Fractional Relaxation of Dielectric Materials: Adomian Decomposition Method

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Abstract: This paper gives an analytical solution on dielectric relaxation processes. Here, Adomian decomposition method is used for solving fractional diffusion equation obtained from evolution of Ising Model, where fractional derivative is based on Riemann-Liouville definition. Then this solution, which is valid at low temperatures, is applied to the dielectric relaxation processes. The solution leads to Cole-Cole dispersion relation in frequency domain. It also reaches to KWW (Kolraush-William-Watts) and algebraic decay relaxation functions in some approximations.

Key Words: Dielectric Relaxation, Fractional Calculus, Decomposition Method, Ising Model

1. INTRODUCTION

Fractional Calculus, which is the field of mathematical analysis dealing with the investigation and applications of integrals and derivatives of arbitrary order, has attracted in recent years a considerable interest in many disciplines. It has been found that the behavior of many physical systems can be more properly defined by using the fractional theory. Flexibility of degree of freedom, which is very easily obtained in the fractional theory, is one of the most important advantages of the fractional order modeling. Moreover, in all these studies, analysis of fractional diffusion equations has been a field of increasing interest [Mainardi (1997), (2001) - Metzler *et al*. (1999), (2000) - Schneider *et al*. (1989) - Ray (2008) - Das (2009)]

1.1. The fractional integral and Riemann-Liouville fractional derivative

According to the Riemann–Liouville approach the fractional integral of order $\alpha > 0$ is defined as

$$ {}_aJ_t^{-\alpha} U(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} U(\tau)\ d\tau \qquad (1.1)$$

$$ {}_aJ_t^{0} U(t) = U(t) \qquad (1.2)$$

Moreover, for $\alpha, \beta > 0$, $t > 0$ and $\nu > -1$ it has properties:

$$J_t^{-\alpha} J_t^{-\beta} U(t) = J_t^{-(\alpha+\beta)} U(t) \qquad (1.3a)$$

or

$$J_t^{-\beta} J_t^{-\alpha} U(t) = J_t^{-(\beta+\alpha)} U(t) \qquad (1.3b)$$

and

$$J_t^{-\alpha} t^{\nu} = \frac{\Gamma(\nu+1)}{\Gamma(\nu+1+\alpha)} t^{\nu+\alpha} \qquad (1.4)$$

Also,

$$ {}_aD_t^{p} U(t) = \left(\frac{d}{dt}\right)^{m+1} \int_a^t (t-\tau)^{m-p} U(\tau) d\tau \qquad (1.5)$$

The expression (1.5) it is the most widely known definition of the fractional derivative and is usually called the Riemann-Liouville fractional definition. Maybe, the most important property of the Riemann-Liouville fractional approach is that

$$ {}_aD_t^{\alpha} \left({}_aJ_t^{-\alpha} U(t) \right) = U(t) \qquad (1.6)$$

The Riemann-Liouville fractional differentiation operator is a left inverse to Riemann-Liouville fractional integration operator of the same order α. More details and properties of the operator J^{α} and D^{p} can be found in [Miller *et al*. (1993)-Oldham *et al*. (1974)-Podlubny (1999),]

1.2. Adomian Decomposition Method

Adomian decomposition method introduced by Adomian in 1980, has proved to be a very useful tool on solution of nonlinear functional equations. The decomposition method consists in finding the solution in the form

$$U(x,t) = \sum_{n=0}^{\infty} U_n(x,t) \qquad (1.8)$$

where the components $U_n(x,t)$ will be determined recursively. More information about ADM can be found in [Adomian (1994)].

2. DIELECTRIC RELAXATION PROCESSES

Relaxation properties are generally expressed in terms of time-domain response function $f(t)$ or of the frequency-dependent real and imaginary components of its Fourier transform [Uchaikin (2003)]:

$$\tilde{f}(i\omega) = \int_0^\infty e^{-i\omega t} f(t)dt = \varphi'(\omega) - i\varphi''(\omega). \qquad (2.1)$$

Classically, relaxation processes are described in terms of the exponential function;

$$\phi(t) = \exp(-t/\tau)\ ,\ t \geq 0 \qquad (2.2)$$

which is generally referred to as Maxwell–Debye relaxation. However, in many systems the dynamical behavior shows conspicuous deviations from the ideal exponential pattern. Experimental results in the time domain are often described in terms of the Kohlrausch-Williams-Watts (KWW) or stretched exponential function [Metzler *et al.* (2002)]

$$\phi(t) = e^{-(t/\tau)^\beta}\ ,\ 0 < \beta < 1 \qquad (2.4)$$

or through asymptotic power-laws

$$\phi(t) = \frac{1}{1+(t/\tau)^\delta}\qquad ,\ \delta > 0 \qquad (2.5)$$

Usually three general relaxation laws are encountered in the experimental studies of complex systems:

(i) stretched exponential (KWW function) [William *et al.* (1971)]

$$f(t) \approx \exp\left[-\left(\frac{t}{\tau}\right)^\alpha\right],\ 0 < \alpha < 1\ ,\ t > \tau \qquad (2.6)$$

(ii) exponential–logarithmic function

$$f(t) \approx \exp[-Bln^\alpha(t/\tau)] \qquad (2.7)$$

(iii) algebraic decay

$$f(t) \approx (t/\tau)^{-\alpha} \qquad (2.8)$$

where α, τ and B are the appropriate fitting parameters [Schneider *et al.* (1989)].

By definition, $\chi(\omega)$ is connected to the temporal relaxation function through the relation

$$\chi(\omega) = \int_0^\infty e^{-i\omega t}\, d(-\phi(t)) = 1 - i\omega \int_0^\infty e^{-i\omega t}\, \Phi(t)dt \qquad (2.9)$$

where $\Phi(t) = \phi(t)/\phi(0)$. Significant amount of experimental data on disordered systems supports the following empirical expressions for dielectric loss spectra, namely, the Cole-Cole equation [Cole and Cole, (1941)]

$$\chi(\omega) = \frac{\chi_0}{1+(i\omega\tau)^\alpha}\ ,\ 0 < \alpha \leq 1 \qquad (2.10)$$

the Cole-Davidson equation [Davidson *et al.* (1951)]

$$\chi(\omega) = \frac{\chi_0}{(1+i\omega\tau)^\beta}\ ,\ 0 < \beta \leq 1 \qquad (2.11)$$

and the Havriliak–Negami equation [Havriliak *et al.* (1966)] considered as a general expression for the universal relaxation law [Jonscher (1983)]

$$\chi(\omega) = \frac{\chi_0}{(1+(i\omega\tau)^\alpha)^\beta}\ ,\ 0 < \alpha \leq 1\ ,\ 0 < \beta \leq 1 \qquad (2.12)$$

Havriliak–Negami equation is a combination of the Cole–Cole and Cole–Davidson equations.

3. THE ISING MODEL AND FRACTIONAL RELAXATION

The decay of the spin-spin time correlation functions in a one-dimensional Ising model [XX] with Glauber [Glauber (1963)] dynamics was studied by Brey and Parados [Brey *at al.* (1996)]. They started that the energy of the system in the one-dimensional Ising model for a configuration σ is

$$H(\sigma) = -J\sum_i \sigma_i\sigma_{i+1} \qquad (3.1)$$

with J a positive constant. The state of the system is specified by the spin vector $\sigma = \{\sigma_i\}$, where $\sigma_i = \pm 1$ is the spin at site i. The evolution of the system is described by Markov process with Glauber dynamics. So, the conditional probability $P_{1/1}(\sigma,t/\sigma',t')$ of finding the system in the state σ at time t, given it was in the state σ' at time t' obeys the master equation

$$\frac{\partial P_{1/1}(\sigma,t/\sigma',t')}{\partial t} = \sum_{i=-\infty}^{\infty}[\omega_i(R_i\sigma)P_{1/1}(R_i\sigma,t/\sigma',t') - \omega_i(\sigma)P_{1/1}(\sigma,t/\sigma',t')] \qquad (3.2)$$

where $R_i\sigma$ is the configuration obtained from σ by flipping the i.th spin and $\omega_i(\sigma)$ is the transition rate for the flip. Following, in the low temperature limit, spin-spin time correlation function was found by Brey and Parados in form of a diffusion type equation

$$\frac{\partial f(x,t)}{\partial t} = (\alpha\gamma - \alpha) f(x,t) + \frac{\alpha\gamma}{2}\frac{\partial^2 f(x,t)}{\partial x^2}. \qquad (3.3)$$

If equation (3.3) is evaluated to fractional differential equation form, the one can be expressed as

$$D_t^{\xi} f(x,t) = (\alpha\gamma - \alpha) f(x,t) + \frac{\alpha\gamma}{2}\frac{\partial^2 f(x,t)}{\partial x^2}. \qquad (3.4)$$

Where D_t^{ξ} is the Riemann-Liouville fractional differentiation operator, and the initial condition for this equation is

$$f(x,0) = e^{-|x|}. \qquad (3.5)$$

We adopt Adomian decomposition method for solving Eq. (3.4). According to this method we assume that

$$f(x,t) = \sum_{n=0}^{\infty} f_n(x,t) \qquad (3.6)$$

Now, the fractional differential equation (3.4) can be written as, for $\nu + \xi = 1$,

$$D_t^{\nu}\left(D_t^{\xi} f(x,t)\right) = (\alpha\gamma - \alpha) D_t^{\nu} f(x,t) + \frac{\alpha\gamma}{2} D_t^{\nu}\frac{\partial^2 f(x,t)}{\partial x^2} \qquad (3.7)$$

If we operate both sides of this relation with integral operator $\mho_t^{-1}$, we reach to

$$\mho_t^{-1} D_t^{\nu}\left(D_t^{\xi} f(x,t)\right) = (\alpha\gamma - \alpha)\mho_t^{-1}\left(D_t^{\nu} f(x,t)\right) + \frac{\alpha\gamma}{2}\mho_t^{-1}\left(D_t^{\nu}\frac{\partial^2 f(x,t)}{\partial x^2}\right) \qquad (3.8.a)$$

$$f(x,t) = (\alpha\gamma - \alpha)\mho_t^{-1}\left(D_t^{\nu} f(x,t)\right) + \frac{\alpha\gamma}{2}\mho_t^{-1}\left(D_t^{\nu}\frac{\partial^2 f(x,t)}{\partial x^2}\right) \qquad (3.8.b)$$

Moreover, where recursive relations is

$$\begin{aligned}
f(0) &= f(x,0) = e^{-x} \\
f(1) &= (\alpha\gamma - \alpha) D_t^{-\xi} f(0) + \frac{\alpha\gamma}{2} D_t^{-\xi}\frac{\partial^2 f(0)}{\partial x^2} \\
&= \left(\alpha\gamma - \alpha + \frac{\alpha\gamma}{2}\right)\frac{e^{-|x|} t^{\xi}}{\Gamma(\xi+1)} \\
f(2) &= (\alpha\gamma - \alpha) D_t^{-\xi} f(1) + \frac{\alpha\gamma}{2} D_t^{-\xi}\frac{\partial^2 f(1)}{\partial x^2} \\
&= \left(\alpha\gamma - \alpha + \frac{\alpha\gamma}{2}\right)^2\frac{e^{-|x|} t^{2\xi}}{\Gamma(2\xi+1)} \\
f(3) &= (\alpha\gamma - \alpha) D_t^{-\xi} f(2) + \frac{\alpha\gamma}{2} D_t^{-\xi}\frac{\partial^2 f(2)}{\partial x^2} \\
&= \left(\alpha\gamma - \alpha + \frac{\alpha\gamma}{2}\right)^3\frac{e^{-|x|} t^{3\xi}}{\Gamma(3\xi+1)}
\end{aligned}$$

and so on. Therefore the solution is

$$\begin{aligned}
f(x,t) &= \sum_{n=0}^{\infty}\left(\alpha\gamma - \alpha + \frac{\alpha\gamma}{2}\right)^n\frac{e^{-|x|} t^{n\xi}}{\Gamma(n\xi+1)} \\
&= e^{-|x|} E_{\xi}\left\{\alpha\left(-1 + \frac{3\gamma}{2}\right) t^{\xi}\right\}, \quad 0 < \xi < 1 \qquad (3.9)
\end{aligned}$$

Where $E_{\xi}\{.\}$ is the Mittag–Leffler function given by

$$E_{\nu}(z) = \sum_{n=0}^{\infty}\frac{z^n}{\Gamma(\nu n+1)} \qquad (3.10)$$

If we assume that situation of dipoles located between x and $x + x_0$ have a probability density given by

$$f(x) = \frac{1}{x_0} e^{(-x/x_0)}, \qquad (3.11)$$

Thus, integrating the dipole correlation function (3.9) over the all space we can reach to the time dependent correlation function

$$\begin{aligned}
f(t) &= \int_0^{\infty}\frac{1}{x_0} e^{(-x/x_0)} e^{-|x|} E_{\xi}\left\{\alpha\left(-1 + \frac{3\gamma}{2}\right) t^{\xi}\right\} dx \\
&= \frac{E_{\xi}\left\{\alpha\left(-1+\frac{3\gamma}{2}\right) t^{\xi}\right\}}{1+x_0} \qquad (3.12)
\end{aligned}$$

where x_0 is the average value of x and $1/2x_0$ is average number of dipoles per unit length.

If equation (3.12) substituted into equation (2.9),

$$\chi(\omega) = 1 - i\omega\int_0^{\infty} e^{-i\omega t}\frac{E_{\xi}\left\{\alpha\left(-1+\frac{3\gamma}{2}\right) t^{\xi}\right\}}{1+x_0} dt, \qquad (3.13)$$

at frequency zone, empiric Cole-Cole type equation is obtained simply as:

$$\chi(\omega) = \frac{\chi_0}{1+(i\omega\tau)^{\xi}}, \quad 0 < \xi < 1 \qquad (3.14)$$

Where we take $\tau = \left(\alpha(-1 + 3\gamma/2)\right)^{-\xi}$, $\chi_0 = 1 + \lambda(i\omega\tau)^{\xi}$ and $\lambda = 1 - 1/(1 + x_0)$.

Moreover, for sufficiently small times Mittag-Leffler function exhibits the same behavior with a stretched exponential [Mainardi *at al.* (2000)] :

$$\begin{aligned}
f(t) &\approx 1 - \frac{(t/\tau)^{\xi}}{\Gamma(\xi+1)} + \cdots \\
&\approx exp\left[-\frac{(t/\tau)^{\xi}}{\Gamma(\xi+1)}\right], \quad 0 \le t \ll 1 \qquad (3.15)
\end{aligned}$$

which is KWW (Kolraush-William-Watts) function. Also, using the asymptotic expansions it can be written

$$f(t) \approx \frac{\Gamma(\xi) sin(\xi\pi)}{\pi}(t/\tau)^{-\xi}, \quad t \to \infty \qquad (3.16)$$

which has same form with empirical algebraic decay function (2.8). When the equation (3.3) is solved by generation function method at appropriate boundary condition, which was done by [Brey *at al.* (1996)],

$$\chi(\omega) = \alpha\frac{1-\eta^2}{1+\eta^2}\frac{1}{[(i\omega+\alpha)^2 - \alpha^2\gamma^2]^{1/2}} \qquad (3.17)$$

is obtained. This expression, at low temperature, converts to Cole-Davidson distribution:

$$\chi(\omega) = \frac{1}{(1 + i\omega\tau_{CD})^{\beta_{CD}}} \tag{3.18}$$

where τ_{CD} is constant and $\beta_{CD} = 1/2$ [Brey *at al.* (1996)].

4. CONCLUSION

In this study it is shown that fractional solution of the diffusion equation obtained from Ising model, where we used the Adomian decomposition method that has prove successful in deriving analytical solutions of linear and nonlinear differential equations, is more comprehensive than many other approaches. A flexible α parameter, which is especially used in the forming of the differential equations within fractional order modeling, exhibits that the space of physical processes has a fractional form, and irregularity (or chaos) in the nature compels us to use the fractional theory.

We have seen that the order of the differential equations which is compatible with the most experiment is generally smaller than the integer order differential equations. Likely, in medium the nearest neigbour interaction between particles has not the same times and velocities because of the time (or energy) is fractionally changing. The local spaces of charged particles which have different time and energy intervals should be resulted to have different order differential equations. Moreover, maybe, we say that in the atomic levels (or electronic, or molecular) the flow of the time is quantized. Interaction between particles may be also quantized in time space. That is, quantization of the energy may be result of the time quantization.A result of these processes, the order of differential equations should be changed during the interaction time.

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