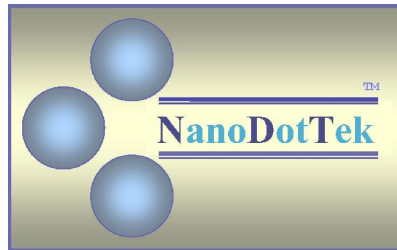


## **What is Fractance and why is it Useful?**

Report NDT24-11-2007  
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## 1. Introduction

The capacitor is a device well-known to the electrical engineer. Capacitors are ubiquitous, and electrical and electronic systems often contain many such devices. At the very least circuits are often modeled and designed accounting for the behavior of such devices even if they are not actually present by design (e.g., modeling “parasitics”). The capacitor is deceptively simple consisting as it does of a dielectric material sandwiched between two metal electrodes that make up the device terminals. Simple physical models for the capacitor appear early within introductory texts about the device (e.g., Chapter 5 of Hayt [1]). And simple dynamic models for the terminal behavior of the device are presented quite early in first courses on electric circuits.

However, it is increasingly clear that these simplified treatments of the device can be inadequate. A way in which problems with simplified models have arisen is in the context of wideband systems analysis and design (e.g., ultra-wideband (UWB) wireless systems). The traditional undergraduate treatment of the capacitor usually neglects nonlinear effects, dielectric anisotropy, and the possible hysteretic relationship between dielectric material polarization and the applied electric field such as would arise in ferroelectric materials and devices. But even if we accept that these particular effects may be ignored, for wideband applications the frequency dependence of the dielectric constant, and therefore of the dielectric material permittivity, simply cannot be ignored. The assumption that device capacitance (which depends on the permittivity of the dielectric) is not a function of frequency is implicitly a narrowband assumption.

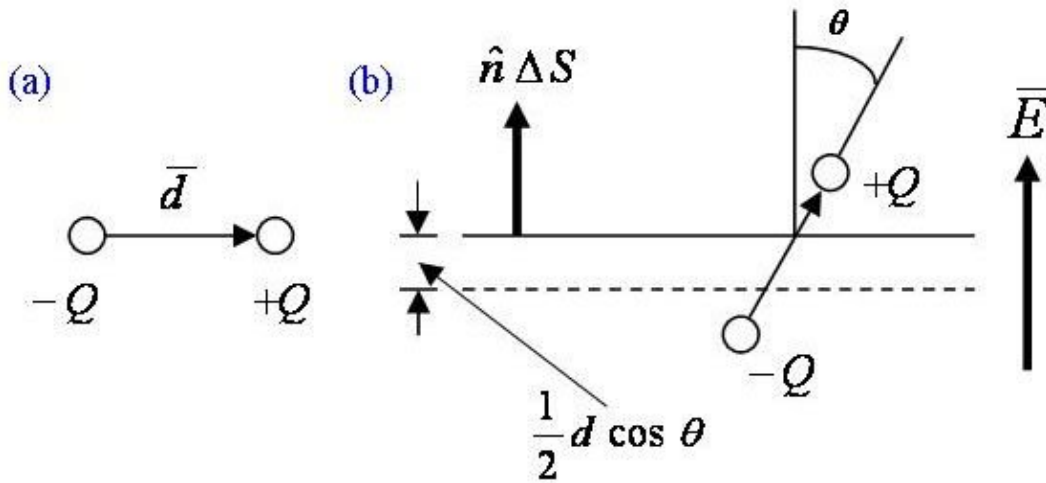
But the situation regarding the frequency dependence of capacitance is even more complicated than this. In particular, in basic circuit models for the terminal behavior of the device it is usually assumed that the current through the device is directly proportional to the time rate of change of the electrical potential between the device terminals, and the constant of proportionality is the device’s capacitance. It is known that this dynamic relationship is not strictly true, though of course manufacturers of capacitors generally strive to make it so. In fact, for example, Westerlund and Ekstam [2] have pointed out that a more accurate description of device terminal current-voltage ( $i$ - $v$ ) behavior is the *Curie law* known since at least 1889. If this law is “translated” into a general relationship between the current through the device and the potential between the device terminals then the need to work with *fractional calculus* immediately arises. The dynamical model familiar to most electrical engineers involving the simple first derivative is at best a special case of this more general (and more accurate) model. Moreover, a deeper inquiry into the implications of the standard undergraduate textbook model reveals that the first derivative special case cannot even physically exist ! This is because the “ideal” capacitor of the textbook is a lossless system. And this implies that all real-world capacitors are already to some degree *fractance devices* implementing a fractional calculus operation relating device current and terminal voltage. However, as already noted, the goal in most capacitor fabrications is to make the derivative as close to a first derivative (ideal case) as possible.

And yet there exist *many* engineering applications where one would want to realize non-integer (fractional) calculus operations. In other words, there is actually a need for *lossy* capacitors with *prescribed* losses not at all close to the ideal lossless case noted above. Therefore, this report provides a review of the physical basis for fractance, and makes a case for the development of capacitors *deliberately* engineered to be lossy. This is for the purpose of realizing analog fractional calculus operations within a *single device*. The notion of realizing a controlled (or “tunable”) fractance within a single device is believed to be preferable to approximating desired fractional calculus operations via complicated networks of nominally ideal circuit elements be they active or passive elements.

Note that the subject of this report is extremely ambitious, as the field of dielectric science and engineering is vast. Thus, this report is incomplete in many important ways. But the cited references will give the reader an idea of where to go for other sources of information.

## 2. An Elementary View of the Capacitor

This section provides a quick summary of an elementary physical model for a capacitor. We follow Hayt [1] (Chapter 5). Approaching an understanding of the physical basis for fractance is easier if we begin in such a simple way.



**Figure 1:** (a) The electric dipole. (b) Rotation of an electric dipole in an applied static electric field  $\vec{E}$ .

In Fig. 1(a) (above) we see a symbolic representation of an *electric dipole*. This is two charges each of magnitude  $Q$  but of opposite sign with a distance vector  $\vec{d}$  directed from the negative charge towards the positive charge. From Section 4.7 of [1] we recall that the *dipole moment* is defined to be

$$\vec{p} = Q\vec{d} \tag{2.1}$$

The electrical potential in space due to the dipole can be written in terms of (2.1), but this is not essential for our purpose here. Of more immediate importance is the following.

The dielectric properties of matter are determined by its molecular structure. Matter (liquid, solid, or gas) has the ability to store energy due to shifting the relative position of internal positive and negative charges against the normal electromagnetic forces within the material. How this arises varies from one type of material to the next. For example, in some materials there is a permanent separation of charges into the form of a dipole as in Fig. 1(a). These are *polar materials*. By contrast in *non-polar materials* this kind of charge separation can only arise if there is an applied field.

As one may expect the application of an external electric field such as  $\vec{E}$  in Fig. 1(b) will result in the dipoles trying to align themselves with this field. In general the alignment will not be “perfect.” In Fig. 1(b) the incremental surface element  $\overline{\Delta S} = \hat{n} \Delta S$  ( $\hat{n}$  is a unit vector) is considered to be collinear with  $\vec{E}$ . The surface element is perpendicular to the plane of the page and is indicated by the solid horizontal line. From the direction of the applied electric field the dipole will make an angle  $\theta$  with this plane as indicated. The dashed horizontal line represents another (parallel) plane a distance  $\frac{1}{2} \cdot d \cos \theta$  below the plane denoted by the solid horizontal line, where  $d = |\vec{d}|$  is the distance between the *bound charges* of the dipole. As a result, any molecule whose center was originally within the volume element bounded by the two planes gives a movement of charge  $+Q$  upwards and across  $\Delta S$ . There is a similar motion of charge  $-Q$  across  $\Delta S$  directed downwards. If we assume that there are  $N$  electric dipoles per unit of volume then the total net charge that crosses the surface element in the upward direction is given by

$$\Delta Q_b = N Q d \cos \theta \Delta S = N Q \vec{d} \cdot \hat{n} \Delta S \quad (2.2)$$

The subscript “b” emphasizes that the charges are *bound* charges and so are not free to move as, say, conduction band electrons within a conductor. Now, the material *polarization* is the *electric dipole moment per unit of volume* of material and is the vector denoted  $\vec{P}$ . Thus, (2.2) can be rewritten as

$$\Delta Q_b = \vec{P} \cdot \overline{\Delta S} \quad (2.3)$$

Now assume that the surface element is a part of a closed surface. The motion of the bound charges is directed outwards from the enclosed volume, and so the net *increase* of bound charge within the volume must be

$$Q_b = - \oint_S \vec{P} \cdot d\vec{S} \quad (2.4)$$

This bound charge is distributed with a volume charge density denoted  $\rho_b$ , and hence

$$Q_b = \int_V \rho_b dV \quad (2.5)$$

Combining (2.5) with (2.4) it is apparent that

$$-\oint_S \bar{P} \cdot d\bar{S} = \int_V \rho_b dV \quad (2.6)$$

Applying the divergence theorem of vector calculus yields

$$\nabla \cdot \bar{P} = -\rho_b \quad (2.7)$$

Now, *Gauss's law* relates electric field intensity  $\bar{E}$  to the total volume charge density denoted by  $\rho_t$ . That is,

$$\nabla \cdot \varepsilon_0 \bar{E} = \rho_t \quad (2.8)$$

( $\varepsilon_0$  = permittivity of vacuum). At this point the total volume charge density is now regarded as being composed of *free charges* of density  $\rho_f$ , and bound charges of density  $\rho_b$ . Thus, (2.8) is now

$$\nabla \cdot \varepsilon_0 \bar{E} = \rho_f + \rho_b \quad (2.9)$$

But from (2.7) this is also

$$\nabla \cdot \varepsilon_0 \bar{E} = \rho_f - \nabla \cdot \bar{P} \quad (2.10)$$

or alternatively

$$\nabla \cdot (\varepsilon_0 \bar{E} + \bar{P}) = \rho_f \quad (2.11)$$

The *electric flux density* is therefore given as

$$\bar{D} = \varepsilon_0 \bar{E} + \bar{P} \quad (2.12)$$

and so

$$\nabla \cdot \bar{D} = \rho_f \quad (2.13)$$

The polarization  $\bar{P}$  arises in response to the applied electric field  $\bar{E}$ . The simplest relationship to assume is the linear one

$$\bar{P} = \chi \epsilon_0 \bar{E} \quad (2.14)$$

where  $\chi$  is the *electric susceptibility* of the dielectric material. Equation (2.14) neglects the possibility of material nonlinearity, anisotropy, frequency dependence, and hysteresis. In what follows we shall only consider generalizations accounting for frequency dependence.

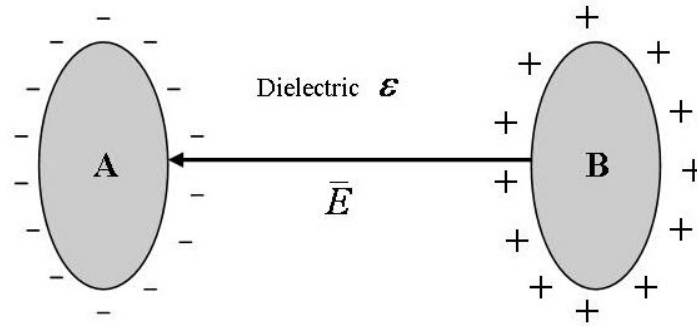
The electric susceptibility is often defined in terms of *relative permittivity* which is also known as the *dielectric constant* here denoted as  $\epsilon_r$ . Specifically,

$$\chi = \epsilon_r - 1 \quad (2.15)$$

Combining (2.12), (2.14) and (2.15) we easily see that

$$\bar{D} = \epsilon_r \epsilon_0 \bar{E} = \epsilon \bar{E} \quad (2.16)$$

Because so far the field  $\bar{E}$  is static the relative permittivity should properly be called the *static* relative permittivity. Similar language should also apply to the electric susceptibility.



**Figure 2:** Conducting bodies A and B are separated by a homogeneous dielectric material of permittivity  $\epsilon$ . This “device” is a capacitor.

Now consider Fig. 2. Symbols A and B denote ideal conducting bodies with static charges upon their surfaces, where A is negatively charged and B is positively charged. Since the electric field  $\bar{E}$  between the bodies is static and free charges cannot exist within the conducting bodies their surfaces are equipotential surfaces. The total charge within a closed surface  $S$  enclosing B is given by the integral form of Gauss’s law

$$Q = \oint_S \bar{D} \cdot d\bar{S} \quad (2.17)$$

Of course, the charge on body A is  $-Q$ . The potential difference between the conductors may be obtained by integrating along any path from a point on the surface of A to a point on the surface of B, and is therefore of the form

$$V = -\int_A^B \vec{E} \cdot d\vec{l} \quad (2.18)$$

The *capacitance* of the capacitor in Fig. 2 is defined to be

$$C = \frac{Q}{V} = \frac{\oint_S \epsilon \vec{E} \cdot d\vec{S}}{-\int_A^B \vec{E} \cdot d\vec{l}} \quad (2.19)$$

Of course, Equation (2.19) employs Equation (2.16). Plainly, the capacitance of the capacitor depends on the permittivity of the dielectric (a homogeneous medium here), and also upon the geometry of the system.

If we assume that capacitance is a constant with respect to time, but the charge on the conducting bodies (i.e., capacitor plates) varies with time, then the potential difference between the conductors and the current flow into the device will be time-varying as well. From (2.19) then

$$q(t) = Cv(t) \quad (2.20)$$

where now  $v(t)$  replaces  $V$ , and  $q(t)$  replaces  $Q$  to emphasize the introduction of time into our problem. Electrical current is the time rate of change of electric charge and so (2.20) yields upon differentiating with respect to time  $t$

$$i(t) = \frac{dq(t)}{dt} = C \frac{dv(t)}{dt} \quad (2.21)$$

Physically, the current flow is due to the accumulation of charge upon the capacitor plates during charging. Equation (2.21) is, of course, the usual electric circuit textbook description of the device terminal iv-relationship.

The derivations of this section worked with a *static* applied electric field, but the situation for a *time-varying* applied electric field is really quite different. Originally, classical physics was used to create a model for dielectric polarization accounting for time-variations in the applied electric field. These results are sometimes called *Drude models*. A summary account appears in Amos [3] with respect to the insight such models can give concerning chemical bonds. Drude models can also “explain” the frequency dependence of magnetic susceptibility [3], and electrical conductivity (Ashcroft and Mermin [4]).

More recently, Drude models have been used to understand double-negative metamaterials (e.g., Ziolkowski and Kipple [5], Ziolkowski and Heyman [6]). This is sometimes in association with understanding such exotic notions as flat lenses and cloaking devices. It is noteworthy that although Drude models have their original formulation via classical physics that these models can be arrived at by quantum mechanical reasoning. This is a more fundamental and correct approach, and an illustration of this is provided in the next section.

### 3. The Quantum Mechanical Basis for the Frequency-dependence of Permittivity

In the previous section it was noted that classical physics has been used to understand the frequency dependence of dielectric permittivity. But it was not long after the inception of quantum mechanical theory that this physics was applied to understanding dielectric phenomena. Yet, contingent upon certain assumptions (e.g., electrons are non-interacting, Pauli exclusion is ignored) the quantum theoretic approach yields much that same end result as the classical Drude approach. However, in this section we present a sketch of the elementary theory of the dielectric constant based on quantum mechanical reasoning. This approach is technically correct, and more advanced forms of the theory yield more accurate results than are available from attempts to extend classical theory. What follows borrows from Greiner [7] (Section 11.11), but we will begin with a review of more basic material.

#### A Review of Basic Ideas from Quantum Theory

We begin with a consideration of the Schrödinger equation assuming a time-varying potential field<sup>1</sup>

$$j\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\vec{r}, t) \Psi \quad (3.1)$$

Here  $j = \sqrt{-1}$ <sup>2</sup>,  $\Psi \equiv \Psi(\vec{r}, t)$  is the *wave function*,  $m$  is the particle mass,  $V(\vec{r}, t)$  is the *potential function* (such as due to an applied electric field), and the *Laplacian operator* is

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (3.2)$$

Vector  $\vec{r}$  is a position vector within the Cartesian frame of reference and so is the point  $(x, y, z)$ , or alternatively we can write

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k} \quad (3.3)$$

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<sup>1</sup> The time-varying potential will be important in the theory of the dielectric as will be seen later on.

<sup>2</sup> Physicists like to use “i” instead of “j,” but this risks confusion with electrical current.

The unit vectors  $\hat{i}, \hat{j}, \hat{k}$  define the reference frame and are mutually orthonormal. Also,  $\hbar (= 1.05457 \times 10^{-34}$  Joule-seconds) is called *Planck's constant*.

We further recall that quantum theory is an example of applied probability theory. In particular, the wave function has a probabilistic interpretation which will now be summarized beginning with a consideration of the form of the solution to (3.1).

If we define the *Hamiltonian operator*

$$H \equiv -\frac{\hbar^2}{2m} \nabla^2 + V(\bar{r}, t) \quad (3.4)$$

then (3.1) is now

$$j\hbar \frac{\partial \Psi}{\partial t} = H\Psi \quad (3.5)$$

Assume for the moment that the potential function is *time-independent*:  $V(\bar{r}, t) = V(\bar{r})$ . The first line of attack in solving a partial differential equation (PDE) such as the Schrödinger equation is separation of variables, and thus we assume that

$$\Psi(\bar{r}, t) = \psi(\bar{r})f(t) \quad (3.6)$$

Substituting Equation (3.6) into (3.1) results in the PDE reducing to an equivalent system of two ordinary differential equations (ODEs). Skipping the details<sup>3</sup> the general form of the solution can be shown to be

$$\Psi(\bar{r}, t) = \psi(\bar{r})e^{-jEt/\hbar} \quad (3.7)$$

Moreover, the time-independent part of (3.7) satisfies the eigensystem

$$H\psi = E\psi \quad (3.8)$$

The constant  $E$  is an eigenvalue with the physical interpretation of energy. For a so-called *bound system* (the case of interest to us in this report) a countable infinity of eigenfunctions satisfies (3.8). Assuming for the  $n$ th eigenvalue (*eigenenergy*)  $E_n$  that the corresponding eigenfunction is unique<sup>4</sup> and denoted by  $\psi_n(\bar{r})$  then

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<sup>3</sup> A very approachable presentation of the details appears in the text D. J. Griffiths, *Introduction to Quantum Mechanics*, Prentice Hall, 1995. This book is even more approachable after a study of basic function space ideas to be found in C. J. Zarowski, *An Introduction to Numerical Analysis for Electrical and Computer Engineers*, John Wiley and Sons, 2004 (see Chapter 1).

<sup>4</sup> This is the assumption of a *non-degenerate* system.

$$H\psi_n = E_n\psi_n \quad (3.9)$$

The general solution to the wave equation will be a superposition of the functions

$$\Psi_n(\vec{r}, t) = \psi_n(\vec{r})e^{-jE_n t / \hbar} \quad (3.10)$$

That is, the general form of the solution to the Schrödinger equation (again, we are assuming a time-invariant potential function, and non-degeneracy within a bound system) must be

$$\Psi(\vec{r}, t) = \sum_n c_n \psi_n(\vec{r})e^{-jE_n t / \hbar} \quad (3.11)$$

The constants  $c_n$  are selected to *normalize* the system. This notion arises with respect to the probabilistic interpretation of the wave function. Specifically, the probability that the mass  $m$  particle is within the infinitesimal volume element  $d^3\vec{r} = dx dy dz$  at time  $t$  is given by  $|\Psi(\vec{r}, t)|^2 d^3\vec{r}$ . Therefore, the constants  $c_n$  are selected to ensure

$$\int |\Psi(\vec{r}, t)|^2 d^3\vec{r} = 1 \quad (3.12)$$

The integral is taken over all space. In practice, the initial wave function<sup>5</sup>  $\Psi(\vec{r}, 0)$  can be used to determine the constants  $c_n$ . The form of the potential function and boundary conditions determines the mathematical form of the wave functions. For example, in analyzing the hydrogen atom the potential function will be Coulomb's, and is

$$V(r) = -\frac{e^2}{4\pi \epsilon_0} \frac{1}{r} \quad (3.13)$$

where  $e$  is the *electron charge*, and  $r = |\vec{r}|$  is the Euclidean distance from the “center” of the nucleus of the atom. To analyze the hydrogen atom it is best to convert to spherical coordinates and solve Schrödinger's equation within that system. The eigenfunctions will then be expressed in terms of special functions such as radial wave functions and associated Laguerre polynomials. Most realistic problems have no analytic solution forcing the use of numerical methods, or approximation methods perhaps involving perturbation techniques. In fact, a perturbation theory is needed to establish the elementary theory of the dielectric constant.

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<sup>5</sup> Solving the Schrödinger equation from a given initial wave function amounts to determining the evolution through time of the quantum mechanical system. But results are expressed in terms of probabilities or of statistical averages.

The perturbation method of analysis for quantum mechanical systems assumes that the real system of interest is described by a small change in an easily solvable idealized system. If the Hamiltonian of the idealized system (unperturbed system) is denoted by  $H_0$  then the system of interest has Hamiltonian

$$H = H_0 + \delta W \quad (3.14)$$

The perturbation term  $\delta W$  (a product of constant  $\delta$  and operator  $W$ ) is assumed to be “small.” The notion of “small” is not necessarily rigorously defined. Constant  $\delta$  is the *perturbation parameter*. The perturbation solution wave functions and associated energies are considered to be series expansions in this parameter. The next sub-section applies this sort of thinking to obtaining a theory of the dielectric constant.

### Elementary Theory of the Dielectric Constant

In the absence of an applied field the Hamiltonian  $H_0$  of an electron bound within a molecule has a *ground state*<sup>6</sup>  $\psi_0(\vec{r})$  with corresponding energy  $E_0$ . The charge on the electron is  $Q = -e$  ( $= -1.60218 \times 10^{-19}$  C). Recalling Section 2 the dipole moment of this system is  $\vec{p} = -e\vec{r}$ . Atomic scale (microscopic) entities such as this relate to classical (macroscopic) entities through the taking of statistical averages. It is the statistical averages that correspond to “lab bench” observables. If the molecule is in the ground state and there is no applied field then there will be no observed dipole moment, which means that the *average dipole moment* is

$$\langle \vec{p} \rangle_0 = -e \int \psi_0^* \vec{r} \psi_0 dV = 0 \quad (dV \equiv d^3\vec{r}) \quad (3.15)$$

( $\psi_0^*$  is the complex-conjugate of  $\psi_0$ ). The wave function for the ground state is a special case of (3.11), and is considered to be

$$\Psi_0(\vec{r}, t) = \psi_0(\vec{r}) e^{-jE_0 t / \hbar} \quad (3.16)$$

Now, assume that the molecule experiences a time-varying electrical potential field<sup>7</sup>

$$V(\vec{r}, t) = -e\phi(\vec{r}, t) = e z A \sin(\omega t) \quad (3.17)$$

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<sup>6</sup> The ground state is the lowest possible energy state of a quantum mechanical system. In contrast with classical physics the energy is non-zero.

<sup>7</sup> A propagating electromagnetic wave not only has an electric field but a magnetic one as well. The present analysis neglects the magnetic component. The error due to neglecting the time-varying magnetic field can be formally shown to be negligible.

This is due to the application of a plane monochromatic and linearly polarized electric field of frequency  $\omega$  (radians/second), i.e.,

$$\bar{E} = -\nabla\phi = -\frac{\partial}{\partial z}[-zA\sin(\omega t)]\hat{k} = A\sin(\omega t)\hat{k} \quad (3.18)$$

This field perturbs an otherwise “stationary” system. The Schrödinger equation for the perturbed system is therefore

$$[H_0 + ezA\sin(\omega t)]\Psi(\bar{r}, t) = j\hbar \frac{\partial}{\partial t} \Psi(\bar{r}, t) \quad (3.19)$$

Of course, the term “ $ezA\sin(\omega t)$ ” corresponds to the perturbation term in (3.14) with  $A \equiv \delta$ . The solution to the perturbed “problem” of (3.19) is considered to have the general form

$$\Psi(\bar{r}, t) = \psi_0(\bar{r})e^{-jE_0t/\hbar} + A\Psi^1(\bar{r}, t) \quad (3.20)$$

The function  $\Psi^1(\bar{r}, t)$  is called the *first correction* to the stationary ground state in the time-varying electrical potential field. Equation (3.20) must satisfy (3.19). To carry the solution process out one must assume a reasonable form for the perturbation (correction) term in (3.20). In particular, it is assumed that

$$\Psi^1(\bar{r}, t) = w_+(\bar{r})e^{-j(E_0 + \hbar\omega)t/\hbar} + w_-(\bar{r})e^{-j(E_0 - \hbar\omega)t/\hbar} \quad (3.21)$$

Equation (3.20) is substituted into (3.19). Terms that are linear in the perturbation parameter  $A$  are compared leading to the conclusion that

$$\left[ H_0 - j\hbar \frac{\partial}{\partial t} \right] \Psi^1(\bar{r}, t) = -ez\sin(\omega t)\psi_0(\bar{r}) \exp\left[ -\frac{jE_0t}{\hbar} \right] \quad (3.22)$$

Working with (3.21), (3.22) and the elementary identity

$$\sin(\omega t) = \frac{1}{2j} \left[ e^{j\omega t} - e^{-j\omega t} \right] \quad (3.23)$$

it is next discovered that

$$\begin{aligned} H_0 w_+ - (E_0 + \hbar\omega)w_+ &= \frac{ez}{2j}\psi_0 \\ H_0 w_- - (E_0 - \hbar\omega)w_- &= -\frac{ez}{2j}\psi_0 \end{aligned} \quad (3.24)$$

The energies  $E_0 \pm \hbar\omega$  are not eigenvalues of the Hamiltonian  $H_0$ . In particular,  $E_0 + \hbar\omega$  is not an eigenvalue because  $\omega$  is not an absorption frequency for the system, and  $E_0 - \hbar\omega$  cannot be an eigenvalue since  $E_0$  is the ground state energy. Thus, the system (3.24) is not homogeneous and has an unambiguous solution.

It is now assumed that the eigenvalues and corresponding eigenfunctions of the Hamiltonian  $H_0$  are, respectively,  $E_j$  and  $\psi_j(\bar{r})$  for  $j = 0, 1, 2, \dots$ . These eigenfunctions are assumed to represent an orthogonal basis for a space of functions that includes the coefficients  $w_+(\bar{r})$ , and  $w_-(\bar{r})$  in (3.21). This implies that there are expansion coefficients  $c_k^+$  and  $c_k^-$  such that

$$\begin{aligned} w_+(\bar{r}) &= \sum_{k=0}^{\infty} c_k^+ \psi_k(\bar{r}) \\ w_-(\bar{r}) &= \sum_{k=0}^{\infty} c_k^- \psi_k(\bar{r}) \end{aligned} \quad (3.25)$$

respectively<sup>8</sup>. The next step is to substitute (3.25) into (3.24), multiply by  $\psi_j^*(\bar{r})$  and then integrate over all space to obtain expressions for the expansion coefficients. The end result is found to be

$$\begin{aligned} w_+(\bar{r}) &= \frac{e}{2j} \sum_{k=1}^{\infty} \frac{\langle \psi_k | z | \psi_0 \rangle}{E_k - E_0 - \hbar\omega} \psi_k(\bar{r}) \\ w_-(\bar{r}) &= -\frac{e}{2j} \sum_{k=1}^{\infty} \frac{\langle \psi_k | z | \psi_0 \rangle}{E_k - E_0 + \hbar\omega} \psi_k(\bar{r}) \end{aligned} \quad (3.26)$$

The terms  $k = 0$  have vanished on account of (3.15)<sup>9</sup>. There is no average dipole moment for the ground state system. Moments only arise due to the presence of the perturbing field. We have found our (approximate) solution to (3.19) which is

$$\Psi(\bar{r}, t) = \left[ \psi_0(\bar{r}) + \frac{Ae}{2j} \sum_{k=1}^{\infty} \psi_k(\bar{r}) \langle \psi_k | z | \psi_0 \rangle \left\{ \frac{e^{-j\alpha t}}{E_k - E_0 - \hbar\omega} - \frac{e^{j\alpha t}}{E_k - E_0 + \hbar\omega} \right\} \right] e^{-jE_0 t/\hbar} \quad (3.27)$$

The applied electric field is in the z-direction. Thus, the mean dipole moment in this direction is obtained by evaluating  $\tilde{p} = e \langle \Psi | z | \Psi \rangle$ . So, from (3.27) we find that

<sup>8</sup> An introduction to thinking about bases in this manner is to be found in C. J. Zarowski, *An Introduction to Numerical Analysis for Electrical and Computer Engineers*, John Wiley and Sons, 2004.

<sup>9</sup> Note that  $\langle \psi_k | z | \psi_0 \rangle = \int \psi_k^* z \psi_0 dV$ .

$$\tilde{p} = 2e^2 A \sin(\omega t) \sum_{k=1}^{\infty} |\langle \psi_k | z | \psi_0 \rangle|^2 \frac{E_k - E_0}{(E_k - E_0)^2 - (\hbar\omega)^2} \quad (3.28)$$

If there is no electric field then  $A = 0$ . Only the ground state is populated and there is no net dipole moment (recall again Equation (3.15)). If there is an applied time-varying electric field it partly polarizes the molecules, which is consistent with our intuition about the system as argued in an elementary manner in Section 2.

Let the electron mass be denoted by  $m_e (=9.10939 \times 10^{-31} \text{ kg})$ . We may define the transition energies  $\hbar\omega_k = E_k - E_0$ , and the *dipole strength*<sup>10</sup>

$$f_k = \frac{2m_e}{\epsilon_0 \hbar} |\langle \psi_k | z | \psi_0 \rangle|^2 \omega_k \quad (3.29)$$

If the electron makes a jump from ground state  $E_0$  to the higher energy state  $E_k$  then this requires absorbing a photon of energy  $\hbar\omega_k$ . Conversely, in dropping from the higher energy state to the ground state a photon of this energy will be emitted. From Equation (3.29) we see that (3.28) is now

$$\tilde{p} = \frac{e^2 \epsilon_0 A}{m_e} \sin(\omega t) \sum_{k=1}^{\infty} \frac{f_k}{\omega_k^2 - \omega^2} \quad (3.30)$$

Now the polarization in the z-direction is (recalling the classical argument in Section 2)

$$\bar{P} = P\hat{k} = N\tilde{p}\hat{k} \quad (3.31)$$

As before  $N$  is the number of dipoles per unit of volume of dielectric material. From (2.16) and (3.18) we now see that

$$\bar{D} = \epsilon\bar{E} = \epsilon A \sin(\omega t) \hat{k} \quad (3.32)$$

But also

$$\bar{D} = \epsilon_0 \bar{E} + \bar{P} = \epsilon_0 A \sin(\omega t) \hat{k} + \frac{Ne^2 A \epsilon_0}{m_e} \sin(\omega t) \sum_{k=1}^{\infty} \frac{f_k}{\omega_k^2 - \omega^2} \hat{k} \quad (3.33)$$

Comparing (3.33) with (3.32) the factor  $A \sin(\omega t)$  drops out revealing that

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<sup>10</sup> Defining dipole strength results in an expression for the dielectric constant in terms of classically familiar quantities. It “disguises” the quantum mechanical basis for polarization.

$$\varepsilon = \varepsilon(\omega) = \left[ 1 + \frac{Ne^2}{m_e} \sum_{k=1}^{\infty} \frac{f_k}{\omega_k^2 - \omega^2} \right] \varepsilon_0 \quad (3.34)$$

That is, the dielectric constant is now manifestly dependent upon frequency and from (3.34) is

$$\varepsilon_r(\omega) = 1 + \frac{Ne^2}{m_e} \sum_{k=1}^{\infty} \frac{f_k}{\omega_k^2 - \omega^2} \quad (3.35)$$

This is a minor variation on Equation (23) of Section 11.11 in Greiner [7]. Differences between (3.35) and (23) in [7] are due to working within a different system of units.

In the more realistic scenario of systems containing many interacting electrons in a molecule the general features of (3.35) are preserved. This is discussed, for example, in Milonni [8]. Formulae such as these are sometimes called *Kramers-Heisenberg* expressions for polarizability. The expression (3.35) is an infinite series of rational functions in frequency  $\omega$ . Classically obtained Drude models are only finite series. A question arises as to what a series such as (3.35) converges to. For example, is the limit a rational or irrational function of frequency ?

#### 4. Causality and the Kramers-Kronig Integrals

Here we show that the physical requirement of causality constrains the relationship between the real and imaginary parts of the dielectric constant. However, before getting into this it is necessary to consider an important shortcoming of the frequency-dependent model for the dielectric constant in (3.35).

The model for the dielectric constant in (3.35) has some problems owing to the simplified derivation. Aside from the consequences of other simplifications noted in Section 3 the expression (3.35) diverges for  $\omega \rightarrow \omega_k$  which is non-physical behavior. In essence this difficulty has arisen because the model does not account for *losses*. The classical approach to dealing with this was to view the electric dipole as analogous to two masses in a mechanical system connected by a spring with (linear) mechanical damping present. In the electronic systems we consider in this report this suggests modifying (3.35) according to

$$\varepsilon_r(\omega) = 1 + \sum_{k=1}^{\infty} \frac{A_k}{\omega_k^2 + 2(j\omega)\Gamma_k + (j\omega)^2} \quad (4.1)$$

The new constants  $\Gamma_k$  model the losses (damping) that are really present within any real-world dielectric material. If the series in (4.1) were truncated to work with only a finite number of terms, perhaps as an approximation, then the resulting model is often called a

*Drude-Lorentz model.* However, quantum mechanics would insist that a better model is to retain all terms in the series (4.1).

Electrical engineers are comfortable with Laplace transforms and we may wish to view (4.1) as a complex-valued transfer function for some linear dynamic system. Therefore, we may analytically continue (4.1) from the  $j\omega$ -axis to the rest of the complex  $s$ -plane simply by replacing  $j\omega$  with  $s$ . Thus, instead of (4.1) we now have

$$\varepsilon_r(s) = 1 + \sum_{k=1}^{\infty} \frac{A_k}{\omega_k^2 + 2\Gamma_k s + s^2} \quad (4.2)$$

Suppose this is viewed as the Laplace transform of the impulse response of some dynamic system. Then the poles of the  $k$ th term of (4.2) may be assumed to be of the form  $p_k = a_k + jb_k$ , and  $p_k^* = a_k - jb_k$ , which are a complex-conjugate pair. The constants  $a_k, b_k$  are always real-valued. Therefore,

$$(s - p_k)(s - p_k^*) = s^2 - 2\operatorname{Re}[p_k]s + |p_k|^2 = s^2 + 2\Gamma_k s + \omega_k^2 \quad (4.3)$$

( $\operatorname{Re}[\ ]$  means take the real part of the argument.) Inverse transforming (4.2) will result in an expression containing the exponentials

$$e^{p_k t}, e^{p_k^* t} \Rightarrow e^{a_k t} e^{jb_k t}, e^{a_k t} e^{-jb_k t} \quad (4.4)$$

The only way to prevent explosive growth in these entities for  $t \rightarrow \infty$  is if  $a_k < 0$  from which we infer that  $\Gamma_k > 0$  for all  $k$ .

We have inferred that a *lossy dielectric must* possess a non-trivially complex-valued dielectric constant since (4.1) has non-trivial real and imaginary parts that depend on  $\omega$ . Moreover, the need for causality constrains the relationship between the real and imaginary parts of the dielectric constant. This relationship is specified via the famous *Kramers-Kronig integrals*. It is also worth noting that signal processing engineers are already familiar with Kramers-Kronig relations, except that these are more usually called *Hilbert transform relations*. For example, Oppenheim and Schaffer [9] discuss the discrete-time version of the Hilbert transform relations (see Chapter 7).

The Kramers-Kronig integrals may be expressed in various ways. Milonni [8] gives the Kramers-Kronig integrals relating the real and imaginary parts of the *refractive index* of a material. Although there is a simple relationship between the dielectric constant and the refractive index we have begun by a consideration of the dielectric constant, and so we shall follow the derivational approach in Johnson [10].

A few mathematical preliminaries (definitions) now follow. If we are given a frequency domain (Fourier domain) function  $F(\omega)$  then the corresponding time-domain function (if it exists) is given as

$$f(t) = F^{-1}\{F(\omega)\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) e^{j\omega t} d\omega \quad (4.5)$$

This is the *inverse Fourier transform (IFT)*. Of course, given (4.5) the *Fourier transform (FT)* is

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-j\omega t} dt \quad (4.6)$$

Below we are faced with the need to integrate a function, say  $f(x)$ , such that it goes to infinity at  $x = a$ . That is,

$$\lim_{x \rightarrow a} |f(x)| = \infty \quad (4.7)$$

From Kreyszig [11] for  $\delta > 0$

$$P \int_{-\infty}^{\infty} f(x) dx = \lim_{\delta \rightarrow 0} \left[ \int_{-\infty}^{a-\delta} f(x) dx + \int_{a+\delta}^{\infty} f(x) dx \right] \quad (4.8)$$

is the *Cauchy principal value* of the integral which allows us to handle the singularity in the integrand at  $x = a$ . Equation (4.8) implicitly assumes that  $f(x)$  is sufficiently well-behaved at infinity.

The real part and the imaginary part of the dielectric constant are, respectively,

$$\varepsilon_R(\omega) = \text{Re}[\varepsilon_r(\omega)], \quad \varepsilon_I(\omega) = \text{Im}[\varepsilon_r(\omega)] \quad (4.9)$$

( $\text{Im}[\ ]$  means take the imaginary part of the argument.) Therefore,

$$\varepsilon_r(\omega) = \varepsilon_R(\omega) + j\varepsilon_I(\omega) \Rightarrow \chi(\omega) = [\varepsilon_R(\omega) - 1] + j\varepsilon_I(\omega) \quad (4.10)$$

Here  $\chi(\omega)$  is the electric susceptibility (recall (2.15)) with the frequency-dependence explicitly indicated. The dielectric is a causal physical system and its dynamic response to an applied field is determined by its susceptibility. This must mean that

$$\chi(t) = \varepsilon_r(t) - \delta(t) = 0 \quad \text{for } t < 0 \quad (4.11)$$

Recall that the inverse Fourier transform of unity is the Dirac impulse  $\delta(t)$ :

$$F\{\delta(t)\} = \int_{-\infty}^{\infty} \delta(t)e^{-j\omega t} dt = 1 \quad (4.12)$$

The theory of distributions (generalized functions) can be used to formally justify these things. Although the Fourier transform  $\chi(\omega)$  is complex-valued, the inverse transform is real-valued. It is possible to express  $\chi(t)$  as the sum of an even and an odd function

$$\chi(t) = e(t) + o(t) \quad \text{with} \quad e(t) = e(-t), o(t) = -o(-t) \quad (4.13)$$

( $e(t)$  is even, and  $o(t)$  is odd and both are real-valued). It is useful to define the *sign function*

$$\text{sgn}(x) = \begin{cases} +1, & x > 0 \\ 0, & x = 0 \\ -1, & x < 0 \end{cases} \quad (4.14)$$

Sometimes this is considered undefined at  $x = 0$ . From (4.11) and (4.13) we have

$$e(t) = \text{sgn}(t)o(t) \quad \text{for} \quad t \neq 0 \quad (4.15)$$

We need to consider  $t = 0$ . First of all,  $o(t)$  is odd so immediately  $o(0) = 0$ . Now assume that (4.15) *doesn't* apply at  $t = 0$ . This means that for all  $t$

$$e(t) = \text{sgn}(t)o(t) + x(t) \quad (4.16)$$

where  $x(t) = 0$  for  $t \neq 0$ . If  $x(0)$  were nonzero the Fourier transform  $E(\omega) = F\{e(t)\}$  would be the same as that for  $x(0) = 0$ , and the only forms of  $x(t)$  that affect  $E(\omega)$  are  $\delta(t)$  or perhaps a derivative of  $\delta(t)$ . But  $e(t)$  must be finite for all  $t$ , or  $\chi(\omega)$  must be square-integrable. This prevents  $x(t)$  from being a Dirac impulse or a derivative of such an entity. All of this implies that  $x(t) = 0$  for all  $t$ , and thus  $e(0) = 0$ . This implies that (4.15) is actually valid for *all* times  $t$ .

According to Papoulis [12] (see Equation (3-49)) the sign function has the Fourier transform

$$F\{\text{sgn}(t)\} = \frac{2}{j\omega} \quad (4.17)$$

Hence from (4.5) and (4.8) we must have

$$\text{sgn}(t) = \frac{1}{2\pi} P \int_{-\infty}^{\infty} \frac{2}{j\omega} e^{j\omega t} d\omega \quad (4.18)$$

Equation (4.15) relates the even and odd parts of the time-domain form of the electric susceptibility through a time-domain product of functions. Another basic result of analog (continuous-time) Fourier theory is the transform pair

$$x(t)h(t) \leftrightarrow \frac{1}{2\pi} \int_{-\infty}^{\infty} X(\nu)H(\omega - \nu) d\nu = \frac{1}{2\pi} X(\omega) * H(\omega) \quad (4.19)$$

The integral is a convolution in the Fourier domain. This result is the dual of the time-domain convolution result

$$x(t) * h(t) = \int_{-\infty}^{\infty} x(\tau)h(t - \tau) d\tau \leftrightarrow X(\omega)H(\omega) \quad (4.20)$$

Additionally, if  $x(t)$  is an even function then it is easy to confirm that

$$X(\omega) = 2 \int_0^{\infty} x(t) \cos(\omega t) dt \quad (4.21)$$

This is real-valued for all frequencies. Similarly, if  $x(t)$  is an odd function then

$$X(\omega) = -2j \int_0^{\infty} x(t) \sin(\omega t) dt \quad (4.22)$$

This is purely imaginary for all frequencies. These notions are covered in detail in Papoulis [12] as well as in many other more recent textbooks pertaining to signal processing or to signals and systems.

Taking into account (4.21) and (4.22) then from (4.13) we must be able to write

$$\chi(\omega) = E(\omega) + O(\omega) = E(\omega) + jO'(\omega) \quad (4.23)$$

for which  $E(\omega)$ , and  $O'(\omega)$  are real-valued at all frequencies. From (4.10) and (4.23) we make the identifications

$$E(\omega) = \varepsilon_R(\omega) - 1, \quad \varepsilon_I(\omega) = O'(\omega) \quad (4.24)$$

If we apply (4.17) and (4.19) to (4.15) (which includes making use of (4.8)) we find that

$$E(\omega) = -\frac{j}{\pi} P \int_{-\infty}^{\infty} \frac{O(\nu)}{\omega - \nu} d\nu \quad (4.25)$$

But because of (4.24) and (4.23) Equation (4.25) finally becomes

$$\varepsilon_R(\omega) - 1 = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\varepsilon_I(\nu)}{\omega - \nu} d\nu \quad (4.26)$$

This is a *Kramers-Kronig integral*. Another similar integral can be found expressing the imaginary part of the dielectric constant as an integral in terms of the real part of the dielectric constant.

It is emphasized that the relationship between the real and imaginary parts of the dielectric constant arose as a direct consequence of the physical necessity for causality. Johnson [10] continues by showing how to numerically compute the real part of the dielectric constant when given the imaginary part (or vice versa) by Fourier series expansions and expediting the calculation through the use of the *fast Fourier transform (FFT)*. The Kramers-Kronig integral relations can be important in *dielectric spectroscopy* as they can permit the inference of dielectric properties from limited experimental data (e.g., see Axelrod et al. [13]). Finally, we mention that Tip [14] shows that the Kramers-Kronig relations continue to apply even in the limit as damping goes to zero (i.e.,  $\Gamma_k \rightarrow 0$ ). Tip [14] begins with the (lossy) Drude-Lorentz model.

## 5. Approximations for Permittivity

Previously (Sections 3 and 4) we have seen expressions for the dielectric constant, hence the permittivity, involving *rational* functions of the frequency variable. However, it has long been known that rational functions of frequency do not usually provide a good fit to permittivity values derived by experiments except perhaps over a sufficiently narrow frequency band. In this section we summarize a few of the empirical models for permittivity as a function of frequency that are in common use. We make a distinction between *Debye relaxation* processes, and *non-Debye relaxation* processes.

Suppose that we try to approximate electric susceptibility with but a single term of (4.2). That is, assume

$$\chi(s) = \frac{A_1}{s^2 + 2\Gamma_1 s + \omega_1^2} \quad (5.1)$$

For suitable  $\alpha = j\alpha_i$ ,  $p = a + jb$  (constants  $\alpha_i, a, b$  are real-valued) via partial fraction expansion this may be rewritten as

$$\chi(s) = \frac{\alpha}{s-p} + \frac{\alpha^*}{s-p^*} \quad (5.2)$$

If  $u(t)$  is the (Heaviside) unit step function then we should also recall the Laplace transform [11]

$$L\{e^{at}u(t)\} = \int_{-\infty}^{\infty} [e^{at}u(t)]e^{-st} dt = \frac{1}{s-a} \quad (5.3)$$

This is a linear transform and may be used to invert (5.2). The resulting time-domain expression for susceptibility is therefore

$$\chi(t) = -2\alpha_i e^{at} \sin(bt)u(t) \quad (5.4)$$

The dielectric response never displays unbounded growth for  $t \rightarrow \infty$  and so the dielectric is both a causal and *stable* system. We have noted before that this implies  $a < 0$  for which  $\Gamma_1 > 0$ . This type of *relaxation process* is plainly an exponential one, and is often called a *Debye relaxation process*.

It is clear that the exponential relaxation of polarization (Debye relaxation) is merely a consequence of our approximation to infinite series such as (3.35) or (4.1). But there is no reason to believe that such infinite series always converge to a limit that is rational in frequency. It may be that the limiting function is a non-rational function of frequency. And indeed this is strongly suggested (if not definitively confirmed) by numerous experimental results going back to the 19<sup>th</sup> century. Neglecting the sinusoidal component and the constant factor involving  $\alpha_i$  of (5.4) a Debye relaxation has the general form

$$\phi(t) = e^{-t/\tau}u(t) \quad (5.5)$$

for which  $\tau$  is the time-constant for the system. However, for example, Metzler and Klafter [15] have noted that either the *stretched exponential model*

$$\phi(t) = e^{-(t/\tau)^\beta} \quad (0 < \beta < 1) \quad (5.6)$$

or the *power law model*

$$\phi(t) = \frac{1}{1 + \left(\frac{t}{\tau}\right)^\delta} \quad (\delta > 0) \quad (5.7)$$

are far more agreeable with lab-bench reality. Expressions such as (5.6) and (5.7) correspond to *non-Debye relaxation processes*.

The power law behavior of (5.7) is generally associated with the frequency domain Cole–Cole model ([16] and [17]) for the *complex* permittivity which is commonly denoted by  $\varepsilon^*(\omega) = \varepsilon'(\omega) - j\varepsilon''(\omega)$ . In fact Cole and Cole specifically suggest the model

$$\varepsilon^*(\omega) - \varepsilon_\infty = \frac{\varepsilon_s - \varepsilon_\infty}{1 + (j\omega\tau)^{1-\alpha}} \quad (5.8)$$

This is for  $0 \leq \alpha < 1$  and is generally *non-rational* in frequency  $\omega$ . The special case  $\alpha = 0$  corresponds to a Debye process, and in this case we observe that

$$\begin{aligned} \varepsilon'(\omega) &= \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + (\omega\tau)^2} \\ \varepsilon''(\omega) &= \frac{(\varepsilon_s - \varepsilon_\infty)\omega\tau}{1 + (\omega\tau)^2} \end{aligned} \quad (5.9)$$

From (5.8) observe that  $\varepsilon^*(0) = \varepsilon_s$  which is the low frequency limit of (5.8) while  $\varepsilon^*(\infty) = \varepsilon_\infty$  is the high frequency limit.

Table 2 of the Ph. D. thesis by Bohannan [18] summarizes other complex permittivity models. It is possible that series such as (3.35) and (4.1) or any reasonable generalization thereof will converge to any one of these alternatives.

Finally, note that for  $0 < \alpha < 1$  the complex permittivity involves fractional powers of the frequency. This is automatically associating the physics of the dielectric with the mathematics of fractional calculus.

## 6. The Curie Law and Fractance Defined

So far we have developed an understanding of the capacitor with respect to considering the permittivity of the dielectric material. However, an alternative is to treat the device as an integrated system consisting of the dielectric *and* the terminals, and further to only consider the relationship between the current through and voltage drop across the entire system. This leads to a consideration of the Curie law, and what follows is based on the presentation in Westerlund and Ekstam [2].

### Fractance

The *Curie law* [19] is as follows. Suppose that the voltage  $v(t) = Uu(t)$  is applied to a capacitor possessing no initially stored charged. That is, there is no energy stored in the

device before applying the DC voltage  $U$ . The current through the device will have the general form

$$i(t) = \frac{U}{ht^n} \quad \text{for } t > 0, \text{ and } 0 < n < 1 \quad (6.1)$$

( $h$  and  $U$  are real-valued). This is a power law dependence of terminal current upon the input voltage. The Laplace transform of the input voltage is

$$V(s) = \frac{U}{s} \quad (6.2)$$

which is just a special case of the transform (5.3). However, the Laplace transform of (6.1) is [20]

$$I(s) = \frac{\Gamma(1-n)U}{hs^{1-n}} \quad (6.3)$$

Here  $\Gamma(x)$  is the *gamma function*<sup>11</sup>. If we take the Laplace transform of (2.21) then

$$I(s) = CsV(s) = Cs \cdot \frac{U}{s} = UC \quad (6.4)$$

( $v(0) = 0$ ). Comparing (6.4) with (6.3) we see that for the *ideal* capacitor we must have  $n = 1$  (even though  $\Gamma(0)$  is *undefined*). Of course, inverse transforming (6.4) gives

$$i(t) = UC \delta(t) \quad (6.5)$$

This current is “impulsive” hence non-physical, a consequence of the ideality inherent in (2.21). This is routinely tolerated by engineers since the relationship (2.21) is so easy to work with, and in many cases produces an acceptably accurate result. But this report is about what to do when this simple model is no longer useful.

Normally, the *impedance* of a two-terminal linear time-invariant (LTI) circuit element is defined to be

$$Z(s) = \frac{V(s)}{I(s)} \quad (6.6)$$

---

<sup>11</sup> The gamma function is defined to be  $\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t} dt$ .

The *admittance* is  $Y(s) = 1/Z(s)$ . For the Curie law device of (6.3) from (6.6) we see that

$$Z(s) = \frac{h}{\Gamma(1-n)} \frac{1}{s^n} \quad (6.7)$$

Of course, the ideal capacitor has impedance

$$Z(s) = \frac{1}{C} \frac{1}{s} \quad (6.8)$$

In (6.7)  $0 < n < 1$  and so (6.7) is considered a *fractional impedance*, or *fractance* for short. A device with impedance (6.7) may be called a *fractor* (Bohannan [21]). For  $n = 1$  (exactly) we call the device, as always, a capacitor.

As noted in the Introduction capacitor manufacturers invariably strive for  $n = 1$ . But we have established that perfection in this respect will never be achieved, although it is possible to get pretty close in practice (e.g.,  $n = 0.999952$  for polypropylene [2]). And thus real-world devices are fractance devices (fractors) to some degree in all cases.

As in [2] in order to make (6.7) look more like (6.8) we define the real-valued constant<sup>12</sup>

$$C_{\circ} = \frac{\Gamma(1-n)}{h} \quad (0 < n < 1) \quad (6.9)$$

Thus, for the fractor

$$I(s) = C_{\circ} s^n V(s) \quad (6.10)$$

We now wish to consider the steady-state behavior of the fractor modeled according to (6.10). This implies considering  $s = j\omega$ . From Euler's identity<sup>13</sup>

$$(j\omega)^n = \omega^n \exp\left[j\frac{\pi}{2}n\right] = \omega^n \left[ \cos\left(\frac{\pi}{2}n\right) + j \sin\left(\frac{\pi}{2}n\right) \right] \quad (6.11)$$

Therefore, applying (6.11) to (6.10) yields

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<sup>12</sup> Intuitively (6.9) should behave in a reasonable manner for  $n \rightarrow 1$  in spite of the fact that  $\Gamma(0)$  is undefined. The experimentally confirmed finiteness of  $C_{\circ}$  suggests that  $h$  is implicitly a function of  $n$  and

thus  $\lim_{n \rightarrow 1} \frac{\Gamma(1-n)}{h(n)} = \text{constant}$ .

<sup>13</sup> This identity is reviewed and extensively employed in C. J. Zarowski, *An Introduction to Numerical Analysis for Electrical and Computer Engineers*, John Wiley and Sons, 2004.

$$\begin{aligned}
I(j\omega) &= C_{\circ} \omega^n \sin\left(\frac{\pi}{2}n\right) \left[ j + \frac{\cos\left(\frac{\pi}{2}n\right)}{\sin\left(\frac{\pi}{2}n\right)} \right] V(j\omega) \\
&= C_{\circ} j \omega^n \sin\left(\frac{\pi}{2}n\right) \left[ 1 - j \cot\left(\frac{\pi}{2}n\right) \right] V(j\omega)
\end{aligned} \tag{6.12}$$

From basic trigonometry  $\tan\left(\frac{\pi}{2} - x\right) = \cot(x)$ , and so alternatively

$$I(j\omega) = C_{\circ} j \omega^n \sin\left(\frac{\pi}{2}n\right) \left[ 1 - j \tan\left(\frac{\pi}{2}(1-n)\right) \right] V(j\omega) \tag{6.13}$$

Now define the *loss tangent*

$$\tan \delta = \tan\left(\frac{\pi}{2}(1-n)\right) \tag{6.14}$$

Therefore,

$$I(j\omega) = C_{\circ} j \omega^n \sin\left(\frac{\pi}{2}n\right) [1 - j \tan \delta] V(j\omega) \tag{6.15}$$

We observe that for  $n = 1$  the loss tangent is zero and (6.15) reduces to  $I(j\omega) = j\omega C_{\circ} V(j\omega)$  which is consistent with the ideal (lossless) model for a capacitor. For  $0 < n < 1$  the loss tangent is nonzero and (6.15) has a non-zero real part. In fact, we may write

$$I(j\omega) = [ \underbrace{C_{\circ} \omega^n \tan \delta \sin(\pi n / 2)}_{=G(\omega)} + j \underbrace{C_{\circ} \omega^n \sin(\pi n / 2)}_{\equiv \omega C(\omega)} ] V(j\omega) \tag{6.16}$$

That is,  $I(j\omega) = [G(\omega) + j\omega C(\omega)] V(j\omega)$ . Here we are thinking of the non-ideal (lossy) fractor as being equivalent to the parallel<sup>14</sup> combination of a frequency-dependent conductance  $G(\omega)$  and a frequency-dependent *ideal* capacitance  $C(\omega)$ . The term containing conductance  $G(\omega)$  models the fractor's losses which are *non-Ohmic*<sup>15</sup>.

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<sup>14</sup> A series equivalent circuit model is possible too (see [2]).

<sup>15</sup> See the remarks immediately following (3.29). Excited dipole electrons must eventually give up energy received from the perturbing electric field. This is in the form of a *radiative* loss. Ohmic losses are conduction band electrons losing energy by scattering with the atoms in the material through which they move. This involves an exchange of *phonons*. The lost energy is in the form of heat.

As directly stated in [2] it is impossible to realize a fractor with the interconnection of a *finite* number of ideal circuit elements  $R$ ,  $C$ , and/or  $L$ . However, approximations do exist and this is discussed in the next section.

### Fractional Calculus

We now wish to consider the *dynamic* behavior of a fractor. This involves discovering a time-domain relationship which generalizes (2.21). This immediately implies the need to work with fractional calculus, and in particular requires an adequate definition of the fractional derivative associated with a Fourier/Laplace domain representation that is consistent with a result such as (6.15). Various definitions of the fractional derivative exist and may be expressed in varied forms. Bohannan [18] considers various possibilities drawing on the content of the 1974 textbook by Oldham and Spanier. We wish to deduce *fractional ordinary differential equations (FODEs)* allowing us to set up initial value problems for networks of interconnected fractors and other electronic devices. At least from an engineering point of view it is argued in Debnath [22] that a good definition is the *Caputo derivative ( $\alpha$ th order)*

$$D^\alpha f(t) = \frac{1}{\Gamma(m-\alpha)} \int_0^t \frac{f^{(m)}(\tau)}{(t-\tau)^{\alpha+1-m}} d\tau \quad (6.17)$$

where  $m-1 < \alpha < m$  ( $m$  is an integer), and  $f^{(m)}(t)$  is the “usual”  $m$ th-order derivative of the real-valued function  $f(t)$ . Diethelm et al. [23] also recommend working with this sort of definition due in part to the availability of suitable numerical methods where analytical solutions are unavailable.

The Caputo derivative has nice properties. For example, if  $f(t) = A$  (constant) then

$$D^\alpha A = 0$$

That is, the Caputo derivative of a constant is zero. Westerlund and Ekstam [2] state that the fractional derivative of a constant is not zero. But this appears to be due to their definition of the fractional derivative<sup>16</sup>. Another very important feature of the Caputo form of the fractional derivative is that if

$$F(s) = L\{f(t)\} = \int_0^\infty f(t)e^{-st} dt \quad (6.18)$$

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<sup>16</sup> From Equation (19) in [2]  $D^n f(t) = \frac{1}{\Gamma(1-n)} \left[ \int_0^t \frac{f^{(1)}(\tau)}{(t-\tau)^n} d\tau + \frac{f(0)}{t^n} \right]$  for  $t > 0$  with  $0 < n < 1$ .

(which presumes that  $f(t)$  is not defined for  $t < 0$ ) then

$$L\{D^\alpha f(t)\} = s^\alpha F(s) - \sum_{k=0}^{m-1} f^{(k)}(0) s^{\alpha-k-1} \quad (6.19)$$

We see in (6.19) that the Laplace domain representation of the Caputo derivative uses initial conditions  $f^{(k)}(0)$  only for *integer*  $k$ . This is important as other definitions of the fractional derivative generally need to work with *fractional*  $k$  and these do not possess any easy physical interpretation. Moreover, if the initial conditions are null then (6.19) reduces to  $L\{D^\alpha f(t)\} = s^\alpha F(s)$  which is perfectly consistent with the usual Laplace domain form of the differentiation operator when  $\alpha$  is an integer.

A general FODE may have the form

$$\sum_{k=0}^m a_k D^{\alpha_k} f(t) = g(t) \quad (6.20)$$

where  $\alpha_k > \alpha_{k-1}$  can be any real numbers, and  $a_k$  are arbitrary constants. We might interpret  $g(t)$  as the driving function for some system modeled by (6.20). From the above an initial attempt at an analytical solution to (6.20) would involve the Laplace transform approach.

As in illustration we might consider the example of a fractor with an initial voltage  $v(0)$  in series with an ideal resistor of resistance  $R$ . From (6.10)  $i(t) = C_\circ D^n v(t)$  is the fractor current while via Kirchoff's voltage law (KVL) we obtain the FODE for this system as

$$v(t) + Ri(t) = 0 \Rightarrow v(t) + RC_\circ D^n v(t) = 0 \quad (6.21)$$

If we apply (6.19) to (6.21) we obtain

$$V(s) + RC_\circ [s^n V(s) - v(0)s^{n-1}] = 0 \quad (6.22)$$

Therefore, the Laplace domain solution is

$$V(s) = \frac{v(0)RC_\circ s^{n-1}}{1 + RC_\circ s^n} = v(0) \frac{s^{n-1}}{s^n + \frac{1}{RC_\circ}} \quad (6.23)$$

The special case  $n = 1$  yields the familiar solution for an ideal capacitor discharging through the resistor  $R$ . That is,

$$v(t) = v(0)e^{-t/RC_0} u(t) \quad (6.24)$$

The inverse transform of (6.23) for  $0 < n < 1$  is a bit more difficult and requires the introduction of a special function. The *Mittag-Leffler function* is defined to be

$$E_{a,b}(t) = \sum_{m=0}^{\infty} \frac{t^m}{\Gamma(am+b)} \quad (a, b > 0) \quad (6.25)$$

Observe<sup>17</sup> that

$$E_{1,1}(t) = \sum_{m=0}^{\infty} \frac{t^m}{\Gamma(m+1)} = \sum_{m=0}^{\infty} \frac{t^m}{m!} = e^t \quad (6.26)$$

Thus, the Mittag-Leffler function includes the exponential function as a special case. It turns out that the inverse transform of (6.23) is

$$v(t) = v(0) E_{n,1}(-kt^n) u(t) \quad (6.27)$$

for  $k = 1/RC_0$ . We may informally arrive at this result as follows. Recall that<sup>18</sup>

$$\frac{1}{1+x} = \sum_{m=0}^{\infty} (-1)^m x^m \quad (\text{if } |x| < 1) \quad (6.28)$$

Now observe that because of this and provided that  $|s|$  is big enough we have

$$\frac{s^{n-1}}{s^n + k} = \frac{1}{s} \left[ \frac{1}{1 + \frac{k}{s^n}} \right] = \sum_{m=0}^{\infty} (-k)^m s^{-(nm+1)} \quad (6.29)$$

From [20]

$$L\{t^{k-1}u(t)\} = \frac{\Gamma(k)}{s^k} \quad \text{if } k > 0 \quad (6.30)$$

---

<sup>17</sup>  $E_{a,1}(t)$  has behavior ranging from  $e^t$  to  $1/(1-t)$  for  $0 < a < 1$ . Thus, it displays a range of behavior from exponential to power-law. And thus the Mittag-Leffler function accommodates mathematical descriptions of both Debye and non-Debye relaxation phenomena.

<sup>18</sup> See Equation (3.83) in C. J. Zarowski, *An Introduction to Numerical Analysis for Electrical and Computer Engineers*, John Wiley and Sons, 2004.

If we assume that we may inverse transform (6.29) term-by-term then from (6.30)

$$L^{-1}\left\{\frac{s^{n-1}}{s^n+k}\right\} = \sum_{m=0}^{\infty} (-k)^m L^{-1}\left\{\frac{1}{s^{mn+1}}\right\} = \sum_{m=0}^{\infty} (-k)^m \frac{t^{nm}}{\Gamma(nm+1)} = E_{n,1}(-kt^n) \quad (6.31)$$

for  $t \geq 0$ . Immediately this gives us the stated result in (6.27) which generalizes (6.24).

The previous example is suggestive of a general truth. This is that the Mittag-Leffler function is as important to the theory of FODEs as the exponential function is to the classical theory of ODEs. Recall that classical ODEs (ordinary differential equations) only work with derivatives of integer order.

If a step-voltage is applied to the fractor possessing no initial stored energy then the charge on the device must be

$$q(t) = \int_0^t i(\tau) d\tau \quad (6.32)$$

for  $t \geq 0$ . In the Laplace domain from (6.3)

$$Q(s) = \frac{1}{s} I(s) = \frac{\Gamma(1-n)U}{hs^{2-n}} \quad (6.33)$$

From (6.30) this has the inverse Laplace transform

$$q(t) = \frac{U}{h(1-n)} t^{1-n} u(t) \quad (6.34)$$

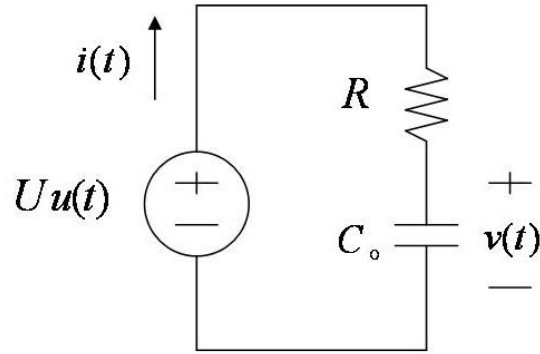
This was arrived at also by making use of the gamma function identity

$$\Gamma(x+1) = x\Gamma(x) \quad (6.35)$$

Equation (6.34) gives the curious result that a fractor's charge builds up indefinitely as  $t \rightarrow \infty$ . Reference [12] in [2] provides experimental confirmation of this. Of course, in practice, charge cannot accumulate indefinitely since dielectric breakdown will arise at some point for any real-world material.

As another example consider the series connection of a fractor and an ideal resistor in Fig. 3 where the system is driven by an ideal step-voltage source. The FODE for this system is easily shown to be

$$RC_{\circ}D^n v(t) + v(t) = Uu(t) \quad (6.36)$$



**Figure 3:** A simple voltage divider circuit containing a fractor and an ideal resistor driven by an ideal step-voltage source.

Similarly to (6.22)

$$RC_o[s^n V(s) - s^{n-1}v(0)] + V(s) = \frac{U}{s} \quad (6.37)$$

Thus, the Laplace domain voltage drop across the fractor is given by

$$V(s) = \frac{v(0)RC_o s^{n-1}}{1 + RC_o s^n} + \frac{U}{s[1 + RC_o s^n]} \quad (6.38)$$

We see that the first term of (6.38) is (6.23) and thus the inverse Laplace transform of our present problem is already partly determined. Again, if we let  $k = 1/RC_o$ , then the second term of (6.38) can be expressed as

$$V_f(s) = \frac{U}{s[1 + RC_o s^n]} = \frac{kU}{s^{n+1}} \frac{1}{1 + \frac{k}{s^n}} \quad (6.39)$$

This is the part of the solution due to the forcing function which is the ideal step-voltage source. Following the same process that gave us (6.31) we readily discover that

$$v_f(t) = U[1 - E_{n,1}(-kt^n)]u(t) \quad (6.40)$$

For the special case of the ideal device for which  $n = 1$  this reduces to the familiar

$$v_f(t) = U[1 - \exp(-t/RC_o)]u(t) \quad (6.41)$$

Equation (6.40) corresponds to Equation (30) of [2].

The dynamic models of this section can be used to understand *insulation resistance*, and *dielectric absorption*. However, the reader is referred to Westerlund and Ekstam [2] for the details.

## 7. Network Approximations for Fractance

The impedance of a fractor was seen in Section 6 to be of the form  $Z(s) = 1/C_o s^n$  for  $n$  such that  $0 < n < 1$ . The ideal capacitor arose for  $n = 1$ . Presently it seems that one cannot “buy” a single device with a prescribed  $n$  (*fractance order*). Thus, if one wishes to realize such a device then it must be *approximated* using a network of interconnected passive or active circuit elements that are nominally “ideal.” The problem of approximating a fractor is analogous to such problems as approximating a fractional delay element in a digital signal processing system (e.g., Laakso et al. [24]). In fact, *digital* (that is, discrete-time) approximations are sometimes also sought for  $s^n$  when  $n$  is fractional (e.g., Maione [25] for  $n = 0.5$ ). It all boils down to seeking *rational* functions in the complex variable to approximate irrational functions of this variable. Podlubny et al. [26] summarizes various approximation techniques. The interest in rationally approximating  $s^n$  is also quite old, and the paper by Carlson and Halijak [27] from 1964 cites even earlier work by O. Heaviside regarding RC transmission line approximations. The approximation theory in [27] is based on the application of Newton-Raphson iterations<sup>19</sup>. And there is similar interest in rationally approximating transfer functions of the form  $H(s) = A/(1 + as)^n$  for fractional  $n$ , and for which the constants  $a$ , and  $A$  are positive real numbers. For this problem Sun et al. [28] suggest a scheme based on Padé approximation. However, in this section we will quickly review the method in [27] to give the reader an idea of the complexity of practical network realizations.

As derived in [27] and summarized in [26] a rational approximation to a fractional power of the complex variable  $s$  begins with applying the Newton-Raphson iterations to solving for  $H(s)$  when given  $G(s)$  in the nonlinear equation

$$[H(s)]^p - G(s) = 0 \quad (7.1)$$

for which  $p = 2, 3, 4, \dots$ . If  $m = p/2$  then the  $k$ th rational approximant to  $H(s) = [G(s)]^{1/p}$  is obtained by executing the following recursive process

$$H_k(s) = H_{k-1}(s) \frac{(p-m)[H_{k-1}(s)]^2 + (p+m)G(s)}{(p+m)[H_{k-1}(s)]^2 + (p-m)G(s)} \quad (7.2)$$

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<sup>19</sup> The Newton-Raphson iterations are a standard method for root-finding. The method is discussed in Chapter 7 of C. J. Zarowski, *An Introduction to Numerical Analysis for Electrical and Computer Engineers*, John Wiley and Sons, 2004.

where  $H_0(s) = 1$  initializes the recursion. For example, if  $p = 2$  with  $G(s) = 1/s$  then we are seeking a rational approximation to  $H(s) = 1/s^{1/2}$ . In this special case (7.2) reduces to

$$H_k(s) = H_{k-1}(s) \frac{H_{k-1}^2(s) + 3s^{-1}}{3H_{k-1}^2(s) + s^{-1}} \quad (7.3)$$

After one iteration of Equation (7.3) we have approximation

$$H_1(s) = \frac{s+3}{3s+1} \approx \frac{1}{s^{1/2}} \quad (7.4)$$

After two iterations of Equation (7.3) we now have the approximation

$$H_2(s) = \frac{s^4 + 36s^3 + 126s^2 + 84s + 9}{9s^4 + 84s^3 + 126s^2 + 36s + 1} \approx \frac{1}{s^{1/2}} \quad (7.5)$$

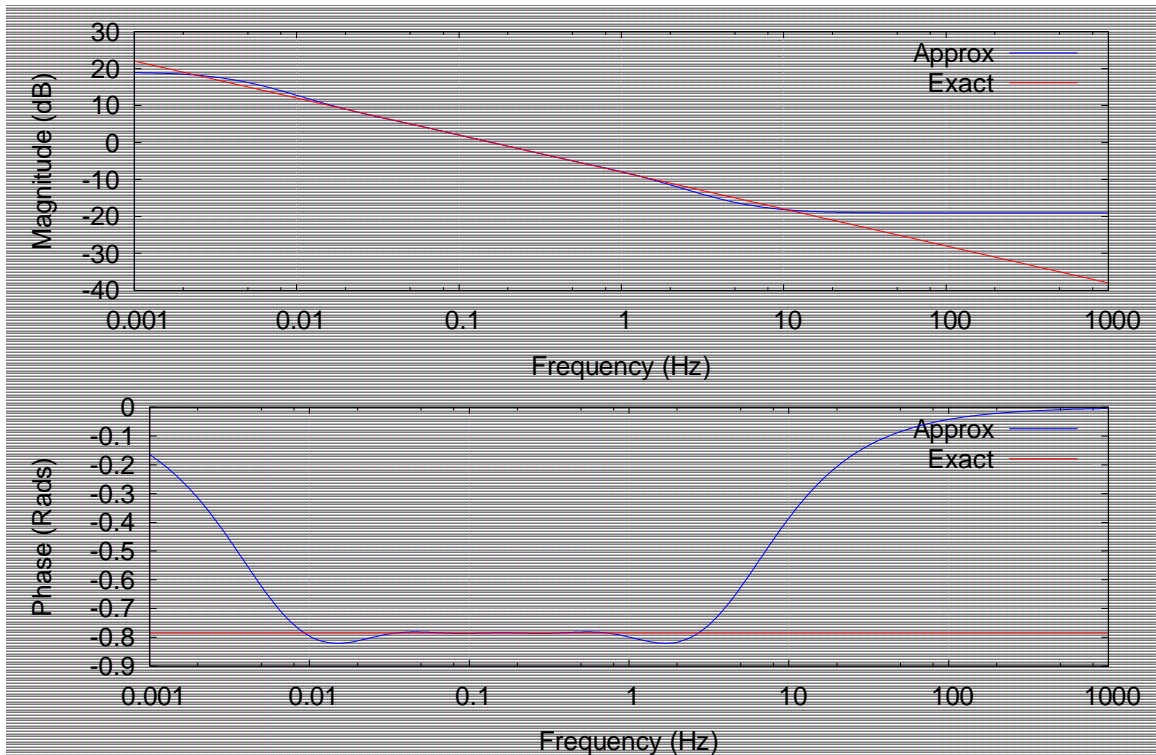
It is shown in [27] how to realize an approximate fractor as a driving-point impedance involving the interconnection of “ideal” resistors, capacitors and inductors based on suitably manipulating  $H_k(s)$ .

Figure 4 (below) displays the magnitude and phase response plots of both  $H(s) = 1/s^{1/2}$  and the approximation  $H_2(s)$  given by (7.5). It is clear that the approximation is only “good” over a limited range of frequencies. It also appears that there is no clear statement about the accuracy of the approximation as a function of the number of iterations of (7.3) published in the open literature. Simple “tricks” involving component scaling can be used to move the band of frequencies over which the approximation is useful<sup>20</sup>. However, in a practical application a lot of trial-and-error may be involved in arriving at a satisfactory solution based on the methodology in [27].

We remark that the phase response of a fractor is independent of frequency. This is clearly illustrated in the bottom plot of Fig. 4. Consequently, such a device is sometimes also called a *constant phase-angle element* in published literature pertaining to fractance.

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<sup>20</sup> The basics of this are covered in various texts such as D. E. Johnson, *Introduction to Filter Theory*, Prentice-Hall, 1976.



**Figure 4:** The top plot is of the magnitude response of  $H_2(s)$  (Approx) versus the magnitude response of  $H(s) = 1/s^{1/2}$  (Exact). Similarly, the bottom plot is of the phase responses of each of these entities.

## 8. Concluding Remarks

This report takes the position that there is *now* a need for a *single device* realization of fractance for the *user's choice* of fractance order  $n$  in  $1/s^n$  such that  $0 < n < 1$ . This call for development is not new as it was also made by Bohannan [21]. As indicated in Section 7 over many decades now people have sought to approximately realize fractance by networks of nominally ideal circuit elements. However, Bohannan [21] has noted that this approach is only effective over a relatively narrow band of frequencies since the nominally ideal circuit components only behave (approximately) ideally over a narrow frequency range. Here “narrow” could mean with respect to the needs of ultrawideband (UWB) technologies such as wireless.

For example, it was suggested in NDT17<sup>21</sup> that fractional calculus be employed to shape signaling pulses for UWB transceivers. In general, this was to maximize transmitter power while maintaining compliance with legally imposed restrictions on the use of UWB technology. However, this idea is not really a practical solution unless the mathematical operation can be efficiently implemented in the frequency range of roughly

<sup>21</sup> “The Gaussian Monocycle Pulses, Fractional Derivatives, UWB Wireless, and the FCC Part 15 Spectral Masks,” Technical Report NDT17-09-2007, 5 September 2007, NanoDotTek (18 pages).

1 to 10 GHz. Of course, this is not the only application area where a single fractance device would be a good thing to have.

Bohannon [21] emphasized the utility of a single device realization to efficiently implement  $PI^\lambda D^\mu$  feedback control systems which generalize classical PID<sup>22</sup> controllers. The underlying theory of control here is considered in Podlubny [29] with earlier work in the field by A. Oustaloup and other contributors. It has been shown that such generalized controllers can produce better results compared to classical controllers when the problem is one of controlling dynamic systems possessing fractional dynamics such as systems involving diffusive processes, viscoelastic mechanical systems, or certain biomedical systems. It has recently been asserted that fractional order controllers can be used to stabilize delay-differential systems (Cheng and Hwang [30]). Fractional calculus is being used to generalize classical state-space theory (Daftardar-Gejji and Babakhani [31]) and so may have a significant impact on state-variable control systems in the future.

Where the need to implement a fractor arises, even if the rational approximation approach works technically, it remains desirable to replace a “complicated” space-consuming and power-consuming electrical or electronic system with but a single device. This would be particularly true in the context of integrated circuit implementations where even with the current extremely high levels of integration chip real-estate is always at a premium, and the need to reduce power consumption is always pressing.

### Acknowledgment

The free online file-type conversion service PDF Online<sup>TM</sup> was used to convert the original MS Word form of this report into pdf format. GNU Octave 2.1.73 running under Windows XP did the “number crunching” that yielded Figure 4. MS Publisher in combination with the software for a Minolta E323 digital camera was used to prepare the other figures of this report.

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<sup>22</sup> PID stands for “proportional-integral-derivative.” PID control is a “classical” methodology that is the subject of basic texts regarding control systems design (e.g., R. C. Dorf, *Modern Control Systems* (3<sup>rd</sup> edition), Addison-Wesley, 1980).

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