ON THE ELECTROSTATIC POTENTIAL OF A POINT CHARGE IN A DIELECTRIC SOLID

R. D. MINDLIN

Department of Civil Engineering, Columbia University, New York

THE electrostatic potential of a point charge, q, in an unbounded vacuum, is

$$\varphi = q/4\pi\varepsilon_0 r, \tag{1}$$

where ε_0 is the permittivity of the vacuum and r is the distance from the point charge. If the vacuum is replaced by an isotropic dielectric, the point charge polarizes the atoms of of the dielectric and, according to the classical theory of electrostatics, the potential is modified to

$$\varphi = q/4\pi\varepsilon_0(1+\eta)r = q/4\pi\varepsilon r, \tag{2}$$

where η is the dielectric susceptibility and ε is the permittivity of the dielectric. The result (2) is based on the assumption, fundamental to the classical theory, that the stored energy of polarization depends only on the local polarization. In terms of the shell model of the atom (a core, comprising the nucleus and inner electrons, surrounded by a shell of outer electrons) this corresponds to a contribution to the stored energy solely from the interaction between the shell of an atom and its own core. It is interesting to calculate the effect of the interaction between the shells of adjacent atoms, which is known to be important in the calculation of phonon dispersion relations in dielectric crystal lattices. In a continuum, the shell–shell interaction is represented by the contribution of the polarization gradient [1] to the stored energy of polarization. The appropriate field equations may be derived by means of a slight modification of Toupin's [2] variational principle for the classical theory of elastic dielectrics. Essentially, it is only necessary to replace the strain by the polarization gradient.

For a dielectric material occupying a volume V, bounded by a surface S separating V from an outer vacuum V', the variational principle, for the linear case, is

$$\delta \int_{V+V'} H \, dV + \int_V \rho\delta\varphi \, dV = 0, \tag{3}$$

where ρ is the charge density and H is the electric enthalpy density:

$$H = W^L(P_i, P_{j,i}) - \tfrac{1}{2}\varepsilon_0 \varphi_{,i}\varphi_{,i} + \varphi_{,i}P_i. \tag{4}$$

In (4), $W^L(P_i, P_{j,i})$ is the stored energy of polarization: a function of both the polarization and the polarization gradient. The polarization and the charge density are zero outside V whereas φ exists in V and V'.

Now,

$$\delta H = -E_i^L \delta P_i + E_{ij} \delta P_{j,i} - \varepsilon_0 \varphi_{,i} \delta \varphi_{,i} + \varphi_{,i} \delta P_i + P_i \delta \varphi_{,i} \tag{5}$$

where

$$E_i^L \equiv -\partial W^L/\partial P_i, \qquad E_{ij} \equiv \partial W^L/\partial P_{j,i}. \tag{6}$$

By the chain rule of differentiation,

$$\delta H = -(E_{ij,i} + E_j^L - \varphi_{,j})\delta P_j - (-\varepsilon_0 \varphi_{,ii} + P_{i,i})\delta \varphi + (E_{ij}\delta P_j)_{,i} + [(-\varepsilon_0 \varphi_{,i} + P_i)\delta \varphi]_{,i}. \tag{7}$$

Inserting this result in (3) and applying the divergence theorem, we have

$$-\int_V [(E_{ij,i} + E_j^L - \varphi_{,i})\delta P_i + (-\varepsilon_0 \varphi_{,ii} + P_{i,i} - \rho)\delta \varphi]\, \mathrm{d}V + \int_{V'} \varepsilon_0 \varphi_{,ii}\delta \varphi\, \mathrm{d}V$$

$$+ \int_S [n_i E_{ij}\delta P_j + n_i(\varepsilon_0[\varphi_{,i}] + P_i)\delta \varphi]\, \mathrm{d}S = 0, \tag{8}$$

where $[\varphi_{,i}]$ is the jump in $\varphi_{,i}$ across S. Thus, the field equations in V, which are all we need for the present application, are

$$E_{ij,i} + E_i^L - \varphi_{,i} = 0, \qquad \varepsilon_0 \varphi_{,ii} - P_{i,i} + \rho = 0. \tag{9}$$

The stored energy of polarization is taken to be

$$W^L = \tfrac{1}{2}\alpha_{ij}P_iP_j + \tfrac{1}{2}\beta_{ijkl}P_{j,i}P_{l,k} + \gamma_{ijk}P_iP_{k,j}. \tag{10}$$

We shall consider only centrosymmetric, isotropic materials—in which case

$$\alpha_{ij} = \varepsilon_0^{-1}\eta^{-1}\delta_{ij},$$
$$\beta_{ijkl} = \beta_1\delta_{ij}\delta_{kl} + \beta_2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \beta_3(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}), \tag{11}$$
$$\gamma_{ijk} = 0,$$

where δ_{ij} is the Kronecker delta and β_1, β_2, β_3 are constants associated with the polarization gradient.

From (6), (10) and (11), we have

$$E_i^L = -\varepsilon_0^{-1}\eta^{-1}P_i,$$
$$E_{ij} = \beta_1\delta_{ij}P_{k,k} + \beta_2(P_{j,i} + P_{i,j}) + \beta_3(P_{j,i} - P_{i,j}). \tag{12}$$

Substituting these constitutive equations into (9) and converting to vector notation, we find the field equations for the centrosymmetric, isotropic dielectric:

$$(\beta_2 + \beta_3)\nabla^2\mathbf{P} + (\beta_1 + \beta_2 - \beta_3)\nabla\nabla\cdot\mathbf{P} - \varepsilon_0^{-1}\eta^{-1}\mathbf{P} - \nabla\varphi = 0, \qquad -\varepsilon_0\nabla^2\varphi + \nabla\cdot\mathbf{P} = \rho. \tag{13}$$

To eliminate $\mathbf{P}$ from (13), operate on the first of the two equations with the divergence, to get

$$(\beta_1 + 2\beta_2)\nabla^2\nabla\cdot\mathbf{P} - \varepsilon_0^{-1}\eta^{-1}\nabla\cdot\mathbf{P} - \nabla^2\varphi = 0$$

and then use the second of (13) to eliminate $\nabla\cdot\mathbf{P}$ with the result, after some manipulations,

$$\varepsilon(1 - l^2\nabla^2)\nabla^2\varphi = -[1 + (1 + \eta)l^2\nabla^2]\rho, \tag{15}$$

where

$$l = [\varepsilon_0 \eta (\beta_1 + 2\beta_2)/(1+\eta)]^{\frac{1}{2}}. \tag{16}$$

The constant l has the dimension of length and is estimated to be of the order of the distance between adjacent atoms or molecules.

A particular integral of (15) is

$$4\pi\varepsilon\varphi = \int_V \psi[1 + (1+\eta)l^2 \nabla^2]\rho \, dV, \tag{17}$$

where

$$\psi = (1 - e^{-r_1/l})/r_1 \tag{18}$$

and r_1 is the distance between a field point and a source point.

By Green's second identity,

$$\int_V \psi \nabla^2 \rho \, dV = \int_S \mathbf{n} \cdot (\psi \nabla \rho - \rho \nabla \psi) \, dS + \int_V \rho \nabla^2 \psi \, dV. \tag{19}$$

Also,

$$l^2 \nabla^2 \psi = e^{-r_1/l}/r_1. \tag{20}$$

Hence

$$4\pi\varepsilon\varphi = \varepsilon \int_S \mathbf{n} \cdot (\psi \nabla \rho - \rho \nabla \psi) \, dS + \int_V \rho r_1^{-1}(1 + \eta \, e^{-r_1/l}) \, dV. \tag{21}$$

Accordingly, for a point charge, q, in an infinite dielectric,

$$\varphi = q(1 + \eta \, e^{-r/l})/4\pi\varepsilon r, \tag{22}$$

where r is the distance from the point charge.

For materials with high dielectric susceptibility, the exponential correction term, in (22), can be significant even at distances of several times l from the point charge, where the continuum approximation is probably valid. A comparable result has been obtained from atomic considerations [3].

REFERENCES

[1] R. D. Mindlin, *Int. J. Solids Struct.* 4, 637 (1968); 5, 1197 (1969).
[2] R. A. Toupin, *J. ration. Mech. Analysis* 5, 849 (1956).
[3] G. D. Mahan and R. M. Mazo, *Phys. Rev.* 175, 1191 (1968).