where the subscripts on the functions Ω indicate the case for which they are to be used, i.e., $j_3\neq 0$ or $j_3=0$.

We will now treat the dipole summation over the plane which contains the origin. The z component of the field due to these dipoles oriented in the z direction is given by:

$$S_{j_1,j_2,0}^{0}(z,p_z)=-a_1^{-3}\sum_{\lambda_1,\lambda_2}\sigma_{\lambda,j}^{-3}. \quad (26)$$

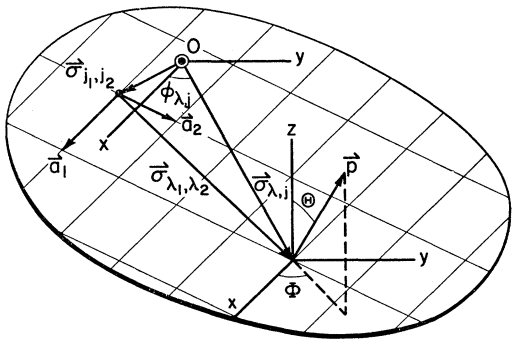

FIG. 4. Vectors and angles pertinent for the treatment of lattice sums with origin in the $\mathbf{a}_1$, $\mathbf{a}_2$ plane.

The decomposition of the vector $\boldsymbol{\sigma}_{\lambda,j}$, which lies in the $\mathbf{a}_1$, $\mathbf{a}_2$ plane is shown in Fig. 4.

As we mentioned earlier, in order to find a rapidly converging expression for this sum we have to use the first method outlined in Sec. IIB. A suitable choice for the auxiliary convergence function $\mathfrak{F}(\sigma)$ is the incomplete gamma function[14]: $\mathfrak{F}(\sigma)=\Gamma(\frac{3}{2},\pi\sigma^2)/\Gamma(\frac{3}{2})$. Introducing this $\mathfrak{F}(\sigma)$ into (26) we have

$$S_{j_1,j_2,0}{}^0(z,p_z)=-\frac{1}{a_1{}^3}\left\{\frac{1}{\Gamma(\frac{3}{2})}\sum_{\lambda_1,\lambda_2}\Gamma(\tfrac{3}{2},\pi\sigma_{\lambda,j}{}^2)\sigma_{\lambda,j}{}^{-3}+\frac{1}{\Gamma(\frac{3}{2})}\int d^2\sigma[\textstyle\sum_{\lambda_1,\lambda_2}\delta(\boldsymbol{\sigma}-\boldsymbol{\sigma}_{j_1,j_2}-\boldsymbol{\sigma}_{\lambda_1,\lambda_2})][\gamma(\tfrac{3}{2},\pi\sigma^2)\sigma^{-3}]\right\}, \quad (27)$$

where we have written the second series in the form of an integral. The function γ is defined by $\gamma(n,x)=\Gamma(n)-\Gamma(n,x)$. The first sum is rapidly converging and the second can be converted into a rapidly converging sum over the reciprocal lattice by the use of Parseval's formula. The method has been worked out in Ref. 7, and the calculation will not be repeated here. The final result is

$$S_{j_1,j_2,0}{}^0(z,p_z)=-\frac{1}{a_1{}^3}\left\{\frac{4\pi}{O_a}+\frac{2}{\sqrt{\pi}}\sum_{\lambda_1,\lambda_2}\Gamma(\tfrac{3}{2},\pi\sigma_{\lambda,j}{}^2)\sigma_{\lambda,j}{}^{-3}+\frac{2\pi^{3/2}}{O_a}\sum{}'_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\Gamma(-\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^2)\right.$$
$$\left.\times\exp[-2\pi i(j_1\mu_1+j_2\mu_2)]\right\}, \quad (28)$$

where we have used $\Gamma(\frac{3}{2})=\frac{1}{2}\sqrt{\pi}$. The λ_1, λ_2 summation is over the two-dimensional real lattice; the μ_1, μ_2 summation is over the two-dimensional reciprocal lattice. For convenience the term $\mu_1=\mu_2=0$ ($h_{\mu_1,\mu_2}=0$) is separated from the rest of the summation (indicated by the prime on the summation sign), this term being $-4\pi/O_a$.

If, in addition to $j_3=0$ also $j_1=j_2=0$, we are performing the summation over the sublattice to which the origin belongs. This means that we have to exclude the dipole at the origin, i.e., we have to subtract out the term for $\lambda_1=\lambda_2=0$, which is $-(4\pi/3)$ (see Ref. 10). We thus have

$$S_{0,0,0}{}^0(z,p_z)=-\frac{1}{a_1{}^3}\left\{-\frac{4\pi}{3}+\frac{4\pi}{O_a}+\frac{2}{\sqrt{\pi}}\sum{}'_{\lambda_1,\lambda_2}\Gamma(\tfrac{3}{2},\pi\sigma_\lambda{}^2)\sigma_\lambda{}^{-3}+\frac{2\pi^{3/2}}{O_a}\sum{}'_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\Gamma(-\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^2)\right\}. \quad (29)$$

The total sum at the origin for the case $j_3=0$ is

$$S_{j_1,j_2,0}(z,p_z)=S_{j_1,j_2,0}{}^{\lambda_3}(z,p_z)+S_{j_1,j_2,0}{}^0(z,p_z), \quad (30)$$

if either j_1 or j_2 (or both) $\neq 0$, and

$$S_{0,0,0}(z,p_z)=S_{0,0,0}{}^{\lambda_3}(z,p_z)+S_{0,0,0}{}^0(z,p_z), \quad (31)$$

if $j_1=j_2=j_3=0$. $S_{0,0,0}{}^{\lambda_3}$ follows immediately from (25) by substituting $j_1=j_2=0$.

For $j_3\neq 0$ the complete sum is always given by (24).

IV. GENERAL DIPOLE ORIENTATION

We decompose the dipole moment $\mathbf{p}$ into its components along the x, y, and z axes, then calculate the x, y, and z components of the field due to each dipole component, obtaining a total of nine sums. This may at first seem to be a rather cumbersome approach to the problem, but it turns out to simplify the calculations and the use of the final results. Referring to Fig. 5, the dipole moment is decomposed as follows:

$$\begin{aligned}\mathbf{p}_x&=p\mathbf{n}_x\sin\Theta\cos\Phi,\\ \mathbf{p}_y&=p\mathbf{n}_y\sin\Theta\sin\Phi,\\ \mathbf{p}_z&=p\mathbf{n}_z\cos\Theta,\end{aligned} \quad (32)$$

where $\mathbf{n}_x$, $\mathbf{n}_y$, and $\mathbf{n}_z$ are the unit vectors in the x, y, and z directions.

The field component in the κ-direction due to a unit dipole in the ν direction (κ, ν indicate x, y, or z) at a

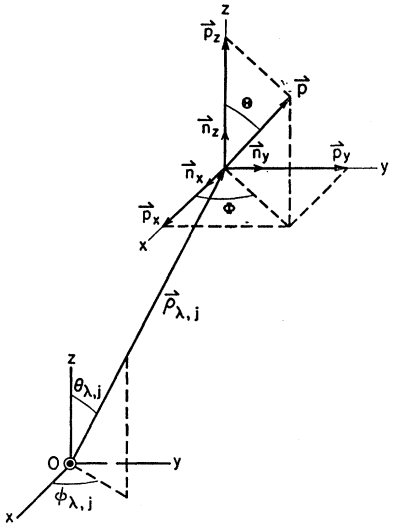

FIG. 5. Decomposition of a dipole $\mathbf{p}$ of arbitrary orientation into $\mathbf{p}_x$, $\mathbf{p}_y$, $\mathbf{p}_z$.

[14] The incomplete gamma function $\Gamma(\alpha,x)$ is defined for $\mathrm{Re}(\alpha)>0$ by

$$\Gamma(\alpha,x)=\int_x^\infty e^{-t}t^{\alpha-1}dt.$$

However, in connection with the convergence difficulties for $\mathrm{Re}(\alpha)\leq 0$ of the complement function $\gamma(\alpha,x)=\Gamma(\alpha)-\Gamma(\alpha,x)$, the definitions in terms of the confluent hypergeometric functions are to be preferred. Cf. Bateman Manuscript Project: *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, Chap. IX, p. 133.

distance $\mathbf{r}$ is given by

$$E(\kappa,\mathbf{p}_\nu)=3\frac{(\mathbf{p}_\nu\cdot\mathbf{r})(\mathbf{r}\cdot\mathbf{n}_\kappa)}{r^5}-\frac{\mathbf{p}_\nu\cdot\mathbf{n}_\kappa}{r^3}, \tag{33}$$

where $\mathbf{p}_\nu=\mathbf{n}_\nu$. The nine corresponding sums for unit dipoles in the x, y, and z directions become

$$S(x,p_x)=a_1^{-3}\sum_\lambda\{3(\boldsymbol{\sigma}_{\lambda,j})_x^2\rho_{\lambda,j}^{-5}-\rho_{\lambda,j}^{-3}\}, \tag{34}$$

$$S(y,p_y)=a_1^{-3}\sum_\lambda\{3(\boldsymbol{\sigma}_{\lambda,j})_y^2\rho_{\lambda,j}^{-5}-\rho_{\lambda,j}^{-3}\}, \tag{35}$$

$$S(z,p_z)=a_1^{-3}\sum_\lambda\{3(\lambda_3+j_3)^2(a_3/a_1)^2(\cos^2\delta)\rho_{\lambda,j}^{-5}-\rho_{\lambda,j}^{-3}\}, \tag{36}$$

$$S(x,p_y)=S(y,p_x)=a_1^{-3}\sum_\lambda 3(\boldsymbol{\sigma}_{\lambda,j})_x(\boldsymbol{\sigma}_{\lambda,j})_y\rho_{\lambda,j}^{-5}, \tag{37}$$

$$S(x,p_z)=S(z,p_x)=a_1^{-3}\sum_\lambda 3(\boldsymbol{\sigma}_{\lambda,j})_x(\lambda_3+j_3)(a_3/a_1)(\cos\delta)\rho_{\lambda,j}^{-5}, \tag{38}$$

$$S(y,p_z)=S(z,p_y)=a_1^{-3}\sum_\lambda 3(\boldsymbol{\sigma}_{\lambda,j})_y(\lambda_3+j_3)(a_3/a_1)(\cos\delta)\rho_{\lambda,j}^{-5}, \tag{39}$$

where we have suppressed the subscripts j_1, j_2, j_3 on S.

The derivations to obtain rapidly converging expressions for S are completely analogous to the derivation given for $S(z,p_z)$ in Sec. III. We will therefore merely quote the results. As in Sec. III, we consider the cases $j_3\neq 0$ and $j_3=0$ separately.

A. Case 1: $j_3\neq 0$

As in the corresponding case in Sec. III, the two-dimensional λ_1, λ_2 summation can in its entirety be equated to a summation over the two-dimensional reciprocal lattice by the use of Parseval's formula. The necessary Fourier transforms are given in Ref. 13 [cf. (I.12); (I.15)–(I.17) of Ref. 13]. We obtain:

$$S_{j_1,j_2,j_3}(x,p_x)=-4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_x^2h_{\mu_1,\mu_2}^{-1}\Omega_{j_3}(\mu_1,\mu_2), \tag{40}$$

$$S_{j_1,j_2,j_3}(y,p_y)=-4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_y^2h_{\mu_1,\mu_2}^{-1}\Omega_{j_3}(\mu_1,\mu_2), \tag{41}$$

$$S_{j_1,j_2,j_3}(z,p_z)=4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\Omega_{j_3}(\mu_1,\mu_2), \tag{42}$$

$$\begin{aligned}S_{j_1,j_2,j_3}(x,p_y)&=S_{j_1,j_2,j_3}(y,p_x)\\&=-4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_x(\mathbf{h}_{\mu_1,\mu_2})_yh_{\mu_1,\mu_2}^{-1}\Omega_{j_3}(\mu_1,\mu_2),\end{aligned} \tag{43}$$

$$\begin{aligned}S_{j_1,j_2,j_3}(x,p_z)&=S_{j_1,j_2,j_3}(z,p_x)\\&=i4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_x\Omega_{j_3}(\mu_1,\mu_2),\end{aligned} \tag{44}$$

$$\begin{aligned}S_{j_1,j_2,j_3}(y,p_z)&=S_{j_1,j_2,j_3}(z,p_y)\\&=i4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_y\Omega_{j_3}(\mu_1,\mu_2).\end{aligned} \tag{45}$$

$S_{j_1,j_2,j_3}(z,p_z)$, which was evaluated in Sec. III [cf. (24) and (24a)], is repeated here for the sake of completeness. From the form of (44) and (45) it is not immediately obvious that the sums are real, as they must be. However, one can show the reality of end results in the same fashion as outlined for (24) in Sec. III.

For a dipole $\mathbf{p}$ with arbitrary direction, the three field components along the coordinate directions are given by [cf. (32) and Fig. 5]

$$E_{j_1,j_2,j_3}(\kappa,\mathbf{p})=p\{S_{j_1,j_2,j_3}(\kappa,p_x)\sin\Theta\cos\Phi+S_{j_1,j_2,j_3}(\kappa,p_y)\sin\Theta\sin\Phi+S_{j_1,j_2,j_3}(\kappa,p_z)\cos\Theta\} \tag{46}$$

(κ indicates x, y, z).

B. Case 2: $j_3=0$

The field components due to all dipoles other than those in the plane containing the origin are obtained by the same method as used in Case 1, but omitting the term $\lambda_3=0$ in the λ_3 summation. The resultant formulas are obtained from (40)–(45) by replacing $\Omega_{j_3}(\mu_1,\mu_2)$ by $\Omega_0(\mu_1,\mu_2)$:

$$S_{j_1,j_2,0}{}^{\lambda_3}(x,p_x)=-4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_x^2h_{\mu_1,\mu_2}^{-1}\Omega_0(\mu_1,\mu_2), \tag{47}$$

$$S_{j_1,j_2,0}{}^{\lambda_3}(y,p_y)=-4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_y^2h_{\mu_1,\mu_2}^{-1}\Omega_0(\mu_1,\mu_2), \tag{48}$$

$$S_{j_1,j_2,0}{}^{\lambda_3}(z,p_z)=4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\Omega_0(\mu_1,\mu_2), \tag{49}$$

$$\begin{aligned}S_{j_1,j_2,0}{}^{\lambda_3}(x,p_y)&=S_{j_1,j_2,0}{}^{\lambda_3}(y,p_x)\\&=-4\pi^2O_a^{-1}a_1^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_x(\mathbf{h}_{\mu_1,\mu_2})_yh_{\mu_1,\mu_2}^{-1}\Omega_0(\mu_1,\mu_2),\end{aligned} \tag{50}$$

$$S_{j_1,j_2,0}{}^{\lambda_3}(x,p_z)=S_{j_1,j_2,0}{}^{\lambda_3}(z,p_x)$$
$$=i4\pi^2O_a{}^{-1}a_1{}^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_x\Omega_0(\mu_1,\mu_2), \tag{51}$$

$$S_{j_1,j_2,0}{}^{\lambda_3}(y,p_z)=S_{j_1,j_2,0}{}^{\lambda_3}(z,p_y)$$
$$=i4\pi^2O_a{}^{-1}a_1{}^{-3}\sum_{\mu_1,\mu_2}(\mathbf{h}_{\mu_1,\mu_2})_y\Omega_0(\mu_1,\mu_2). \tag{52}$$

$S_{j_1,j_2,0}{}^{\lambda_3}(z,p_z)$, which was evaluated in Sec. III [cf. (25) and (25a)], is repeated here for the sake of completeness.

We now evaluate the field components $S_{j_1,j_2,0}{}^{0}(\kappa,p_\nu)$ due to the dipoles in the plane which contains the origin. For these calculations it will be easier to express the functions to be summed in terms of $\phi_{\lambda,j}$ and $\sigma_{\lambda,j}$ (see Fig. 4) rather than in terms of $(\boldsymbol{\sigma}_{\lambda,j})_x$ and $(\boldsymbol{\sigma}_{\lambda,j})_y$. However, the final results will be written in terms of $(\boldsymbol{\sigma}_{\lambda,j})_x$, $(\boldsymbol{\sigma}_{\lambda,j})_y$, $(\mathbf{h}_{\mu_1,\mu_2})_x$ and $(\mathbf{h}_{\mu_1,\mu_2})_y$ to preserve a consistent notation.

Since the z direction is perpendicular to the plane containing the origin (x, y plane), it follows immediately from (33) that

$$E(x,p_z)=E(z,p_x)=E(y,p_z)=E(z,p_y)=0; \tag{53}$$

hence the corresponding sums $S_{j_1,j_2,0}{}^{0}(\kappa,p_z)$ and $S_{j_1,j_2,0}{}^{0}(z,p_\kappa)$ are zero (κ is x or y). The remaining sums are

$$S_{j_1,j_2,0}{}^{0}(z,p_z)=-a_1{}^{-3}\sum_{\lambda_1,\lambda_2}\sigma_{\lambda,j}{}^{-3},$$

which was evaluated in Sec. III [cf. Eqs. (26) and (27)], and

$$S_{j_1,j_2,0}{}^{0}(x,p_x)=a_1{}^{-3}\sum_{\lambda_1,\lambda_2}(3\cos^2\phi_{\lambda,j}-1)/\sigma_{\lambda,j}{}^{3}$$
$$=\tfrac{3}{2}a_1{}^{-3}\sum_{\lambda_1,\lambda_2}\cos2\phi_{\lambda,j}/\sigma_{\lambda,j}{}^{3}+\tfrac{1}{2}a_1{}^{-3}\sum_{\lambda_1,\lambda_2}\sigma_{\lambda,j}{}^{-3}, \tag{54}$$

$$S_{j_1,j_2,0}{}^{0}(y,p_y)=a_1{}^{-3}\sum_{\lambda_1,\lambda_2}(3\sin^2\phi_{\lambda,j}-1)/\sigma_{\lambda,j}{}^{3}$$
$$=-\tfrac{3}{2}a_1{}^{-3}\sum_{\lambda_1,\lambda_2}\cos2\phi_{\lambda,j}/\sigma_{\lambda,j}{}^{3}+\tfrac{1}{2}a_1{}^{-3}\sum_{\lambda_1,\lambda_2}\sigma_{\lambda,j}{}^{-3}, \tag{55}$$

$$S_{j_1,j_2,0}{}^{0}(x,p_y)=S_{j_1,j_2,0}{}^{0}(y,p_x)=3a_1{}^{-3}\sum_{\lambda_1,\lambda_2}\sin\phi_{\lambda,j}\cos\phi_{\lambda,j}/\sigma_{\lambda,j}{}^{3}$$
$$=\tfrac{3}{2}a_1{}^{-3}\sum_{\lambda_1,\lambda_2}\sin2\phi_{\lambda,j}/\sigma_{\lambda,j}{}^{3}. \tag{56}$$

Equations (54)–(56) are expressed in terms of $\cos2\phi_{\lambda,j}$ and $\sin2\phi_{\lambda,j}$ to facilitate the evaluation of the necessary integrals. Notice that the second sum in both (54) and (55) has been evaluated in Part B of Sec. III [cf. (26) and (28)]. Because the summand in the first sum of (54) and (55) depends on $\sigma_{\lambda,j}{}^{-5}$, we use for these sums the auxiliary convergence function $\Gamma(\frac{5}{2},\pi\sigma^2)/\Gamma(\frac{5}{2})$. The method is completely analogous to the one that leads from (27) to (28). The necessary Fourier transforms are evaluated in Ref. 13. Using $\Gamma(\frac{5}{2})=\frac{3}{2}\Gamma(\frac{3}{2})=\frac{3}{2}\cdot\frac{1}{2}\sqrt{\pi}$, we have

$$S_{j_1,j_2,0}{}^{0}(x,p_x)=\frac{1}{a_1{}^{3}}\left\{\frac{2\pi}{O_a}+\frac{2}{\sqrt{\pi}}\sum_{\lambda_1,\lambda_2}[\Gamma(\tfrac{5}{2},\pi\sigma_{\lambda,j}{}^{2})\cos2\phi_{\lambda,j}+\tfrac{1}{2}\Gamma(\tfrac{3}{2},\pi\sigma_{\lambda,j}{}^{2})]\sigma_{\lambda,j}{}^{-3}\right.$$
$$\left.-\frac{2\pi^{3/2}}{O_a}\sum{}'_{\mu_1,\mu_2}h_{\mu_1,\mu_2}[\Gamma(\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^{2})\cos2\varphi_{\mu_1,\mu_2}-\tfrac{1}{2}\Gamma(-\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^{2})]\exp[-2\pi i(j_1\mu_1+j_2\mu_2)]\right\}, \tag{57}$$

in which the result (28) for the second sum in (54) has been incorporated. The prime on the μ_1, μ_2 summation is justified since $\lim_{h\to0}h\Gamma(\frac{1}{2},\pi h^2)=0$, as is easily verified.

For an actual evaluation of the sums in (57) it will be found more convenient to make the substitution $\cos2\phi=2\cos^2\phi-1$, with $\cos^2\phi_{\lambda,j}=(\boldsymbol{\sigma}_{\lambda,j})_x{}^2\sigma_{\lambda,j}{}^{-2}$, $\cos^2\varphi_{\mu_1,\mu_2}=(\mathbf{h}_{\mu_1,\mu_2})_x{}^2h_{\mu_1,\mu_2}{}^{-2}$. Since the expression for $S_{j_1,j_2,0}{}^{0}(y,p_y)$ is obtained from $S_{j_1,j_2,0}{}^{0}(x,p_x)$ by simply replacing $(\boldsymbol{\sigma}_{\lambda,j})_x$ by $(\boldsymbol{\sigma}_{\lambda,j})_y$, and $(\mathbf{h}_{\mu_1,\mu_2})_x$ by $(\mathbf{h}_{\mu_1,\mu_2})_y$, we can use the following combined expression for both these sums:

$$S_{j_1,j_2,0}{}^{0}(\kappa,p_\kappa)=\frac{1}{a_1{}^{3}}\left\{\frac{2\pi}{O_a}+\frac{2}{\sqrt{\pi}}\sum_{\lambda_1,\lambda_2}[\Gamma(\tfrac{5}{2},\pi\sigma_{\lambda,j}{}^{2})(2(\boldsymbol{\sigma}_{\lambda,j})_\kappa{}^2\sigma_{\lambda,j}{}^{-2}-1)+\tfrac{1}{2}\Gamma(\tfrac{3}{2},\pi\sigma_{\lambda,j}{}^{2})]\sigma_{\lambda,j}{}^{-3}\right.$$
$$\left.-\frac{2\pi^{3/2}}{O_a}\sum{}'_{\mu_1,\mu_2}h_{\mu_1,\mu_2}[\Gamma(\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^{2})(2(\mathbf{h}_{\mu_1,\mu_2})_\kappa{}^2h_{\mu_1,\mu_2}{}^{-2}-1)-\tfrac{1}{2}\Gamma(-\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^{2})]\exp[-2\pi i(j_1\mu_1+j_2\mu_2)]\right\}, \tag{58}$$

where κ is either x or y.

The expression for $S_{j_1,j_2,0}{}^{0}(x,p_y)=S_{j_1,j_2,0}{}^{0}(y,p_x)$ is obtained from (56) by an analogous derivation. (For the necessary Fourier transform see Ref. 13.) Using $\sin2\phi_{\lambda,j}=2(\boldsymbol{\sigma}_{\lambda,j})_x(\boldsymbol{\sigma}_{\lambda,j})_y\sigma_{\lambda,j}{}^{-2}$ and $\sin2\varphi_{\mu_1,\mu_2}=2(\mathbf{h}_{\mu_1,\mu_2})_x(\mathbf{h}_{\mu_1,\mu_2})_y$

$\times h_{\mu_1,\mu_2}{}^{-2}$, we obtain

$$S_{j_1,j_2,0}{}^0(x,p_y)=S_{j_1,j_2,0}{}^0(y,p_x)$$
$$=\frac{1}{a_1{}^3}\left\{\frac{4}{\sqrt{\pi}}\sum_{\lambda_1,\lambda_2}\Gamma(\tfrac{5}{2},\pi\sigma_{\lambda,j}{}^2)(\boldsymbol{\sigma}_{\lambda,j})_x(\boldsymbol{\sigma}_{\lambda,j})_y\sigma_{\lambda,j}{}^{-5}-\frac{4\pi^{3/2}}{O_a}\sum'_{\mu_1,\mu_2}\Gamma(\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^2)(\mathbf{h}_{\mu_1,\mu_2})_x(\mathbf{h}_{\mu_1,\mu_2})_y h_{\mu_1,\mu_2}{}^{-1}\right.$$
$$\left.\times\exp[-2\pi i(j_1\mu_1+j_2\mu_2)]\right\}. \quad (59)$$

If, in addition to $j_3=0$ also $j_1=j_2=0$, we are performing the summation over the sublattice to which the origin belongs. This means that we have to exclude the term $\lambda_1=\lambda_2=0$ from the summations in (54)–(56). The expressions for $S_{0,0,0}{}^0(\kappa,p_\kappa)$ and $S_{0,0,0}{}^0(\kappa,p_\nu)$ (κ, ν indicate x or y) are then obtained from (58) and (59) by priming the λ_1, λ_2 summations, and in the case of (58) by also subtracting the term $2\pi/3$, which results from "priming" the sum $\frac{1}{2}\sum_{\lambda_1,\lambda_2}\sigma_\lambda{}^{-3}$ [cf. (29)]. Priming of the sums involving $\cos 2\phi$ and $\sin 2\phi$ in (54)–(56) does not give any extra terms. We thus have

$$S_{0,0,0}{}^0(\kappa,p_\kappa)=\frac{1}{a_1{}^3}\left\{-\frac{2\pi}{3}+\frac{2\pi}{O_a}+\frac{2}{\sqrt{\pi}}\sum'_{\lambda_1,\lambda_2}[\Gamma(\tfrac{5}{2},\pi\sigma_\lambda{}^2)(2(\boldsymbol{\sigma}_\lambda)_\kappa{}^2\sigma_\lambda{}^{-2}-1)+\tfrac{1}{2}\Gamma(\tfrac{3}{2},\pi\sigma_\lambda{}^2)]\sigma_\lambda{}^{-3}\right.$$
$$\left.-\frac{2\pi^{3/2}}{O_a}\sum'_{\mu_1,\mu_2}h_{\mu_1,\mu_2}[\Gamma(\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^2)(2(\mathbf{h}_{\mu_1,\mu_2})_\kappa{}^2 h_{\mu_1,\mu_2}{}^{-2}-1)-\tfrac{1}{2}\Gamma(-\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^2)]\right\}, \quad (60)$$

where κ is either x or y, and

$$S_{0,0,0}{}^0(x,p_y)=S_{0,0,0}{}^0(y,p_x)$$
$$=\frac{1}{a_1{}^3}\left\{\frac{4}{\sqrt{\pi}}\sum'_{\lambda_1,\lambda_2}\Gamma(\tfrac{5}{2},\pi\sigma_\lambda{}^2)(\boldsymbol{\sigma}_\lambda)_x(\boldsymbol{\sigma}_\lambda)_y\sigma_\lambda{}^{-5}-\frac{4\pi^{3/2}}{O_a}\sum'_{\mu_1,\mu_2}\Gamma(\tfrac{1}{2},\pi h_{\mu_1,\mu_2}{}^2)(\mathbf{h}_{\mu_1,\mu_2})_x(\mathbf{h}_{\mu_1,\mu_2})_y h_{\mu_1,\mu_2}{}^{-1}\right\}. \quad (61)$$

The total sum at the origin for the case $j_3=0$ is

$$S_{j_1,j_2,0}(\kappa,p_\nu)=S_{j_1,j_2,0}{}^{\lambda_3}(\kappa,p_\nu)+S_{j_1,j_2,0}{}^0(\kappa,p_\nu), \quad (62)$$

(κ, ν indicate x, y, or z) if either j_1 or $j_2\neq 0$ (or both), and

$$S_{0,0,0}(\kappa,p_\nu)=S_{0,0,0}{}^{\lambda_3}(\kappa,p_\nu)+S_{0,0,0}{}^0(\kappa,p_\nu), \quad (63)$$

if $j_1=j_2=j_3=0$.

For $j_3\neq 0$ the complete sums are given by (40)–(45).

Simplifications

We conclude this section by noting a general relation between dipole sums, and by listing some simplifications which occur when the lattice symmetry is higher than the triclinic symmetry, for which the expressions in this and the previous section were derived.

(1) We notice that

$$S(x,p_x)+S(y,p_y)+S(z,p_z)=0 \quad (64)$$

for any set of subscripts and superscripts. In other words, this relation is valid for the sums S_{j_1,j_2,j_3}, $S_{j_1,j_2,0}{}^{\lambda_3}$, $S_{j_1,j_2,0}{}^0$, or $S_{0,0,0}{}^0$. Relation (64) follows directly from the fact that for given λ, the corresponding terms in (34)–(36) add up to zero. For the sums S_{j_1,j_2,j_3}, Eq. (64) can be verified by adding (40), (41), and (42); for the sums $S_{j_1,j_2,0}{}^{\lambda_3}$ by adding (47), (48), and (49), and similarly for $S_{j_1,j_2,0}{}^0$ and $S_{0,0,0}{}^0$.

(2) For lattices of *monoclinic* or higher symmetry, the quantities δ, ξ_1, and ξ_2 [cf. (16a) and (16b)] are all zero and the equations simplify accordingly.

(3) For lattices of orthorhombic, tetragonal, and cubic symmetry a number of sums vanish, as can be easily deduced from (37)–(39).

$$S_{j_1,j_2,j_3}(x,p_\kappa)=S_{j_1,j_2,j_3}(\kappa,p_x)=0, \quad \text{for} \quad j_1=0,\tfrac{1}{2} \quad \text{if} \quad \kappa \text{ is } y \text{ or } z. \quad (65)$$

$$S_{j_1,j_2,j_3}(y,p_\kappa)=S_{j_1,j_2,j_3}(\kappa,p_y)=0, \quad \text{for} \quad j_2=0,\tfrac{1}{2} \quad \text{if} \quad \kappa \text{ is } x \text{ or } z. \quad (66)$$

$$S_{j_1,j_2,j_3}(z,p_\kappa)=S_{j_1,j_2,j_3}(\kappa,p_z)=0, \quad \text{for} \quad j_3=0,\tfrac{1}{2} \quad \text{if} \quad \kappa \text{ is } x \text{ or } y. \quad (67)$$

$$S_{j_1,j_2,0}{}^{\lambda_3}(z,p_\kappa)=S_{j_1,j_2,0}{}^{\lambda_3}(\kappa,p_z)$$
$$=S_{j_1,j_2,0}{}^{0}(z,p_\kappa)=S_{j_1,j_2,0}{}^{0}(\kappa,p_z)=0 \quad \text{if } \kappa \text{ is } x \text{ or } y, \tag{68}$$

$$S_{0,0,0}(\kappa,p_\nu)=S_{0,0,0}{}^{\lambda_3}(\kappa,p_\nu)=S_{0,0,0}{}^{0}(\kappa,p_\nu)=0,$$
$$S_{1/2,1/2,1/2}(\kappa,p_\nu)=0, \tag{69}$$

where κ, ν are x, y, or z and $\kappa\neq\nu$.

(4) For *square two-dimensional lattices*, which occur in the case of tetragonal lattices (if the z axis is chosen along the c axis), and of cubic lattices, (58) simplifies for cases for which $j_1=j_2=j$, to

$$S_{j,j,0}{}^{0}(\kappa,p_\kappa)=\frac{1}{a_1{}^3}\left\{\frac{2\pi}{O_a}+\frac{1}{\sqrt{\pi}}\sum_{\lambda_1,\lambda_2}\Gamma(\tfrac{3}{2},\pi\sigma_{\lambda,j}{}^2)\sigma_{\lambda,j}{}^{-3}-\frac{\pi^{3/2}}{O_a}\sum{}'_{\mu_1,\mu_2}h_{\mu_1,\mu_2}\Gamma(-\tfrac{1}{2},h_{\mu_1,\mu_2}{}^2)\exp[-2\pi ij(\mu_1+\mu_2)]\right\}, \tag{70}$$

(κ is x or y). The corresponding expression for $S_{0,0,0}{}^{0}(\kappa,p_\kappa)$ is obtained by priming the λ_1, λ_2 summation and adding the term $-2\pi/3$ inside the curly brackets.

V. DIPOLE-WAVE SUMS

In this section we briefly mention a type of dipole sums of a slightly more general form than the sums (34)–(39), namely

$$S=\sum_\lambda f(x_{\lambda,j},y_{\lambda,j},z_{\lambda,j})\exp[2\pi i\mathbf{k}\cdot\boldsymbol{\varrho}_\lambda], \tag{71}$$

where $\mathbf{k}$ is a reciprocal space vector, and f is any one of the summands in (34)–(39) [$\boldsymbol{\varrho}=\boldsymbol{\varrho}(x,y,z)$]. These sums, which for instance appear in the theory of crystal spectra, and the theory of dipolar ferromagnetism, have been called *dipole-wave sums* by Cohen and Keffer.[15]

The practical importance of the factor $\exp[2\pi i\mathbf{k}\cdot\boldsymbol{\varrho}_\lambda]$ is that it allows for a wave-type variation of the dipole strength through the lattice. A description of a lattice in which the dipole *orientation* varies in a wave-like fashion, can be obtained by multiplying the summands in $S(\kappa,p_x)$, $S(\kappa,p_y)$, and $S(\kappa,p_z)$ (κ indicates x, y, or z) by exponentials with the proper phase differences.

The way in which the exponential factor modifies the lattice summation formulas is as follows. In the sums over the ordinary lattice the exponential factor simply enters as it is. In the sums over the two-dimensional reciprocal lattice, the exponential factor gives rise to a shift in the origin, as well as to a phase factor. This is easily seen by combining the exponential factor with the δ functions when the Fourier transform is taken. Writing $\boldsymbol{\varrho}_\lambda=\boldsymbol{\sigma}_{\lambda_1,\lambda_2}+\lambda_3\mathbf{a}_3a_1{}^{-1}$, and $\mathbf{k}=\boldsymbol{\kappa}+k_3\mathbf{b}_3$, so that $\mathbf{k}\cdot\boldsymbol{\varrho}_\lambda=\boldsymbol{\kappa}\cdot\boldsymbol{\sigma}_{\lambda_1,\lambda_2}+k_3\lambda_3$ ($\boldsymbol{\kappa}$ is the projection of $\mathbf{k}$ in the two-dimensional reciprocal space), we have instead of (20)

$$[\mathrm{FT}_2\{\textstyle\sum_{\lambda_1,\lambda_2}\delta(\boldsymbol{\sigma}-\boldsymbol{\sigma}_{j_1,j_2}-\boldsymbol{\sigma}_{(\lambda_3+j_3)\xi_1,(\lambda_3+j_3)\xi_2}-\boldsymbol{\sigma}_{\lambda_1,\lambda_2})\times\exp(2\pi i\mathbf{k}\cdot\boldsymbol{\varrho}_\lambda)\}]^*=O_a{}^{-1}\textstyle\sum_{\mu_1,\mu_2}\exp[-2\pi i\times\{[j_1+(\lambda_3+j_3)\xi_1]\mu_1+[j_2+(\lambda_3+j_3)\mu_2+k_3\lambda_3\}]\times\delta\{\mathbf{h}-(\mathbf{h}_{\mu_1,\mu_2}-\boldsymbol{\kappa})\}. \tag{72}$$

The final result, corresponding to (24), which we denote by $S_{j_1,j_2,j_3}(z,p_z|k)$, is obtained from (24) by making the following changes: (1) replace h_{μ_1,μ_2} everywhere by $|\mathbf{h}_{\mu_1,\mu_2}-\boldsymbol{\kappa}|$, (2) replace $(\xi_1\mu_1+\xi_2\mu_2)$ by $(\xi_1\mu_1+\xi_2\mu_2+k_3)$. Corresponding changes are to be made in the expressions (40)–(45), and (47)–(52) if these sums contain exponential factors. In the sums (58)–(61), one only has to make the change (1).

In Sec. VII we mention an example in which an exponential factor can be used.

VI. USE OF THE SUMMATION FORMULAS

With the summation formulas given in the preceding sections one can evaluate dipole fields in arbitrary dipole lattices. Owing to their generality these formulas look rather formidable, but they are actually rather easy to use, especially since summing over 3 or 4 shells of neighbors is normally sufficient to obtain accuracy within 0.1%. And of course, as we mentioned above, for lattices of higher than triclinic symmetry, the equations simplify greatly. Fortunately, triclinic systems are not encountered too often.

The lattice sums over the plane containing the origin are the most troublesome to evaluate, since one must use incomplete gamma functions, which are not extensively tabulated, as is the exponential function. For that reason we have tabulated in Ref. 13 those incomplete gamma functions that enter in the lattice summation expressions, which were derived above. In the table we have chosen a reasonable density of values of the argument. However, in most cases interpolation will have to be used which necessarily limits the accuracy of the calculation.

In some cases it is possible to avoid these difficulties by rechoosing the $\mathbf{a}_1$, $\mathbf{a}_2$ planes, so that none of the planes pass through the origin. As stated previously, if differently oriented sets of $\mathbf{a}_1$, $\mathbf{a}_2$ planes are used for different sublattices, corrections for the different depolarization fields of these sublattices have to be made, so that all correspond to the same crystal shape when they are added together.

In these derivations all lengths have been normalized to the length of the sublattice basis vector $\mathbf{a}_1$, which at the same time indicates the x direction. The lengths of the two-dimensional lattice vector and the reciprocal lattice vector are given by $\sigma_{\lambda,j}=[(\sigma_{\lambda,j})_x{}^2+(\sigma_{\lambda,j})_y{}^2]^{1/2}$

[15] M. H. Cohen and F. Keffer, Phys. Rev. **99**, 1128 (1955).

TABLE I. Quantities used in the evaluation of lattice sums for lattices of various symmetry. The symbols are explained in the text. λ stands for the two indices λ_1 and λ_2. For j_1 and/or j_2 unequal to zero, they must be added to λ_1 and λ_2, respectively.

Lattice symmetry	$(\sigma_\lambda)_x$	$(\sigma_\lambda)_y$	$(\mathbf{h}_{\mu_1,\mu_2})_x$	$(\mathbf{h}_{\mu_1,\mu_2})_y$	O_a	V_a
Cubic	λ_1	λ_2	μ_1	μ_2	1	1
Tetragonal[a]	λ_1	λ_2	μ_1	μ_2	1	a_3/a_1
Orthorhombic	λ_1	$\lambda_2 a_2/a_1$	μ_1	$\mu_2 a_1/a_2$	a_2/a_1	a_2a_3/a_1^2
Hexagonal[b] $\gamma=60°$	$\lambda_1+\frac{1}{2}\lambda_2$	$\frac{1}{2}\sqrt{3}\lambda_2$	μ_1	$(-\mu_1+2\mu_2)/\sqrt{3}$	$\frac{1}{2}\sqrt{3}$	$\frac{1}{2}\sqrt{3}a_3/a_1$
$\gamma=120°$	$\lambda_1-\frac{1}{2}\lambda_2$	$\frac{1}{2}\sqrt{3}\lambda_2$	μ_1	$(\mu_1+2\mu_2)/\sqrt{3}$	$\frac{1}{2}\sqrt{3}$	$\frac{1}{2}\sqrt{3}a_3/a_1$
Monoclinic	$\lambda_1+\lambda_2(a_2/a_1)\cos\gamma$	$\lambda_2(a_2/a_1)\sin\gamma$	μ_1	$-\mu_1\cot\gamma+\mu_2(a_1/a_2)\csc\gamma$	$(a_2/a_1)\sin\gamma$	$(a_2a_3/a_1^2)\sin\gamma$
Triclinic	$\lambda_1+\lambda_2(a_2/a_1)\cos\gamma$	$\lambda_2(a_2/a_1)\sin\gamma$	μ_1	$-\mu_1\cot\gamma+\mu_2(a_1/a_2)\csc\gamma$	$(a_2/a_1)\sin\gamma$	$(a_2a_3/a_1^2)\sin\gamma\cos\delta$

[a] For the case in which the z axis is chosen along the a_3 axis (c axis) of the crystal. If the z axis is chosen along the a_2 axis, use the expressions for the orthorhombic lattice with $a_3=1$.
[b] We have listed the quantities for two different choices of the unit cell.

and $h_{\mu_1,\mu_2}=[(\mathbf{h}_{\mu_1,\mu_2})_x^2+(\mathbf{h}_{\mu_1,\mu_2})_y^2]^{1/2}$, respectively. Since the summations are carried out over λ_1 and λ_2, and μ_1 and μ_2, which measure distances along the basis vectors of the ordinary two-dimensional lattice, and the reciprocal two-dimensional lattice, respectively, the x and y components of $\boldsymbol{\sigma}_{\lambda,j}$ have to be expressed in terms of λ_1 and λ_2, and those of $\mathbf{h}_{\mu_1,\mu_2}$ in terms of μ_1 and μ_2. This has been done in Table I for the various lattices. For simplicity it has been assumed that j_1 and j_2 are zero. For nonzero j_1 and/or j_2 simply add their values to λ_1 and λ_2, respectively. Further, we have listed the values of O_a, which is the area of the untransformed two-dimensional lattice unit cell in the $\mathbf{a}_1$, $\mathbf{a}_2$ planes (in units a_1^2), and V_a, which is the unit cell volume of the ordinary space lattice (in units a_1^3).

The evaluation of the lattice sums has now become a relatively simple matter. One chooses the proper expressions from Table I for the sublattice symmetry under consideration, substitutes these into the appropriate lattice summation expression, and performs the straightforward arithmetic calculation.

VII. EXAMPLE: POTASSIUM FERROCYANIDE

As an example we calculate the dipole field at the dipole positions in potassium ferrocyanide. This compound, $K_4Fe(CN)_6\cdot 3H_2O$, is monoclinic, pseudotetragonal, with basis vectors[16] $a_0=c_0=9.32$ Å, and $b_0=16.84$ Å.[17] The electric dipoles under consideration are those of the water molecules. The water molecules are located and their dipole moments are oriented in the a, c planes which occur at the positions $z=0$, $\pm\frac{1}{2}b_0$, $\pm b_0$, etc. The positions and orientations[18] of the dipoles in the planes $z=0$, $\pm b_0$, $\pm 2b_0$, etc., are shown in Fig. 6, while the dipoles in the planes $z=\pm\frac{1}{2}b_0$, $\pm\frac{3}{2}b_0$, etc., are shifted an amount $\frac{1}{2}a_0$ in the a direction from the locations shown in Fig. 6, preserving the orientations.

In Fig. 6, the solid lines outline the a, c face of the unit cell, while the broken lines outline the a, c faces of three of the sublattice unit cells which are used in the calculation. The sublattices are chosen so that each contains dipoles of one orientation only. The designations e, f_1, and f_2 indicate dipole positions as well as dipole orientations for these three sublattices (e and f are the occupied positions in the C_{2h}^6 symmetry). Since the dipoles in the planes $z=\pm\frac{1}{2}b_0$, $\pm\frac{3}{2}b_0$, etc., are shifted a distance $\frac{1}{2}a_0$ in the a direction three more sublattices must be introduced to include these dipoles, giving a total of six sublattices. For all sublattices the basis vectors are $\mathbf{a}_1=\frac{1}{2}\mathbf{c}_0$, $\mathbf{a}_2=\mathbf{a}_0$, and $\mathbf{a}_3=\mathbf{b}_0$. Normalizing to a_1 we have $a_2/a_1=2.00$ and $a_3/a_1=3.614$. Further,

$$\sigma_{\lambda,j}=[(\lambda_1+j_1)^2+4(\lambda_2+j_2)^2]^{1/2}$$

and

$$h_{\mu_1,\mu_2}=[\mu_1^2+\tfrac{1}{4}\mu_2^2]^{1/2}.$$

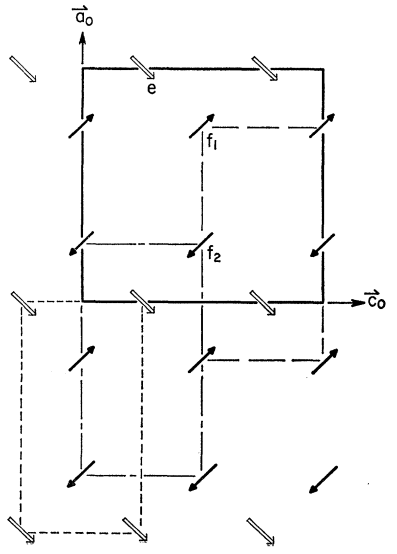

FIG. 6. Location and orientation of the dipole moments of the water molecules in a plane $z=0$ of potassium ferrocyanide.

[16] Cf. *Structure Reports*, edited by A. J. C. Wilson (Oosthoek, Utrecht, 1952), Vol. VI, p. 421.
[17] We use the customary designation a_0, b_0, c_0 for the unit cell basis vectors, to distinguish them from the sublattice basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$.
[18] T. Tsang, G. K. McCormick, D. E. O'Reilly, and G. E. Schacher, Bull. Am. Phys. Soc. 9, 503 (1964). The dipole orientations used here are derived from high-temperature NMR data.

TABLE II. Values of the dipole sums $O_a a_1^3 S_{j_1,j_2,j_3}(x,p_x)$, $O_a a_1^3 S_{j_1,j_2,j_3}(y,p_y)$, $O_a a_1^3 S_{j_1,j_2,j_3}(z,p_z)$ for selected points in the sublattice unit cell of potassium ferrocyanide. $a_2/a_1=2.00$, $a_3/a_1=3.614$.

Point[a]	j_1	j_2	j_3	$O_a a_1^3 S_{j_1,j_2,j_3}(x,p_x)$	$O_a a_1^3 S_{j_1,j_2,j_3}(y,p_y)$	$O_a a_1^3 S_{j_1,j_2,j_3}(z,p_z)$
1	0	0	0	9.6126	−1.5136	−8.1015
2	$\frac{1}{2}$	$\frac{1}{4}$	0	8.2585	8.2585	−14.0996
3	0	$\frac{1}{2}$	0	−0.5791	10.5559	20.5406
4	$\frac{1}{2}$	$\frac{3}{4}$	0	8.2585	8.2585	−14.0996
5	0	0	$\frac{1}{2}$	−0.0016	−0.2732	0.2748
6	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	0.0016	0.0016	−0.0032
7	0	$\frac{1}{2}$	$\frac{1}{2}$	−0.0016	0.2700	0.2685
8	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{1}{2}$	0.0016	0.0016	−0.0032

[a] The numbering of the points corresponds to that in Fig. 7.

The dipole orientations are given by

$$\mathbf{p}_e = p(\mathbf{n}_1 - \mathbf{n}_2)/\sqrt{2}, \tag{73a}$$

$$\mathbf{p}_{f_1} = -\mathbf{p}_{f_2} = p(\mathbf{n}_1 + \mathbf{n}_2)/\sqrt{2}, \tag{73b}$$

where p is the strength of the permanent dipole moment of a water molecule, and $\mathbf{n}_1$ and $\mathbf{n}_2$ are the unit vectors in the $\mathbf{a}_1$ and $\mathbf{a}_2$ directions, respectively. Since there are six sublattices and we want to calculate the field at the six dipole positions, it would, in general, be necessary to perform 36 separate calculations. However, since all six sublattices have the same basis vectors the problem can be reduced to evaluating lattice sums for the eight points in the sublattice unit cell which are shown in Fig. 7. Further, because the sublattice unit cell is orthorhombic and because the points at which the sums are to be evaluated are located in reflection planes in the sublattice unit cell, all the "mixed" sums vanish [cf. (65)–(67)] and the only sums left to evaluate are $S_{j_1,j_2,j_3}(\kappa,p_\kappa)$, where κ is x, y, or z. The results of the calculations are compiled in Table II, where we have listed the indices j_1, j_2, j_3 of the eight points and the values of the sums at these points. At this point we re-emphasize the fact that the value of $S_{j_1,j_2,j_3}(z,p_z)$ contains a depolarization contribution, while $S_{j_1,j_2,j_3}(\kappa,p_\kappa)$ for $\kappa=x$ or y does not contain such a contribution. This, as we recall, is due to the fact that the planewise summation is carried out over the x, y planes, which corresponds to summation over a slab-shaped crystal perpendicular to the z axis. Consequently, the electric fields in the x and y directions, given in Tables III and IV, do not contain a depolarization field. For any other shape of the crystal one has to correct the numbers in the tables with the appropriate depolarization contributions.

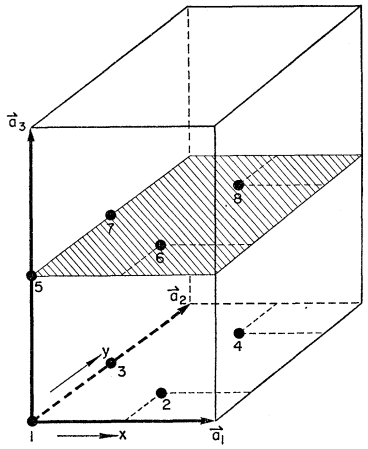

FIG. 7. Points in the sublattice unit cell of potassium ferrocyanide at which the sums $O_a a_1^3 S_{j_1,j_2,j_3}(\kappa,p_\kappa)$ (κ indicates x, y or z) have been evaluated.

We are now in a position to evaluate the components of the electric field at each dipole site. The e dipoles in the plane $z=\frac{1}{2}b_0$ are related by a lattice symmetry operation to the e dipoles in the plane $z=0$; the same is true for the f_1 and f_2 dipoles. Therefore, in tabulating the results we need not consider the planes $z=0$ and $z=\frac{1}{2}b_0$ separately (it should be pointed out, however, that this does not mean that the calculations could have been carried out with three sublattices rather than six). In Tables III and IV we give the x and y components of the electric field at each dipole site, listed according to the dipoles that produce the field. Since the dipoles have no component in the z direction, the z component of the electric field is zero. As an example of how the numbers in the tables are obtained we have

$$E_x(\text{at } e, \text{ due to } f_1) = (\mathbf{p}_{f_1})_x[S_{\text{site } 2}(x,p_x) + S_{\text{site } 8}(x,p_x)],$$

where $(\mathbf{p}_{f_1})_x = p/\sqrt{2}$. The numbers in the Tables III and IV are in units of $p/(\sqrt{2}O_a a_1^3)$.

We note that the f_1 and f_2 dipoles together produce a zero net field at the e sites. This is due to the fact that the f_1 and f_2 sites are related by inversion with respect to any e site, and the fact that the f_1 and f_2 dipoles are antiparallel.

TABLE III. x component of the dipole field in potassium ferrocyanide at the e, f_1, and f_2 positions (see text). The numbers are in units $p/(\sqrt{2}O_a a_1^3)$.

Field point \ Source dipoles	e	f_1	f_2
e	9.6110	8.2601	−8.2601
f_1	8.2601	9.6110	0.5807
f_2	8.2601	−0.5807	−9.6110

TABLE IV. y component of the dipole field in potassium ferrocyanide at the e, f_1, and f_2 positions (see text). The numbers are in units $p/(\sqrt{2}O_a a_1^3)$.

Field point \ Source dipoles	e	f_1	f_2
e	1.2436	8.2601	−8.2601
f_1	−8.2601	−1.2436	−10.2827
f_2	−8.2601	10.2827	1.2436

Example of the Use of the Factor $\exp[2\pi i\mathbf{k}\cdot\varrho_\lambda]$

The f_1 and f_2 sublattices in potassium ferrocyanide may be combined into one single sublattice by the use of an exponential factor, as introduced in Sec. V. It is seen in Fig. 6 that, starting from either an f_1 or f_2 site, the dipole direction reverses when going a distance $\frac{1}{2}a_0$ in either the $\mathbf{a}_0$ or $\mathbf{c}_0$ direction. If we choose new sublattice basis vectors $\mathbf{a}_1'=\mathbf{a}_1$, $\mathbf{a}_2'=\frac{1}{2}\mathbf{a}_2$ (cf. Fig. 7), then the choice of the reciprocal space vector $\mathbf{k}=\frac{1}{2}(\mathbf{b}_1'+\mathbf{b}_2')$, where the $\mathbf{b}'$'s are related to the $\mathbf{a}'$'s according to (21), gives rise to the exponential factor

$$\exp[2\pi i\mathbf{k}\cdot\varrho_\lambda']=(-1)^{(\lambda_1+\lambda_2)},$$

where ϱ_λ' is expressed in the basis vectors $\mathbf{a}_1'$, $\mathbf{a}_2'$, $\mathbf{a}_3$ (normalized to a_1'). In the lattice sum this factor has the effect of changing the sign when going from an f_1 to an f_2 site and vice versa. This properly represents the reversal of the dipole direction. The choice of $\mathbf{a}_1'$ and $\mathbf{a}_2'$ means that we have two-dimensional sums over square lattices. Furthermore, the sum over the reciprocal lattice has to be performed with respect to the point $\mathbf{k}=\frac{1}{2}(\mathbf{b}_1'+\mathbf{b}_2')$, which is the center of the square.

Note added in proof. Recent dielectric measurements and NMR results indicate that the water molecule dipole orientations shown in Fig. 6 for potassium ferrocyanide are incorrect. The values of the dipole sums presented in Table II are of course valid since they do not depend on the dipole orientations. However, the values of the field components presented in Table III are incorrect, since they are dependent on the dipole orientations. Of course all results are valid for the model shown in Fig. 6.

One of the authors (G. E. S.) is in the process of writing a comprehensive FORTRAN program for the numerical evaluation of the lattice sums treated in this paper. Information concerning the program may be obtained from this author.

APPENDIX: THE LORENTZ-FACTOR MATRIX

In this Appendix we express the elements $\gamma_{\kappa,\nu}{}^{i,j}$ of the Lorentz-factor matrix in terms of the dipole sums $S(\kappa,p_\nu)$ which were treated in this paper (κ, ν indicate x, y, z). For brevity we are suppressing the subscripts on S, but in each case it will be evident which subscripts are appropriate.

First, we consider a system with parallel dipoles $\mathbf{p}(p_x,p_y,p_z)$ of one kind only [i.e., there is only one sublattice; the complete notation for S is $S_{0,0,0}(\kappa,p_\nu)$]. In the absence of external charges the components of the internal electric field, in a slab-shaped crystal perpendicular to the z axis, are

$$E_{\text{int},\kappa}=V_a\sum_\nu S(\kappa,p_\nu)P_\nu, \tag{A1}$$

where $P_\nu=p_\nu/V_a$ are the components of the polarization (V_a is the volume of the sublattice unit cell). On the other hand, expressed in the Lorentz form [cf. Eq. (1)] we have for the internal field components

$$E_{\text{int},\kappa}=E_\kappa+\sum_\nu\gamma_{\kappa,\nu}P_\nu. \tag{A2}$$

In deriving the rapidly converging expressions for the dipole sums $S(\kappa,p_\nu)$ we have carried out the summations over a slab-shaped crystal perpendicular to the z axis. Since there are no external charges the only sources of the field $\mathbf{E}$ are the polarization charges on the faces of the slab, hence $E_x=E_y=0$, $E_z=-4\pi P_z$. Equating Eqs. (A1) and (A2) we thus find

$$\gamma_{\kappa,\nu}=V_aS(\kappa,p_\nu)\quad(\kappa=\nu=z\text{ excluded}) \tag{A3}$$

$$\gamma_{z,z}=V_aS(z,p_z)+4\pi. \tag{A4}$$

The tensor $\gamma_{\kappa,\nu}$ has the following properties:

(1) $\gamma_{\kappa,\nu}$ is symmetric, because $S(\kappa,p_\nu)=S(\nu,p_\kappa)$,
(2) $\mathrm{Tr}(\gamma_{\kappa,\nu})=\sum_\kappa\gamma_{\kappa,\kappa}=4\pi$, because of Eq. (64).

As we have pointed out in the introduction, the Lorentz factors $\gamma_{\kappa,\nu}$ are independent of the crystal shape; they are exclusively determined by the crystal symmetry. Equations (A3) and (A4) relate the shape-dependent dipole sums $S(\kappa,p_\nu)$ as evaluated by the method of planewise summation to the shape-independent Lorentz factors $\gamma_{\kappa,\nu}$.

For the case of many sublattices we have for the κ component of the internal field at a lattice position of sublattice i

$$E^{(i)}{}_{\text{int},\kappa}=\sum_{j(\text{sublattices})}V_a{}^{(j)}\sum_\nu S_{j_1,j_2,j_3}(\kappa,p_\nu)P^{(j)}{}_\nu. \tag{A5}$$

The index j labels the sublattices, $V_a{}^{(j)}$ is the volume of the sublattice unit cell and $P^{(j)}{}_\nu=p^{(j)}{}_\nu/V_a{}^{(j)}$ is the polarization of sublattice j. The subscripts j_1, j_2, j_3 on S, however, indicate the origin of the unit cell of sublattice j with respect to the origin of sublattice i. Equation (A2) is replaced by

$$E^{(i)}{}_{\text{int},\kappa}=E_\kappa+\sum_{j(\text{sublattices})}\sum_\nu\gamma_{k,\nu}{}^{i,j}P^{(j)}{}_\nu. \tag{A6}$$

Again $E_x=E_y=0$, $E_z=-4\pi\sum_j P^{(j)}{}_z$, hence

$$\gamma_{\kappa,\nu}{}^{i,j}=V_a{}^{(j)}S_{j_1,j_2,j_3}(\kappa,p_\nu)\quad(\kappa=\nu=z\text{ excluded}) \tag{A7}$$

$$\gamma_{z,z}{}^{i,j}=V_a{}^{(j)}S_{j_1,j_2,j_3}(z,p_z)+4\pi. \tag{A8}$$