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Fractional drude model of electrons in a metal

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In the present work we analyse the behaviour of electrons in a metal placed into uniform electric field, E, from its fractional differential equation. We show that the velocity and the current density of the electrons not only depend on the time t, but also on the order of the fractional differential equation γ, the Drude model is a particular case. This fact could have interesting consequences in the study of electrical properties of metals.

Keywords: Fractional derivative; drude model; Mittag-Leffler function.

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1. Introduction

Fractional calculus (FC) is the generalization of the ordinary integer calculus that deals with operators having non-integer order: fractional derivatives and fractional integrals [1-4]. The FC provide an excellent instrument for the description of memory and hereditary properties of various materials and processes [5-9];. This is the main advantage of FC in comparison with ordinary integer calculus, in which such effects are in fact neglected. In the last few decades the FC and fractional differential equations have found applications in science and various engineering disciplines [10-13].

Recently, at the work [14] it was shown that the fractional order Gompertz model of order 0.68 produced a better fit to experimental dataset than the well-known Gompertz model. On the other hand, at [15] charging and discharging processes of different capacitors in electrical RC circuit has been considered theoretically and experimentally. It was shown that, the measured experimental results could be exactly obtained within the fractional calculus approach for the order 0.998.

In the present work we analyse the behaviour of electrons in a metal placed into uniform electric field from its fractional differential equation. We show that its behavior depends on the fractional order of the differential equation and its solutions are given by the Mittag-Leffler function. We consider here both DC and AC electric field.

2. Basic Concepts of Fractional Calculus

In this work we use the Caputo fractional derivative defined as [2]

$$\frac{d^\gamma f(t)}{dt^\gamma} = {}_0^C D_t^\gamma f(t) = \frac{1}{\Gamma(n-\gamma)} \int_0^t \frac{f^{(n)}(\eta)}{(t-\eta)^{\gamma-n+1}} d\eta \quad (1)$$

where $\Gamma(\cdot)$ denotes the Euler Gamma function, $n = 1, 2, \ldots \in N$ and $n-1 < \gamma \leq n$, where γ is the fractional order derivative. In this definition $f^{(n)}$ is an ordinary derivative. The Laplace transform of the Caputo's fractional derivative has the form [2]

$$\mathcal{L}\Big[{}_0^C D_t^\gamma f(t)\Big] = s^\gamma F(s) - \sum_{k=0}^{n-1} s^{\gamma-k-1} f^{(k)}(0) \quad (2)$$

The classical Mittag-Leffler function is a complex function depending on a complex parameter and was defined and studied by Mittag-Leffler [16-18], as

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)} \qquad \mathrm{Re}(\alpha > 0) \quad (3)$$

This function is a generalization of the exponential function since for $\alpha = 1$ we have e^z. The generalization of the function (3) is given by

$$E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + \beta)}$$
$$\mathrm{Re}(\alpha > 0) \qquad \mathrm{Re}(\beta > 0) \quad (4)$$

Note that $E_{\alpha,1} = E_\alpha$. This generalization was studied by Wiman [19]. The Laplace transform of the function $t^{\beta-1}E_{\alpha,\beta}(at^\alpha)$ is given by

$$\int_0^\infty e^{-st} t^{\beta-1} E_{\alpha,\beta}(\pm a t^\alpha) dt = \frac{s^{\alpha-\beta}}{s^\alpha \mp a} \quad (5)$$

Consequently, the inverse Laplace transform is

$$\mathcal{L}^{-1}\Big[\frac{s^{\alpha-\beta}}{s^\alpha \mp a}\Big] = t^{\beta-1} E_{\alpha,\beta}(\pm a t^\alpha) \quad (6)$$

Some useful here Laplace transform are [2]

$$\mathcal{L}\Big[1 - E_\alpha(-at^\alpha)\Big] = \frac{a}{s(s^\alpha + a)}$$
$$\mathcal{L}\Big[\frac{t^{\alpha-1}}{\Gamma(\alpha)}\Big] = \frac{1}{s^\alpha}$$
$$\mathcal{L}\Big[E_\alpha(\pm a t^\alpha)\Big] = \frac{s^{\alpha-1}}{s^\alpha \pm a} \quad (7)$$

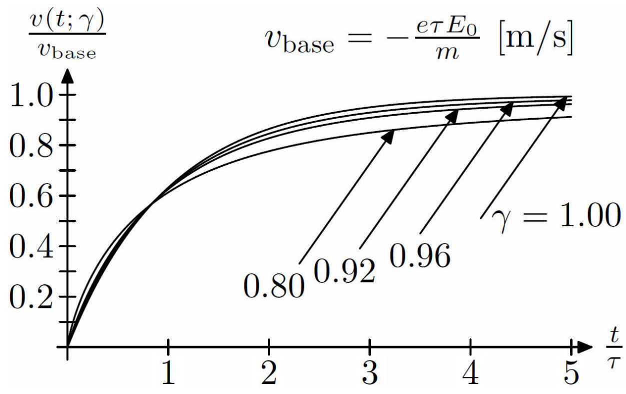


FIGURE 1. Fractional Drude model.

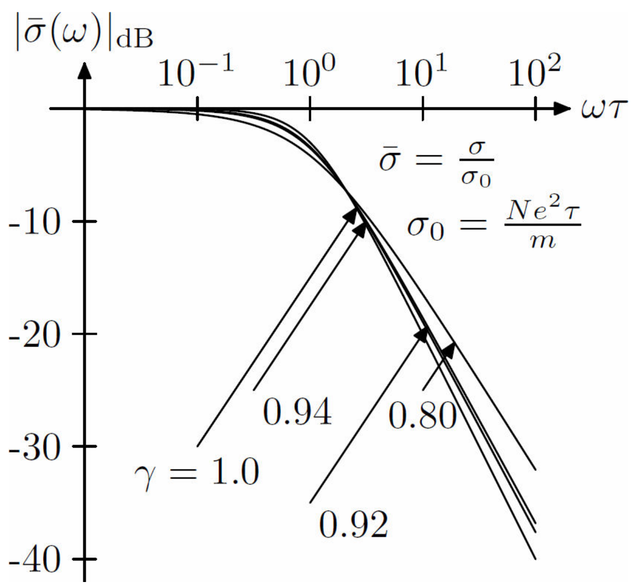


FIGURE 2. Bode diagram of conductivity for some value of γ.

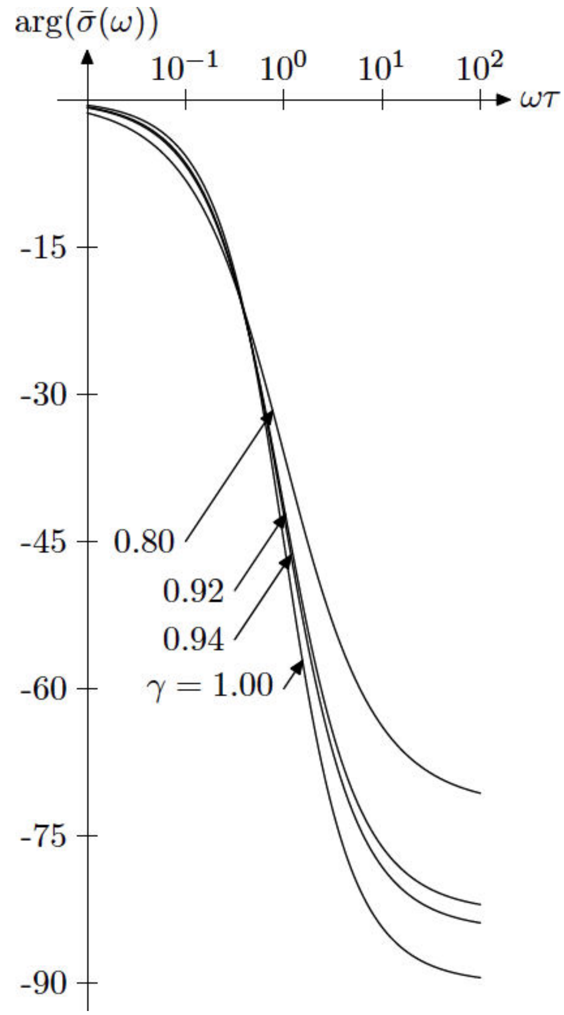


FIGURE 3. Bode diagram of the phase for different value of γ.

3. Fractional DC Drude model

The first realistic model for a metal is due to Drude. He simply treated a metal as a free-electron gas and neglected the positive-ion background. Although the model is quite simple, yet the simple ideas are still useful in the interpretation of the optical properties of metals [20].

The one-dimensional equation of motion for a charged particle of mass m and charge e affected by an external electric field E is given by [20]

$$m\frac{dv}{dt} + \frac{m}{\tau}v = -eE \tag{8}$$

where v is the drift velocity, t is the time and $E = E_0$ is a constant electric field. Besides the electrostatic force that accelerates electrons in the electric field, the expression (8) contains a phenomenological damping (relaxation) term that describes how collisions hinder the free motion of electrons and how the drift velocity relaxes to zero.

In order to give a fractional character to the equation (8) we make the following redefinition

$$u(t) = -\frac{m}{eE_0\tau}v(t) \tag{9}$$

Then, we have a fractional dimensionless equation

$$\frac{d^\gamma u}{d\bar{t}^\gamma} + u = 1, \qquad 0 < \gamma \leq 1 \tag{10}$$

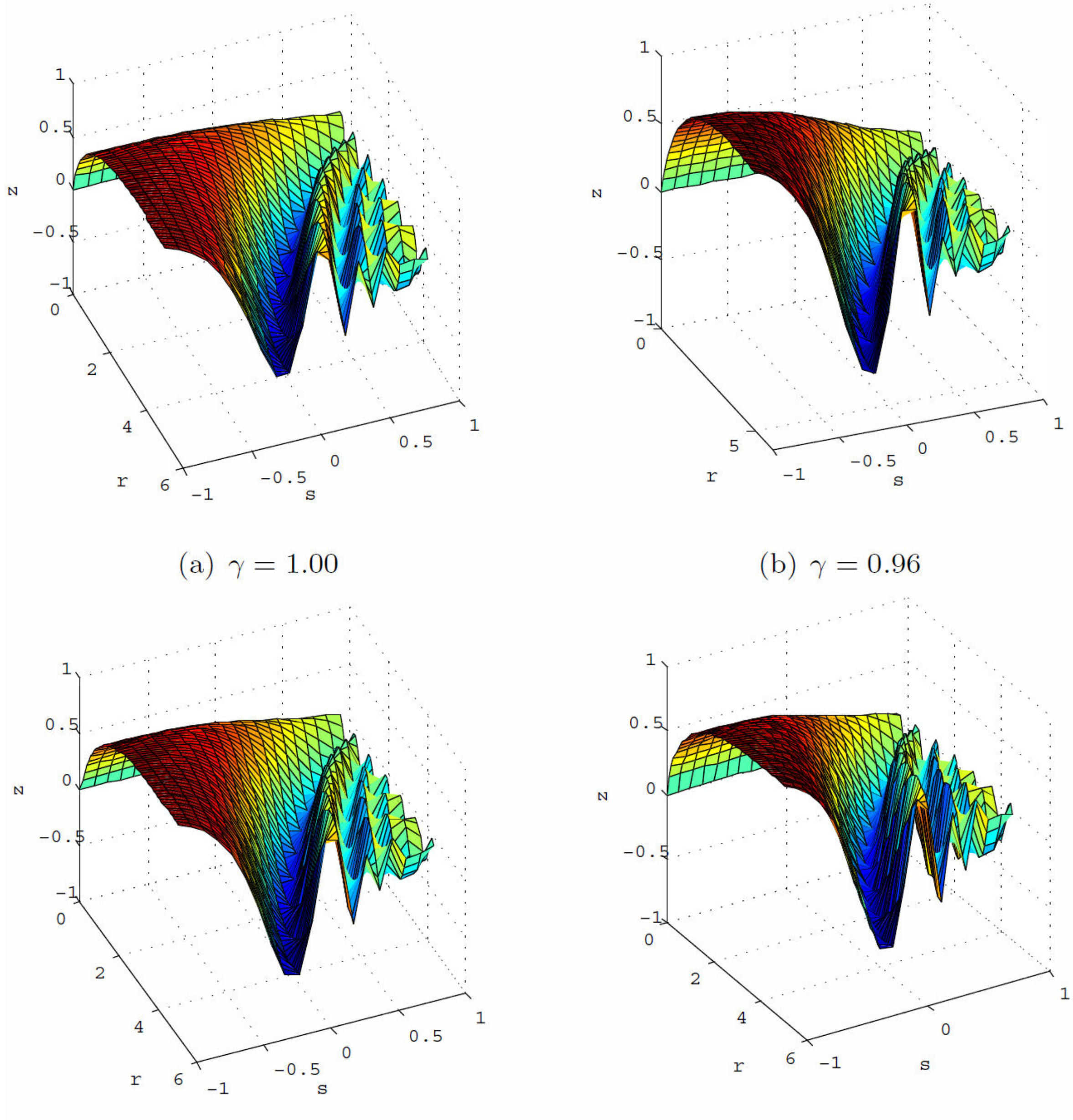
where $\bar{t} = t/\tau$. Taking the condition $u(0) = 0$ and using the Laplace transform (2) we have

$$U(s) = \frac{1}{s[(\tau s)^\gamma + 1]} \tag{11}$$

To take the inverse Laplace transform we use the first equation in (7) and using the expression (9) we have

$$v(\bar{t};\gamma) = -\frac{e\tau}{m}\left[1 - E_\gamma\left(-\bar{t}^\gamma\right)\right]E_0 \tag{12}$$

where $E_\gamma(\cdot)$ is defined in (3). This expression depends on the time t and on the fractional parameter γ. For a conductor that obeys the Ohm's law with a number N of electrons per



(a) $\gamma = 1.00$ (b) $\gamma = 0.96$

(c) $\gamma = 0.92$ (d) $\gamma = 0.80$

FIGURA 4. Plot of the equation (23) or (24) for different values of γ. With $\omega\tau = 10^s$ and $t = r \times \tau$. The value of $v(t;\gamma)$ and $j(t;\gamma)$ may be determined multiplying z by $-eE_0\tau/m$ or $e^2NE_0\tau/m$, respectively.

unit volume moving at the same velocity can be written the current density as $j = -eNv$. Hence, we have the fractional current density of electrons given by

$$j(\bar{t};\gamma) = \sigma_0 \left[1 - E_\gamma\left(-\bar{t}^\gamma\right)\right] E_0 \qquad 0 < \gamma \leq 1 \qquad (13)$$

where $\sigma_0 = e^2N\tau/m$ is the static Drude conductivity. We can see that in the case when $\gamma = 1$ the expressions (12) and (13) become the ordinary Drude formulae. Asymptotic approximations to the Mittag-Leffler function for small $t \to 0$ and large $t \to \infty$ times, in the first approximation, are [21]

$$E_\gamma(-\bar{t}) \sim e^{-\frac{\bar{t}^\gamma}{\Gamma(1-\gamma)}}, \qquad t \to 0 \qquad (14)$$

$$E_\gamma(-\bar{t}) \sim \frac{\bar{t}^{-\gamma}}{\Gamma(1-\gamma)}, \qquad t \to \infty \qquad (15)$$

As a consequence the Mittag-Leffler function interpolates for intermediate time $\bar{t}$ between the stretched exponential and the negative power law. The stretched exponential models the very fast decay for small time $\bar{t}$, whereas the asymptotic power law is due to the very slow decay for large time $\bar{t}$ as can be seen in Fig. (1), showing the behaviour of (12) for different value of γ, taking some typical values

$e = -1.602 \cdot 10^{-19}$ C, $m_e = 9.109 \cdot 10^{-31}$ kg, $E_0 = 100$ V/m and $\tau = 1 \cdot 10^{-14}$ s.

The fractional conductivity in the frequency domain is given by

$$\sigma(s) = \frac{e^2 N\tau}{m}\frac{1}{1+(s\tau)^\gamma} = \frac{\sigma_0}{1+(s\tau)^\gamma} \tag{16}$$

where σ_0 is the static Drude conductivity, and its magnitude depending on frequency $\sigma(\omega)$ expressed in decibels is

$$|\bar{\sigma}(\omega)|_{dB} = 20\log\left|\frac{1}{1+(j\omega\tau)^\gamma}\right| \tag{17}$$

This equation may be written as follow

$$|\bar{\sigma}(\omega)|_{dB} = -10\log\left|1+(\omega\tau)^{2\gamma}+2(\omega\tau)^\gamma\cos\frac{\gamma\pi}{2}\right| \tag{18}$$

The behaviour of the conductivity in the frequency domain can be better visualized by Bode diagrams of magnitude and phase. From 2, we can see how increase the slope of the high frequency asymptote as the order of the fractional derivative γ decreases, with a minimun of -20 dB/dec, for $\gamma = 1.0$. The wavelength of electric field, λ, in the case of $\omega\tau = 10^2$ is of the order of hundreds of milimiters; much larger than the intermolecular distances. Attenuation of low frequency conductivity is higher with decreasing the order γ of the derivative.

The Drude phase for conductivity may be obtained from (16) as follow

$$\begin{aligned}\arg\bar{\sigma}(\omega) &= \arg\frac{1}{1+(j\omega\tau)^\gamma}\\ &= -\arctan\frac{(\omega\tau)^\gamma\sin\frac{\gamma\pi}{2}}{1+(\omega\tau)^\gamma\cos\frac{\gamma\pi}{2}}\end{aligned} \tag{19}$$

See Fig. (3).

4. The Fractional AC Drude Model

Now, we will consider a varying electric field $E = E_0\cos\omega t$, where E_0 is its constant amplitude and ω its frequency. Hence, the fractional differential equation has the form

$$m\frac{dv}{dt} + \frac{m}{\tau}v = -eE_0\cos\omega t \tag{20}$$

Making $u = -mv/eE_0\tau$ in (20) and $\bar{t} = t/\tau$

$$\frac{\mathrm{d}^\gamma u}{\mathrm{d}\bar{t}^\gamma} + u = \cos(\omega\tau\bar{t}) \tag{21}$$

If the condition is $u(0) = 0$, then, applying the Laplace transform, we have

$$U(s) = \frac{s}{[(\tau s)^\gamma + 1](s^2+\omega^2)} \tag{22}$$

We take the highest power of s as a common factor from the denominator and then expanding it in an alternating geometric series, we have [22]

$$\begin{aligned}v(t;\gamma) &= -\frac{eE_0\tau}{m}\\ &\times\sum_{k,\,l=0}^{\infty}\frac{(-1)^{k+l}(\omega\tau)^{2k}}{\Gamma[\gamma(l+1)+2k+1]}\left(\frac{t}{\tau}\right)^{\gamma(l+1)+2k}\end{aligned} \tag{23}$$

In this case we have the fractional current density given by

$$\begin{aligned}j(t;\gamma) &= \frac{e^2NE_0\tau}{m}\\ &\times\sum_{k,\,l=0}^{\infty}\frac{(-1)^{k+l}(\omega\tau)^{2k}}{\Gamma[\gamma(l+1)+2k+1]}\left(\frac{t}{\tau}\right)^{\gamma(l+1)+2k}\end{aligned} \tag{24}$$

The corresponding plots are given in the Fig. (4), for different value of γ.

5. Conclusions

As mentioned before, there are strong evidences that the fractional models describe better the physical processes. In this communication, using the fractional Caputo derivative we have extended the classical Drude model for electrons in a metal. We have obtained that the velocity and the current density of the electrons not only depend on the time t, but also on the order of the fractional differential equation γ. This fact could have interesting consequences in the study of electrical properties of metals.

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