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Surface effects in the response of a polarisable lattice to an external field

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Abstract. We consider surface effects in the response of a plane slab shaped sample of a simple cubic lattice of polarisable points with unit spacing to an applied constant external electric field $\boldsymbol{E}$. In the bulk interior, with the polarisability α of a point less than a critical value $\alpha_c = 3/4\pi$, the response is that of a plane slab of continuum dielectric with dielectric constant $\varepsilon = (1+2x)/(1-x)$ with $x = \alpha/\alpha_c$, the value $\alpha = \alpha_c$ corresponding to the usual polarisation catastrophe. If $\boldsymbol{E}$ is normal to the plane surface of the slab, there is almost no difference between the surface and the bulk interior. However if $\boldsymbol{E}$ is parallel to the plane surface then there are marked surface effects which can decay slowly as α becomes large. There is a second critical polarisability α_{c2} for this reponse which signals the onset of surface effects which propagate undiminished into the bulk of the lattice.

1. Introduction

The response of insulating crystals to applied electric fields has been studied rather extensively. Much recent work has been devoted to the distortion of (particularly ionic) crystal structures by impurity charges and dipoles and some effects of external applied fields have also been studied. Because the potential close to an impurity charge or dipole can be large, the response (shift of position) of ions to such an impurity is often nonlinear in the distorting field, at least close to the impurity. Thus understanding of such point impurities requires extensive numerical investigation if the insights gained are to be applicable to the distortion of real ionic crystals. However, it must be remembered that there are other problems besides the nonlinearity of the short-ranged response which can be important in studying the distortion of crystals. One such class of problems is that of how to deal with the long-ranged forces which occur between charges and dipoles associated with ions and impurities. Accordingly it is of considerable interest to consider simple models of crystals in an attempt to understand some of the effects of these long-ranged forces.

In earlier papers (Smith 1980, Wielopolski 1981 and Smith and Wielopolski 1982) we considered the response of a large sample of a simple cubic lattice of unit spacing with a point of polarisability α at each lattice vertex to various applied electric fields. Smith and Wielopolski (1982) (referred to hereafter as I) considered the response of the lattice to point charges and point dipoles deep within the lattice. Far from these point defects (but still in the deep interior of the sample), the polarisation response was that of a continuum dielectric with a rescaled point charge or dipole embedded

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in it. The dielectric constant is $\varepsilon(x)=(1+2x)/(1-x)$, with $x=4\pi\alpha/3=\alpha/\alpha_c$, where $\alpha_c=3/4\pi$ is the critical polarisability for the usual polarisation catastrophe. We found no obvious way to interpret the rescaled dipole moment in terms of the usual cavity fields and the renormalisations they induce (Bottcher 1973). Another problem considered in I was the response of a large lattice sample of given shape to a constant applied electric field. Deep within the sample the response was that of a sample of continuum dielectric of the same shape as the lattice sample and of dielectric constant $\varepsilon(x)$. The lattice problem showed the same shape dependence as the Laplace equation solutions for the continuum problem. These calculations made a clear connection between the electrostatics of continuous media and a simple (zero temperature) model of a polarisable lattice. Munn and Eisenstein (1983) have made extensions of the work of I to lattices other than simple cubic ones, and have investigated the notion of cavity fields further, giving interpretations of how the lattice can renormalise an impurity point dipole. Earlier work by Bellemans and Plaitin (1975) considered the change in bulk dielectric constant of a medium caused by inclusion of a finite concentration of impurities of different polarisability in the lattice. All of these treatments have concentrated on bulk properties. Lehnen and Bruch (1980) used such a polarisable lattice as a model of noble gas crystals and studied the response of a crystal surface to a static point charge near the surface and were able to show good agreement between their models and experimental results of charged particle scattering by such crystal surfaces. In this paper we make some contact between that work and our earlier studies by considering the polarisation response of the surface region of a plane slab of simple cubic lattice of polarisable point atoms when a constant electric field is applied to the system.

Consider then a simple cubic lattice Λ with unit spacing so that the lattice vertices are $\boldsymbol{n}=(l,m,n)$ with l, m and n being integers. The sums of electric fields which arise in the problems we consider can be conditionally convergent so that to make contact with a physical picture, a summation order must be defined. Accordingly we consider parallelipiped shaped samples $\Lambda(\boldsymbol{N})$ defined by

$$\Lambda(\boldsymbol{N})=\{\boldsymbol{n}=(l,m,n): 0\leqslant l\leqslant N_1, -N_2\leqslant m\leqslant N_2, -N_3\leqslant n\leqslant N_3\}.$$

Each vertex $\boldsymbol{n}\in\Lambda(\boldsymbol{N})$ carries a point atom of polarisability α.

A dipole $\boldsymbol{\mu}$ at $\boldsymbol{r}_1$ sets up an electric field $\boldsymbol{e}(\boldsymbol{r}_2)$ at $\boldsymbol{r}_2$ which is

$$\boldsymbol{e}(\boldsymbol{r}_2)=-\boldsymbol{t}(\boldsymbol{r}_2-\boldsymbol{r}_1)\cdot\boldsymbol{\mu}, \tag{1.1}$$

if $\boldsymbol{r}_2\neq\boldsymbol{r}_1$ and zero if $\boldsymbol{r}_2=\boldsymbol{r}_1$. Here then,

$$t(r)=\begin{cases}\dfrac{1}{|\boldsymbol{r}|^3}[1-3\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}] & \boldsymbol{r}\neq\boldsymbol{0}\\ 0 & \boldsymbol{r}=\boldsymbol{0}.\end{cases} \tag{1.2}$$

Under the influence of that field, a point of polarisability α at $\boldsymbol{r}_2$ develops a dipole moment $\alpha\boldsymbol{e}(\boldsymbol{r}_2)$. Suppose then that the lattice sample is exposed to a constant electric field $\boldsymbol{E}$. The electric field at a lattice site $\boldsymbol{m}\in\Lambda(\boldsymbol{N})$ is then the sum of $\boldsymbol{E}$ and the fields at $\boldsymbol{m}$ due to each of the other induced dipoles in $\Lambda(\boldsymbol{N})$. Thus the polarisation $\boldsymbol{\mu}(\boldsymbol{m})$ of the polarisable point at $\boldsymbol{m}\in\Lambda(\boldsymbol{N})$ may be written

$$\boldsymbol{\mu}(\boldsymbol{m})=\alpha\boldsymbol{E}-\alpha\sum_{\boldsymbol{n}\in\Lambda(\boldsymbol{N})}t(\boldsymbol{m}-\boldsymbol{n})\cdot\boldsymbol{\mu}(\boldsymbol{n}). \tag{1.3}$$

To study the response near a surface of a plane slab, we consider the limit $N_2 = N_3 \to \infty$ and then $N_1 \to \infty$ of equation (1.3) and calculate $\boldsymbol{\mu}(l) = \boldsymbol{\mu}((l, 0, 0))$.

The bulk response of this plane slab has a polarisation catastrophe. This catastrophe may be seen by considering a simpler system of two points of polarisability α, one at $\mathbf{0}$ and the second at $\boldsymbol{r}$. The dipoles $\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$ produced when an external field is applied are given by

$$\boldsymbol{\mu}_2 = \alpha \boldsymbol{E} - \alpha t(\boldsymbol{r}) \cdot \boldsymbol{\mu}_1, \qquad \boldsymbol{\mu}_1 = \alpha \boldsymbol{E} - \alpha t(\boldsymbol{r}) \cdot \boldsymbol{\mu}_2, \tag{1.4}$$

so that

$$\boldsymbol{\mu}_j = \alpha Q(\boldsymbol{r}) \cdot \boldsymbol{E}, \tag{1.5}$$

where simple algebra gives by cancellation of the matrix $[I - \alpha T(\boldsymbol{r})]$

$$Q(\boldsymbol{r}) = [I + \alpha t(\boldsymbol{r})]^{-1}. \tag{1.6}$$

The eigenvalues of $[I \mp \alpha t(\boldsymbol{r})]$ are $1 \pm 2\alpha/|\boldsymbol{r}|^3$ (eigenvector $\hat{\boldsymbol{r}}$) and $1 \mp \alpha/|\boldsymbol{r}|^3$ (two eigenvectors, both normal to $\hat{\boldsymbol{r}}$) so that Q diverges as $\alpha \to 2|\boldsymbol{r}|^{-3}-$. This divergence of $\boldsymbol{\mu}_j$ is the polarisation catastrophe. It is unphysical because it assumes that polarisation is linear in the applied field. Normally we could expect the susceptibility of a polarisable atom or molecule to saturate as the polarisation becomes large, so that the catastrophe is not reached. The main task of the next section is to give an outline of a method of solution of (1.3) written in the plane slab limit (PSL). To begin the equation can be put into its PSL form by starting with a given $\boldsymbol{N}$. Then

$$\boldsymbol{\mu}(\boldsymbol{m}; \boldsymbol{N}) = \alpha \boldsymbol{E} - \alpha \sum_{l=0}^{N_1} \left(\sum_{m=-N_2}^{N_2} \sum_{n=-N_3}^{N_3} t(\boldsymbol{m} - (l, m, n)) \cdot \boldsymbol{\mu}((l, m, n); \boldsymbol{N}) \right). \tag{1.7}$$

Now let $N_2 = N_3$ and let both tend to infinity. Assume that the solution depends only on $\boldsymbol{m} \cdot (1, 0, 0)$ and so define

$$\boldsymbol{\mu}(l) = \text{PSL}\, \{\boldsymbol{\mu}(l, m, n); \boldsymbol{N})\}. \tag{1.8}$$

Let $\boldsymbol{n} = (n, \rho_y, \rho_z)$ and $\boldsymbol{\rho} = (\rho_y, \rho_z)$ so that (1.7) may be rewritten, when N_1 also tends to $+\infty$ as

$$\boldsymbol{\mu}(m) = \alpha \boldsymbol{E} - \alpha \sum_{n=0}^{\infty} \left(\sum_{\rho \in Z^2}^{*} t(m - n, \rho_y, \rho_z) \right) \cdot \boldsymbol{\mu}(n). \tag{1.9}$$

The asterisk on the sum on $\boldsymbol{\rho}$ here indicates that for $\rho_y = \rho_z = 0$, the $m = n$ term is omitted (cf (1.2)). The problem solved in the next section is thus the Weiner-Hopf sum equation given by (1.9).

2. Solution of the sum equations

It is useful to make the substitution

$$\boldsymbol{\mu}(m) = \boldsymbol{\mu}_0 + \boldsymbol{\nu}'(m) \tag{2.1}$$

where $\boldsymbol{\mu}_0$ is the polarisation expected deep in the interior of a plane slab exposed to the electric field. In I we found

$$\mu_0 = \frac{\alpha}{1+2x}\begin{pmatrix} \frac{1-x}{1+2x} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \boldsymbol{E} \tag{2.2}$$

where $x = 4\pi\alpha/3$. We may put this result and (2.1) into (1.9) and obtain

$$\boldsymbol{\nu}'(m) = \alpha\boldsymbol{\tau}'(m) - \alpha \sum_{n=0}^{\infty} T(m-n)\cdot\boldsymbol{\nu}'(n) \qquad \text{for } m \geq 0 \tag{2.3}$$

where

$$T(m) = \begin{cases} \displaystyle\sum_{m_2=-\infty}^{\infty}\sum_{m_3=-\infty}^{\infty} t((m, m_2, m_3)), & m \neq 0 \\ \displaystyle\sum_{m_2=-\infty}^{\infty}\sum_{\substack{m_3=-\infty \\ (m_2,m_3)\neq(0,0)}}^{\infty} t((0, m_2, m_3)), & m = 0 \end{cases} \tag{2.4}$$

and

$$\boldsymbol{\tau}'(m) = \sum_{n=1}^{\infty} T(m+n)\cdot\boldsymbol{\mu}_0. \tag{2.5}$$

We expect $\boldsymbol{\nu}'(m)$ to decay to zero as $m \to +\infty$. General methods for the solution of the Wiener-Hopf sum equation (2.3) have been given by Widom (1965) for the case when $\boldsymbol{\nu}'(m)$ is square summable. They do not apply to (1.9) because the inhomogeneous term $\alpha\boldsymbol{E}$ in (1.9) is not square summable. We require summability of $T(m)$ and $\boldsymbol{\tau}'(m)$ on $[0, \infty)$. We implement these methods on equations for the components of $\boldsymbol{\nu}'(m) = (\nu(m), \lambda(m), \kappa(m))$, with $\boldsymbol{E} = (E_x, E_y, E_z)$, $\mu_0 = (\mu_{0x}, \mu_{0y}, \mu_{0z})$ and $\boldsymbol{\tau}'(m) = (\tau_1(m), \tau_2(m), t_3(m))$. The equation for $\nu(m)$ may be written

$$\nu(m) = \alpha\sigma(m)\mu_{0x} - \alpha \sum_{m=0}^{\infty} T_{11}(m-n)\nu(n) \tag{2.6}$$

where $T_{11}(m)$ is the (1, 1) element of $T(m)$ and

$$\sigma(m) = \sum_{n=1}^{\infty} T_{11}(|m|+n) \qquad \forall m. \tag{2.7}$$

Notice that the two-dimensional lattice sum for $T(m)$ is absolutely convergent and the summand is traceless. Thus

$$T_{22}(m) = T_{33}(m) = \tfrac{1}{2}T_{11}(m) \qquad \forall m. \tag{2.8}$$

The other components of $\boldsymbol{\nu}'(m)$ are essentially the same, and (2.8) may be used to give

$$\lambda(m) = -\alpha\sigma(m)\mu_{0y} + \tfrac{1}{2}\alpha \sum_{n=0}^{\infty} T_{11}(m-n)\lambda(n). \tag{2.9}$$

We need to simplify the lattice sums for $T(m)$. We use a method for lattice sums of electrostatic potentials which was developed by de Wette and Nijboer (1958) and Nijboer and de Wette (1957, 1958) and used by Massidda (1976, 1978) and Nijboer (1984) to examine lattice sums by planewise summation. This method gives more tractable forms than those introduced by Ewald (1921) and used by Smith (1983) to study potentials at coulombic crystal surfaces. We consider

$$F(x) = \lim_{N\to\infty} \sum_{l=-N}^{N} \sum_{k=-N}^{N} (x^2 + l^2 + k^2)^{-3/2} \tag{2.10}$$

so that for $m \neq 0$,

$$T_{11}(m) = \frac{\mathrm{d}}{\mathrm{d}x} xF(x)\big|_{x=m}. \tag{2.11}$$

The method of de Wette and Nijober gives

$$F(x) = \frac{2\pi}{|x|} \sum_{\underline{k}\in Z^2} \exp(-2\pi|x|\,|\boldsymbol{k}|) \tag{2.12}$$

and thus

$$T_{11}(m) = -4\pi^2 \sum_{k\in Z^2} |\underline{k}| \exp(-2\pi|m|\,|\underline{k}|), \qquad m \neq 0. \tag{2.13}$$

This also gives $T_{22}(m) = T_{33}(m)$ by (2.8). The lattice sum for $T_{11}(0)$ is a simple number and is approximately

$$T_{11}(0) = \sum_{\underline{k}\pm\underline{0}} |\underline{k}|^{-3} \simeq 9.0336. \tag{2.14}$$

Further, (2.7) gives

$$\sigma(m) = -4\pi^2 \sum_{\substack{\underline{k}\in Z^2\\ \underline{k}\neq\underline{0}}} |\underline{k}| \exp(-2\pi(|m|+1)|\underline{k}|)\,[1-\exp(-2\pi|\underline{k}|)]^{-1}. \tag{2.15}$$

The lattice sums for $T_{11}(m)$ and $\sigma(m)$ in (2.13) and (2.15) are absolutely (and rapidly) convergent.

We now introduce $\nu_+(m) = \nu(m)$ for $m \geqslant 0$ and $\nu_+(m) = 0$ for $m < 0$ and

$$\nu_-(m) = \alpha\sigma(m)\mu_{0x} - \alpha \sum_{n=-\infty}^{\infty} T_{11}(m-n)\nu_+(n), \qquad m<0 \tag{2.16}$$

while $\nu_-(m) = 0$ for $m \geqslant 0$. Thus for all m

$$\nu_+(m) + \nu_-(m) = \alpha\sigma(m)\mu_{0x} - \alpha \sum_{n=-\infty}^{\infty} T_{11}(m-n)\nu_+(n). \tag{2.17}$$

We define

$$\hat{\nu}_+(z) = \sum_{n=-\infty}^{\infty} \nu_+(n) z^n$$

which must be analytic inside $|z| < 1$ so that

$$\nu_+(n) = \frac{1}{2\pi \mathrm{i}} \oint_{C_+} \hat{\nu}_+\left(\frac{1}{z}\right) z^{n-1}\,\mathrm{d}z \tag{2.18}$$

where the contour C_+ is a circle just outside the unit circle with centre $z = 0$. We now define

$$\hat{T}_{11}(z) = \sum_{m=-\infty}^{\infty} T_{11}(m) z^m, \qquad \hat{\sigma}(z) = \sum_{m=-\infty}^{\infty} \sigma(m) z^m \tag{2.19}$$

and thus

$$\hat{T}_{11}(z)=T_{11}(0)+H(z)+H(1/z), \qquad \hat{\sigma}(z)=\tau(0)+G(z)+G(1/z) \tag{2.20}$$

where

$$H(z)=-4\pi^2 z\sum_{\underline{k}\neq \underline{0}}\frac{|\underline{k}|\exp(-2\pi|\underline{k}|)}{1-z\exp(-2\pi|\underline{k}|)} \tag{2.21}$$

and

$$G(z)=-4\pi^2 z\sum_{\underline{k}\neq \underline{0}}|\underline{k}|\exp(-4\pi|\underline{k}|)\{[1-\exp(-2\pi|\underline{k}|)][1-z\exp(-2\pi|\underline{k}|)]\}^{-1} \tag{2.22}$$

are both analytic in $\exp(-2\pi)<|z|<\exp(2\pi)$. Note that $\hat{T}(z)=\hat{T}(1/z)$, $\hat{\sigma}(z)=\hat{\sigma}(1/z)$. If $\nu_+(m)=O(m^p)$ then a simple argument from (2.16) shows that

$$\hat{\nu}_-(z)=\sum_{m=-\infty}^{\infty}\nu_-(m)z^m \tag{2.23}$$

is analytic in $|z|>\exp(-2\pi)$. Thus we may multiply (2.17) by z^m and sum on m to obtain

$$\hat{\nu}_+(z)+\hat{\nu}_-(z)=\alpha\hat{\sigma}(z)\mu_{0x}-\alpha\hat{T}_{11}(z)\hat{\nu}_+(z) \tag{2.24}$$

in $\exp(-2\pi)<|z|<1$ and hence for all z by analytic continuation. Thus we have

$$\nu_+(m)=\frac{1}{2\pi i}\oint_{C_+}dz\, z^{m-1}\frac{\alpha\hat{\sigma}(z)\mu_{0x}-\hat{\nu}_-(1/z)}{1+\alpha T_{11}(z)}, \qquad m\geqslant 0. \tag{2.25}$$

A similar analysis applies to $\lambda(m)$ and gives

$$\lambda(m)=\frac{1}{2\pi i}\oint_{C_+}dz\, z^{m-1}\frac{[-\frac{1}{2}\alpha\hat{\sigma}(z)\mu_{0y}-\hat{\lambda}_-(1/z)]}{1-\frac{1}{2}\alpha T_{11}(z)}, \qquad m\geqslant 0. \tag{2.26}$$

In the integrand in (2.25), $\hat{\nu}_-(1/z)$ is analytic in $|z|<\exp(2\pi)$ and the only singularities of $\hat{T}_{11}(z)$ are simple poles which are removed by cancellation with poles of $\hat{\sigma}(z)$. The only singularities of the integrand in (2.25) are simple poles at the zeros of $1+\alpha\hat{T}_{11}(z)$. Let those zeros inside C_+ be denoted ζ_j, $j\geqslant 1$ with $|\zeta_{j+1}|\leqslant|\zeta_j|$ to order them. Then

$$\nu_+(m)=\sum_{j=1}^{\infty}A_j\zeta_j^m \tag{2.27}$$

where

$$A_j=\frac{[\alpha\hat{\sigma}(\zeta_j)\mu_{0x}-\hat{\nu}_-(1/\zeta_j)]}{\alpha\zeta_j\hat{T}'_{11}(\xi_j)}. \tag{2.28}$$

These results may now be inserted into (2.24) to give $\hat{\nu}_-(1/\zeta_j)$ in terms of the A_j and ζ_j. If the ζ_j are known, this form of $\hat{\nu}_-(1/\zeta_j)$ may be put into (2.28) and the matrix equation solved for the A_j.

To locate the zeros of $1+\alpha\hat{T}_{11}(z)$ we may approximate the lattice sum for $\hat{T}_{11}(z)$ from (2.19) and (2.21) by including only those $\boldsymbol{k}$ vectors with $|\boldsymbol{k}|$ equal to one of its smallest M possible magnitudes. This gives a $2M$th-order polynomial equation for the zeros. This M-approximant to the function $1+\alpha\hat{T}_{11}(z)$ has M poles on $0<z<1$ and M on $1<z$, so that there are $2(M-1)$ zeros of this approximation on the real axis, $M-1$ of them inside $|z|<1$. Similar conclusions hold for $1-\frac{1}{2}\alpha\hat{T}_{11}(z)$. Note that $\hat{T}_{11}(1)=8\pi/3\simeq 8.3776$ so there is a further zero of the M approximant to $1+\alpha\hat{T}_{11}(z)$

on $\exp(-2\pi) < z < 1$ and one on $1 < z < \exp(2\pi)$. This locates all the zeros of $1 + \alpha\hat{T}_{11}(z)$ as $M \to \infty$. The solution $\nu_+(m)$ may now be calculated numerically using a particular value of M. A larger value of M may then be taken and the procedure repeated until the results are stable in M. The behaviour of $\nu_+(m)$ is dominated by the form

$$\nu_+(m) = A_1\zeta_1^m = A_1 \exp[-m/D_A(\alpha)] \tag{2.29}$$

where ζ_1 is the zero inside $|z| < 1$ closest to $z = 1$ and $D_A(\alpha) = 1/|\log|\zeta_1||$ is a 'correlation length' which measures how far into the plane surface the influence of that surface can be seen in the response of the plane slab to a normal applied electric field.

The solution $\lambda(m)$ to (2.26) for the response to a field imposed parallel to the surface proceeds in the same way as for $\nu(m)$. However while $1 - \frac{1}{2}\alpha\hat{T}_{11}(z)$ has zeros on the real axis in $0 < z < \exp(-2\pi)$ and $\exp(2\pi) < z$, the two zeros on $\exp(-2\pi) < z < \exp(2\pi)$ are no longer present. On $0 < \alpha < \alpha_{c2} \simeq 0.2065$, $1 - \frac{1}{2}\alpha\hat{T}_{11}(-1) < 0$ and so there is a zero on the negative real axis at ζ_1, $-1 < \zeta_1 < 0$, with another zero at $1/\zeta_1$. For $\alpha_{c2} < \alpha < \alpha_c < 3/4\pi$ these two zeros move on to the unit circle and move round the circle to $z = 1$ as $\alpha \to \alpha_c$. For the case $0 < \alpha < \alpha_{c2}$ we then obtain the dominant form

$$\lambda(m) = A_1(-1)^m \exp(-m/D_B(\alpha)) \tag{2.30}$$

with $D_B(a) = 1/[\log|\zeta_1||$ again determining how far the influence of the surface penetrates into the bulk. On $\alpha_{c2} < \alpha < \alpha_c$ the two zeros on the unit circle again dominate the behaviour of the solution. These solutions are not square summable but in fact the above analysis still holds because they are not large enough to affect the analyticity properties of the functions concerned.

3. Discussion

The numerical procedure is fairly easy to implement, merely requiring the inversion of an $M \times M$ matrix to obtain the A_j for some M, although it might be said that the coefficient matrix is fairly complicated. We found that for $M = 5$ the procedure gave results for $\nu(m)$ and $\lambda(m)$ which were stable to five significant figures (which means that significantly increasing M did not change the results to that accuracy). We plot the correlation lengths $D_A(\alpha)$ and $D_B(\alpha)$ in figure 1. We discuss the case of field normal to the plane surface first. The correlation length is rather insensitive to the value of α and remains about 20% of a lattice spacing throughout the range $0 < \alpha < \alpha_c = 3/4\pi \simeq 0.2387$. At $\alpha = 0$, this length (corresponding to a zero of $1 + \alpha\hat{T}_{11}(z)$ which collapses on to the pole of that function at $\zeta_1 = \exp(-2\pi)$ when $\alpha = 0$) is given by $D_A(0) = 1/2\pi$. Thus for the field normal to the surface there is almost no deviation of the polarisation response from the bulk value μ_{0x} except in the first surface layer. For this surface layer, we may consider $\nu(0)/\mu_{0x}$, the fractional deviation of the surface polarisation from its bulk interior value. The solution shows that this is a function which is negative and increasing in α, but which remains less than 0.03 in magnitude. In fact $\nu(0)/\mu_{0x} \simeq -0.024\,07$ at $\alpha = 0.2$. We plot $\nu(0)/\mu_{0x}$ as a function of α in figure 2. We see that the polarisation response normal to the surface shows almost no surface effect. Any surface effects decay by a factor about e^{-5} for each layer into the surface. In the outermost surface layer, the polarisation is more than 97% of its bulk interior value for all values of α on $0 < \alpha < \alpha_c$.

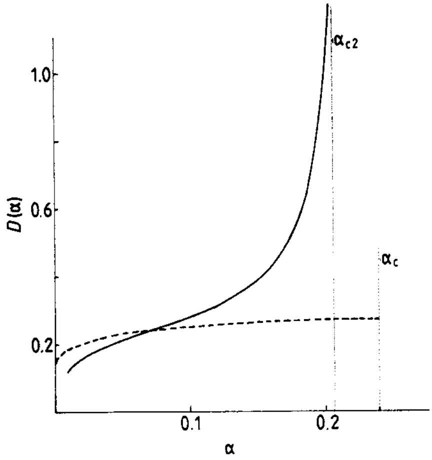

Figure 1. Plots of $D_A(\alpha)$(lower curve, no diverging at α_{c2}) and $D_B(\alpha)$(upper curve) as functions of α.

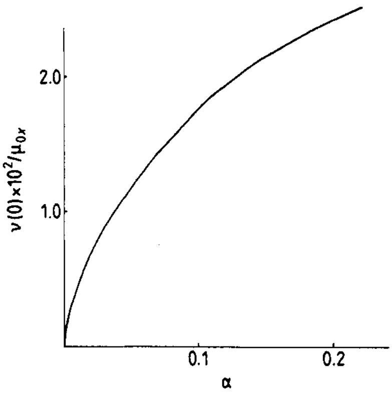

Figure 2. Plot of $-\nu(0)/\mu_{0x}$ as a function of α.

The situation is very different for the response to a field parallel to the plane slab surface, as is shown by our solution $\lambda(m)$. The correlation length $D_B(\alpha)$ is also plotted in figure 1. It diverges as $(\alpha_{c2}-\alpha)^{-1}$ as $\alpha\to\alpha_{c2}^-$. On the range $0<\alpha<\alpha_{c2}$, the polarisation response shows surface effects which alternate in sign, layer by layer, as they propagate in from the surface. For $\alpha_{c2}<\alpha<\alpha_c$, the solution $\lambda(m)$ does not decay as $m\to\infty$. On this range $\alpha_{c2}<\alpha<\alpha_c$, there is no 'bulk interior' where surface effects have decayed away: they propagate right across the slab. In this region the polarisation response appears to be a polarisation wave with a wavelength 2 at $\alpha=\alpha_{c2}$. As α increases from α_{c2} to α_c this wavelength increases so that the polarisation catastrophe occurs at $\alpha=\alpha_c$ with a divergent response uniform across the whole slab.

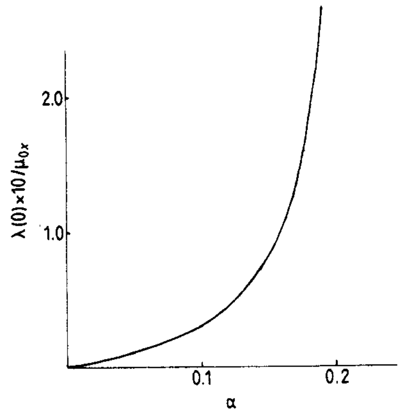

Figure 3. Plot of $\lambda(0)/\mu_{0x}$ as a function of α.

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