Nijboer, B. R. A.
De Wette, F. W.

Physica XXIV
Zernike issue
422–431

THE INTERNAL FIELD IN DIPOLE LATTICES

by B. R. A. NIJBOER and F. W. DE WETTE

Instituut voor theoretische fysica, Rijksuniversiteit te Utrecht, Nederland

Synopsis

The internal field for Bravais lattices of equal parallel dipoles having monoclinic and higher symmetry is evaluated. The electric field at a lattice point due to all the other dipoles in the lattice is given by a conditionally convergent sum. It is shown that, when considering a slab of dielectric material in a parallel plate condensor, this 'dipole sum' should be summed 'plane-wise' in order to obtain the correct contribution to the internal field. Rapidly converging expressions for this contribution are derived. For a simple cubic lattice the resulting expression for the internal field reduces, of course, to that of Lorentz.

§ 1. *Introduction.* In a previous publication [1]) (to be quoted as I) we have presented a convenient method for the calculation of lattice sums of a rather general type. While the evaluation of such sums finds application in many branches of solid state physics, we shall be mainly interested in the calculation of the electric field in multipole lattices. This problem will be discussed in some detail in a forthcoming paper. In the present note we shall be concerned with a particular example of this general problem, namely with the evaluation of the field strength at the position of a lattice point in a lattice consisting of parallel dipoles of equal strength.

In view of the fact that Ornstein and Zernike[2]) were among the first to make explicit calculations for such a dipole lattice with regard to a somewhat similar problem, this paper may perhaps be an appropriate contribution to an issue of Physica dedicated to Zernike at his 70th birthday.

One will have noted that our problem, i.e. the calculation of the field in a lattice point of a lattice of equal, parallel dipoles, is closely related to the problem of the so-called internal field in the theory of the dielectric constant, which, for cubic lattices, was solved many years ago by Lorentz [3]). It is our aim to rederive Lorentz' result for cubic lattices by a direct summation of the contributions of the dipoles. This procedure may elucidate some points which have not always been clearly understood. Furthermore, our method can also be used to evaluate the internal field in non-cubic(tetragonal, hexagonal, orthorhombic and monoclinic) crystals, which cannot be readily treated by Lorentz' method.

Let us recall that the internal field $\mathbf{E}_i$, i.e. the electric field effective in polarizing a particle in a medium, is due partly to the externally applied field

and partly to the dipoles induced in all other particles. Lorentz has shown that for cubic crystals $\mathbf{E}_i$ is given by

$$\mathbf{E}_i = \mathbf{E} + \tfrac{4}{3}\pi \mathbf{P}, \tag{1}$$

where $\mathbf{E}$ is the electric fieldstrength in the dielectric medium and $\mathbf{P}$ the polarization, i.e. the dipole moment per unit volume. ((1) is also valid for isotropic substances such as gases and liquids when correlation effects are neglected). This value for the internal field leads in a direct way to the well-known equations of Clausius-Mossotti for the dielectric constant and of Lorentz-Lorenz for the refractive index.

In the usual derivation of (1) one considers a dielectric medium between the plates of a parallel plate condensor. Further, around the field point a spherical region is considered of dimensions such that, for the purpose of finding the field in the center, the polarization of the medium outside the sphere may be taken as continuous. The internal field $\mathbf{E}_i$ at the center of the sphere then consists of four contributions: $\mathbf{E}_1$, $\mathbf{E}_2$, $\mathbf{E}_3$ and $\mathbf{E}_4$. $\mathbf{E}_1$ is the field due to the real charges on the condensor plates, i.e. $\mathbf{E}_1 = \mathbf{D}$. $\mathbf{E}_2$ gives the field due to the apparent surface charges at the outer boundary of the dielectric slab, so that $\mathbf{E}_2 = -4\pi\mathbf{P}$. $\mathbf{E}_3$ is the field due to the apparent charges on the spherical surface, giving $\mathbf{E}_3 = \frac{4}{3}\pi\,\mathbf{P}$. Finally $\mathbf{E}_4$ is the contribution from the dipoles within the sphere (except from the dipole in the center). For cubic crystals $\mathbf{E}_4$ is easily shown to vanish exactly (see below). Therefore we have

$$\mathbf{E}_i = \mathbf{D} - 4\pi\,\mathbf{P} + \tfrac{4}{3}\pi\,\mathbf{P} = \mathbf{E} + \tfrac{4}{3}\pi\,\mathbf{P}.$$

Clearly, the contribution of all dipoles in the slab of dielectric material is in this case (cubic crystals) given by

$$\mathbf{E}_2 + \mathbf{E}_3 + \mathbf{E}_4 = -\tfrac{8}{3}\pi\mathbf{P}. \tag{2}$$

Evidently, this latter result should also be the outcome of a direct summation of the contributions of all dipoles over the lattice. Now here a difficulty arises.

Let us consider an infinite simple cubic lattice with equal point dipoles $\mathbf{p}$ at the lattice points, all directed parallel to one of the four-fold axes. The direction of $\mathbf{p}$ will be taken as the positive z-direction. The z-component of the electric field at a lattice point due to all the other dipoles in the lattice is then given by the lattice sum

$$S' = p \sum_\lambda{}' 2P_2(\cos\theta_\lambda)/r_\lambda{}^3. \tag{3}$$

λ denotes the three numbers λ_1, λ_2, and λ_3 appearing in the expression for the lattice vector $\mathbf{r}_\lambda = \lambda_1\mathbf{a}_1 + \lambda_2\mathbf{a}_2 + \lambda_3\,\mathbf{a}_3$; $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are the basic vectors determining the unit cell; θ_λ is the polar angle of the lattice vector $\mathbf{r}_\lambda$. A prime on a summation sign means that the term $\lambda = 0$ (i.e. $\lambda_1 = \lambda_2 = \lambda_3 =$

$= 0$) is not included (for notation see I). Now the sum (3), the dipole sum as we shall call it, is only *conditionally convergent* with the consequence that the value of the sum depends on the order of summation. If the summation is carried out "spherically", i.e. if the contributions of successive shells of neighbours are added, the result is zero. Thus

$$S' = 0 \text{ (summed spherically).} \tag{4}$$

For the same reason $\mathbf{E}_4$, i.e. the sum over a finite sphere, also vanishes. In both cases this is due to the fact that the terms belonging to the same shell of neighbours cancel each other. One might also say that it is a consequence of the fact that there exists no linear combination of the spherical harmonics $Y_{2,m}(\theta, \phi)$ which has the cubic symmetry. Evidently, the 'spherical' summation of the dipole sum is not appropriate for the calculation of the internal field in a slab of dielectric material and the question arises which method of summing the dipole sum (3) would yield the value $-\frac{8}{3}\pi P$ (cf. (2)), that leads to the correct expression (1) for the internal field. It may be remarked here that, instead of summing the dipole sum over an infinite lattice (in which case a summation prescription should be provided), one could also consider the dipole sum taken over a finite crystal. Then its value would be shape-dependent, as is well-known from the theory of the demagnetization factor. If one evaluates the dipole sum for a finite lattice of given shape and then goes to the limit of an infinite crystal under conservation of shape, then thereby a summation prescription for the infinite sum has been provided.

Considering this fact of shape dependence of the dipole sum (3), it seems obvious that, in order to obtain the value $-\frac{8}{3}\pi P$ for a *slab* of dielectric material, one should sum (3) "plane-wise", i.e. first calculate the sums in planes perpendicular to the direction of the dipoles (planes parallel to the condensor-plates), and then sum the contributions of all the planes. In other words one should first sum over the indices λ_1 and λ_2, and only then over λ_3. (if $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are chosen along the x-, y- and z-axis respectively). It will be shown below that this procedure gives the correct result. Furthermore it will be seen that it is immaterial that the λ_3-summation is extended to infinity (whereas in an actual condensor the distance between the plates is always macroscopically small), since the convergence with respect to λ_3 is extremely rapid, once that the λ_1, λ_2-summations have been carried out.

Our method can be easily extended to yield the internal field in non-cubic (tetragonal, hexagonal, orthorhombic, monoclinic) crystals. For tetragonal and hexagonal crystals the internal field has been calculated before [4)5)], but according to methods which in our opinion are less satisfactory than the present one.

We have argued above that the contribution of the dipoles to the internal field, i.e. the dipole sum (3), is dependent on the order of summation. This,

of course, does not apply to the expression (1) for the internal field itself. It should be remembered that **E** in (1) stands for the electric fieldstrength in the medium and not for the external field, as is asserted sometimes. **E** is obtained by properly averaging the microscopic electric field. The difference between **E** and $\mathbf{E}_i$, therefore, is a local effect, a point which is brought out much more clearly by Lorentz' original derivation of (1) than by the usual derivation which was given at the beginning of this section. If in a sample of a certain shape the dipoles give a contribution different from that $(-\frac{8}{3}\pi P)$ in a slab between two parallel condensor plates (the dipole contribution in a spherical sample, for instance, is zero as explained above), then also the contribution of the external charges will be different from **D** in such a way that the sum is again given by (1).

§ 2. *Direct evaluation of the dipole sum for a simple cubic lattice.* In this section we will present a direct way of summation of the dipole sum (3) for a simple cubic lattice, which illustrates the convergence properties very nicely. For simplicity we assume that one of the four-fold axes is perpendicular to the condensor-plates. The general case of arbitrary orientation of the four-fold axes can be treated in the same way, giving the same result.

Introducing the dimensionless quantity $\rho = r/a$, where a is the distance between nearest neighbours, we may write

$$S' = P \sum_\lambda' 2P_2(\cos\theta)/\rho_\lambda^3, \tag{5}$$

$p/a^3 = P$ is the polarization. S' which is, except for a multiplying constant, equal to the sum $S'_{2,0}(0|0, \frac{1}{2})$ as defined in I, § 6, is now treated by the method which was developed in I, where a rapid convergence of lattice sums was obtained by means of an auxiliary function (cf. I, § 4). Making use in this case of the function $\Gamma(\frac{5}{2}, \pi\rho^2)/\Gamma(\frac{5}{2})$ we may split (5) into two sums

$$S' = P\left[\sum_\lambda' \frac{\Gamma(\frac{5}{2}, \pi\rho_\lambda^2).2P_2(\cos\theta_\lambda)}{\Gamma(\frac{5}{2})\rho_\lambda^3} + \sum_\lambda' \frac{\gamma(\frac{5}{2}, \pi\rho_\lambda^2).2P_2(\cos\theta_\lambda)}{\Gamma(\frac{5}{2})\rho_\lambda^3}\right], \tag{6}$$

where

$$\Gamma(\alpha, x) = \int_x^\infty e^{-t}\, t^{x-1}\, \mathrm{d}t;\ \gamma(\alpha, x) = \Gamma(\alpha) - \Gamma(\alpha, x).$$

Due to the presence of the rapidly converging function $\Gamma(\frac{5}{2}, \pi\rho^2)$, the first sum is absolutely convergent and therefore may be summed 'spherically'. Now, since there does not exist a linear combination of $Y_{2,m}$'s which has the cubic symmetry ($P_2 = \text{const. } Y_{2,0}$), this sum vanishes for a cubic lattice.

The second sum in (6) is now, by means of three-dimensional Fourier transform (FT_3), converted into an equivalent sum over the reciprocal lattice, which is also simple cubic. We may write

$$S' = P \int \mathrm{d}_3\boldsymbol{\rho} \sum_\lambda^{(')} \delta(\boldsymbol{\rho} - \boldsymbol{\rho}_\lambda)\, \gamma(\tfrac{5}{2}, \pi\rho^2)\ .\ 2P_2(\cos\theta)/\Gamma(\tfrac{5}{2})\rho^3. \tag{7}$$

The prime on the summation may be omitted because the term with $\lambda = 0$ is zero, as is easily verified. For a simple cubic lattice with lattice distance 1 we have

$$FT_3[\Sigma_\lambda \delta(\boldsymbol{\rho} - \boldsymbol{\rho}_\lambda)] = \Sigma_\lambda \delta(\mathbf{h} - \mathbf{h}_\lambda), \text{ (cf. I, appendix 2)} \tag{8}$$

where the summation on the right hand side is extended over the corresponding reciprocal lattice. Furthermore, from I, (41) it follows immediately that

$$FT_3[\gamma(\tfrac{5}{2}, \pi\rho^2) \, . \, 2P_2(\cos\theta)/\Gamma(\tfrac{5}{2})\rho^3] = -\tfrac{8}{3}\pi \, P_2(\cos\vartheta) \, e^{-\pi h^2}, \tag{9}$$

where ϑ is the polar angle of the reciprocal space vector $\mathbf{h}$. By applying Parseval's formula to (7), while using (8) and (9), we obtain

$$S' = P\int \{\Sigma_\lambda \delta(\mathbf{h} - \mathbf{h}_\lambda)\} \{-\tfrac{8}{3}\pi \, P_2(\cos\vartheta) \, e^{-\pi h^2}\} \, \mathrm{d}_3\mathbf{h},$$

or when taking the term $\lambda = 0$ out of the sum

$$S' = P[-\tfrac{8}{3}\pi \lim_{\mathbf{h}\to 0} P_2(\cos\vartheta) \, e^{-\pi h^2} - \tfrac{8}{3}\pi \, \Sigma'_\lambda P_2(\cos\vartheta_\lambda) \, e^{-\pi h^2}]. \tag{10}$$

The sum, which is absolutely convergent, vanishes for the same reason as the first sum in (6), hence

$$S' = -\tfrac{8}{3}\pi \, P \lim_{\mathbf{h}\to 0} P_2(\cos\vartheta) \, e^{-\pi h^2}. \quad *) \tag{11}$$

In this expression for S' the convergence difficulty of the original sum (5) is brought out very clearly, because obviously the value of S' depends on the way in which the origin is approached in the limit. For a slab of dielectric material the origin should evidently be approached along the z-axis ($\vartheta = 0$). Then, because in this case $\lim_{\mathbf{h}\to 0} P_2(\cos\vartheta) \, \mathrm{e}^{-\pi h^2} = 1$, wo obtain $S' = -\frac{8}{3}\pi P$, in accordance with Lorentz' result.

In the case of 'spherical' summation (5) is known to give $S' = 0$. In that case all directions are treated equivalently and the same should then also be done in (11). Since $\overline{\cos^2\vartheta} = \frac{1}{3}$ we have $\overline{P_2(\cos\vartheta)} = 0$, also in the limit, thus giving the correct result $S' = 0$.

This connection between the order of summation in ordinary space and the way of approaching the origin in reciprocal space does seem to be intuitively obvious. A complete mathematical justification can probably be based on theorems relating the asymptotic behaviour of a function to the behaviour near the origin of its Fourier transform, but we did not consider this question any further.

One might ask why the dipole sum (5) was not evaluated by simply applying I, (44). This formula, however, only holds in the case $\mathbf{k} = 0$ for

*) Formula (11) can also be arrived at by directly taking the Fourier transform of the total sum (5) (i.e. without the use of the converging function $\Gamma(\frac{5}{2}, \pi\rho^2)/\Gamma(\frac{5}{2})$), when one uses the formal equality $FT_3[2P_2(\cos\theta)/\rho^3] = (8\pi/3)\{1 - P_2(\cos\vartheta)\}$. The resulting derivation, however, is mathematically less satisfactory.

$2n + l > 3$. This in turn is due to the fact that I, (43*b*) is valid only under this condition *). In the present paper, however, we are treating the case $2n + l = 3$, which requires special attention on account of the conditional convergence of the corresponding sum.

The question of the ambiguity in the value of the dipole sum is closely related to a phenomenon discussed by Cohen and Keffer [6]). These authors find that $S'_{2,0}(0 \mid \mathbf{k}, \frac{1}{2})$ (cf. I, § 6) has a discontinuity at $\mathbf{k} = 0$, i.e. that its value depends on the way in which $\mathbf{k} = 0$ is approached.

The method used in this section for the evaluation of the dipole sum for a simple cubic lattice can also be used for the calculation of this sum for monoclinic lattices. We shall restrict ourselves to the simple case where the dipoles are oriented along the *c*-axis (*i.e.* the axis which is perpendicular to the other two crystal axes), because then the electric field due to the dipoles is also parallel to the *c*-axis. (In the cubic case the electric field is always parallel to the dipole direction, even for arbitrary orientation of the dipoles with respect to the crystal axes). For monoclinic lattices the first sum in (6) and the sum in (10), which vanish in the simple cubic case on account of the symmetry, will not vanish, and the final expression, therefore, will contain both these sums and the limit (11), the latter still depending on the way in which the origin is approached. We will not give the formulae here, they can be easily obtained by generalizing the formulae of this section. Instead, for monoclinic lattices with the special orientation of the dipoles mentioned above, we prefer to use a different method where the plane-wise summation is carried out explicitly (cf. § 3).

In the case of orthorhombic lattices, in which the basic vectors are mutually perpendicular, one can choose the *x*-, *y*- and *z*-axis along these basic vectors. Then one can consider the dipole sums S_x', S_y' and S_z', defined in such a way that they give the internal field when the external field is chosen along the *x*-, *y*- and *z*-axis respectively (*x*-, *y*- and *z*-axis resp. $\perp$ to the condensor plates). S_x', S_y' and S_z' then will in general be different. Using the method indicated in the preceding paragraph one can show that

$$S_x' + S_y' + S_z' = -8\pi P.$$

The proof simply results from the equality

$$P_2(\cos\theta_x) + P_2(\cos\theta_y) + P_2(\cos\theta_z) = 0,$$

where θ_x, θ_y and θ_z are the angles between a certain lattice vector and the *x*-, *y*- and *z*-axis respectively.

§ 3. *Evaluation of the dipole sum by plane-wise summation.* In this section we will derive expressions for S', which are valid for monoclinic lattices and therefore also for all other lattices having higher than monoclinic symmetry.

*) The condition for which I, (43*b*) is valid should read $2n + l > 3$ instead of $n > \frac{3}{2}$ as stated in I.

Again we assume the dipoles to be parallel to the c-axis. The derivation is based on the understanding, expressed in the introduction, that the summation of S' will have to be carried out plane-wise in order to obtain the results for a slab-shaped crystal. As was remarked, we could also have followed the method of § 2, where the plane-wise summation was not carried out explicitly but in an implicit way, viz. by approaching the origin in reciprocal space along the z-axis. However, we prefer to carry out the plane-wise summation more directly, because firstly it leads to an expression for the contribution of each plane, showing a rapid decrease with increasing distance from the reference point, secondly it explicitly verifies the idea that the Lorentz field has to be obtained by plane-wise summation and thirdly it leads to expressions which are well-suited for numerical calculations.

The analysis then is such that in (3) the summation over the z-direction should come after the summation over the x-y-planes. In this connection we consider two contributions to S' separately: S_I' giving the field due to all dipoles in the lattice except those situated in the plane $z = 0$ and S_{II}' giving the contribution of all dipoles in the latter plane.

Starting with S_I' we have

$$S_I' = (p/a^3) \sum_{\lambda_3}{}' \sum_{\lambda_1, \lambda_2} 2P_2(\cos\theta_\lambda)/\rho_\lambda{}^3, \tag{12}$$

in which the order of the summations is essential. (a is the length of one of the unit vectors in the x–y-plane; ρ is dimensionless.) By two-dimensional Fourier transform (FT_2) we now transform the two-dimensional sum into an equivalent sum over the corresponding two-dimensionel reciprocal lattice. Choosing the dimensionless basic vector $\boldsymbol{\alpha}_3 = \mathbf{a}_3/a$ along the z-axis ($\mathbf{a}_3 \perp \mathbf{a}_1$ and $\mathbf{a}_2$ for all monoclinic lattices) we may decompose $\boldsymbol{\rho}_\lambda$ into the vector $\lambda_3\boldsymbol{\alpha}_3$, indicating the plane in which the lattice point is situated and $\boldsymbol{\sigma}_{\lambda_1,\lambda_2}$ giving the location of the point in the plane (in the following λ' will mean λ_1, λ_2): $\rho_\lambda = (\sigma_{\lambda'}{}^2 + \lambda_3{}^2\,\alpha_3{}^2)^{\frac{1}{2}}$.

We may write S_I' partially as an integral

$$S_I' = \frac{p}{a^3} \sum_{\lambda_3}{}' \int \sum_{\lambda'} \delta(\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\lambda'}) \frac{2P_2\{\lambda_3\alpha_3/(\sigma^2 + \lambda_3{}^2\alpha_3{}^2)^{\frac{1}{2}}\}}{(\sigma^2 + \lambda_3{}^2\alpha_3{}^2)^{\frac{3}{2}}} \, \mathrm{d}_2\boldsymbol{\sigma}. \tag{13}$$

It can be shown that

$$FT_2[2(\sigma^2 + \lambda_3{}^2\alpha_3{}^2)^{-\frac{3}{2}} P_2\{\lambda_3\alpha_3/(\sigma^2 + \lambda_3{}^2\alpha_3{}^2)^{\frac{1}{2}}\}] = 4\pi^2 h \exp(-2\pi h\,|\lambda_3|\,\alpha_3) \tag{14}$$

and further that

$$FT_2[\textstyle\sum_{\lambda'} \delta(\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\lambda'})] = (1/o_a) \sum_{\lambda'} \delta(\mathbf{h} - \mathbf{h}_{\lambda'}) \quad \text{(cf. I, appendix 2)}, \tag{15}$$

where o_a is the area of the unit cell in the two-dimensional lattice in the x–y-planes and $\mathbf{h}_{\lambda'}$ the lattice vector in the corresponding two-dimensional reciprocal lattice (measured in units a^2 and $1/a$ respectively). Applying

Parseval's formula to (13) and making use of (14) and (15) we find

$$S_I' = \frac{p}{a_3}\frac{4\pi^2}{o_a}\sum_{\lambda_3}'\int\sum_{\lambda}'\delta(\mathbf{h}-\mathbf{h}_{\lambda'})\,h\,e^{-2\pi h|\lambda_3|\alpha_3}\,\mathrm{d}_2\mathbf{h} =$$

$$= \frac{p}{a_3}\frac{4\pi^2}{o_a}\sum_{\lambda_3}'\sum_{\lambda'}'h_{\lambda'}\,e^{-2\pi h_{\lambda'}|\lambda_3|\alpha_3}.$$

Since the term $\lambda' = 0$ vanishes we may write

$$\sum_{\lambda_3}'\sum_{\lambda'}'h_{\lambda'}\,e^{-2\pi h_{\lambda'}|\lambda_3|\alpha_3} = \sum_{\lambda_3}'\sum_{\lambda'}'h_{\lambda'}\,e^{-2\pi h_{\lambda'}|\lambda_3|\alpha_3} = \sum_{\lambda'}'h_{\lambda'}\sum_{\lambda_3}'e^{-2\pi h_{\lambda'}|\lambda_3|\alpha_3}. \quad (16)$$

The order of summation could be reversed here, because the series is absolutely convergent. The series in λ_3 obtained in this way is a convergent geometrical series and can therefore be summed simply. The extreme rapidity of convergence is obvious from (16); summation over very few planes in the z-direction already gives extremely accurate results. We may therefore extend the λ_3-summation to infinity leading to

$$S_I' = \frac{p}{a^3}\frac{8\pi^2}{o_a}\sum_{\lambda'}'\frac{h_{\lambda'}}{\exp(2\pi h_{\lambda'}\alpha_3)-1}. \quad (17)$$

We now proceed to find a suitable form for the field of the dipoles in the plane $z = 0$. The corresponding sum

$$S_{II}' = -(p/a^3)\sum_{\lambda'}'1/\sigma_{\lambda'}{}^3 \quad (18)$$

can conveniently be treated with the method of I. Using as a converging factor the function $\Gamma(\frac{3}{2},\pi\sigma^2)/\Gamma(\frac{3}{2})$, we find

$$S_{II}' = -\frac{p}{\Gamma(\frac{3}{2})a^3}\left[\sum_{\lambda'}'\frac{\Gamma(\frac{3}{2},\pi\sigma_{\lambda'}{}^2)}{\sigma_{\lambda'}{}^3} - \pi^2\int h\Gamma(-\tfrac{1}{2},\pi h^2)\,\mathrm{d}_2\mathbf{h} + \right.$$

$$\left. + \frac{\pi^2}{o_a}\sum_{\lambda'}'h_{\lambda'}\,\Gamma(-\tfrac{1}{2},\pi h_{\lambda'}{}^2)\right].$$

The integral and the term $\lambda' = 0$ in the second sum can be evaluated right away. One has

$$\{\pi^2/\Gamma(\tfrac{3}{2})\}\int h\Gamma(-\tfrac{1}{2},\pi h^2)\,\mathrm{d}_2\mathbf{h} = 4\pi/3$$

$$\lim_{\mathbf{h}\to 0}\{\pi^2/\Gamma(\tfrac{3}{2})o_a\}h\Gamma(-\tfrac{1}{2},\pi h^2) = 4\pi/o_a,$$

leading to

$$S_{II}' = \frac{p}{a^3}\left[-\frac{4\pi}{o_a}+\frac{4\pi}{3}-\frac{2}{\sqrt{\pi}}\sum_{\lambda'}'\frac{\Gamma(\frac{3}{2},\pi\sigma_{\lambda'}{}^2)}{\sigma_{\lambda'}{}^3} - \right.$$

$$\left. - \frac{2\pi^{\frac{3}{2}}}{o_a}\sum_{\lambda'}'h_{\lambda'}\,\Gamma(-\tfrac{1}{2},\pi h_{\lambda'}{}^2)\right]. \quad (19)$$

Now, adding (17) and (19) we find for the total expression (3)

$$S' = \frac{p}{a^3}\left[-\frac{4\pi}{o_a}+\frac{4\pi}{3}-\frac{2}{\sqrt{\pi}}\sum_{\lambda'}'\frac{\Gamma(\frac{3}{2},\pi\sigma_{\lambda'}{}^2)}{\sigma_{\lambda'}{}^3}-\right.$$
$$\left.-\frac{2\pi^{\frac{3}{2}}}{o_a}\sum_{\lambda'}' h_{\lambda'}\,\Gamma(-\tfrac{1}{2},\pi h_{\lambda'}{}^2)+\frac{8\pi^2}{o_a}\sum_{\lambda'}'\frac{h_{\lambda'}}{\exp(2\pi h_{\lambda'}\alpha_3)-1}\right]. \quad (20)$$

This expression for the electric field in a lattice point of a slab of dielectric material having monoclinic or higher symmetry, is very convenient for the evaluation of the Lorentzfield in such a lattice. As far as we know, an expression for the Lorentzfield valid for such a wide class of lattices has not been given before.

For simple cubic, tetragonal and hexagonal lattices (20) may be simplified by making use of numerical values for (18), which were calculated by Van der Hoff and Benson [7]). These authors find for a two-dimensional

$$\left.\begin{array}{ll}\text{square ('simple cubic') lattice:} & \sum_{\lambda'}' 1/\sigma_{\lambda'}{}^3 = 9.0336217\\ \text{hexagonal lattice:} & \sum_{\lambda'}' 1/\sigma_{\lambda'}{}^3 = 11.0341754\end{array}\right\} \quad (21)$$

both with nearest neighbour distance equal to 1.

Simple cubic lattice. It is natural to choose for a the nearest neighbour distance, then $\alpha_3 = 1$, $o_a = 1$ and $p/a^3 = P$. We then find from (17) and the above numerical value for (18)

$$S'_{sc} = P\,[-\,9.0336217 + 8\pi^2 \sum_{\lambda'}' h_{\lambda'}/\{\exp(2\pi h_{\lambda'}) - 1\}]. \quad (22)$$

From the Lorentz calculation we know that this should be equal to $-\frac{8}{3}\pi P$. A numerical check gives this result to any degree of accuracy. This then is a direct proof of the assertion made in the introduction, that (3) must be summed plane-wise in order to obtain the Lorentz formula (1).

Tetragonal lattice. Here we choose $a = a_1 = a_2$, then again $o_a = 1$. Further $P = Np = p/\alpha_3 a^3$ (N = number of dipoles per unit volume), giving $p/a^3 = \alpha_3 P$. We now find for S'

$$S'_{tetr} = \alpha_3 P\,[-9.0336217 + 8\pi^2 \sum_{\lambda'}' h_{\lambda'}/\{\exp(2\pi h_{\lambda'}\alpha_3) - 1\}] \equiv \alpha_3\, s(\alpha_3)\, P. \quad (23)$$

As in (22) the sum $\sum_{\lambda'}'$ is to be taken over a two-dimensional square lattice with lattice distance 1. The expression (23) can easily be evaluated for arbitrary values of $\alpha_3 (= a_3/a)$. It is seen that for $\alpha_3 > 1$ the main deviation of S' from the cubic value $-\frac{8}{3}\pi P$ arises from the multiplying factor α_3 ($s(\alpha_3)$ varies between $-\frac{8}{3}\pi = -8{,}377\ldots$ and $-9.033\ldots$ for α_3 varying between 1 and ∞). For values of α_3 larger than $\alpha_3{}^0$ (determined by $\alpha_3{}^0\, s(\alpha_3{}^0)/4\pi = -1$, ($\alpha_3{}^0 \simeq 1{,}4$)) the internal field $\mathbf{E}_i$ becomes smaller than the electric field $\mathbf{E}$. For values of α_3 smaller than one, the variation

of $s(\alpha_3)$ becomes important. With (23) we find for the internal field.

$$\mathbf{E}_i = \mathbf{D} + \alpha_3 s(\alpha_3) \mathbf{P} = \mathbf{E} + 4\pi (1 + \alpha_3 s(\alpha_3)/4\pi) \mathbf{P}. \quad (24)$$

These results for tetragonal lattices are not new, an expression like (24) has for the first time been given by Mueller [5]). His method is less straightforward than the present one and hence less suited for numerical computations. Mueller's results were, except for negligibly small differences, completely confirmed by our calculations, carried out with (23). For $\alpha_3 = 1.01$ we find: $1 + \alpha_3 s(\alpha_3)/4\pi = 0{,}323313$, which is in excellent agreement with Mueller's value $L_z = 0{,}32333$.

Hexagonal lattice. Again we choose $a = a_1 = a_2$, but now $o_a = \frac{1}{2}\sqrt{3}\, a^2$. $P = p/\frac{1}{2}\sqrt{3}\, \alpha_3 a^3$ giving $p/a^3 = \frac{1}{2}\sqrt{3}\, \alpha_3 P$. Using the second number given in (19), we find

$$S'_{hex} = \tfrac{1}{2}\sqrt{3}\, \alpha_3 P [- 11.0341754 + 8\pi^2 \textstyle\sum'_{\lambda'} h_{\lambda'}/\{\exp(2\pi h_{\lambda'} \alpha_3) - 1\}]. \quad (25)$$

In this case the sum $\sum_{\lambda'}{}'$ has to be taken over a plane hexagonal lattice with lattice with distance 1. Also (25) leads to numerical results which are in good agreement with Mueller's results.

Received 14-2-58.

REFERENCES

1) Nijboer, B. R. A. and De Wette, F. W., Physica **23** (1957) 309.
2) Ornstein, L. S. and Zernike, F., Proc. kon. Akad. Wetensch. Amsterdam **21** (1918) 911.
3) Lorentz, H. A., *Theory of Electrons*, Dover, New York, p. 137 ff.
4) McKeehan, L. W., Phys. Rev. **43** (1933) 1022, 1025.
5) Mueller, H., Phys. Rev. **47** (1935) 947, **50** (1936) 547.
6) Cohen, M. H. and Keffer, F., Phys. Rev. **99** (1955) 1128.
7) Van der Hoff, B. M. E. and Benson, G. C., Can. J. Phys, **31** (1953) 1087.