Drift-Diffusion: A Model for Teaching Spatial-Dispersion Concepts and the Importance of Screening in Nanoscale Structures

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Abstract

Spatial dispersion has emerged as an extremely important concept in modeling metamaterials, including macro-, micro-, and nano-structured composites. However, the incorporation of spatial dispersion requires a considerable complication of the usual Ohm's law relationship with which students are familiar. In this note, the drift-diffusion equation is shown to be equivalent to the usual form of spatial dispersion in simple isotropic plasmas and metamaterials. It is suggested that the drift-diffusion equation is physically clear and intuitive, and, therefore, can be effectively used to help teach concepts of spatial dispersion to beginning graduate students. Furthermore, the drift-diffusion equation leads to a simple treatment of charge screening, which is important for fundamental understanding, and for the electromagnetics of nanostructures.

Keywords: Metamaterials; local and nonlocal homogenization; spatial dispersion; drift-diffusion equation; electromagnetic propagation in nonhomogeneous media; electromagnetic propagation in plasma media; electromagnetic analysis

1. Introduction

Cpatial dispersion (non-locality) is associated with important Dphysical phenomena, such as natural optical activity, bianisotropy, and excitonic effects [1-3]. However, the effect is very small for many natural materials, and may often be neglected. This is particularly true below THz frequencies. As an example, for ordinary metals at room temperature, spatial dispersion is quite important near the plasma frequency (in the optical or UV range) [3], but far below these frequencies it can usually be ignored (although at low temperature, one encounters the anomalous skin effect [4]). The concept of spatial dispersion has gained great importance in the engineering electromagnetics community in recent years, due to its occurrence in artificial materials (metamaterials) at relatively low GHz frequencies, and to the strength of its contribution [5-10]. For example, in a wire medium consisting of metallic rods, at GHz frequencies we can ignore spatial dispersion in the rods themselves, but not in the effective medium formed by the rods. Moreover, spatial dispersion is important in the electromagnetic analysis of nanostructures, and for the analysis of charge screening. Therefore, there are many different reasons to teach concepts of spatial dispersion to beginning graduate students, or even to advanced undergraduates.

Physical understanding of the non-local nature of spatial dispersion can be difficult to grasp for students accustomed to the usual form of Ohm's law. It is suggested here that the connection between spatial dispersion and the drift-diffusion model of charge transport – more often used in modeling semiconductors [11] – can be exploited to teach concepts of spatial dispersion. It is shown that the most common form of spatial dispersion (associated with a "warm" plasma) is equivalent to the seemingly local drift-diffusion model [12, 13], the latter being straightforward to understand from an intuitive basis.

Aside from explaining spatial dispersion in plasmas, the driftdiffusion equation can be used to quite simply determine static screening from a conductor [14], avoiding more-complicated Thomas-Fermi treatments. One can argue that this topic, which is often absent from electromagnetic textbooks, is too important to ignore in developing an understanding of the electric-field behavior in conductors. Furthermore, for the electromagnetic analysis of nanoscale materials, charge screening is quite important, as sizes may approach the screening length. In the following, a time-harmonic variation, e^{jot} , is assumed and suppressed.

2. Current Due to Diffusion

In much of frequency-domain electromagnetics, we consider the constitutive relation $J(\mathbf{r}, \omega) = \sigma(\omega) \mathbf{E}(\mathbf{r}, \omega)$, Ohm's law, which provides the (drift) current associated with charge movement due to fields. We can also have charge movement due to diffusion, which is charge moving from an area of high charge concentration to an area of low concentration. Diffusion is a natural, fairly intuitive process that is important in many areas of science, including biology and chemistry. The topic of charge-carrier diffusion was nicely presented in [14, Section 11], from which most of the material in this section is taken.

The current associated with charge diffusion is given by Fick's law, $\mathbf{J}_{diff}(\mathbf{r}, \omega) = -D(\omega) \nabla \rho(\mathbf{r}, \omega)$, where D is the diffusion constant (m^2/s) and ρ is the charge density (C/m³). The negative sign is due to the fact that charge moves from an area of high concentration to an area of low concentration, whereas the gradient points from low to high concentration. The total current in the drift-diffusion model for an isotropic, homogeneous medium is thus

$$\mathbf{J}(\mathbf{r},\omega) = \sigma(\omega)\mathbf{E}(\mathbf{r},\omega) - D(\omega)\nabla\rho(\mathbf{r},\omega). \tag{1}$$

The diffusion term is applicable when $\omega < \gamma = 1/\tau$, where γ is the collision frequency and τ is the time between collisions. This condition means that there should be lots of particle collisions in each cycle of oscillation. The drift-diffusion equation is derived in the appendix using a hydrodynamic model (alternatively, it can be derived from Boltzmann's equation).

In terms of frequency dependence, we can write the conductivity and diffusion constants as

$$\sigma(\omega) = \frac{q^2 n_e \tau}{m_e (1 + j\omega\tau)}$$

$$= \frac{\omega_p^2 \tau \varepsilon_0}{(1 + j\omega\tau)}$$

$$= \frac{\sigma_0}{1 + j\omega\tau},$$

$$D(\omega) = \frac{\beta \tau}{1 + j\omega\tau}$$
(2)

$$=\frac{D_0}{1+j\omega\tau},$$
(3)

where $\omega_p^2 = n_e q_e^2 / \varepsilon_0 m_e$ is the plasma frequency. The static diffusion constant for an electron plasma is $D_0 = \beta \tau$, where $\beta = \langle v^2 \rangle / 3$, with $\langle v^2 \rangle$ being the mean-square velocity of the charge carrier. For good metals,

$$\left\langle v^2 \right\rangle = \frac{3}{5} v_F^2, \tag{4}$$

where v_F is the electron Fermi velocity $v_F = \hbar \left(3\pi^2 n_e\right)^{1/3} / m_e$, n_e is the electron density (m⁻³), \hbar is the reduced Planck's constant, and m_e is the electron mass. Therefore,

$$D_0^{metal} = \frac{1}{5} v_F^2 \tau \,. \tag{5}$$

As an example, for copper, $n_e \approx 8.45 \times 10^{28} / \text{m}^3$, $\tau = 2.47 \times 10^{-14} \text{ s}$ (at room temperature), $v_F = 1.57 \times 10^6 \text{ m/s}$, and $D = 0.0122 \text{ m}^2 / \text{s}$.

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For a semiconductor or a low-density plasma, $v = v_{thermal}$, where

$$\frac{1}{2}m_e \left\langle v_{thermal}^2 \right\rangle = \frac{3}{2}k_B T \,, \tag{6}$$

and where k_B is Boltzmann's constant and T is temperature in kelvin. We therefore obtain

$$D_0^{plasma} = \frac{k_B T}{m_e} \tau$$
$$= \frac{k_B T}{e^2 n_e} \sigma_0, \tag{7}$$

where $\sigma_0 = e^2 n_e \tau / m_e$ is the usual dc conductivity (-e is the charge of an electron). In terms of mobility, μ ,

$$D_0^{plasma} = \frac{\mu}{e} k_B T , \qquad (8)$$

which is known as the Einstein relation. For a semiconductor, similar relations can be developed for the hole density.

As an example, at room temperature, intrinsic Si has electron and hole mobilities of $\mu_e = 0.1350 \text{ m}^2/\text{V-s}$ and $\mu_h = 0.045 \text{ m}^2/\text{V-s}$, leading to the diffusion constants $D_e = 0.00349 \text{ m}^2/\text{s}$ and $D_h = 0.00116 \text{ m}^2/\text{s}$. Comparing with $D_{copper} = 0.0122 \text{ m}^2/\text{s}$, we see that D_0 only differs by approximately one order of magnitude between a very good conductor and a fairly poor conductor.

The units of D are m^2/s , and the meaning is that the time taken for a particle to diffuse a distance L is

$$\tau_L = \frac{L^2}{D_0}.$$
(9)

Note that in a good conductor, we typically don't need to consider diffusion, unless we are interested in the screening of fields that occurs over very small (sub-angstrom) distances at the surface of the conductor (as discussed later). From the continuity equation (assuming $J = \sigma E$), we have

$$\rho(t) = \rho(0) e^{-t/\tau_{\rho}},$$

where $\tau_{\rho} = \varepsilon/\sigma$ is the characteristic time for charge to disperse in a material. Assuming $\sigma = 10^7$ S/m and $\varepsilon = \varepsilon_0$ as for a good metal, then $\tau_p \sim 9 \times 10^{-19}$ s. Any excess charge thus moves to the surface almost instantaneously, and we don't have any charge-density gradients in the material bulk (i.e., $\nabla \rho = 0$, unless we are considering times less than 10^{-18} s). In a bulk semiconductor this is not the case, and charge-density gradients are important for times short compared to τ_p . For intrinsic Si, $n_e = n_p = 10^{16}$ m⁻³, so that $\sigma = e\mu_e n_e + e\mu_p n_p = 0.00028$ S/m. Assuming $\varepsilon_{Si} \approx 12$, then we have $\tau_p = 0.379$ µs, thus allowing $\nabla \rho \neq 0$ to exist over moderately long time scales. Perhaps more importantly, in semiconductor junctions (e.g., a pn junction) or metal-semiconductor junctions at equilibrium, there are charge-density gradients over macroscale distances, which do not occur for metal-metal junctions.

3. Connection Between Spatial Dispersion and Drift-Diffusion

For the case of a homogeneous material, a general linear relationship between current density and field is [4]

$$J(\mathbf{r},\omega) = \int \overline{\sigma} (\mathbf{r} - \mathbf{r}', \omega) \cdot \mathbf{E}(\mathbf{r}', \omega) d^3 \mathbf{r}', \qquad (10)$$

with the local case recovered from $\overline{\sigma}(\mathbf{r}-\mathbf{r}',\omega) = \overline{\sigma}(\omega)\delta(\mathbf{r}-\mathbf{r}')$. Upon using a spatial Fourier transform, $\mathbf{r} \leftrightarrow \mathbf{q}$, and the convolution theorem, we have

$$\mathbf{J}(\mathbf{q},\omega) = \overline{\sigma}(\mathbf{q},\omega) \cdot \mathbf{E}(\mathbf{q},\omega). \tag{11}$$

It is shown next that the "local" drift-diffusion relation, Equation (1), leads to an equation of the same form.

Using the continuity equation, $\rho(\mathbf{r},\omega) = -\nabla \cdot \mathbf{J}(\mathbf{r},\omega)/j\omega$, the drift-diffusion equation, Equation (1), becomes

$$\mathbf{J}(\mathbf{r},\omega) = \sigma(\omega)\mathbf{E}(\mathbf{r},\omega) + \frac{D(\omega)}{j\omega}\nabla[\nabla \cdot \mathbf{J}(\mathbf{r},\omega)], \qquad (12)$$

or

$$\left(1 - \frac{D(\omega)}{j\omega} \nabla \nabla\right) \cdot \mathbf{J}(\mathbf{r}, \omega) = \sigma(\omega) \mathbf{E}(\mathbf{r}, \omega), \qquad (13)$$

where 1 is the identity dyadic. Just as the local form of Ohm's law, $\mathbf{E}(\mathbf{r}, \omega) = \sigma(\omega)^{-1} \mathbf{J}(\mathbf{r}, \omega)$, is an extension of the circuit form of Ohm's law $(V(\omega) = G(\omega)^{-1} I(\omega))$, where $G^{-1}(\omega) = Z(\omega)$ is the conductance and Z is the impedance) to vector functions of position, Equation (13) is a non-local extension of Ohm's law. Non-locality is easy to grasp in the differential form of an expression, since the nature of a derivative is to sample the quantity that it acts on not only at the point in question, but also at nearby points. For example, in this sense Faraday's law $\nabla \times \mathbf{E}(\mathbf{r}, \omega) = -j\omega \mathbf{B}(\mathbf{r}, \omega)$ is also non-local, where the magnetic field at **r** depends on the electric field not only at **r**, but at nearby points.

The form of Equation (13) is not particularly surprising, since it says that the electric field at **r** associated with a current density depends not only on the value of the current density at **r**, but also at nearby points. Although this is not the case for the usual local Ohm's law, $\mathbf{E}(\mathbf{r},\omega) = \sigma(\omega)^{-1} \mathbf{J}(\mathbf{r},\omega)$, it is actually a typical case in electromagnetics, and, in particular, in antenna and other sourceexcited problems. For example, consider a homogeneous space characterized by scalar permittivity ε and scalar permeability μ , where the wavenumber is $k = \omega \sqrt{\mu \varepsilon}$. The electric field due to a current $\mathbf{J} \in \Omega$ is

$$\mathbf{E}(\mathbf{r},\omega) = \frac{1}{j\omega\varepsilon} \left(k^2 + \nabla\nabla \cdot\right) \int_{\Omega} \frac{e^{-jkR(\mathbf{r},\mathbf{r}')}}{4\pi R(\mathbf{r},\mathbf{r}')} \mathbf{J}(\mathbf{r}',\omega) d\mathbf{r}', \quad (14)$$

where $R(\mathbf{r}, \mathbf{r}') = |\mathbf{r} - \mathbf{r}'|$ and Ω is the support of the current. In this case, the electric field at \mathbf{r} is the superposition of the response of the current over all points \mathbf{r}' where $\mathbf{J}(\mathbf{r}', \omega) \neq 0$ (and we can have $\mathbf{r} \in \Omega$, and also $\mathbf{r} = \mathbf{r}'$). In a sense, Equation (14) (even without the $\nabla \nabla$ term), or any spatial superposition, is also a non-local relationship. However, spatial superposition is a somewhat trivial form of spatial non-locality.

The real point in understanding non-locality in the sense of spatially-dispersive materials is to invert Equation (13) as

$$\mathbf{J}(\mathbf{r},\omega) = \sigma(\omega) \left[\mathbf{1} - \frac{D(\omega)}{j\omega} \nabla \nabla \right]^{-1} \cdot \mathbf{E}(\mathbf{r},\omega) , \qquad (15)$$

and to view E as the driving field that produces current J. In this form, non-locality means that the response of the current density at r is due not only to the driving field at r, but also to the value of the driving field at points near to r.

We can obtain the form of Equation (11) upon a spatial Fourier transform of the above expression, leading to (see also [15] for a similar expression)

$$\overline{\sigma}(\mathbf{q},\omega) = \sigma(\omega) \left[\mathbf{1} + \frac{D(\omega)}{j\omega} \mathbf{q} \mathbf{q} \right]^{-1}.$$
 (16)

We can easily perform the inversion in Equation (16). The term 1 is the 3×3 identity matrix. Assuming any coordinate direction for \mathbf{q} , $\mathbf{q} = \hat{\alpha}q_{\alpha}$, where $\alpha = x$ or y or z, and the term $\mathbf{q}\mathbf{q}$ is a 3×3 diagonal matrix with one non-zero entry. Adding these two matrices results in a 3×3 diagonal matrix that is trivially inverted, resulting in

$$\overline{\sigma}(\mathbf{q},\omega) = \sigma(\omega) \left[\mathbf{1} - \frac{D(\omega)}{j\omega + D(\omega)q^2} \mathbf{q} \mathbf{q} \right].$$
(17)

Fourier inversion of the expression $J(q, \omega) = \overline{\sigma}(q, \omega) \cdot E(q, \omega)$ obviously leads to the general form of Equation (10). Therefore, starting with the drift-diffusion model for a homogeneous, isotropic medium, we obtain the usual non-local form, Equation (10). Although not shown above, it turns out that, conversely, starting from the non-local form Equation (10), and assuming an isotropic, homogeneous medium in which only the longitudinal response exhibits spatial dispersion (in which case $\bar{\sigma}(\mathbf{q},\omega) = \hat{\mathbf{q}}\hat{\mathbf{q}}\sigma_L(q,\omega) + (1-\hat{\mathbf{q}}\hat{\mathbf{q}})\sigma(\omega)$, which is equivalent to Equation (17) when $\sigma_L(\mathbf{q},\omega) = \alpha(\mathbf{q},\omega)\sigma(\omega)$, one obtains the drift-diffusion equation. For $\bar{\sigma}(\mathbf{q},\omega)$ having a more-general form (including spatial dispersion in the transverse component, which can be important in some plasmas), one obtains a modified driftdiffusion equation.

Parenthetically, it should be noted that the inverse transform of Equation (17) can easily be performed to obtain $\bar{\sigma}(\mathbf{r},\omega)$. The term associated with the identity dyadic is obviously the local term, leading to $\sigma(\omega)\delta(\mathbf{r})\mathbf{1}$. The other term can be evaluated using complex-plane analysis, since the only singularities are simple poles occurring at $q_p = \pm \sqrt{-j\omega/D(\omega)}$.

Since we have taken a spatial Fourier transform, we have a wave propagating in the direction \mathbf{q} . In a homogeneous local medium, there would only be a transverse component of field \mathbf{E} , perpendicular to \mathbf{q} . However, in a homogeneous spatially dispersive medium, we also have a longitudinal component of \mathbf{E} , parallel to \mathbf{q} (we also obtain a longitudinal field component in a local inhomogeneous medium, such as a planar dielectric waveguide or optical fiber, but this is a different matter). This naturally leads to the concepts of a transverse and longitudinal conductivity, which arise from the dyadic quantity of Equation (17). To see this, it becomes necessary to separate currents and fields into transverse and longitudinal (to \mathbf{q}) components,

$$\mathbf{J} = \mathbf{J}_L + \mathbf{J}_T,$$

$$\mathbf{E} = \mathbf{E}_L + \mathbf{E}_T.$$
(18)

Substituting into Equation (15), we obtain

$$\mathbf{J}_{L}(\mathbf{q},\omega) = \sigma_{L}(q,\omega)\mathbf{E}_{L}(\mathbf{q},\omega), \qquad (19)$$

$$\mathbf{J}_{T}(\mathbf{q},\omega) = \sigma_{T}(\omega)\mathbf{E}_{T}(\mathbf{q},\omega), \qquad (20)$$

where

$$\sigma_{L}(q,\omega) = \frac{\sigma(\omega)}{1 + \frac{D(\omega)}{j\omega}q^{2}}$$

$$\sigma_{T}(\omega) = \sigma(\omega).$$
(21)

This shows that spatial dispersion manifests itself in the longitudinal – and not the transverse – conductivity (adding other derivatives to the drift-diffusion model could lead to the transverse conductivity being \mathbf{q} -dependent, but this is beyond the scope of the present treatment).

A more-familiar form is provided by forming the complex effective permittivity. If $\varepsilon_r(\omega) = \varepsilon' - j\varepsilon''$ is the relative permittivity ($\varepsilon = \varepsilon_r \varepsilon_0$) associated with polarization, the associated relative complex permittivity that accounts for polarization and charge movement is

$$\varepsilon_r(\omega) = \varepsilon' - j\varepsilon'' - j\frac{\sigma}{\omega\varepsilon_0}.$$
 (22)

Then, using Equation (2),

$$\varepsilon_r^L(q,\omega) = \varepsilon' - j\varepsilon'' - j\frac{\sigma_L(q,\omega)}{\omega\varepsilon_0}$$
(23)

$$=\varepsilon'-j\varepsilon''-\frac{\omega_p^2}{\omega(\omega-j\gamma)-\beta q^2},$$
(24)

which is the usual form for non-local permittivity. As such, the form for the spatial-dispersion parameter β is $\beta = D_0/\tau$, where

 D_0 is the static diffusion constant. The transverse permittivity arising from $\sigma_T = \sigma$ is the usual local result,

$$\varepsilon_r^T(q,\omega) = \varepsilon_r^T(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega - j\gamma)}.$$
 (25)

Note that up to this point all equations have been exact, and no approximations have been made. For small q, it is sometimes useful to expand the denominator in a power series in q, resulting in

$$\varepsilon_{r}^{L}(q,\omega) = \varepsilon' - j\varepsilon'' - \omega_{p}^{2} \left[\frac{1}{\omega(\omega - j\gamma)} + q^{2} \frac{\beta}{\omega^{2}(\omega - j\gamma)^{2}} + \dots \right],$$
(26)

highlighting the connection between spatial dispersion and spatial derivatives of the response.

In summary, starting with the drift-diffusion model of Equation (1), we can obtain the non-local relation Equation (10), and also identify the transform-domain conductivity tensor Equation (17). From this, we obtain the usual form of the non-local permittivity, Equation (24), used in simple plasma calculations. Since diffusion is an intuitively clear physical process, this approach may be useful in teaching spatial-dispersion concepts.

4. Drift-Diffusion for Artificial Plasmas

The longitudinal permittivity, Equation (24), is also of the form often assumed for the effective permittivity of metamaterial plasmas. For example, for a wire medium, this is the form of the permittivity along the wire's axis [5]. However, in that case we are not interested in what may be viewed as microscopic or electronic spatial dispersion, where ω_p and $\beta = \langle v^2 \rangle / 3$ refer to electron motion, but to macroscopic electromagnetic quantities, where ω_p and β refer to properties of the electromagnetic wave in the artificial medium. For example, in a wire medium, we use $\beta = v_p^2$, where v_p is the phase velocity of the wave in the host medium of the wires, and $k_p = \omega_p / v_p$ is a plasma wavenumber corresponding to the wire-medium's plasma frequency (which is a function of the wire's lattice period and the wire radius). The result for a wire medium consisting of perfectly conducting, infinitely long parallel wires (i.e., an artificial material formed by a two-dimensional lattice of infinite wires with period small compared to wavelength) is [5]

$$\varepsilon_r^L(q,\omega) = 1 - \frac{k_p^2}{k^2 - q^2}, \qquad (27)$$

where $k = \omega/v_p$ and $k_p^2 = (2\pi/a^2)/[\ln(a/2\pi R) + 0.5275]$, where *a* is the lattice period and *R* is the wire's radius. The permittivity transverse to the wire's axis is

$$\varepsilon_r^T(\omega) = \varepsilon_r(\omega), \tag{28}$$

where $\varepsilon_r(\omega)$ is the host medium permittivity. However, this medium is anisotropic, complicating the formation of an equivalent



Figure 1. An example of a homogeneous, isotropic metamaterial consisting of a triple array of connected metal wires.

drift-diffusion equation. Instead, we consider an isotropic metamaterial, such as a triple array of connected wires [16] as depicted in Figure 1. In this case, the effective medium is isotropic and spatially dispersive.

For this type of material, we can form a drift-diffusion equation for the polarization. In simple materials, the relationship between polarization and electric field is

$$\mathbf{P}(\mathbf{r},\omega) = \varepsilon_0 \chi(\omega) \mathbf{E}(\mathbf{r},\omega)$$

$$= \varepsilon_0 [\varepsilon_r(\omega) - 1] \mathbf{E}(\mathbf{r},\omega).$$
(29)

For the polarization in a metamaterial, we will write

$$\mathbf{P}(\mathbf{r},\omega) = \mathbf{P}_{h}(\mathbf{r},\omega) + \mathbf{P}_{eff}(\mathbf{r},\omega), \qquad (30)$$

where \mathbf{P}_h is the dynamic polarization associated with the host material (the dielectric background), and \mathbf{P}_{eff} is the effective polarization that accounts for the presence of the metamaterial inclusions. In analogy with Equation (1), we will assume the form

$$\mathbf{P}(\mathbf{r},\omega) = \varepsilon_0 \chi(\omega) \mathbf{E}(\mathbf{r},\omega) + \varepsilon_0 D(\omega) \nabla \rho_{eff}(\mathbf{r},\omega), \quad (31)$$

where ρ_{eff} is an effective polarization charge density (C/m³) and χ is the susceptibility of the host medium. The relation between current density and polarization is

$$\mathbf{J}(\mathbf{r},t) = \frac{\partial}{\partial t} \mathbf{P}(\mathbf{r},t) \rightarrow \mathbf{J}(\mathbf{r},\omega) = j\omega \mathbf{P}(\mathbf{r},\omega), \qquad (32)$$

and so we can rewrite Equation (31) in terms of polarization current as

$$\mathbf{J}_{p}(\mathbf{r},\omega) = j\omega\varepsilon_{0}\chi(\omega)\mathbf{E}(\mathbf{r},\omega) + j\omega\varepsilon_{0}D(\omega)\nabla\rho_{eff}(\mathbf{r},\omega)$$
(33)
$$= j\omega\varepsilon_{0}\chi(\omega)\mathbf{E}(\mathbf{r},\omega) + D_{p}(\omega)\nabla\rho_{eff}(\mathbf{r},\omega),$$
(34)

where $D_p(\omega) = j\omega\varepsilon_0 D(\omega)$ has units of m^2/s , as expected for a diffusion constant. Therefore, Equation (34) is a drift-diffusion equation for polarization current in a metamaterial.

The drift-diffusion equation for current in conducting media is well established, and the manipulations in the previous section are straightforward consequences of this relationship. For metamaterials, the situation is not so clear. However, since the longitudinal permittivity, Equation (24), often occurs in metamaterials, the ansatz, Equation (31), can be justified if it leads to a non-local permittivity of the known form. So, in the following we will assume the form of Equation (31) and see what material-response function is obtained.

Using

$$\nabla \cdot \mathbf{P}(\mathbf{r}, \omega) = \nabla \cdot \mathbf{P}_{h}(\mathbf{r}, \omega) + \nabla \cdot \mathbf{P}_{eff}(\mathbf{r}, \omega)$$
$$= \nabla \cdot \mathbf{P}_{eff}(\mathbf{r}, \omega)$$
$$= -\rho_{eff}(\mathbf{r}, \omega)$$

(since the uniform background polarization, P_h , is independent of position), then,

$$\mathbf{P}(\mathbf{r},\omega) = \varepsilon_0 \chi(\omega) \mathbf{E}(\mathbf{r},\omega) - \varepsilon_0 D(\omega) \nabla \nabla \cdot \mathbf{P}(\mathbf{r},\omega).$$
(35)

Upon Fourier transformation, we have

$$\mathbf{P}(\mathbf{q},\omega) = \varepsilon_0 \chi(\omega) \mathbf{E}(\mathbf{q},\omega) + \varepsilon_0 D(\omega) \mathbf{q} \mathbf{q} \cdot \mathbf{P}(\mathbf{q},\omega), \quad (36)$$

so that

1

$$\left[\mathbf{1} - \varepsilon_0 D(\omega) \mathbf{q} \mathbf{q}\right] \cdot \mathbf{P}(\mathbf{q}, \omega) = \varepsilon_0 \chi(\omega) \mathbf{E}(\mathbf{q}, \omega), \qquad (37)$$

or

$$\mathbf{P}(\mathbf{q},\omega) = \varepsilon_0 \chi(\omega) [\mathbf{1} - \varepsilon_0 D(\omega) \mathbf{q} \mathbf{q}]^{-1} \cdot \mathbf{E}(\mathbf{q},\omega).$$
(38)

The inversion is easily performed in the same manner as in the last section (inversion of a 3×3 diagonal matrix) to yield

$$\mathbf{P}(\mathbf{q},\omega) = \left(\mathbf{1} + \frac{\varepsilon_0 D}{1 - \varepsilon_0 D q^2} \mathbf{q} \mathbf{q}\right) \cdot \varepsilon_0 \chi(\omega) \mathbf{E}, \qquad (39)$$

or

$$\mathbf{P}(\mathbf{q},\omega) = \varepsilon_0 \overline{\chi}(\mathbf{q},\omega) \cdot \mathbf{E} , \qquad (40)$$

where

$$\overline{\chi}(\mathbf{q},\omega) = \chi(\omega) \left(1 + \frac{\varepsilon_0 D}{1 - \varepsilon_0 D q^2} \mathbf{q} \mathbf{q} \right), \tag{41}$$

analogous to Equation (17).

Defining the relative permittivity as

$$\overline{\varepsilon}(\mathbf{q},\omega) = \mathbf{1} + \overline{\chi}(\mathbf{q},\omega), \qquad (42)$$

we obtain

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$$\overline{\varepsilon}(\mathbf{q},\omega) = \mathbf{1} + \chi(\omega) \left(\mathbf{1} + \frac{\varepsilon_0 D}{1 - \varepsilon_0 D q^2} \mathbf{q} \mathbf{q}\right)$$
(43)

$$= \left\{ \chi(\omega) \frac{\varepsilon_0 D q^2}{1 - \varepsilon_0 D q^2} + \left[\chi(\omega) + 1 \right] \right\} \frac{\mathbf{q}\mathbf{q}}{q^2}$$
(44)

$$+\left[\chi(\omega)+1\right]\left(1-\frac{\mathbf{q}\mathbf{q}}{q^2}\right) \tag{45}$$

$$=\varepsilon^{L}(\mathbf{q},\omega)\frac{\mathbf{q}\mathbf{q}}{q^{2}}+\varepsilon^{T}(\omega)\left(1-\frac{\mathbf{q}\mathbf{q}}{q^{2}}\right),$$
(46)

which is the usual form for the spatially-dispersive permittivity tensor for a homogeneous isotropic medium [4, 16], where we added and subtracted $\mathbf{qq} \left[\chi(\omega) + 1 \right] / qq$ in the second line.

To identify the diffusion constant for a homogeneous wiremesh medium, we compare Equation (46) with the form of $\varepsilon^{T/L}$ given in [16]. In terms of susceptibility,

$$\overline{\chi}(\mathbf{q},\omega) = \overline{\varepsilon}(\mathbf{q},\omega) - \mathbf{1} \tag{47}$$

$$= \left(\varepsilon^{T}(\omega) - 1\right) \left\{ 1 + \frac{\mathbf{q}\mathbf{q}}{q^{2}} \frac{\varepsilon^{T}(\omega)}{\left[\varepsilon^{T}(\omega) - 1\right]} \left[\frac{\varepsilon^{L}(\mathbf{q}, \omega)}{\varepsilon^{T}(\omega)} - 1 \right] \right\}$$
(48)

$$= \chi(\omega) \left[1 + \frac{\mathbf{q}\mathbf{q}}{q^2} \frac{\chi^L(\mathbf{q},\omega) - \chi(\omega)}{\chi(\omega)} \right], \tag{49}$$

where

$$\chi = \frac{1}{A(\omega)},$$

$$\chi^{L} = \frac{1}{A(\omega) + \alpha q^{2}},$$
(50)

with [16]

$$A(\omega) = \frac{1}{\varepsilon_m - 1} \frac{1}{f_V} - \frac{\omega^2}{k_p^2 c^2},$$
(51)

$$\alpha = \frac{1}{l_0 k_p^2}.$$
(52)

In the above expressions, ε_m is the relative permittivity of the wire, $f_V = \pi R^2/a^2$ is the volume fraction of wires where R is the radius of the wire and a is the lattice constant, k_p is the plasma wavenumber defined above, c is the speed of light, and l_0 is a dimensionless geometrical parameter of the lattice $(l_0 \sim 3)$. Then,

$$\frac{\chi^{L}(\mathbf{q},\omega)-\chi(\omega)}{\chi(\omega)} = \frac{-\alpha q^{2}}{A+\alpha q^{2}},$$
(53)

so that

$$\overline{\chi}(\mathbf{q},\omega) = \chi(\omega) \left[1 + \frac{-\alpha}{A(\omega) + \alpha q^2} \mathbf{q} \mathbf{q} \right].$$
 (54)

If we compare this expression with Equation (41), we identify the diffusion constant for a homogeneous wire-mesh medium as

$$D(\omega) = \frac{-\alpha}{A(\omega)\varepsilon_0}.$$
(55)

The dimensions of $\varepsilon_0 D$ are m².

As discussed in [9], spatial dispersion arises from charge accumulation on the wires comprising the metamaterial (more generally, due to charge accumulation on the inclusions). It is therefore not surprising that spatial dispersion can be related to diffusion of polarization charge associated with the inclusions. If no charge build-up occurs, then diffusion will be absent, and spatial dispersion will vanish.

5. Application of Drift-Diffusion to Charge Screening in Spheres

Aside from the usefulness of the drift-diffusion equation in understanding spatial dispersion in plasmas, and its obvious importance in semiconductor modeling, an interesting application of the drift-diffusion equation is to the static screening of fields in conductors. For good conductors, this screening occurs over angstrom distances, which is why it is often ignored in undergraduateengineering electromagnetics textbooks. However, it seems a rather essential process in developing an understanding of how conductors screen electric fields. The usual statement that any conductor, not only perfect conductors, completely screens electric fields is unduly simplistic (the argument being that if electric field penetrated a conductor then current would flow, which is not consistent with static equilibrium). Moreover, as attention is focused on the electromagnetic analysis of nanostructures, this becomes an important consideration. The topic of screening in a planar conductor was covered in [14], and here we consider the case of screening in an imperfectly-conducting sphere as a tractable example assessable to beginning graduate students.

It should be noted that screening is a completely different phenomenon than skin effect. For nanospheres, the radius is much less than the skin depth $\delta = \sqrt{2/\omega\mu_0\sigma}$, even for the best conductors through at least optical frequencies. Therefore, based on skin depth alone, one would gather than a time-varying field is uniform throughout a metallic nanosphere. It turns out that a time-varying field is indeed uniform throughout a small sphere, except in a very thin region near the surface, related to diffusion. As frequency approaches zero, this transition region grows, and eventually the field decreases linearly inside the sphere, yielding the static (diffusion) result. Only when diffusion is absent does the field inside a conductor go to zero. The time-varying case is much more complicated than the static case, and so here we consider the static case arising from the drift-diffusion model, and merely present the time-varying result from another method.

5.1 Screening in Material Spheres from the Drift-Diffusion Equation

Consider a static field $\mathbf{E} = \mathbf{z}E_0$ (leading to $\phi_{applied} = -E_0 \mathbf{z} = -E_0 \mathbf{r} \cos \theta$) applied to an imperfectly conducting

material sphere having permittivity ε_{in} and radius *a*, immersed in a lossless homogeneous medium having permittivity ε_{out} . The Poisson's equation in each region is

$$\nabla^2 \phi_{in} = -\frac{\rho}{\varepsilon_{in}},\tag{56}$$

$$\nabla^2 \phi_{out} = 0 \,, \tag{57}$$

where ρ is free charge. Ignoring diffusion, the solutions for the potential and for the polarizability are the well-known results for a dielectric sphere ($\sigma = 0$),

$$\phi_{in}^{d} = -E_0 r \cos\theta \frac{3\varepsilon_{out}}{\varepsilon_{in} + 2\varepsilon_{out}},$$
(58)

$$\phi_{out}^{d} = -E_0 \cos \theta \left[r - \frac{a^3}{r^2} \left(\frac{\varepsilon_{in} - \varepsilon_{out}}{\varepsilon_{in} + 2\varepsilon_{out}} \right) \right], \tag{59}$$

$$\alpha^{d} = 4\pi a^{3} \varepsilon_{out} \frac{\varepsilon_{in} - \varepsilon_{out}}{\varepsilon_{in} + 2\varepsilon_{out}}, \qquad (60)$$

and for a perfectly conductor sphere ($\sigma \rightarrow \infty$),

$$\phi_{in}^{pc} = 0, \qquad (61)$$

$$\phi_{out}^{pc}(r) = -E_0 \left(1 - \frac{a^3}{r^3} \right) r \cos \theta , \qquad (62)$$

$$\alpha^{pc} = 4\pi a^3 \varepsilon_{out} \,. \tag{63}$$

To see what happens when we include diffusion, using the relationship of Equation (1) with the total current set to zero at static equilibrium, inside the sphere we have

$$\nabla \left(\nabla^2 \phi_{in} \right) = -\frac{1}{\varepsilon_{in}} \nabla \rho$$
$$= -\frac{1}{\varepsilon_{in}} \frac{\sigma}{D} \left(-\nabla \phi_{in} \right)$$
$$= \nabla \left(\frac{1}{\varepsilon_{in}} \frac{\sigma}{D} \phi_{in} \right)$$
(64)

and so

$$\nabla \left(\nabla^2 \phi_{in} - k_D^2 \phi_{in} \right) = 0 , \qquad (65)$$

where $k_D^2 = \sigma/\varepsilon_{in}D = 1/l_D^2$ is called the Debye wavenumber, and l_D is the Debye length. Thus,

$$\nabla^2 \phi_{in} - k_D^2 \phi_{in} = C \,. \tag{66}$$

If we choose C = 0, then $\nabla^2 \phi_{in} = -\rho/\varepsilon_{in} = k^2 \phi_{in}$, so that $\phi_{in} = -\rho/(k^2 \varepsilon_{in})$. Assuming that $\int_V \rho dV = 0$, we then have that the average of ϕ_{in} over the sphere is zero.

If we let $p^2 = -k_D^2$, then the equations to solve are

$$\nabla^2 \phi_{in} + p^2 \phi_{in} = 0, \qquad (67)$$

$$\nabla^2 \phi_{out} = 0. \tag{68}$$

The solution is subject to the usual boundary conditions (i.e., the same boundary conditions as for the local dielectric sphere). There is no need for an additional boundary condition. Specifically, the boundary conditions are that the potential must be finite at r = 0, as $r \to \infty$ the potential must approach the unperturbed potential $\phi_{applied}$, and that the tangential **E** and normal **D** fields must be continuous. The solution is

$$\phi_{in} = -E_0 \frac{3\varepsilon_{out} \left[\frac{aj_1(jk_D r)}{j_1(jk_D a)} \right]}{\varepsilon_{in} \left[jk_D a \frac{j'_1(jk_D a)}{j_1(jk_D a)} \right] + 2\varepsilon_{out}} \cos\theta , \qquad (69)$$

$$\phi_{out} = -E_0 \cos\theta \left[r + \frac{a^3}{r^2} \left\{ \frac{\varepsilon_{out} - \varepsilon_{in} \left[jk_D a \frac{j_1'(jk_D a)}{j_1(jk_D a)} \right]}{2\varepsilon_{out} + \varepsilon_{in} \left[jk_D a \frac{j_1'(jk_D a)}{j_1(jk_D a)} \right]} \right\} \right],$$
(70)

leading to the polarizability

$$\alpha = 4\pi\varepsilon_{out}a^{3}\left\{\frac{\varepsilon_{in}\left[jk_{D}a\frac{j'(jk_{D}a)}{j_{1}(jk_{D}a)}\right] - \varepsilon_{out}}{\varepsilon_{in}\left[jk_{D}a\frac{j'_{1}(jk_{D}a)}{j_{1}(jk_{D}a)}\right] + 2\varepsilon_{out}}\right\}.$$
(71)

Note that the drift-diffusion results, Equations (69)-(71), become those of the dielectric sphere as $k_D \rightarrow 0$ (i.e., $\sigma \rightarrow 0$), and those of the perfectly conducting sphere for $k_D \rightarrow \infty$ ($\sigma \rightarrow \infty$).

The potential ϕ_{in} shows the very thin screening depth in metals associated with the Debye length $l_D = 1/k_D$. By considering that for metals $k_D \sim 10^{10} \text{ m}^{-1}$ (and so $l_D \sim 10^{-10} \text{ m}$), we can assume that $k_D a \gg 1$ through visible frequencies, even for nanoscale spheres. Then,

$$j_{1}(jk_{D}r) = \frac{\sin(ik_{D}r)}{(ik_{D}r)^{2}} - \frac{\cos(ik_{D}r)}{ik_{D}r}$$
(72)

$$=\frac{i}{2rk_{D}}\left(e^{k_{D}r}+e^{-k_{D}r}\right)-\frac{i}{2r^{2}k_{D}^{2}}\left(e^{k_{D}r}-e^{-k_{D}r}\right),$$
(73)

and so the spatial dependence of ϕ_{in} varies as

$$\frac{j_1(jk_Dr)}{j_1(jk_Da)} \approx \left(1 - \frac{1}{k_Dr}\right) \frac{e^{k_Da\left(\frac{r}{a}-1\right)}}{\frac{r}{a}}.$$
(74)

This function is exceedingly small unless r is very close to a (for poorer conductors, the Debye length can be considerably longer). The nonuniform potential arising from the drift-diffusion model is associated with an electric field, which indeed drives currents. However, there is diffusion of charge in the opposite direction, and the net current is zero at static equilibrium. The reason that diffusion is important for this example is that the applied field brings a lot of charge to the surface, but that high concentration of charge tends to diffuse back towards the interior until equilibrium is reached. Results will be shown in Figure 2 in the next section.

The concept of Debye length is familiar from ionospheric propagation, which makes sense since the ionosphere is modeled as a plasma, similar to the simple electron-gas model of a metal (which ignores band theory). In the ionosphere electron densities are much lower than for metals, and so Debye lengths are macro-scopic. Assuming an ionospheric electron density of $n_e = 10^{12} \text{ m}^{-3}$ and $T = 10^3$ [21], the Debye length is $\lambda_D = 2 \times 10^{-3}$ m. Screening is thus a macroscale phenomena for low electron densities, but becomes nanoscopic for metal-like densities.

5.2 Other Non-Local Models

There are a few methods for spheres based on other non-local (spatially dispersive) models. For scattering from spheres or similar objects, these are quite a bit more complicated than the drift-diffusion model presented in the previous section, and require an additional boundary condition. However, they are applicable at arbitrary frequencies. In particular, in [17] Ruppin extended the Mie theory to account for a non-local sphere, and in a series of papers [18-20], Fuchs approximately solved the spatial-transform-domain problem using $\varepsilon_r^L(q,\omega)$. In Fuchs' method, it was shown that the potential varies as

$$\phi_{in}(r) = -\frac{2}{\pi}C\sqrt{\frac{3}{4\pi}}a^2\cos\theta \int_0^\infty \frac{j_1(qa)j_1(qr)}{\varepsilon^L(q,\omega)}dq,\qquad(75)$$

where j_1 is the first-kind spherical Bessel function, and C is a constant (expressions for C and for ϕ_{out} were given in [20]). Numerical agreement between results for the spatial-dispersion model arising from the drift-diffusion equation, Equation (69), and those from Fuchs' spatial dispersion model, Equation (75), in the dc limit was found to be excellent.

In Figure 2, a plot of the static potential normalized by its value at the surface (computed by the drift-diffusion model) is shown for the drift-diffusion model of Equations (69)-(70) (DD); the Fuchs' model, Equation (75); and the simple PEC model for a gold 10 nm radius sphere. The non-local Fuchs' model and the drift-diffusion model showed excellent agreement, whereas the PEC model gave the incorrect field inside the sphere, as expected. The Debye length was $l_D = 0.046$ nm. Note that the Debye wavenumber depends on conductivity, such that the degree of screening varies depending on the density of free electrons, which makes physical sense.

However, it should be kept in mind that despite the form of Equations (2)-(3) and (23), Equation (25), the resulting potentials, Equations (69)-(70), arise from the static Maxwell's equations, and are essentially static results, since $k_D^2 = \sigma(\omega)/\varepsilon_{in} D(\omega) = \sigma_0/\varepsilon_{in} D_0$ is independent of frequency



Figure 2. The static potential $\phi(r)$ normalized by $\phi_s = \phi(r = a)$ for the drift-diffusion model, the Fuchs' model, and the simple PEC model for a gold 10 nm radius sphere.



Figure 3. The quasi-static potential at 10 MHz for a 10 nm radius gold sphere, computed using the drift-diffusion, Fuchs', local conductor, and PEC models.

(other than possibly through $\varepsilon_{in} = \varepsilon_0$ for a typical metal). For example, the quasistatic potential at 10 MHz is shown in Figure 3 for the same gold sphere, where we added the local conductor result obtained from the usual dielectric-sphere case, Equations (58)-(59), using $\varepsilon_{in}(\omega) = (1 - j\sigma/\omega\varepsilon_0)\varepsilon_0$ (on the scale of the plot, the local result may appear discontinuous, but it is not). It can be seen that the Fuchs model captures both the non-locality of the response (associated with the small transition region near the surface of the sphere) and the expected behavior of the quasistatic potential well inside the sphere (i.e., the uniform interior field well inside the sphere, predicted by skin-depth considerations). However, the drift-diffusion model exhibits the static behavior.

The spatially-dispersive model provides a smooth transition between time-varying and time-static cases (here, as above, for the time-varying case we use Fuchs' model). Considering Figure 3, as frequency was lowered, the breakpoint where the Fuchs' model changed from decreasing to essentially constant (note the log scale) moved to the left. For f = 10 MHz, the breakpoint occurred at $r/a \approx 0.91$, as shown in Figure 3, whereas at f = 1 Hz, the breakpoint occurred at approximately r/a = 0.85. At $f = 10^{-3}$ Hz, the breakpoint was at r/a = 0.8. The breakpoint moves progressively to smaller values as frequency is lowered, providing a smooth transition from the time-varying case to the static case shown in Figure 2. A purely local model can not capture these dynamics.

6. Conclusions

The drift-diffusion equation, normally used for semiconductor modeling, was shown to be equivalent to spatial dispersion in a warm plasma, both for natural materials and artificial metamaterials. Given the physical clarity and intuitive nature of the drift-diffusion equation, it was suggested that this can be helpful for teaching the concepts of spatial dispersion to beginning graduate students. Furthermore, the use of the drift-diffusion equation in determining charge screening in imperfect conductors was highlighted, a topic which is important in the emerging area of nanoelectromagnetics.

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8. Appendix: Hydrodynamic Derivation of the Drift-Diffusion Model

The derivation of the drift-diffusion equation, Equation (1), is particularly simple, assuming a hydrodynamic model [14, Section 16; 21]. We assume a neutral warm plasma and ignore the motion of ions and ion-electron interactions. The usual equation of motion for electrons is

$$m_e \frac{d\mathbf{v}_d}{dt} + m_e \gamma \mathbf{v}_d = q_e \left(\mathbf{E} + \mathbf{v}_d \times \mathbf{B} \right), \tag{76}$$

where \mathbf{v}_d is the average electron drift velocity (we neglect the random thermal velocity). We will neglect the small magnetic-field contribution. To account for diffusion, we add a pressure term, which leads to a force (gas pressure on the walls of a container being force per area). From the kinetic theory of gasses, pressure is

$$p = \frac{2}{3} n_e \left(\frac{1}{2} m_e \left\langle v^2 \right\rangle \right), \tag{77}$$

where n_e is the number density and $\langle v^2 \rangle$ is the mean-square velocity. Assuming that pressure changes sufficiently slowly in space (slowly compared to the average separation between particles for a neutral gas, or compared to the screening length), we can use a fluid model for pressure. The pressure force per unit volume is

$$\frac{\mathbf{f}}{V} = -\nabla p$$

$$= -\nabla \frac{2}{3} n_e \left(\frac{1}{2} m_e \left\langle v^2 \right\rangle \right)$$

$$= -\frac{1}{3} \left(m_e \left\langle v^2 \right\rangle \right) \nabla n_e.$$
(78)

Writing the electron number density in terms of charge density, $\nabla \rho = -e \nabla n_{\rho}$, we have

$$\frac{\mathbf{f}}{V} = \frac{m_e \left\langle v^2 \right\rangle}{3e} \nabla \rho \,. \tag{79}$$

We need (average) force per particle, since we're writing a force law for an individual (average) electron, and so

$$\frac{\mathbf{f}}{V}\frac{1}{n_e} = \frac{m_e \langle v^2 \rangle}{3n_e e} \nabla \rho , \qquad (80)$$

such that

$$m_e \frac{d\mathbf{v}_d}{dt} + m_e \gamma \mathbf{v}_d = -e\mathbf{E} + \left(\frac{m_e \langle v^2 \rangle}{3n_e e} \nabla \rho\right). \tag{81}$$

Notice that electric field will drive electrons in one direction, and the pressure will tend to drive electrons in the opposite direction (i.e., the forces are opposing). We can write

$$m_e \frac{d\mathbf{v}_d}{dt} + m_e \gamma \mathbf{v}_d = -e\mathbf{E} + \left(\frac{\beta m_e}{n_e e} \nabla \rho\right). \tag{82}$$

With $\mathbf{J} = -n_e e \mathbf{v}_d$, this becomes

$$m_e \frac{d\mathbf{J}}{dt} + m_e \gamma \mathbf{J} = n_e e^2 \mathbf{E} - \left(\beta m_e \nabla \rho\right), \qquad (83)$$

so that

$$\frac{d\mathbf{J}}{dt} + \gamma \mathbf{J} = \frac{n_e e^2}{m_e} \mathbf{E} - \beta \nabla \rho .$$
(84)

Time-harmonic variation leads to

$$\mathbf{J}(j\omega+\gamma) = \frac{n_e e^2}{m_e} \mathbf{E} - \beta \nabla \rho \,. \tag{85}$$

Obviously,

$$\mathbf{J}(\mathbf{r},\omega) = \frac{n_e e^2}{m_e (j\omega + \gamma)} \mathbf{E}(\mathbf{r},\omega) - \frac{\beta}{j\omega + \gamma} \nabla \rho(\mathbf{r},\omega)$$
(86)

$$=\sigma(\omega)\mathbf{E}(\mathbf{r},\omega)-D(\omega)\nabla\rho(\mathbf{r},\omega), \qquad (87)$$

which is the drift-diffusion model of Equation (1).

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