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Field due to a dipole in a polarisable molecular lattice

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Abstract. The effective electric field due to a permanent dipole in an arbitrary Bravais lattice of polarisable non-polar molecules is expressed exactly, taking account of the different polarisability of the polar guest molecule. The asymptotic behaviour of the field at large distances from the dipole is evaluated. An interpretation is offered for the rescaled dipole moment required to give agreement with continuum dielectric theory.

1. Introduction

Recent papers have derived analytical expressions for the electric field produced in a simple cubic lattice of isotropically polarisable non-polar particles by a permanent dipole at one site, with particular reference to the long-range behaviour and the corresponding continuum approximation (Smith 1980, Wielopolski 1981, Smith and Wielopolski 1982). Information on the range of validity of the continuum approximation is especially useful for calculations on fluids (Pollock and Alder 1977, 1978, Pollock *et al* 1980, Dunmur and Munn 1983). Knowledge of the field produced by the dipole moment of a guest molecule in a lattice is also required to interpret the electronic Stark effect in molecular crystals (Dunmur and Munn 1975, Fox 1976, Munn 1983).

In this paper we point out that work on the electronic Stark effect has provided exact solutions for the electric field produced in a lattice of arbitrary symmetry composed of anisotropically polarisable molecules with permanent dipole moments when some molecules are replaced by guest molecules with different dipole moments and polarisabilities (Dunmur and Munn 1975, Fox 1976, Munn 1983). Related work on the polarisation energy of a localised charge in a perfect or substitutionally imperfect molecular lattice has treated the long-range contribution to the exact microscopic result, showing how this contribution goes over into the continuum result under cubic symmetry (Bounds and Munn 1979, Eisenstein *et al* 1983). Here we combine results from these pieces of work, deriving a general long-range expression for the field due to a polar molecule in a non-polar lattice, and showing how this work relates to that of Smith (1980), Wielopolski (1981) and Smith and Wielopolski (1982). A number of the expressions obtained here were also foreshadowed by work of Mahan (1967).

2. Microscopic theory

For simplicity we treat a crystal with one non-polar molecule per primitive unit cell of volume v and a single polar guest molecule at site 1. The extension to any number of molecules per unit cell and any number of guests is readily deduced from previous

work (Eisenstein *et al* 1983). The effective or local field is efficiently calculated through the inverse dielectric function (Munn 1980), which for the perfect crystal is

$$\mathbf{E}^{-1} = (\mathbf{I} - \mathbf{T} \cdot \mathbf{B})^{-1} \quad (1)$$

corresponding to the quantity \mathbf{A}^0 of Wielopolski (1981). For N unit cells, the quantities in (1) are dimensionless $3N \times 3N$ matrices composed of 3×3 submatrices which in a site representation are

$$\mathbf{I}_{ij} = \mathbf{I} \delta_{ij} \quad (2)$$

$$\mathbf{T}_{ij} = (v/4\pi) \nabla \nabla (1/r)|_{r=r_{ij}} \quad (3)$$

$$\mathbf{B}_{ij} = (\boldsymbol{\alpha}/\epsilon_0 v) \delta_{ij} \equiv \boldsymbol{\beta} \delta_{ij} \quad (4)$$

where r_{ij} is the vector between site i and site j , $\mathbf{T}_{ii} \equiv 0$, and $\boldsymbol{\alpha}$ is the molecular polarisability tensor. When molecule 1 has its polarisability changed to $\boldsymbol{\alpha} + \mathbf{a}$, the dielectric function for the imperfect crystal becomes (Fox 1976, Eisenstein *et al* 1983)

$$\mathcal{E}^{-1} = \mathbf{Q} \cdot \mathbf{E}^{-1} \quad (5)$$

corresponding to the quantity \mathbf{A} of Wielopolski (1981); here (Fox 1976)

$$\mathbf{Q} = (\mathbf{I} - \mathbf{E}^{-1} \cdot \mathbf{T} \cdot \mathbf{B}')^{-1} \quad (6)$$

$$\mathbf{B}'_{ij} = (\mathbf{a}/\epsilon_0 v) \delta_{ij} \delta_{i1} \equiv \mathbf{b} \delta_{ij} \delta_{i1}. \quad (7)$$

The local field at site i in the imperfect crystal due to a guest dipole moment $\boldsymbol{\mu}_1$ at site 1 is

$$\mathbf{F}_i = (\mathcal{E}^{-1} \cdot \mathbf{T})_{i1} \cdot \boldsymbol{\mu}_1 / \epsilon_0 v \quad (8)$$

$$= (\mathbf{Q} \cdot \mathbf{Z})_{i1} \cdot \boldsymbol{\mu}_1 / \epsilon_0 v \quad (9)$$

where $\mathbf{Z} = \mathbf{E}^{-1} \cdot \mathbf{T}$. By expanding the inverse in (6), using (7) and resumming, or more elegantly by using a projection matrix technique (Eisenstein *et al* 1983), we find eventually (Fox 1976)

$$\mathbf{Q}_{11} = (\mathbf{I} - \mathbf{Z}_{11} \cdot \mathbf{b})^{-1} \quad (10)$$

$$\mathbf{Q}_{i1} = \mathbf{Z}_{i1} \cdot \mathbf{b} \cdot \mathbf{Q}_{11} \quad (i \neq 1) \quad (11)$$

$$\mathbf{Q}_{ij} = \mathbf{I} \delta_{ij} \quad (j \neq 1). \quad (12)$$

Substitution in (9) yields the reaction field as

$$\mathbf{F}_1 = \mathbf{Q}_{11} \cdot \mathbf{Z}_{11} \cdot \boldsymbol{\mu}_1 / \epsilon_0 v \quad (13)$$

while the field at site $i \neq 1$ is

$$\mathbf{F}_i = (\mathbf{Q}_{i1} \cdot \mathbf{Z}_{11} + \mathbf{Z}_{i1}) \cdot \boldsymbol{\mu}_1 / \epsilon_0 v \quad (14)$$

$$= \mathbf{Z}_{i1} \cdot (\mathbf{I} + \mathbf{b} \cdot \mathbf{Q}_{11} \cdot \mathbf{Z}_{11}) \cdot \boldsymbol{\mu}_1 / \epsilon_0 v \quad (15)$$

$$= \mathbf{Z}_{i1} \cdot \mathbf{m}_1 / \epsilon_0 v. \quad (16)$$

Here the combination $\mathbf{m}_1 \equiv \boldsymbol{\mu}_1 + \mathbf{a} \cdot \mathbf{F}_1$ is an effective dipole source which also occurs in analysing the Stark effect (Dunmur and Munn 1975, Fox 1976, Munn 1983). By manipulating (10) one can deduce that

$$\mathbf{I} + \mathbf{b} \cdot \mathbf{Q}_{11} \cdot \mathbf{Z}_{11} = \mathbf{Z}_{11}^{-1} \cdot \mathbf{Q}_{11} \cdot \mathbf{Z}_{11} = \mathbf{Q}_{11}^T \quad (17)$$

where the superscript T denotes the transpose, which leads via the compact result $\mathbf{m}_1 = \mathbf{Q}_{11}^T \cdot \boldsymbol{\mu}_1$ to (Fox 1976)

$$\mathbf{F}_i = \mathbf{Z}_{i1} \cdot \mathbf{Q}_{11}^T \cdot \boldsymbol{\mu}_1 / \epsilon_0 v \quad (i \neq 1). \quad (18)$$

Thus it is the effective dipole moment \mathbf{m}_1 which gives the local fields in the crystal when the guest polarisability differs from that of the host. It corresponds to the quantity $\nu(\omega, \alpha)$ of Smith and Wielopolski (1982). The net dipole moment of the guest is

$$\mathbf{p}_1 = \boldsymbol{\mu}_1 + (\mathbf{a} + \mathbf{a}) \cdot \mathbf{F}_1 \quad (19)$$

which with (13), (17) and the result (Munn 1983)

$$\mathbf{B} \cdot \mathbf{E}^{-1} \cdot \mathbf{T} = (\mathbf{E}^{-1})^T - \mathbf{I} \quad (20)$$

leads to

$$\mathbf{p}_1 = (\mathbf{E}^{-1})_{11}^T \cdot \mathbf{m}_1. \quad (21)$$

Equations (18) and (21) correspond to (4.42) and (4.46) with (5.5) of Smith and Wielopolski (1982).

The response matrix \mathbf{Z} is evaluated by Fourier transformation, which yields (Eisenstein *et al* 1983)

$$\mathbf{Z}_{ij} = N^{-1} \sum_{\mathbf{y}} \exp(-2\pi i \mathbf{y} \cdot \mathbf{r}_{ij}) [\mathbf{1} - \mathbf{t}(\mathbf{y}) \cdot \boldsymbol{\beta}]^{-1} \cdot \mathbf{t}(\mathbf{y}) \quad (22)$$

where \mathbf{y} is the wavevector; the quantity in square brackets is the Fourier transformed inverse dielectric function for the perfect crystal, $\boldsymbol{\epsilon}^{-1}(\mathbf{y})$ (Munn (1980); note a transposition error in (3.18)); and

$$\mathbf{t}(\mathbf{y}) = \sum_j \exp(2\pi i \mathbf{y} \cdot \mathbf{r}_{ij}) \mathbf{T}_{ij} \quad (23)$$

is a modulated lattice dipole sum, which can be calculated by standard methods (Cummins *et al* 1976, Bounds and Munn 1979). The expressions (10), (13), (18), (22) and (23) constitute the exact solution for the electric fields. In practice \mathbf{Z}_{ij} would be evaluated by summation over a suitably dense mesh of points \mathbf{y} in the first Brillouin zone or by an equivalent integration; as shown by Smith and Wielopolski (1982), this process is shape independent in the present case.

3. Long-range behaviour

We now consider the asymptotic long-range behaviour of the electric field at site i in the limit $r_{i1} \rightarrow \infty$. Assuming that $\boldsymbol{\epsilon}^{-1}(\mathbf{y}) \cdot \mathbf{t}(\mathbf{y})$ in (22) varies smoothly with \mathbf{y} , we obtain the dominant contributions to \mathbf{Z}_{i1} from the region $\mathbf{y} \rightarrow 0$. In this region

$$\mathbf{t}(\mathbf{y}) \approx \mathbf{L} - \mathbf{y}\mathbf{y}/y^2 \quad (24)$$

where \mathbf{L} is the Lorentz-factor tensor (Cummins *et al* 1976), which is here independent of \mathbf{y} . The inverse required in (22) is then given by (Bounds and Munn 1979, Munn 1980, Smith 1980)

$$\boldsymbol{\beta} \cdot \boldsymbol{\epsilon}^{-1}(\mathbf{y}) = \boldsymbol{\chi} - (\boldsymbol{\chi} \cdot \mathbf{y})(\mathbf{y} \cdot \boldsymbol{\chi})/y \cdot \boldsymbol{\epsilon} \cdot \mathbf{y} \quad (25)$$

$$\boldsymbol{\chi} = (\boldsymbol{\beta}^{-1} - \mathbf{L})^{-1} \quad (26)$$

where χ is the electric susceptibility and $\epsilon = \mathbf{1} + \chi$ is the macroscopic dielectric tensor. Together these results yield after manipulation

$$\epsilon^{-1}(\mathbf{y}) \cdot \mathbf{t}(\mathbf{y}) = \mathbf{d} \cdot \mathbf{L} - (\mathbf{d} \cdot \mathbf{y})(\mathbf{y} \cdot \mathbf{d}^T) / \mathbf{y} \cdot \epsilon \cdot \mathbf{y} \quad (27)$$

where the local field tensor \mathbf{d} defined by

$$\mathbf{d} \equiv \boldsymbol{\beta}^{-1} \cdot \chi = (\mathbf{1} - \mathbf{L} \cdot \boldsymbol{\beta})^{-1} \quad (28)$$

gives the local field produced by a macroscopic field \mathbf{E} as $\mathbf{F} = \mathbf{d} \cdot \mathbf{E}$ (Dunmur and Munn 1975). When (27) is substituted in (22) for $i \neq j$, the term independent of \mathbf{y} gives zero contribution to the sum.

We now transform to new wavevector variables $\boldsymbol{\eta} = \epsilon^{1/2} \cdot \mathbf{y}$ and direct space variables $\boldsymbol{\rho}_{ij} = \epsilon^{-1/2} \cdot \mathbf{r}_{ij}$. Then for $r_{ij} \rightarrow \infty$ we find

$$\mathbf{Z}_{ij} \approx -\mathbf{d} \cdot \epsilon^{-1/2} \cdot \left[N^{-1} \sum_{\boldsymbol{\eta}} \exp(-2\pi i \boldsymbol{\eta} \cdot \boldsymbol{\rho}_{ij}) \boldsymbol{\eta} \boldsymbol{\eta} / \eta^2 \right] \cdot \epsilon^{-1/2} \cdot \mathbf{d}^T. \quad (29)$$

The sum is now over the allowed wavevectors in the first Brillouin zone of the transformed lattice having basic translations \mathbf{A}_i ($i = 1, \dots, 3$) related to those of the original lattice \mathbf{a}_i by $\mathbf{A}_i = \epsilon^{-1/2} \cdot \mathbf{a}_i$. The quantity in square brackets in (29) is minus dipole tensor \mathcal{F}_{ij} in the transformed lattice (Munn 1980), as follows from (24) since the Lorentz-factor tensor is independent of wavevector. Thus we may write

$$\mathbf{Z}_{ij} \approx \mathbf{G} \cdot \mathcal{F}_{ij} \cdot \mathbf{G}^T, \quad (30)$$

where $\mathbf{G} = \mathbf{d} \cdot \epsilon^{-1/2}$. It is also found that

$$\mathcal{F}_{ij} = \mathbf{T}_{ij}(\boldsymbol{\rho}_{ij}) / (\epsilon_1 \epsilon_2 \epsilon_3)^{1/2} \quad (31)$$

where the ϵ_i are the principal components of ϵ and correct for the new unit-cell volume in the transformed lattice compared with that for the original lattice in (3).

Further insight into (30) and (31) can be obtained by using the principal axis system of ϵ with \mathbf{r}_{ij} parallel to the 1 axis. Then $\epsilon^{-1/2} \cdot \mathbf{r}_{ij} = \epsilon_1^{-1/2} \mathbf{r}_{ij}$ and we find

$$\mathbf{Z}_{ij} = (\epsilon_1^3 / \epsilon_1 \epsilon_2 \epsilon_3)^{1/2} \mathbf{d} \cdot \epsilon^{-1} \cdot \mathbf{T}_{ij} \cdot \mathbf{d}^T \quad (32)$$

with analogous expressions for \mathbf{r}_{ij} parallel to the other principal axes. The factor $\epsilon^{-1} \cdot \mathbf{T}_{ij}$ leads to the screened field expected from continuum theory, but the additional factors also require interpretation. The first factor \mathbf{d} takes account of the discrete structure at the field point i by converting the macroscopic field to the local field. The second factor \mathbf{d}^T can be regarded as similarly taking account of the discrete structure at the source point j . The leading factor $(\epsilon_1^3 / \epsilon_1 \epsilon_2 \epsilon_3)^{1/2}$ arises from (31), since $\mathbf{T}_{ij}(\boldsymbol{\rho}_{ij}) \propto \rho_{ij}^{-3}$ and $\rho_{ij} = \epsilon_1^{-1/2} r_{ij}$. With this correction factor, the transformed lattice already mentioned has dielectric properties equivalent to those of the original lattice and takes account of the dielectric anisotropy.

For a general direction of \mathbf{r}_{ij} , \mathbf{T}_{ij} cannot be separated out as in (32) and the full transformation $\mathbf{T}_{ij} \rightarrow \mathcal{F}_{ij}$ is required. However, from (30) it is seen that the local field tensors occur as before. The inverse dielectric tensor ϵ^{-1} occurs as factors $\epsilon^{-1/2}$ to the left and right of \mathcal{F}_{ij} , thus treating the field and source points symmetrically.

Under cubic symmetry, the tensors $\boldsymbol{\beta}$, χ and ϵ become isotropic, with magnitudes β , χ and ϵ respectively. Then \mathbf{G} also becomes isotropic, with magnitude $\chi / \beta \epsilon^{1/2}$, and \mathcal{F}_{ij} reduces to $\mathbf{T}_{ij}(\mathbf{r}_{ij})$ or simply \mathbf{T}_{ij} , so that

$$\mathbf{Z}_{i1} \approx \mathbf{T}_{i1} / (\epsilon \beta^2 / \chi^2) = \mathbf{T}_{i1} d^2 / \epsilon. \quad (33)$$

From (26) we find results which correspond to the Clausius–Mossotti equation:

$$\beta/\chi = 1 - x \quad (34)$$

$$\epsilon = (1 + 2x)/(1 - x) \quad (35)$$

where $x = \beta/3$ is equivalent to the quantity x of Smith and Wielopolski (1982). The field at site i as $r_{ij} \rightarrow \infty$ can therefore be written as

$$\mathbf{F}_i = \mathbf{T}_{i1} \cdot \mathbf{m}_1 / (1 + 2x)(1 - x)\epsilon_0 v \quad (36)$$

in agreement with (4.45) of Smith and Wielopolski (1982); compare also Mahan (1967). Note that although the host polarisability is isotropic in this case, the polarisability of a polar guest will normally be anisotropic. The effect of this anisotropy is incorporated in the effective dipole \mathbf{m}_1 .

For the reaction field \mathbf{F}_1 it is not appropriate to take $y \rightarrow 0$, since (22) shows that for $i = j = 1$ we must obtain \mathbf{Z}_{11} by a sum over all y . However, a knowledge of the approximate reaction field obtained for $y = 0$ may be useful in interpreting other results. For instance, under cubic symmetry where $\mathbf{L} = \frac{1}{3}\mathbf{I}$, the $y = 0$ approximation \mathbf{Z}_{11}^0 follows from (22) and (27) as

$$\mathbf{Z}_{11}^0 = \frac{1}{3}d(1 - d/\epsilon) = 2d(d - 1)/3\epsilon \quad (37)$$

$$= 2x/3(1 + 2x)(1 - x) \quad (38)$$

where we have used $\mathbf{T}_{ii} = 0$ and (28). Corresponding $y = 0$ approximations follow, giving \mathbf{Q}_{11}^0 from (10) and \mathbf{F}_1^0 from (13). A number of papers have treated the field due to a non-polarisable dipole in a fluid (Pollock and Alder 1977, Pollock *et al* 1980, 1981, Keyes 1980). Then $b = -\beta$ and we obtain

$$\mathbf{F}_1^0 = 2x\boldsymbol{\mu}_1/3(1 + x)\epsilon_0 v, \quad (39)$$

in agreement with (5.9) of Smith and Wielopolski (1982) with $\omega = 0$. The corresponding approximation for the effective dipole source is

$$\mathbf{m}_1^0 = \boldsymbol{\mu}_1 - \alpha\mathbf{F}_1^0 \quad (40)$$

$$= (1 + 2x)(1 - x)\boldsymbol{\mu}_1/(1 + x). \quad (41)$$

If the true source is written as $\mathbf{m}_1 = \lambda\mathbf{m}_1^0$, where λ is a correction factor, the field (36) becomes

$$\mathbf{F}_i = \mathbf{T}_{i1} \cdot \boldsymbol{\mu}_1\lambda/(1 + x)\epsilon_0 v. \quad (42)$$

This is equivalent to the result obtained by Pollock *et al* (1980, 1981), and allows their effective dipole moment $\boldsymbol{\mu}_{\text{eff}}$ to be identified as $\lambda\boldsymbol{\mu}_1$ in the present notation.

4. Discussion

We have shown how previous work on molecular crystals provides exact expressions for the electric field due to a dipole in a non-polar molecular lattice. The extension to a polar lattice with more than one molecule per primitive unit cell is straightforward. Molecular size, shape and orientation can also be taken into account by a submolecule treatment (Luty 1976, Bounds and Munn 1981, Eisenstein *et al* 1983).

We have also derived the asymptotic behaviour of the electric field at large distances from the dipole. Under cubic symmetry, appropriate results of Smith and Wielopolski (1982) are regained. As can be seen from (16) and (32), our results give a field screened by the dielectric tensor ϵ as expected from continuum theory, but there are other changes. The proper source is not the bare dipole moment μ_1 but $m_1 = \mu_1 + a \cdot F_1$, because the guest polarisability differs by a from the host polarisability in the non-zero reaction field F_1 (Smith and Wielopolski 1982). Two local field factors are required to take account of the discrete structure at both the field and source points. Writing d^T as $\epsilon_0 v \chi \cdot a^{-1}$, we can interpret $a^{-1} \cdot m_1$ as the equivalent field required to induce the dipole source m_1 in a host molecule, $\epsilon_0 \chi \cdot E'$ as the polarisation P which would result if the macroscopic field E' were applied to the pure host crystal, and vP as the corresponding dipole moment of the unit cell 1. Thus $d^T \cdot m_1$ can be regarded as an equivalent dipole source in the pure host crystal treated as a continuum. The results also require a further factor to take account of the anisotropic dielectric properties of the crystal, which give more complicated results for the field at points not on the principal dielectric axes.

Note that more than one expression may be regarded as embodying continuum theory. For instance, the local field F_1 as $r_{i1} \rightarrow \infty$ is given by the alternative expressions (36) and (42). In (36) all allowance for the effect of the reaction field is included in the replacement of μ_1 by the effective source m_1 . As we have seen, this conversion depends on the polarisability difference a . In (42) the $y = 0$ approximation for the reaction field in the particular case of a non-polarisable source is included explicitly, and the factor λ allows for the error in this approximation. This difference of approach explains why (36) can be rewritten using (35) to obtain the usual screening factor $1/\epsilon$, whereas rewriting (42) similarly gives a factor $1/(2\epsilon + 1)$ instead (cf Keyes 1980).

Algebraic results like those here do not show at what distance the long-range continuum dominates. Such information can be extracted from numerical microscopic calculations. These include the polarisation energy due to a single charge in a fluid (Pollock and Alder 1978, Pollock *et al* 1980) or in a molecular crystal (Bounds and Munn 1979, 1981) or that due to a pair of opposite charges in a molecular crystal (Bounds *et al* 1981), or calculations of the change in polarisation energy of a single charge due to a vacancy in a crystal (Eisenstein *et al* 1983). These calculations suggest that continuum models provide a good approximation at distances greater than one or two molecular diameters. The behaviour can be quite complex, but when the continuum r^{-n} dependence on distance is obtained (where the integer n depends on the problem considered) it is governed by the same apparent dielectric constant along a given direction (Eisenstein *et al* 1983). The present results for the anisotropic continuum indicate how this occurs if one evaluates \mathcal{F}_{ij} in (31) by taking a coordinate system aligned with the direction concerned. Microscopic calculations of dielectric properties of lattices do therefore agree with continuum theory in suitable limits, but to show this may require rather complicated manipulations.

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