

Universal electromagnetic waves in dielectric

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Abstract

The dielectric susceptibility of a wide class of dielectric materials follows, over extended frequency ranges, a fractional power-law frequency dependence that is called the ‘universal’ response. The electromagnetic fields in such dielectric media are described by fractional differential equations with time derivatives of non-integer order. An exact solution of the fractional equations for a magnetic field is derived. The electromagnetic fields in the dielectric materials demonstrate fractional damping. The typical features of ‘universal’ electromagnetic waves in dielectric are common to a wide class of materials, regardless of the type of physical structure, chemical composition, or of the nature of the polarizing species, whether dipoles, electrons, or ions.

1. Introduction

A growing number of dielectric relaxation data show that the classical Debye behavior [1] is hardly ever observed experimentally [2–4]. The fact that different dielectric spectra are described by the power laws is confirmed in dielectric measurements realized by Jonscher [2, 3] for a wide class of various substances. The dielectric susceptibility of most materials follows, over extended frequency ranges, a fractional power-law frequency dependence, which is called the law of ‘universal’ response [2, 3]. This law is found both in dipolar materials beyond their loss-peak frequency, and in materials where the polarization arises from movements of either ionic or electronic hopping charge carriers. It has been found [5, 6] that the frequency dependence of the dielectric susceptibility $\tilde{\chi}(\omega) = \chi'(\omega) - i\chi''(\omega)$ follows a common universal pattern for virtually all kinds of materials. Namely, the behavior

$$\chi'(\omega) \sim \omega^{n-1}, \quad \chi''(\omega) \sim \omega^{n-1},$$

$$(0 < n < 1, \quad \omega \gg \omega_p), \quad (1)$$

and

$$\chi'(0) - \chi'(\omega) \sim \omega^m, \quad \chi''(\omega) \sim \omega^m,$$

$$(0 < m < 1, \quad \omega \ll \omega_p), \quad (2)$$

where $\chi'(0)$ is the static polarization and ω_p the loss-peak frequency, is observed over many decades of frequency. Note that the ratio of the imaginary to the real component of the susceptibility is independent of frequency. The frequency dependence given by equation (1) implies that the real and

imaginary components of the complex susceptibility obey at high frequencies the relation

$$\frac{\chi''(\omega)}{\chi'(\omega)} = \cot\left(\frac{\pi n}{2}\right), \quad (\omega \gg \omega_p). \quad (3)$$

The experimental behavior (2) leads to a similar frequency-independent rule for the low-frequency polarization decrement:

$$\frac{\chi''(\omega)}{\chi'(0) - \chi'(\omega)} = \tan\left(\frac{\pi m}{2}\right), \quad (\omega \ll \omega_p). \quad (4)$$

There are many models that describe and explain the universal response laws. Let us note some of them. A general equation for the susceptibility of disordered systems is proposed in [7]. It is shown [7] that this equation is a good frequency domain representation of the time domain Kohlrausch–Williams–Watts stretched exponential. In [8], the authors have derived a general two-power-law relaxation function for heterogeneous materials using the maximum entropy principle for nonextensive systems. The asymptotic power-law behaviors coincide with those of the Weron generalized dielectric function derived in the stochastic theory from an extension of the Lévy central limit theorem. These results [8] are in agreement with the Jonscher universality principle. The memory function approach and scaling relationships can be used [9] as a basis for the dynamic model of symmetric dielectric spectrum broadening. For the correspondence between the relaxation time, the geometrical

properties, the self-diffusion coefficient and the exponent of power-law wings was established in [9]. In [10], a memory function equation and scaling relationships were used for the physical interpretation of the Cole–Cole exponent. The correspondence between the relaxation time, the geometrical properties, the self-diffusion coefficient and the Cole–Cole exponent was considered in [10]. The fractional power laws frequently observed in dielectric measurements can be interpreted [11] in terms of regular singular points of the underlying rate equation for the process giving rise to the dielectric response. The review [3] presents a wide-ranging broad-brush picture of dielectric relaxation in solids, making use of the existence of a ‘universality’ of dielectric response regardless of a wide diversity of materials and structures, with dipolar as well as charge-carrier polarization.

The theory of integrals and derivatives of non-integer order goes back to Leibniz, Liouville, Riemann, Grunwald, and Letnikov [12, 13]. Fractional analysis has found many applications in recent studies in mechanics and physics. The interest in fractional equations has been growing continually during the last few years because of numerous applications. In a short period of time the list of applications has become long (see for example [14–19]). Note also the application of fractional calculus to the problems of classical electrodynamics [20, 21].

In [23] fractional calculus has been undertaken in order to understand the nature of one type of nonexponential relaxation. An equation containing operators of fractional integration and differentiation is obtained and solved [23], which the relaxation function obeys in this case. In [23], the potential of the fractional derivative technique is demonstrated using the example of the derivation of all three known patterns of anomalous, nonexponential dielectric relaxation of an inhomogeneous medium in the time domain. It is explicitly assumed [23] that the fractional derivative is related to the dimensionality of a temporal fractal ensemble in a sense that the relaxation times are distributed over a self-similar fractal system. In [24], the model of dielectric relaxation based on the fractional kinetics containing the complex power-law exponents was used to received a confirmation in description of the real part of the complex conductivity by the fitting function. The coincidence between the suggested model and measured data gives [24] the possibility to suggest a more reliable physical picture of the swelling process that takes place in neutral and charged gels. The real process of dielectric relaxation during the polymerization reaction can be described [25] in terms of the fractional kinetic equations containing complex-power-law exponents. Based on the physical and geometrical meanings of the fractional integral with complex exponents there is a possibility [25] of developing a model of dielectric relaxation based on the self-similar fractal character of the averaged microprocesses that take place in the mesoscale region.

In this paper, we prove that in a time domain the fractional power-law frequency dependence gives differential equations with derivatives and integrals of non-integer order. We obtain equations that describe ‘universal’ electromagnetic waves for such dielectric materials. The power laws are presented by

fractional differential equations such that the electromagnetic fields in the materials demonstrate ‘universal’ fractional damping. An exact solution of the fractional equations for magnetic field is derived. The electromagnetic fields in the dielectric materials demonstrate fractional damping. The suggested fractional equations are common (universal) to a wide class of materials, regardless of the type of physical structure, chemical composition or of the nature of the polarizing species, whether dipoles, electrons, or ions. A possible link between dielectric response and structure of low-loss dielectrics is discussed.

2. Fractional equations for universal laws

For the region $\omega \gg \omega_p$, the universal fractional power law (1) can be presented in the form

$$\tilde{\chi}(\omega) = \chi_\alpha (i\omega)^{-\alpha}, \quad (0 < \alpha < 1) \quad (5)$$

with some positive constant χ_α and $\alpha = 1 - n$. Here

$$(i\omega)^\alpha = |\omega|^\alpha e^{i\alpha\pi \operatorname{sgn}(\omega)/2}.$$

It is easy to see that relation (3) is satisfied.

The polarization density can be written as

$$\begin{aligned} \mathbf{P}(t, r) &= \mathcal{F}^{-1} \left(\tilde{\mathbf{P}}(\omega, r) \right) = \varepsilon_0 \mathcal{F}^{-1} \left(\tilde{\chi}(\omega) \tilde{\mathbf{E}}(\omega, r) \right) \\ &= \varepsilon_0 \chi_\alpha \mathcal{F}^{-1} \left((i\omega)^{-\alpha} \tilde{\mathbf{E}}(\omega, r) \right), \end{aligned}$$

where $\tilde{\mathbf{P}}(\omega, r)$ is a Fourier transform \mathcal{F} of $\mathbf{P}(t, r)$.

Note that the Fourier transform \mathcal{F} of the fractional Liouville integral [12, 13]

$$(I_+^\alpha f)(t) = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^t \frac{f(t') dt'}{(t-t')^{1-\alpha}}$$

is given by the following result (see theorem 7.1. in [12] and theorem 2.15 in [13]):

$$(\mathcal{F} I_+^\alpha f)(\omega) = \frac{1}{(i\omega)^\alpha} (\mathcal{F} f)(\omega).$$

Using the fractional Liouville integral, the fractional power-law (5) for $\tilde{\chi}(\omega)$ in the frequency domain gives

$$\mathbf{P}(t, r) = \varepsilon_0 \chi_\alpha (I_+^\alpha \mathbf{E})(t, r), \quad (0 < \alpha < 1). \quad (6)$$

This equation means that the polarization density $\mathbf{P}(t, r)$ for the high-frequency region is proportional to the fractional Liouville integral of the electric field.

For the region $\omega \ll \omega_p$, the universal fractional power law (2) can be presented as

$$\tilde{\chi}(\omega) = \tilde{\chi}(0) - \chi_\beta (i\omega)^\beta, \quad (0 < \beta < 1) \quad (7)$$

with some positive constants χ_β , $\tilde{\chi}(0)$, and $\beta = m$. It is not hard to prove that equation (4) is satisfied.

Note that the Fourier transforms \mathcal{F} of the fractional Liouville derivative [12, 13]

$$\begin{aligned} (D_+^\beta f)(t) &= \frac{\partial^k}{\partial t^k} (I_+^{k-\beta} f)(t) = \frac{1}{\Gamma(k-\beta)} \\ &\times \frac{\partial^k}{\partial t^k} \int_{-\infty}^t \frac{f(t') dt'}{(t-t')^{\beta-k+1}}, \quad (k-1 < \beta < k) \end{aligned}$$

are given by the following result (see theorem 7.1. in [12] and theorem 2.15 in [13]):

$$(\mathcal{F}D_+^\beta f)(\omega) = (i\omega)^\beta (\mathcal{F}f)(\omega).$$

Using the definition of the fractional Liouville derivative, the fractional power laws (7) give the polarization density

$$\mathbf{P}(t, r) = \varepsilon_0 \mathcal{F}^{-1} \left(\tilde{\chi}(\omega) \tilde{\mathbf{E}}(\omega, r) \right)$$

in the form

$$\mathbf{P}(t, r) = \varepsilon_0 \tilde{\chi}(0) \mathbf{E}(t, r) - \varepsilon_0 \chi_\beta (D_+^\beta \mathbf{E})(t, r), \quad (0 < \beta < 1). \quad (8)$$

This equation means that polarization density $\mathbf{P}(t, r)$ for the low-frequency region is defined by the fractional Liouville derivative of the electric field.

Equations (6) and (8) can be considered as the universal laws in the time domain. These equations allow us to derive fractional wave equations for electric and magnetic fields.

3. Universal electromagnetic wave equation

Using the Maxwell equations, it is easy to obtain the equation

$$\varepsilon_0 \frac{\partial^2 \mathbf{E}(t, r)}{\partial t^2} + \frac{\partial^2 \mathbf{P}(t, r)}{\partial t^2} + \frac{1}{\mu} (\text{grad div } \mathbf{E} - \nabla^2 \mathbf{E}) + \frac{\partial \mathbf{j}(t, r)}{\partial t} = 0. \quad (9)$$

For the region $\omega \gg \omega_p$, the polarization density $\mathbf{P}(t, r)$ is related with $\mathbf{E}(t, r)$ by equation (6). Substituting (6) into (9), we obtain the fractional equation for electric field

$$\frac{1}{v^2} \frac{\partial^2 \mathbf{E}(t, r)}{\partial t^2} + \frac{\chi_\alpha}{v^2} (D_+^{2-\alpha} \mathbf{E})(t, r) + (\text{grad div } \mathbf{E} - \nabla^2 \mathbf{E}) = -\mu \frac{\partial \mathbf{j}(t, r)}{\partial t}, \quad (0 < \alpha < 1), \quad (10)$$

where $v^2 = 1/(\varepsilon_0 \mu)$. Note that $\text{div } \mathbf{E} \neq 0$ for $\rho(t, r) = 0$.

For the region $\omega \ll \omega_p$, the fields $\mathbf{P}(t, r)$ and $\mathbf{E}(t, r)$ are connected by equation (8). Then equation (9) gives

$$\frac{1}{v_\beta^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} - \frac{a_\beta}{v_\beta^2} (D_+^{2+\beta} \mathbf{E}) + (\text{grad div } \mathbf{E} - \nabla^2 \mathbf{E}) = -\mu \frac{\partial \mathbf{j}}{\partial t}, \quad (0 < \beta < 1), \quad (11)$$

where

$$v_\beta^2 = \frac{1}{\varepsilon_0 \mu [1 + \tilde{\chi}(0)]}, \quad a_\beta = \frac{\chi_\beta}{1 + \tilde{\chi}(0)}.$$

Equations (10) and (11) describe the time-evolution of the electric field in the dielectric materials. These equations are fractional differential equations.

Using the Maxwell equations, it is not hard to obtain the equation for a magnetic field

$$\frac{\partial^2 \mathbf{B}(t, r)}{\partial t^2} = \frac{1}{\varepsilon_0 \mu} \nabla^2 \mathbf{B}(t, r) + \frac{1}{\varepsilon_0} \frac{\partial}{\partial t} \text{curl } \mathbf{P}(t, r) + \frac{1}{\varepsilon_0} \text{curl } \mathbf{j}(t, r). \quad (12)$$

The experimental applied field $\mathbf{B}(t, r)$ can be presented as

$$\mathbf{B}(t, r) = \begin{cases} 0, & t \leq 0, \\ \mathbf{B}(t, r), & t > 0. \end{cases}$$

For the region $\omega \gg \omega_p$, the polarization density $\mathbf{P}(t, r)$ is related to $\mathbf{E}(t, r)$ by equation (6), and we obtain the fractional equation for magnetic field

$$\frac{1}{v^2} \frac{\partial^2 \mathbf{B}(t, r)}{\partial t^2} + \frac{\chi_\alpha}{v^2} ({}_0 D_+^{2-\alpha} \mathbf{B})(t, r) - \nabla^2 \mathbf{B}(t, r) = \mu \text{curl } \mathbf{j}(t, r), \quad (0 < \alpha < 1), \quad (13)$$

where $v^2 = 1/(\varepsilon_0 \mu)$, and ${}_0 D_+^{2-\alpha}$ is the Riemann–Liouville derivative [13] on $[0, \infty)$ such that

$$({}_0 D_+^{2-\alpha} f)(t) = \frac{1}{\Gamma(\alpha)} \frac{\partial^2}{\partial t^2} \int_0^t \frac{f(t') dt'}{(t-t')^{1-\alpha}}, \quad (0 < \alpha < 1).$$

For the region $\omega \ll \omega_p$, we obtain

$$\frac{1}{v_\beta^2} \frac{\partial^2 \mathbf{B}(t, r)}{\partial t^2} - \frac{a_\beta}{v_\beta^2} ({}_0 D_+^{2+\beta} \mathbf{B})(t, r) - \nabla^2 \mathbf{B}(t, r) = \mu \text{curl } \mathbf{j}(t, r), \quad (0 < \beta < 1), \quad (14)$$

where

$$v_\beta^2 = \frac{1}{\varepsilon_0 \mu [1 + \tilde{\chi}(0)]}, \quad a_\beta = \frac{\chi_\beta}{1 + \tilde{\chi}(0)}.$$

Equation (14) is a fractional differential equation that describes magnetic field in dielectric media.

4. Fractional damping of magnetic field

Let us obtain a solution of equations (13) and (14). These equations can be represented in a general form. This general form of the fractional equations for magnetic field is

$$({}_a D_t^\alpha \mathbf{B})(t, r) - \lambda_1 ({}_a D_t^\beta \mathbf{B})(t, r) - \lambda_2 \nabla^2 \mathbf{B}(t, r) = \mathbf{f}(t, r), \quad (1 \leq \beta < \alpha < 3), \quad (15)$$

where $\mathbf{B}(a, r) = 0$, and the curl of current density of free charges is considered as an external source term:

$$\mathbf{f}(t, r) = \mu \lambda_2 \text{curl } \mathbf{j}(t, r).$$

Equation (15) gives equation (13) for $\alpha = 2, 1 < \beta < 2$, and

$$\lambda_1 = -\chi_\alpha, \quad \lambda_2 = v^2 = 1/(\varepsilon_0 \mu).$$

Equation (14) can be derived from (15) with $2 < \alpha < 3, \beta = 2$, and

$$\lambda_1 = \frac{1}{a_\beta} = \frac{1 + \tilde{\chi}(0)}{\chi_\beta}, \quad \lambda_2 = -\frac{v_\beta^2}{a_\beta} = \frac{-1}{\varepsilon_0 \mu \chi_\beta}.$$

An exact solution of (15) can be presented in terms of the Wright functions [13, 26]. Using the three-dimensional Fourier transform of equation (15) with respect to coordinates and theorem 5.5 in [13], we obtain the solution

$$\mathbf{B}(t, r) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d^3 k \int_0^t dt' e^{ikr} \tilde{\mathbf{f}}(t', k) G(t-t', k), \quad (16)$$

where

$$G(t - t', k) = \sum_{s=0}^{\infty} \frac{(-k^2 \lambda_2)^s}{s!} (t - t')^{\alpha s + \alpha - 1} \times {}_1\Psi_1 \left[\frac{(s + 1, 1)}{(\alpha s + \alpha, \alpha - \beta)} \middle| \lambda_1 (t - t')^{\alpha - \beta} \right]. \quad (17)$$

Here, ${}_1\Psi_1$ is the Wright function

$${}_1\Psi_1 \left[\frac{(s + 1, 1)}{(\alpha s + \beta, \alpha)} \middle| z \right] = \sum_{j=0}^{\infty} \frac{\Gamma(s + j + 1)}{\Gamma(\alpha s + \beta + \alpha j)} \frac{z^j}{j!}$$

that can be derived as $\partial^s E_{\alpha, \beta}[z] / \partial z^s$ of the Mittag-Leffler function $E_{\alpha, \beta}[z]$ (see [13, 26]). Equation (16) describes the fractional field damping of magnetic field in the dielectric media. An important property of the evolution described by the fractional equations for electromagnetic waves is that the solutions have power-like tails.

5. Possible link between dielectric response and molecular structure of dielectric

An interesting problem of considerable practical importance is the link between the dielectric loss of low-loss materials and the identifiable physical and structural features in the material. The following questions relating to this subject can be formulated. What material conditions must be satisfied for the low-loss property to be observed? What are the physical interpretations of this type of behavior?

Jonscher has suggested in [2, 29, 30] that the key to the understanding of low-loss behavior lies in dipolar screening which leads to interactions between dipoles in materials with sufficiently low dipole densities. In other words, the Jonscher's proposition is that electrostatic interactions between dipoles even at large distances from one another lock these dipoles so that their response to external alternating fields is weakened. The physical basis of low-loss dielectrics can be connected [2, 29, 30] with the effect of dipolar screening which produces interaction between neighboring dipoles, thereby preventing a significant part of them from following external alternating fields. It is evident that the case of complete screening must correspond to Debye relaxation, because there is no interaction between any of the dipoles. The result of dipole-dipole interactions with incomplete screening extending over many dipoles is that the system becomes insensitive in the sense that the fields generated by the interacting dipoles are stronger than externally applied fields [30].

We can also assume that the effect of screening is very important for dipolar relaxation. In [30], the Debye screening of the static fields is considered, but the form of dipole-dipole interaction is not discussed. In this section, we consider a possible form of screening dipole-dipole interaction for low-loss dielectric materials. In general, the dipole feels an electric field both from the permanent charges of the system and from the other induced dipoles. To describe low-loss dielectrics, we suggest using a modification of the molecular polarization method. This polarizable point dipoles method has been applied to a wide variety of atomic and molecular

systems, ranging from noble gases and water to amorphous materials and to proteins. Let us note the main features of the polarization methods and a possible generalization to describe low-loss dielectrics. In the point dipoles method, a polarizability α is associated to one or more sites [33]. This method for treating polarizability is to add point inducible dipoles on some or all sites.

The total electric field acting on each site is produced by the external charges and by induced dipole moments [31–34, 37, 41], such that

$$\mathbf{E}_n = \mathbf{E}_n^0 - \sum_{m \neq n} \mathbf{T}_{nm} \mathbf{p}_m, \quad (18)$$

where \mathbf{p}_m is a dipole moment, \mathbf{T}_{nm} denotes the dipole field tensor, and \mathbf{E}_n^0 is the static field at site n due to the permanent charges

$$\mathbf{E}_n^0 = \sum_{m \neq n} \frac{q_m \mathbf{r}_{nm}}{r_{nm}^3}, \quad (19)$$

where q_m is the charge at site m and $r_{nm} = |\mathbf{r}_{nm}|$ is the distance between n and m . The induced dipoles interact through the dipole field tensor

$$\mathbf{T}_{nm} = \frac{1}{r_{nm}^3} \mathbf{I} - \frac{3}{r_{nm}^5} \mathbf{r} \otimes \mathbf{r}, \quad (20)$$

where \mathbf{I} is the unit tensor (identity matrix). Here $\mathbf{r} \otimes \mathbf{r}$ is the tensor with elements $x_k x_l$, where x_k ($k, l = 1, 2, 3$) are the Cartesian components of the vector \mathbf{r}_{nm} between n and m . The dipole moment, \mathbf{p}_n , induced on a site n is proportional to the electric field \mathbf{E}_n at that site,

$$\mathbf{p}_n = \alpha_n \mathbf{E}_n.$$

The proportionality constant is the polarizability tensor α_n . The induced point dipole on site n can be computed iteratively until a given threshold of convergence for the induced dipole is reached (for example, see [34] for issues concerning the efficiency of the different methods for liquid state simulations). The energy of the dipole-induced dipole interaction has the form

$$U_{pp} = \frac{1}{2} \sum_m \sum_{m \neq n} \mathbf{p}_n \mathbf{T}_{nm} \mathbf{p}_m.$$

Here we consider that all the dipoles will interact through the dipole field tensor. The method of Applequist *et al* [35, 36] for calculating molecular polarizabilities uses this approach. One problem with coupling all the dipoles with the interaction given by equation (20) is the 'polarization catastrophe'. As pointed out by Applequist *et al* [35] and Thole [37], the polarization \mathbf{p}_n , and therefore the induced dipole moment, may become infinite at small distances. The polarization catastrophe is avoided by screening (attenuating) the dipole-dipole interaction [37]. As with the screening of the static field, screening of the dipole-dipole interaction can be physically interpreted as correcting for the fact that the electronic distribution is not well represented by point charges and dipoles [35, 37, 38]. The Thole approach for screening is to introduce the screening (damping) functions.

Equations (18)–(20) retain their validity [41] with the only change being that both the electric field created by a fixed charge and that created by a point dipole (depending on the molecular model) are screening by functions $f_1(r)$ and $f_2(r)$,

$$\mathbf{E}_n^0 = \sum_{m \neq n} f_1(r_{nm}) \frac{q_m \mathbf{r}_{nm}}{r_{nm}^3} \quad (21)$$

and

$$\mathbf{T}_{nm} = f_1(r_{nm}) \frac{1}{r_{nm}^3} \mathbf{I} - f_2(r_{nm}) \frac{3}{r_{nm}^5} \mathbf{r} \otimes \mathbf{r}. \quad (22)$$

In the limit of point charges and point dipoles, we have $f_1(r) = f_2(r) = 1$, and the usual expressions (19) and (20) are obtained. If, on the contrary, they are thought to be spatially extended, the form of the screening depends on the charge distribution assumed. Thole concluded that a linear decrease of charge density (up to a cutoff a) was ideal for the purpose of fitting of the molecular polarizability, for which it had been designed. In this approximation we have for the screening functions

$$f_1(r) = 4 \left| \frac{r}{a} \right|^3 - 3 \left| \frac{r}{a} \right|^4, \quad f_2(r) = \left| \frac{r}{a} \right|^4. \quad (23)$$

The possible alternative is an exponential distribution [39–41]. Note that various computer simulations with different screening functions have been used.

We assume that Thole linear decreasing should be replaced by fractional power-law dependence for low-loss dielectrics. Therefore we suggest that dipolar screening in low-loss dielectric materials can be described by the screening functions

$$f_1(r) = \alpha_2 \left| \frac{r}{a} \right|^{\alpha_1} - \alpha_1 \left| \frac{r}{a} \right|^{\alpha_2}, \quad f_2(r) = \left| \frac{r}{a} \right|^{\alpha_2}, \quad (24)$$

where α_1 and α_2 are non-integer positive numbers that define the fractional parameters $\alpha = 1 - n$ and $\beta = m$ of laws (1) and (2). The simplest possible dependences are

$$\alpha_1 = 3 - \alpha, \quad \alpha_2 = 4 + \beta. \quad (25)$$

For $\alpha_1 = 3$ and $\alpha_2 = 4$, equations (24) give the Thole screening functions (23). Using functions (24), we obtain the field from the permanent charges in the form

$$\mathbf{E}_n^0 = \sum_{m \neq n} \frac{q_m \mathbf{r}_{nm}}{a^2 r_{nm}} \left\{ \alpha_2 \left| \frac{r_{nm}}{a} \right|^{\alpha_1 - 2} - \alpha_1 \left| \frac{r_{nm}}{a} \right|^{\alpha_2 - 2} \right\}, \quad (26)$$

and the induced dipoles interact through the dipole field tensor

$$\mathbf{T}_{nm} = \sum_{m \neq n} \left\{ \frac{\alpha_2}{a^3} \left| \frac{r_{nm}}{a} \right|^{\alpha_1 - 3} \mathbf{I} - \frac{\alpha_1 r_{nm}^2 \mathbf{I} + 3 \mathbf{r} \otimes \mathbf{r}}{a^3 r_{nm}^2} \left| \frac{r_{nm}}{a} \right|^{\alpha_2 - 3} \right\}. \quad (27)$$

For $\alpha_1 = 3$ and $\alpha_2 = 4$, equations (26) and (27) give the usual Thole screening. For treating polarizability of low-loss dielectric, we suggest using the fractional values of the parameters α_1 and α_2 . A possible generalization of exponential screening is discussed in the appendix.

Our suggestion to use fractional power laws in (24) is based on the mathematical results that have been obtained

in [42]. In this paper, we consider the vectors \mathbf{r}_n that define sites as in solid state physics [43], i.e.

$$\mathbf{r}_n = \sum_{i=1}^3 n_i \mathbf{a}_i,$$

where \mathbf{a}_i are the translational vectors of the lattice, then

$$\mathbf{r}_{nm} = \mathbf{r}_n - \mathbf{r}_m = \sum_i^3 (n_i - m_i) \mathbf{a}_i.$$

Note that this representation can be used as an approximation, and, in general, should be generalized for amorphous materials. As a result, equations (26) and (27) describe power-law long-range interactions of the type $|n - m|^{-s-1}$ with fractional values of s . In the continuous limit, these interactions are described by fractional integro-differentiation [42]. Using the results of [42], we can state that dipole–dipole interactions with fractional screening are connected with integro-differentiation of non-integer order.

As a result, we assume that the link between the dielectric loss of low-loss materials and the physical and structural features in the material can be realized by the generalized polarizable point dipoles method with fractional screening in molecular dynamics and Monte Carlo simulations. Using these simulations the presence of identified defects in the structure of low-loss materials can also be taken into account. To realize this suggested approach additional investigations are required.

6. Conclusion

In conclusion, the electromagnetic fields and waves in a wide class of dielectric materials must be described by fractional differential equations with derivatives of order $2 - \alpha$ and $2 + \beta$, where $0 < \alpha < 1$ and $0 < \beta < 1$. The parameters $\alpha = 1 - n$ and $\beta = m$ are defined by exponents n and m of the ‘universal’ response laws for the frequency dependence of the dielectric susceptibility. A remarkable property of the dynamics described by the fractional equations for electromagnetic fields is that the solutions have power-like tails. The typical features of ‘universal’ electromagnetic waves in dielectric are common to a wide class of materials, regardless of the type of physical structure, chemical composition, or of the nature of the polarizing species, whether dipoles, electrons, or ions. We assume that the link between the dielectric loss of low-loss materials and the physical/structural features in the material can be obtained by the polarizable point dipoles method with fractional screening of dipole–dipole interactions in the molecular dynamics and Monte Carlo simulations.

For small fractionality of α (or β), it is possible to use ε -expansion [27] over the small parameter $\varepsilon = \alpha$ (or $\varepsilon = 1 - \beta$). There are several numerical methods to solve fractional equations (see for example [28]). Note that the suggested fractional differential equations, which describe the electromagnetic field in dielectric media with power-law response, can be solved numerically. For example, the Grunwald–Letnikov discretization scheme can be used [12] to compute fractional equations for electromagnetic field in dielectric.

Appendix

In section 5, we consider the Thole screening functions and their fractional generalizations. The alternative distributions that are used in the polarizable point dipole method are the exponential screening functions

$$f_1(r) = 1 - \exp\left\{-\left(\frac{r}{a}\right)^3\right\} \quad (28)$$

$$f_2(r) = 1 - \left[1 + \left(\frac{r}{a}\right)^3\right] \exp\left\{-\left(\frac{r}{a}\right)^3\right\}. \quad (29)$$

If we consider the modification of $f_1(r)$ of the form

$$f_1(r) = \left(1 - \exp\left\{-b\left(\frac{r}{a}\right)^3\right\}\right) \exp\left\{-c\frac{r}{a}\right\}, \quad (30)$$

then for $r \ll a$ and $b = 4$, $c = 3/4$, we obtain the Thole function for the electric field created by fixed charge. For $b = 1$ and $c = 0$, equation (30) gives (28). For $r \gg a$, we can use the approximation

$$f_1(r) = \exp\left\{-\frac{3}{4}\frac{r}{a}\right\} \quad (31)$$

that is the Debye screening function with $\lambda_D = 4a/3$ used by Jonscher in [2, 29, 30].

Note that the suggested fractional screening function $f_1(r)$ of the form (24) can be an approximation of the screening function

$$f_1(r) = \left(1 - \exp\left\{-b\left(\frac{r}{a}\right)^{\alpha_1}\right\}\right) \exp\left\{-\frac{\alpha_1}{\alpha_2}\left(\frac{r}{a}\right)^{\alpha_2-\alpha_1}\right\}. \quad (32)$$

If $\alpha_1 = 3$ and $\alpha_2 = 4$, then equation (32) gives (30). For $b = \alpha_2$ and $c = \alpha_1/\alpha_2$ with non-integer values of α_1 and α_2 , we have the fractional screening function (24).

As a result, the exponential functions can be used in the generalized polarizable point dipoles method for molecular dynamics and Monte Carlo simulations of low-loss dielectric materials.

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