Uniqueness of a class of nonlinear electrostatic field problems

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Abstract: The uniqueness properties of a class of nonlinear electrostatic field problems are investigated. The study was motivated by the development of numerical algorithms to analyse the performance of nonlinear semiconducting electron devices. Here, existence and uniqueness of the solution are prerequisites for the numerical results to have any meaning at all.

1 Introduction

Theoretical methods to analyse electrostatic field problems of the type that occur in nonlinear dielectric or nonlinear semiconducting electron devices invariably make use of computational techniques of an iterative nature. Even if a particular technique of this kind proves to converge numerically to a certain answer, the question remains whether this answer is the correct one and not depending on the particular numerical algorithm (including its starting values) employed. A possible ambiguity of this nature can only be resolved if the problem at hand can be shown to have a unique solution. For the case of linear media, the uniqueness properties of the solution of electromagnetic field problems in general have been studied extensively in the literature (see, for example, [1] for dynamic fields and [2, 3] for static and stationary fields). All these proofs essentially rely on the use of the superposition principle. In the presence of nonlinear media, however, the governing equations become nonlinear and the superposition principle fails to hold.

No general uniqueness proof for the solution of the electromagnetic field equations in the case of arbitrarily nonlinear media seems to exist. Sufficient conditions for uniqueness can only be derived for certain classes of problems for which additional assumptions as regards the constitutive properties of the media involved are made.

In this paper we shall present some criteria that ensure the uniqueness of the solution of a class of problems that refer to the computation of electrostatic fields of the type that occurs in nonlinear dielectric and nonlinear semiconducting electron devices. The relevant criteria are applicable to a wide range of problems met in electrical and electronic engineering practice.

The configurations to be considered are inhomogeneous in their electrical constitution, with possible jump discontinuities in their constitutive properties. They can be activated by a variety of 'external' means. Included are, in this respect, the presence of 'impressed' electric volume charges and 'impressed' electric polarisation. Of the former, we mention as an example the electric charges that are due to mechanical friction, accumulate in insulating parts of a configuration, and then can give rise to electrostatic discharges (ESDs). An example of the latter are objects consisting of permanently electrically polarised ceramics (electrets). Electric polarisation can also be used to represent the electrochemical action of a battery. In addition, the configuration can be excited electrically via a finite number of electrodes to which 'external' electric potentials are applied (as in the measuring equipment for electric capacitance tomography). It is important to notice that, due to the nonlinearity in the configuration's electrical behaviour, the fields associated with these different excitation mechanisms cannot be constructed with the aid of the superposition principle (as would be a natural way to do in the case of a configuration with linear electrical properties).

A rather detailed description is given of the admissible class of inhomogeneity and the admissible distributions in space of the source quantities. This description is not only necessary for stating the uniqueness theorem and constructing its proof, but it also serves as a guideline as to what features are to be accommodated in a numerical algorithm for solving field problems of the kind under consideration.

Most of the conditions that are invoked are sufficient conditions that have to do with existence of solutions of the partial differential equations and the associated boundary conditions involved (although we refrain from entering into the difficult area of existence proofs themselves), the applicability of Gauss' divergence theorem, and the kind of conditions for uniqueness. Moreover, some emphasis is placed on the so-called 'compatibility relations' (the term stems from the theory of elasticity, [4], p. 49). These are consequential relations that are automatically satisfied by any exact solution to the problem. However, as soon as solutions are constructed with the aid of numerical algorithms (which is almost a necessity in the case of nonlinear problems), a compatibility relation is no longer automatically satisfied. Experience with the computation of both dynamic and static electromagnetic fields has shown that a numerical solution can fail to converge and be highly erroneous if the relevant compatibility relations are not (numerically) taken into account as separate (and independent) condi-

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tions [5, 6]. A clear explanation for this phenomenon is not yet known, but the facts are there.

The cases for configurations of bounded extent (where the field exterior to the configuration is negligibly small), as in a large class of (shielded) electronic devices, and for configurations embedded in a vacuum exterior domain (where the exterior field extends to infinity) will be investigated separately.

2 Formulation of field problem

In the formulation of the problem, the following constituents are distinguished: the description of the configuration, the nomenclature of the field quantities, the nomenclature of the impressed volume source quantities, the (partial differential) field equations, the specification of the interface boundary conditions and the boundary conditions at the electrodes, and the description of the pertaining constitutive operators. As a corollary, the compatibility relation associated with the field equations is given.

2.1 Description of configuration

The configuration to be analysed is present in three-dimensional Euclidean space $\mathbf{R}^3$. Position in this space is specified by the Cartesian position vector $\boldsymbol{r}$. The material parts of the devices to be considered are contained in a bounded subdomain $\mathcal{D}$ of $\mathbf{R}^3$. The boundary surface of $\mathcal{D}$ is denoted as $\partial\mathcal{D}$. The (unbounded) complement of $\mathcal{D} \cup \partial\mathcal{D}$ in $\mathbf{R}^3$ is the vacuum domain denoted as $\mathcal{D}^\infty$. The domain $\mathcal{D}$ is partitioned into a, presumably finite, number N ($N \geq 1$) of subdomains $\mathcal{D}_n$, $n = 1, ..., N$, in such a manner that, in the interior of each $\mathcal{D}_n$, the impressed volume source densities values and the constitutive operators are continuous functions of position (Cartesian scalar, vector or tensor functions, as appropriate), while their limiting values on approaching the closed boundary surface $\partial\mathcal{D}_n$ of $\mathcal{D}_n$ via its interior are assumed to exist. Then, the only admissible discontinuities are jump discontinuities which may occur across common interfaces between adjacent subdomains of $\mathcal{D}$ and/or at interfaces of the latter with $\mathcal{D}^\infty$. The boundary surfaces $\partial\mathcal{D}$ and $\partial\mathcal{D}_n$, $n = 1, ..., N$, are assumed to be piecewise smooth.

Furthermore, in $\mathcal{D}$ a finite number $M + 1$ ($M \geq 1$) of disjoint electrodes, occupying the surfaces $\mathcal{S}_m$, $m = 0, 1, ..., M$, is present. Through them, the configuration is electrically accessible for acting as an electric or electronic device. Each $\mathcal{S}_m$ is assumed to be either a closed surface or a two-sided, non-closed surface of vanishing thickness. For both cases, the surfaces are assumed to be piecewise smooth. For closed electrode surfaces, their interior is excluded from $\mathcal{D}$. In the special case of a perfectly shielded configuration, we take $\mathcal{S}_0 = \partial\mathcal{D}$, in which case the interior of $\mathcal{S}_0$ coincides with $\mathcal{D}$, while now $\mathcal{D}^\infty$ plays no role in the analysis.

2.2 Impressed volume source quantities

The impressed volume source quantities are: the impressed electric polarisation $\boldsymbol{P}^{\text{imp}} = \boldsymbol{P}^{\text{imp}}(\boldsymbol{r})$ and the impressed volume source density of electric charge $\rho^{\text{imp}} = \rho^{\text{imp}}(\boldsymbol{r})$. Here, $\boldsymbol{P}^{\text{imp}}(\boldsymbol{r})$ is assumed to be a piecewise continuous vector function of position, $\boldsymbol{P}^{\text{imp}}$ having the bounded support $\mathcal{D}\boldsymbol{P} \subset \mathcal{D}$, while $\rho^{\text{imp}}(\boldsymbol{r})$ is assumed to be a piecewise continuous scalar function of position, ρ^{imp} having the bounded support $\mathcal{D}_\rho \subset \mathcal{D}$.

2.3 Electrostatic field quantities

The field quantities that characterise the electrostatic field are: the electric potential $\Phi = \Phi(\boldsymbol{r})$, the electric field strength $\boldsymbol{E} = \boldsymbol{E}(\boldsymbol{r})$, the electric flux density $\boldsymbol{D} = \boldsymbol{D}(\boldsymbol{r})$ and the volume density of charge $\rho = \rho(\boldsymbol{r})$. Under the assumptions stated in Subsections 2.1 and 2.2, it may be conjectured that there exists a solution to the field problem, in which the field quantities are continuously differentiable throughout each subdomain $\mathcal{D}_n$, $n = 1, ..., N$, (and $\mathcal{D}^\infty$, if applicable), while their limiting values on approaching the closed boundary surface $\partial\mathcal{D}_n$ of each subdomain $\mathcal{D}_n$, via its interior, exist. The relevant existence proof is hard to give and is beyond the scope of the present paper.

2.4 Field equations

In any subdomain $\mathcal{D}_n$, $n = 1, ..., N$, of the configuration and $\mathcal{D}^\infty$, the field quantities are to satisfy the partial differential equations

$$-\nabla\Phi(\boldsymbol{r}) = \boldsymbol{E}(\boldsymbol{r}) \tag{1}$$

and

$$\nabla \cdot \boldsymbol{D}(\boldsymbol{r}) = \rho(\boldsymbol{r}) \tag{2}$$

The total electric field strength $\boldsymbol{E}$ consists of the already specified (field-value independent) impressed part $\boldsymbol{E}^{\text{imp}} = -\varepsilon_0^{-1}\,\boldsymbol{P}^{\text{imp}}$ (active part) and a (field-value dependent) induced part $\boldsymbol{E}^{\text{ind}}$ (passive part), i.e.

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}^{\text{ind}}(\boldsymbol{r}) - \varepsilon_0^{-1}\boldsymbol{P}^{\text{imp}}(\boldsymbol{r}) \tag{3}$$

Here, ε_0 is the permittivity of vacuum ($\varepsilon_0^{-1} = \mu_0\, c_0^2$, where $\mu_0 = 4\pi \times 10^{-7}$H/m is the permeability of a vacuum and c_0 = 299792458m/s is the electromagnetic wave speed in a vacuum, both quantities dictated by SI [7]), while the minus sign and the factor ε_0^{-1} are dictated by the conventions in physics. Similarly, the total volume density of electric charge ρ consists of a (field-value independent) impressed part ρ^{imp} (active part) and a (field-value dependent) induced part ρ^{ind} (passive part), i.e.

$$\rho(\boldsymbol{r}) = \rho^{\text{ind}}(\boldsymbol{r}) + \rho^{\text{imp}}(\boldsymbol{r}) \tag{4}$$

2.5 Interface boundary conditions

Across the open, smooth parts of the interfaces where the constitutive properties jump by finite amounts, the following interface boundary conditions are to be satisfied:

$$\Phi = \text{continuous across the interface} \tag{5}$$

and

$$\boldsymbol{\nu} \cdot \boldsymbol{D} = \text{continuous across the interface} \tag{6}$$

where $\boldsymbol{\nu}$ is the unit vector along the normal to the interface.

2.6 Boundary conditions on electrodes

On the electrodes, the activating electric potentials have the constant values

$$\Phi = V_m \text{ on } \mathcal{S}_m, \quad m = 1, \ldots, M \tag{7}$$

while on $\mathcal{S}_0$ (the reference electrode) the electric potential is held at the value zero:

$$\Phi = 0 \text{ on } \mathcal{S}_0 \tag{8}$$

2.7 Constitutive operators

For a large class of materials in use in electric and electronic devices, the electrostatic constitutive behaviour can be described by operators that locally map $\boldsymbol{D}(\boldsymbol{r})$ to $\boldsymbol{E}^{\text{ind}}(\boldsymbol{r})$ and $\Phi(\boldsymbol{r})$ to $\rho^{\text{ind}}(\boldsymbol{r})$. The relevant operators are the field constitutive operator and the volume charge constitutive operator, respectively.

Field constitutive operator:

$$\mathsf{M}_F(\boldsymbol{r}) : \boldsymbol{D}(\boldsymbol{r}) \to \boldsymbol{E}^{\text{ind}}(\boldsymbol{r}) \tag{9}$$

is defined for any $\boldsymbol{r} \in \mathcal{D}_n$, n, ..., N, and in $\mathcal{D}^\infty$. For the generally anisotropic dielectric medium it is a Cartesian tensorial operator of rank two. For a medium with isotropic dielectric behaviour, the tensorial operator M_F has non-zero, identical, diagonal elements only, and $\boldsymbol{D}(\boldsymbol{r})$ and $\boldsymbol{E}^{\text{ind}}(\boldsymbol{r})$ have the same direction in space. The mapping $\mathsf{M}_F(\boldsymbol{r})$ is injective, in most cases of practical interest bijective. Physical models for $\mathsf{M}_F(\boldsymbol{r})$ are provided by, for example, the Lorentz theory of electrons ([8], p. 642).

Volume charge constitutive operator:

$$\mathsf{M}_\rho(\boldsymbol{r}) : \Phi(\boldsymbol{r}) \to \rho^{\text{ind}}(\boldsymbol{r}) \tag{10}$$

is defined for any $\boldsymbol{r} \in \mathcal{D}_n$, $n = 1, \ldots, N$, while in $\mathcal{D}^\infty$ we assume that $\rho^{\text{ind}} = 0$. This operator is a scalar operator. The mapping M_ρ is injective, in many cases of practical interest bijective. A physical model for M_ρ is provided by the quantum-statistical theory of semiconductors. In the relevant expressions for the local equilibrium number densities of the (negatively charged) electrons and (positively charged) holes, the quantum mechanical Fermi potential is, by an argument of an energetic nature, equated to the local value of the electric potential of the energising electric field. This procedure is justified by experimental data. Details of the analysis are given in, for example, [9] (Section 7.2) or [10]. Figs. 1 and 2 show the relevant functional relationship for holes and electrons, respectively. Note that, in semiconducting devices, one particular electrode always serves as the reference electrode. This electrode is chosen to be the one that ensures the desired electronic operation of the device. In the interior of the semiconducting material, the pertaining Fermi levels then adjust themselves to the electronic potential distribution generated by this operational choice.

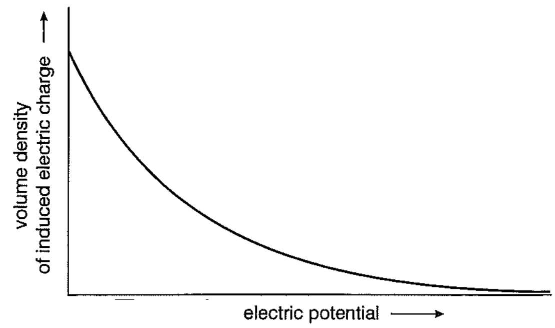

Fig. 1 *Volume density of induced electric charge in a semiconductor as a function of electric potential (holes)*

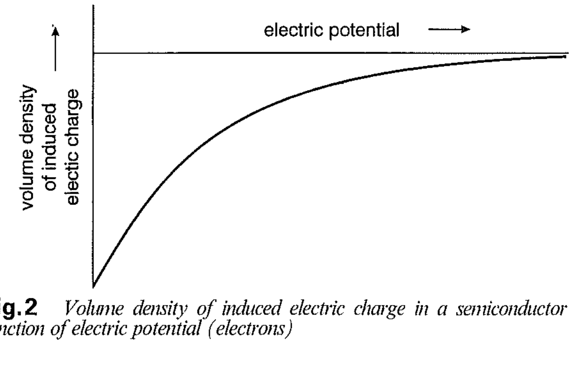

Fig. 2 *Volume density of induced electric charge in a semiconductor as a function of electric potential (electrons)*

It is assumed that $\mathsf{M}_F(\boldsymbol{r})$ and $\mathsf{M}_\rho(\boldsymbol{r})$ are continuous in $\boldsymbol{r}$ in the interior of each $\mathcal{D}_n$, $n = 1, \ldots, N$, and approach finite limiting values at $\partial\mathcal{D}_n$, $n = 1, \ldots, N$, while $\boldsymbol{E}^{\text{ind}}(\boldsymbol{r}) = \varepsilon_0^{-1}\boldsymbol{D}(\boldsymbol{r})$ and $\rho^{\text{ind}}(\boldsymbol{r}) = 0$ for $\boldsymbol{r} \in \mathcal{D}^\infty$. Across interfaces between adjacent subdomains of $\mathcal{D}$, M_F and M_ρ may show a jump discontinuity.

2.8 Compatibility relations

Eqn. 1 entails the compatibility relation

$$\int_{\mathcal{S}} \boldsymbol{n} \times \boldsymbol{E}\, dA = \boldsymbol{0} \tag{11}$$

for any piecewise smooth, closed surface $\mathcal{S}$ with unit vector $\boldsymbol{n} = \boldsymbol{n}(\boldsymbol{r})$ along its outward normal. Eqn. 11 follows from eqn. 1 by integrating $\boldsymbol{n} \times \nabla\Phi(\boldsymbol{r})$ over $\mathcal{S}$ and dividing $\mathcal{S}$ arbitrarily into two parts $\mathcal{S}'$ and $\mathcal{S}''$, both of which are delimited by the same, piecewise smooth, closed curve. Subsequent application of Stokes' circulation theorem to $\mathcal{S}'$ and $\mathcal{S}''$ shows that the two partial surface integrals cancel each other.

Eqn. 2 entails the compatibility relation

$$\int_{\partial\Omega} \boldsymbol{n} \cdot \boldsymbol{D}\, dA = \int_{\Omega} \rho\, dV \tag{12}$$

for any bounded domain Ω with piecewise smooth boundary surface $\partial\Omega$ and unit vector $\boldsymbol{n} = \boldsymbol{n}(\boldsymbol{r})$ along the outward normal. Eqn. 12 follows from eqn. 2 by the application of Gauss' divergence theorem.

As elucidated in the introduction, the compatibility relations are automatically satisfied by any exact solution to the partial differential eqns. 1 and 2. In numerical (or other nonexact) procedures they play, however, a role of importance on their own.

2.9 Field properties in exterior domain

Finally, the field properties in the exterior domain $\mathcal{D}^\infty$ have to be specified. Here, two possibilities arise:

(i) the case where proper electrical shielding or dielectric packaging of a device prevents the leakage of the field into its exterior, in which case the exterior field is negligibly small (see Figs. 3 and 4)

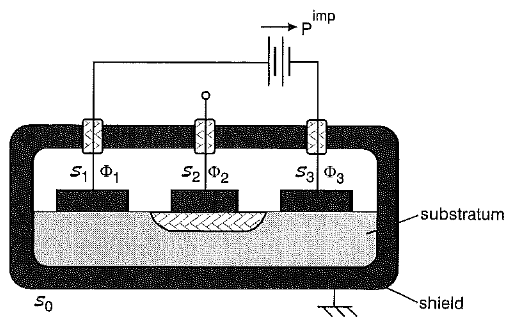

Fig. 3 *Electrically shielded electron device with negligible exterior field*

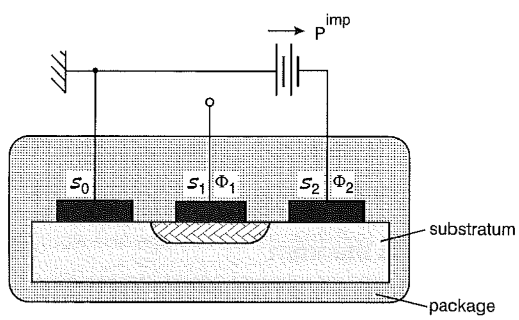

Fig. 4 *Packaged electron device with negligible exterior field*

(ii) the case where the exterior field is not negligibly small, in which case the latter's limiting behaviour as $|\boldsymbol{r}| \to \infty$ in $\mathcal{D}^\infty$ has to be specified (see Fig. 5).

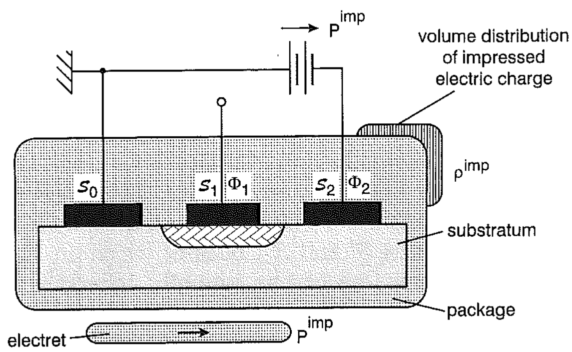

Fig. 5 *Packaged electron device with with non-negligible exterior field*

Configurations with negligible exterior field: The analysis of configurations with negligible exterior field is covered by prescribing explicit boundary conditions on $\partial\mathcal{D}$. Let $\partial\mathcal{D}'$ be the part of $\partial\mathcal{D}$ that takes care of the electrical shielding of the device and let $\partial\mathcal{D}''$ be the part of $\partial\mathcal{D}$ that takes care of its dielectric packaging. Then, the nonleakage of the field into $\mathcal{D}^\infty$ is mathematically covered by the boundary conditions

$$\Phi(\boldsymbol{r}) = 0 \text{ for } \boldsymbol{r} \in \partial\mathcal{D}' \tag{13}$$

and

$$\boldsymbol{n}(\boldsymbol{r}) \cdot \boldsymbol{D}(\boldsymbol{r}) = 0 \text{ for } \boldsymbol{r} \in \partial\mathcal{D}'' \tag{14}$$

where $\boldsymbol{n}$ is the unit vector along the outward normal to $\partial\mathcal{D}$.

Configurations with non-negligible exterior field: If the previous case does not apply, the behaviour of the field as $|\boldsymbol{r}| \to \infty$ in $\mathcal{D}^\infty$ has to be prescribed. As is proven in the Appendix (Section 7), the weakest *a priori* sufficient condition in this respect is

$$\Phi(\boldsymbol{r}) = o(1) \text{ as } |\boldsymbol{r}| \to \infty, \quad \text{uniformly in all directions in } \mathcal{D}^\infty \tag{15}$$

which involves the Landau symbol $o(1)$, ([8], p. 1020), meaning that $|\Phi(\boldsymbol{r})| \to 0$ as $|\boldsymbol{r}| \to \infty$. Because of the special structure of the field in the (vacuum) domain $\mathcal{D}^\infty$, entailed by the equations

$$-\nabla\Phi = \boldsymbol{E}^{\text{ind}} \tag{16}$$

$$\nabla \cdot \boldsymbol{D} = 0 \tag{17}$$

and

$$\boldsymbol{E}^{\text{ind}} = \varepsilon_0^{-1}\boldsymbol{D} \tag{18}$$

where use was made of the fact that (cf. Eqn. 3) $\boldsymbol{P}^{\text{imp}} = \boldsymbol{0}$ and $\rho = 0$ in the (vacuum) domain $\mathcal{D}^\infty$, the condition in eqn. 15 entails the properties (see the Appendix)

$$\Phi(\boldsymbol{r}) = \mathrm{O}(|\boldsymbol{r}|^{-1}) \text{ as } |\boldsymbol{r}| \to \infty, \quad \text{uniformly in all directions in } \mathcal{D}^\infty \tag{19}$$

and

$$\boldsymbol{D}(\boldsymbol{r}) = \mathrm{O}(|\boldsymbol{r}|^{-2}) \text{ as } |\boldsymbol{r}| \to \infty, \quad \text{uniformly in all directions in } \mathcal{D}^\infty \tag{20}$$

which involves the Landau order symbol O, ([8], p. 1019).

3 Uniqueness theorem

For the field problem formulated in Section 2, the following uniqueness theorem will be proven.

Theorem 1: For given values of the volume source quantities $\boldsymbol{P}^{\text{imp}}(\boldsymbol{r})$ and $\rho^{\text{imp}}(\boldsymbol{r})$ and given values V_m, $m = 1, \ldots, M$, of the electric potential Φ at the electrodes $\mathcal{S}_m$, $m = 1, \ldots, M$ (together with $\Phi = 0$ at the reference electrode $\mathcal{S}_0$), there exists at most one electrostatic field with field quantities $\{\Phi, \boldsymbol{D}, \rho^{\text{ind}}, \boldsymbol{E}^{\text{ind}}\}$ in $\cup_{n=1}^N \mathcal{D}_n$ (for the case of negligible exterior field) or $\{\cup_{n=1}^N \mathcal{D}_n\} \cup \mathcal{D}^\infty$ (for the case of non-negligible exterior field) provided that the constitutive operator M_F entails at each point $\boldsymbol{r} \in \cup_{n=1}^N \mathcal{D}_n$ the monotonicity relation

$$[\boldsymbol{D}_2(\boldsymbol{r}) - \boldsymbol{D}_1(\boldsymbol{r})] \cdot \left[\boldsymbol{E}_2^{\text{ind}}(\boldsymbol{r}) - \boldsymbol{E}_1^{\text{ind}}(\boldsymbol{r})\right] > 0 \quad \text{for any } \left\{\boldsymbol{D}_2(\boldsymbol{r}), \boldsymbol{E}_2^{\text{ind}}(\boldsymbol{r})\right\} \neq \left\{\boldsymbol{D}_1(\boldsymbol{r}), \boldsymbol{E}_1^{\text{ind}}(\boldsymbol{r})\right\} \tag{21}$$

and the constitutive operator M_ρ entails at each point $\boldsymbol{r} \in \cup_{n=1}^N \mathcal{D}_n$ where $\rho^{\text{ind}}(\boldsymbol{r}) \neq 0$ the monotonicity relation

$$[\Phi_2(\boldsymbol{r}) - \Phi_1(\boldsymbol{r})]\left[\rho_2^{\text{ind}}(\boldsymbol{r}) - \rho_1^{\text{ind}}(\boldsymbol{r})\right] < 0 \quad \text{for any } \left\{\Phi_2(\boldsymbol{r}), \rho_2^{\text{ind}}(\boldsymbol{r})\right\} \neq \left\{\Phi_1(\boldsymbol{r}), \rho_1^{\text{ind}}(\boldsymbol{r})\right\} \tag{22}$$

Proof: The proof starts in the standard manner by assuming that, for $\{\cup_{n=1}^N \mathcal{D}_n\} \cup \mathcal{D}^\infty$ and corresponding to the same set of prescribed excitation quantities, two non-identical fields $\{\Phi_1(\boldsymbol{r}), \boldsymbol{D}_1(\boldsymbol{r}), \rho_1^{\text{ind}}(\boldsymbol{r}), \boldsymbol{E}_1^{\text{ind}}(\boldsymbol{r})\}$ and $\{\Phi_2(\boldsymbol{r}), \boldsymbol{D}_2(\boldsymbol{r}), \rho_2^{\text{ind}}(\boldsymbol{r}), \boldsymbol{E}_2^{\text{ind}}(\boldsymbol{r})\}$ exist. Then, by subtracting the relevant eqns. 1 and 2 for the two fields, we obtain

$$-\nabla(\Phi_2 - \Phi_1) = \boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}} \tag{23}$$

and

$$\nabla \cdot (\boldsymbol{D}_2 - \boldsymbol{D}_1) = \rho_2^{\text{ind}} - \rho_1^{\text{ind}} \tag{24}$$

Now, consider the expression that results on multiplying eqn. 23 by $\boldsymbol{D}_2 - \boldsymbol{D}_1$ and eqn. 24 by $\Phi_2 - \Phi_1$ and subtracting the results. This yields

$$-\nabla \cdot \left[(\Phi_2 - \Phi_1)(\boldsymbol{D}_2 - \boldsymbol{D}_1)\right] = (\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot \left(\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}}\right) - (\Phi_2 - \Phi_1)\left(\rho_2^{\text{ind}} - \rho_1^{\text{ind}}\right) \tag{25}$$

For the difference field, the interface boundary conditions

$$\Phi_2 - \Phi_1 = \text{continuous across interfaces} \tag{26}$$

and

$$\boldsymbol{\nu} \cdot (\boldsymbol{D}_1 - \boldsymbol{D}_2) = \text{continuous across interfaces} \tag{27}$$

hold, while on the electrodes (including the reference one) we have

$$\Phi_2 - \Phi_1 = 0 \text{ on } \mathcal{S}_m, \quad m = 0, \ldots, M \tag{28}$$

The further proof runs differently for the two cases of negligible and non-negligible exterior fields.

Configurations with negligible exterior field: For configurations with negligible exterior field, the boundary conditions

$$\Phi_2(\boldsymbol{r}) - \Phi_1(\boldsymbol{r}) = 0 \text{ for } \boldsymbol{r} \in \partial\mathcal{D}' \tag{29}$$

and

$$\boldsymbol{\nu} \cdot [\boldsymbol{D}_1(\boldsymbol{r}) - \boldsymbol{D}_2(\boldsymbol{r})] = 0 \text{ for } \boldsymbol{r} \in \mathcal{D}'' \tag{30}$$

apply (cf. eqns. 13 and 14). Then, integrating eqn. 25 over $\mathcal{D}_n$, $n = 1, \ldots, N$, applying Gauss' divergence theorem, adding the results and using the interface boundary conditions, eqns. 26 and 27, the explicit boundary conditions eqn. 28 on the electrodes and eqns. 29 and 30 on the boundary surface $\partial\mathcal{D}$, it follows that

$$\sum_{n=1}^{N} \int_{\mathcal{D}_n} \left[(\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot \left(\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}}\right) - (\Phi_2 - \Phi_1)\left(\rho_2^{\text{ind}} - \rho_1^{\text{ind}}\right)\right] dV = 0 \tag{31}$$

This relation leads to eqns. 21 and 22 as sufficient conditions for uniqueness, since if eqns. 22 and 21 are satisfied, the left-hand side of eqn. 31 would be positive unless $\{\Phi_2(\boldsymbol{r}), \boldsymbol{D}_2(\boldsymbol{r}), \rho_2^{\text{ind}}(\boldsymbol{r}), \boldsymbol{E}_2^{\text{ind}}(\boldsymbol{r})\} = \{\Phi_1(\boldsymbol{r}), \boldsymbol{D}_1(\boldsymbol{r}), \rho_1^{\text{ind}}(\boldsymbol{r}), \boldsymbol{E}_1^{\text{ind}}(\boldsymbol{r})\}$ for all $\boldsymbol{r} \in \cup_{n=1}^{N} \mathcal{D}_n$.

Configurations with non-negligible exterior field: To investigate the conditions for uniqueness for the case of non-negligible exterior fields, first eqn. 25 is integrated over $\mathcal{D}_n$, $n = 1, ..., N$, Gauss' divergence theorem is applied, the results are added and the interface boundary conditions (eqns. 26 and 27) and the explicit boundary conditions (eqn. 28) on the electrodes are used. This leads to

$$\sum_{n=1}^{N} \int_{\mathcal{D}_n} \left[(\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot \left(\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}} \right) - (\Phi_2 - \Phi_1) \left(\rho_2^{\text{ind}} - \rho_1^{\text{ind}} \right) \right] dV = - \int_{\partial\mathcal{D}} \boldsymbol{n} \cdot [(\Phi_2 - \Phi_1)(\boldsymbol{D}_2 - \boldsymbol{D}_1)] \, dA \quad (32)$$

where $\boldsymbol{n}$ is the unit vector along the outward normal to $\partial\mathcal{D}$. In $\mathcal{D}^\infty$, the electrostatic field equations in vacuum eqns. 16–18 hold and hence

$$-\nabla(\Phi_2 - \Phi_1) = \left(\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}} \right) \quad (33)$$

$$\nabla \cdot (\boldsymbol{D}_2 - \boldsymbol{D}_1) = 0 \quad (34)$$

and

$$\left(\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}} \right) = \varepsilon_0^{-1} (\boldsymbol{D}_2 - \boldsymbol{D}_1) \quad (35)$$

Multiplying eqn. 33 by $\boldsymbol{D}_2 - \boldsymbol{D}_1$ and eqn. 34 by $\Phi_2 - \Phi_1$, subtracting the results and invoking eqn. 35 yields

$$-\nabla \cdot [(\Phi_2 - \Phi_1)(\boldsymbol{D}_2 - \boldsymbol{D}_1)] = \varepsilon_0^{-1} (\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot (\boldsymbol{D}_2 - \boldsymbol{D}_1) \text{ for all } \boldsymbol{r} \in \mathcal{D}^\infty \quad (36)$$

Eqn. 36 is integrated over the domain $\mathcal{D}_\Delta$ interior to the sphere $\mathcal{S}_\Delta = \{\boldsymbol{r}' \in \mathbf{R}^3; |\boldsymbol{r} - \boldsymbol{r}'| = \Delta\}$ and exterior to the boundary surface $\partial\mathcal{D}$. It is assumed that Δ is so large that $\partial\mathcal{D}$ is entirely interior to $\mathcal{S}_\Delta$. Next, Gauss' divergence theorem is applied. The limiting behaviour stated in eqns. 19 and 20 ensures that

$$\int_{\mathcal{S}_\Delta} \boldsymbol{n} \cdot [(\Phi_2 - \Phi_1)(\boldsymbol{D}_2 - \boldsymbol{D}_1)] \, dA = \mathrm{O}(\Delta^{-1}) \text{ as } \Delta \to \infty \quad (37)$$

Hence, taking the limit $\Delta \to \infty$ and using eqn. 35, it then follows that

$$\int_{\partial\mathcal{D}} \boldsymbol{n} \cdot [(\Phi_2 - \Phi_1)(\boldsymbol{D}_2 - \boldsymbol{D}_1)] \, dA = \int_{\mathcal{D}^\infty} (\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot \left(\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}} \right) dV \quad (38)$$

Addition of eqns. 32 and 38 and using the continuity of $\Phi_2 - \Phi_1$ and $\boldsymbol{n} \cdot (\boldsymbol{D}_2 - \boldsymbol{D}_1)$ across $\partial\mathcal{D}$ then yields

$$\sum_{n=1}^{N} \int_{\mathcal{D}_n} \left[(\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot \left(\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}} \right) - (\Phi_2 - \Phi_1) \left(\rho_2^{\text{ind}} - \rho_1^{\text{ind}} \right) \right] dV + \int_{\mathcal{D}^\infty} \varepsilon_0^{-1} (\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot (\boldsymbol{D}_2 - \boldsymbol{D}_1) dV = 0 \quad (39)$$

Now $(\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot (\boldsymbol{D}_2 - \boldsymbol{D}_1) > 0$ for all $\boldsymbol{r} \in \mathcal{D}^\infty$ and any $\boldsymbol{D}_2 \neq \boldsymbol{D}_1$. Hence, employing a similar argument as for the case of negligible exterior fields, again eqns. 21 and 22 follow as sufficient conditions for uniqueness, which concludes our proof.

A final observation has to be made with regard to those subdomains of $\mathcal{D}$ throughout which $\rho^{\text{ind}} = 0$. Here, the uniqueness condition eqn. 21 and the condition eqn. 31 lead to $\boldsymbol{E}_2 = \boldsymbol{E}_1$, and hence $\nabla\Phi_2 = \nabla\Phi_1$, thoughout such a domain, i.e. Φ_2 and Φ_1 may differ by a non-zero constant. In this case, we have to invoke the continuity of the electric potential throughout $\mathcal{D}$ and its vanishing at the surface of the electrode $\mathcal{S}_0$ to arrive at the uniqueness of Φ.

Corollary with regard to the field constitutive operator: First, it should be noted that the condition eqn. 21 holds for linear isotropic dielectrics with positive permittivity ([8], p. 618) and for linear anisotropic dielectrics with a symmetric, positive definite tensorial permittivity ([8], p. 619) of rank two.

For nonlinear isotropic dielectrics, a sufficient condition for eqn. 21 to be satisfied is the monotonicity relation

$$|\boldsymbol{E}_2^{\text{ind}}| \gtrless |\boldsymbol{E}_1^{\text{ind}}| \text{ for } |\boldsymbol{D}_2| \gtrless |\boldsymbol{D}_1| \quad (40)$$

To show this, we observe that for isotropic media

$$(\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot (\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}}) = (|\boldsymbol{D}_2| - |\boldsymbol{D}_1|)(|\boldsymbol{E}_2^{\text{ind}}| - |\boldsymbol{E}_1^{\text{ind}}|) + |\boldsymbol{D}_1||\boldsymbol{E}_2^{\text{ind}}| - \boldsymbol{D}_1 \cdot \boldsymbol{E}_2^{\text{ind}} + |\boldsymbol{D}_2||\boldsymbol{E}_1^{\text{ind}}| - \boldsymbol{D}_2 \cdot \boldsymbol{E}_1^{\text{ind}} \quad (41)$$

where we have used the properties that $\boldsymbol{E}_2^{\text{ind}}$ has the same direction as $\boldsymbol{D}_2$ and $\boldsymbol{E}_1^{\text{ind}}$ the same direction as $\boldsymbol{D}_1$. However, in view of the Cauchy–Schwarz inequality,

$$|\boldsymbol{D}_1||\boldsymbol{E}_2^{\text{ind}}| \geq |\boldsymbol{D}_1 \cdot \boldsymbol{E}_2^{\text{ind}}| \quad (42)$$

and

$$|\boldsymbol{D}_2||\boldsymbol{E}_1^{\text{ind}}| \geq |\boldsymbol{D}_2 \cdot \boldsymbol{E}_1^{\text{ind}}| \quad (43)$$

which leads to

$$(\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot (\boldsymbol{E}_2^{\text{ind}} - \boldsymbol{E}_1^{\text{ind}}) \geq (|\boldsymbol{D}_2| - |\boldsymbol{D}_1|)(|\boldsymbol{E}_2^{\text{ind}}| - |\boldsymbol{E}_1^{\text{ind}}|) \quad (44)$$

Hence, the condition in eqn. 40 implies eqn. 21. It should be noted that the condition in eqn. 40 is, for example, satisfied by the field constitutive operator illustrated in Fig. 6*a*, representing the relationship between $|\boldsymbol{E}_1^{\text{ind}}|$ and $|\boldsymbol{D}|$ for an isotropic, nonlinear dielectric whose material component to the constitutive relation follows from the well known Langevin function, i.e. $|\varepsilon_0^{-1} \boldsymbol{D} - \boldsymbol{E}^{\text{ind}}|$ as a function of $|\boldsymbol{E}^{\text{ind}}|$ ([10], pp. 558–559; see Fig. 6*b*). The latter is representative for the orientation of a collection of permanent electric dipoles under the influence of an external electric field as it follows from the application of the laws of classical statistical mechanics. Finally, it is mentioned that a condition similar to the one stated in eqn. 21 has previously been used in [11].

For nonlinear anisotropic dielectrics, no simpler sufficient condition for eqn. 21 to be satisfied seems to exlst.

Corollary with regard to the volume charge constitutive operator: A sufficient condition for eqn. 22 to be satisfied is here the monotonicity relation

$$|\rho_2^{\text{ind}}| \lesseqgtr |\rho_1^{\text{ind}}| \text{ for } |\Phi_2| \gtrless |\Phi_1| \quad (45)$$

It should be noted that the condition in eqn. 45 is standardly met in semiconducting electron devices for the volume densities of the electric charge of electrons and holes in their dependence on the electric potential ([10], pp. 572–573; [9], p. 89; see Figs. 1 and 2).

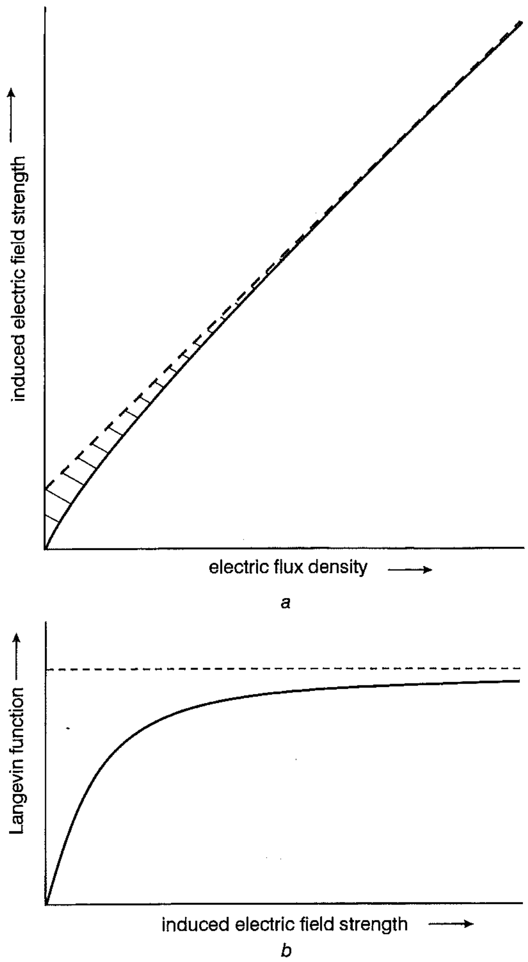

Fig. 6 *Induced electric field strength (magnitude) as a function of electric flux density (magnitude)*

4 Conclusions

A set of sufficient conditions for the uniqueness properties of the electrostatic field equations in a class of nonlinear electric and electronic devices has been derived. The materials show nonlinear electric and/or nonlinear semiconducting electronic properties. The conditions are of importance in the realm of the computational modelling of the electrostatic field in nonlinear electric and electronic devices.

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7 Appendix: Field behaviour in exterior vacuum domain

For the uniqueness proof pertaining to configurations where the field in the exterior vacuum domain is non-negligible, conditions for the behaviour of the electrostatic field at infinity must be specified. To this end, the field is investigated in the vacuum domain $\mathcal{D}^\infty$ exterior to the closed surface $\partial\mathcal{D}$. In $\mathcal{D}^\infty$, the equations

$$-\nabla\Phi = \boldsymbol{E}^{\text{ind}} \tag{46}$$

$$\nabla \cdot \boldsymbol{D} = 0 \tag{47}$$

$$\boldsymbol{E}^{\text{ind}} = \varepsilon_0^{-1}\boldsymbol{D} \tag{48}$$

hold. As a consequence, Φ satisfies Laplace's equation

$$\nabla^2\Phi = 0 \text{ for } \boldsymbol{r} \in \mathcal{D}^\infty \tag{49}$$

Now, let $\boldsymbol{r}$ be a point of observation located in $\mathcal{D}^\infty$. By applying Green's third identity ([1], p. 167) to the bounded domain exterior to $\partial\mathcal{D}$ and interior to the sphere $\mathcal{S}_\Delta = \{\boldsymbol{r}' \in \mathbf{R}^3;\ |\boldsymbol{r} - \boldsymbol{r}'| = \Delta\}$, where Δ is taken so large that $\mathcal{S}_\Delta$ completely surrounds $\partial\mathcal{D}$, it is found that

$$\begin{aligned}\Phi(\boldsymbol{r}) = &- \int_{\partial\mathcal{D}} \Big\{G(\boldsymbol{r},\boldsymbol{r}')[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')] \\ &\qquad - [\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla' G(\boldsymbol{r},\boldsymbol{r}')]\Phi(\boldsymbol{r}')\Big\}dA(\boldsymbol{r}') \\ &+ \int_{\mathcal{S}_\Delta} \Big\{G(\boldsymbol{r},\boldsymbol{r}')[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')] \\ &\qquad - [\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla' G(\boldsymbol{r},\boldsymbol{r}')]\Phi(\boldsymbol{r}')\Big\}dA(\boldsymbol{r}')\end{aligned} \tag{50}$$

where $\boldsymbol{n}$ is the unit vector along the outward normal to the relevant surface, the notation ∇' indicates that the spatial derivatives are taken with respect to the position vector $\boldsymbol{r}'$, and

$$G(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} \text{ for } \boldsymbol{r} \neq \boldsymbol{r}' \tag{51}$$

is the Green function of Laplace's equation (eqn. 49). Since on $\mathcal{S}_\Delta$ we have $|\boldsymbol{r} - \boldsymbol{r}'| = \Delta$, the integrals in the second term on the right-hand side of eqn. 50 can be rewritten as

$$\begin{aligned}&\int_{\mathcal{S}_\Delta} G(\boldsymbol{r},\boldsymbol{r}')[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')]dA(\boldsymbol{r}') \\ &\qquad = \frac{1}{4\pi\Delta}\int_{\mathcal{S}_\Delta} \boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')dA(\boldsymbol{r}')\end{aligned} \tag{52}$$

and

$$\begin{aligned}&\int_{\mathcal{S}_\Delta} [\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla' G(\boldsymbol{r},\boldsymbol{r}')]\Phi(\boldsymbol{r}')dA(\boldsymbol{r}') \\ &\qquad = \frac{-1}{4\pi\Delta^2}\int_{\mathcal{S}_\Delta} \Phi(\boldsymbol{r}')dA(\boldsymbol{r}')\end{aligned} \tag{53}$$

However,

$$\int_{S_\Delta} \boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')dA(\boldsymbol{r}') = \int_{\partial\mathcal{D}} \boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')dA(\boldsymbol{r}') \quad (54)$$

which follows on applying Gauss' integral theorem to the domain $\mathcal{D}_\Delta$ and using eqn. 49. Combining this with eqn. 52, it follows that

$$\int_{S_\Delta} G(\boldsymbol{r},\boldsymbol{r}')[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')]dA(\boldsymbol{r}') = \mathrm{O}(\Delta^{-1}) \quad \text{as } \Delta \to \infty \quad (55)$$

since the integral on the right-hand side of eqn. 54 is bounded. Next, imposing the condition

$$\Phi(\boldsymbol{r}) = \mathrm{o}(1) \text{ as } |\boldsymbol{r}| \to \infty, \quad \text{uniformly in all directions in } \mathcal{D}^\infty \quad (56)$$

we have from eqn. 53

$$-\int_{S_\Delta}[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'G(\boldsymbol{r},\boldsymbol{r}')]\Phi(\boldsymbol{r}')dA(\boldsymbol{r}') = \mathrm{o}(1) \text{ as } \Delta \to \infty \quad (57)$$

Hence, taking the limit $\Delta \to \infty$, it follows from eqn. 50 that, subject to the condition eqn. 56, the electric potential admits, in the entire domain exterior to $\partial\mathcal{D}$, the surface source representation

$$\Phi(\boldsymbol{r}) = -\int_{\partial\mathcal{D}} \Big\{G(\boldsymbol{r},\boldsymbol{r}')[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')] - [\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'G(\boldsymbol{r},\boldsymbol{r}')]\Phi(\boldsymbol{r}')\Big\}dA(\boldsymbol{r}') \quad \text{for } \boldsymbol{r} \in \mathcal{D}^\infty \quad (58)$$

Using in this representation the asymptotic expansions

$$G(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{4\pi|\boldsymbol{r}|}[1 + \mathrm{O}(|\boldsymbol{r}|^{-1})] \text{ as } |\boldsymbol{r}| \to \infty \quad \text{for } \boldsymbol{r}' \in \partial\mathcal{D} \quad (59)$$

and

$$\nabla'G(\boldsymbol{r},\boldsymbol{r}') = \frac{\boldsymbol{r}}{4\pi|\boldsymbol{r}|^3}[1 + \mathrm{O}(|\boldsymbol{r}|^{-1})] \text{ as } |\boldsymbol{r}| \to \infty \quad \text{for } \boldsymbol{r}' \in \partial\mathcal{D} \quad (60)$$

it follows that

$$\Phi(\boldsymbol{r}) = \mathrm{O}(|\boldsymbol{r}|^{-1}) \text{ as } |\boldsymbol{r}| \to \infty, \quad \text{uniformly in all directions in } \mathcal{D}^\infty \quad (61)$$

which is consistent with eqn. 56.

To obtain the asymptotic representation as $|\boldsymbol{r}| \to \infty$ for $\boldsymbol{D}$ in the domain exterior to $\partial\mathcal{D}$, we observe that in this region

$$\boldsymbol{D} = -\varepsilon_0\nabla\Phi \quad (62)$$

and, hence, from eqn. 58 it follows that

$$\boldsymbol{D}(\boldsymbol{r}) = \varepsilon_0\nabla\int_{\partial\mathcal{D}} \Big\{G(\boldsymbol{r},\boldsymbol{r}')[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'\Phi(\boldsymbol{r}')] - [\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'G(\boldsymbol{r},\boldsymbol{r}')]\Phi(\boldsymbol{r}')\Big\}dA(\boldsymbol{r}') \quad \text{for } \boldsymbol{r} \in \mathcal{D}^\infty \quad (63)$$

Using in this representation the asymptotic expansions

$$\nabla G(\boldsymbol{r},\boldsymbol{r}') = -\frac{\boldsymbol{r}}{4\pi|\boldsymbol{r}|^3}[1 + \mathrm{O}(|\boldsymbol{r}|^{-1})] \text{ as } |\boldsymbol{r}| \to \infty \quad \text{for } \boldsymbol{r}' \in \partial\mathcal{D} \quad (64)$$

and

$$\nabla[\boldsymbol{n}(\boldsymbol{r}')\cdot\nabla'G(\boldsymbol{r},\boldsymbol{r}')] = \left[\frac{\boldsymbol{n}(\boldsymbol{r}')}{4\pi|\boldsymbol{r}|^3} - \frac{3[\boldsymbol{n}(\boldsymbol{r}')\cdot\boldsymbol{r}]\boldsymbol{r}}{4\pi|\boldsymbol{r}|^5}\right][1 + \mathrm{O}(|\boldsymbol{r}|^{-1})] \quad \text{as } |\boldsymbol{r}| \to \infty \text{ for } \boldsymbol{r}' \in \partial\mathcal{D} \quad (65)$$

it follows that

$$\boldsymbol{D}(\boldsymbol{r}) = \mathrm{O}(|\boldsymbol{r}|^{-2}) \text{ as } |\boldsymbol{r}| \to \infty, \quad \text{uniformly in all directions in } \mathcal{D}^\infty \quad (66)$$

Eqns. 61 and 66 are used in the main text. Note that eqn. 66 is compatible with a differentiation of eqn. 61, but since termwise differentiation of an asymptotic expansion is in general not permitted ([12], p. 17), eqn. 66 had to be derived independently.