

## A FORTRAN Program for Calculating Internal Fields in General Dipole Lattices

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The calculation of the internal field at some point in a lattice of electric dipoles is a problem that often occurs in dielectric theory. A mathematically equivalent problem is calculating the electric field gradient tensor in a lattice of point charges. The internal field is obtained by summing the contributions due to all dipoles in the lattice. The problem is complicated by the fact that the necessary sums converge only conditionally, that is, the result one obtains depends on the order in which the sum is carried out. This mathematical difficulty corresponds physically to the fact that the internal field in a polarized material depends on the external shape of the sample because of the depolarization field. Thus, when performing a calculation a regular summation, order must be used and one must know to what physical shape the result corresponds.

The FORTRAN program here reported is based on the "plane-wise summation method" [1-3]. In Ref. [2] equations are developed with this method which allow one to easily calculate the electric field at an arbitrary point in a lattice of any symmetry, where the lattice may contain dipoles of varying magnitudes and orientations. Normally when one is treating a lattice that contains inequivalent dipoles the lattice is divided into sublattices, each of which has dipoles of equal strength and orientation at the sublattice unit cell corners. It is not necessary to divide into sublattices to perform a calculation; however, doing so greatly simplifies the necessary input information for a computer program and is the method on which the program presented here is based. Each sublattice is treated by a separate calculation and the resultant field contributions at the point in question added together. The sublattices may not all have the same shape or the shape of the lattice; also the field point will normally be at a different location in the different sublattice unit cells.

The end result of a calculation for a sublattice is a set of nine numbers  $S_{ij}$ ;  $i, j = x, y, z$ . These numbers depend only on the symmetry of the sublattice and on the location of field point within the sublattice unit cell. They do not depend on the strength or orientation of the dipoles, a fact which simplifies calculations where

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one wishes to find how the field varies with dipole orientation.  $S_{ij}$  gives the  $i$ th field component at the field point due to dipoles pointing in the  $j$ -direction. Thus the  $i$ th component of the field is given by

$$E_i = \sum_j S_{ij} p_j,$$

where  $p_j$  is the  $j$ th component of the dipole moment at the sublattice unit cell corner. When obtaining the total field care must be taken in adding the contributions of different sublattices because of the depolarization field contribution, which will be discussed below.

A brief description of the "plane-wise summation" method is as follows: A convenient  $z$ -direction is chosen such that the  $z$ -axis is perpendicular to the plane formed by two sublattice basis vectors. The field due to all dipoles in an  $x$ - $y$  plane is first obtained by summing over the plane immediately below the field point. (All  $x$ - $y$  planes are identical due to the nature of the sublattice.) This slowly convergent two-dimensional summation is converted into a rapidly convergent form by Fourier transformation. Fourier transformation converts the summation to a summation over the reciprocal lattice. After performing the two-dimensional summation the contributions due to all planes are obtained by summing over the  $z$ -direction. It is found that after the Fourier transformation the  $z$  summation may be performed analytically so that, in the final analysis, the only sums that need to be carried out are the two-dimensional sums in reciprocal space. Since the  $x$ - $y$  summation is carried out before the  $z$  summation the final result corresponds to a slab-shaped crystal with the slab faces perpendicular to the  $z$ -axis. Thus, the  $z$ -component of the calculated field includes the depolarization field  $-4\pi P_z$ , where  $P_z$  is the  $z$ -component of the polarization. Since the summation is carried out over a sublattice which contains only one dipole per unit cell volume,  $P_z$  is just the  $z$ -component of the dipole moment. The depolarization factor appears in the term  $S_{zz}$ , the number calculated including  $-4\pi$ .

When more than one sublattice must be used to cover the dipoles in a lattice it may be found convenient to use  $z$ -axes which do not coincide. If this is the case the field contributions from the various sublattices cannot be added together until corrections are made for the depolarization factors. This is easily done by adding or subtracting  $-4\pi$  where appropriate so that all results refer to the same slab-shaped crystal. When the electric field gradient tensor for a point charge lattice is calculated, the depolarization factors will automatically cancel due to charge neutrality as long as all sublattices are referred to the same  $z$ -axis, i.e., the sublattices will contain charges of different signs, and the depolarization factors that are introduced by the mechanics of the calculation will cancel in pairs.

The computer program has a much shorter running time than conventional lattice sum programs because of the transformation to summation over the reciprocal lattice. The program is written in FORTRAN 60. The only inputs required

are: the lengths of the three sublattice basis vectors, the angles between them, the three parameters that specify the point in the unit cell at which the field is to be evaluated, the desired accuracy, and a cut-off parameter that stops the calculation in case of nonconvergence due to error. The outputs are the nine numbers  $S_{ij}$  and a statement of the subroutines used in the summation procedure. In case of input error or nonconvergence the reason for the calculation being stopped is automatically printed out to facilitate correction. The basis vectors are entered in the program in units of Å and the output is in units of Å<sup>-3</sup>.

A copy of the thesis on which this program is based may be obtained from the authors (GES) or from the Defense Documentation Center, Cameron Station, Alexandria, Virginia, 22314; ask for "A Computer Program for Evaluating Lattice Sums," by David B. Dickmann. The thesis contains the complete program, its explanation, and a sample calculation. A card deck may be obtained by writing to Control Data Corporation, Co-Op Distribution Center, 3145 Porter Drive, Palo Alto, California. Ask for program Z1-NPGS-LATSUM.

#### REFERENCES

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