The Fractional Virial Theorem

Cristina Mihaela-Baleanu

National Mihail Sadoveanu High School, District 2, Bucharest, Romania
(e-mail: crisbaleanu@yahoo.com).

Abstract: Fractional calculus is an emerging field and its has many applications in several fields of science and engineering. In this paper the fractional generalization of the classical virial theorem is presented.

Keywords: Fractional calculus, virial theorem, classical mechanics, Riemann-Liouville fractional derivatives.

1. INTRODUCTION

During the last decades the fractional calculus, which deals with fractional derivatives and integrals of any order (Oldham, Spanier (1974); Samko et al (1993); Podlubny (1999); Kilbas et al (2006); Magin (2006); Zaslavsky (2005)); West et al (2003); Sabatier et al (2007); Metzler et al (1995); Hilfer (2000), started to be applied intensively in various fields of science and engineering (Glöckle, Nonnenmacher (1991, 1995); Caputo (1967); Carpinteri-Mainardi (1997); Gorenflo-Mainardi (1997); Tenreiro-Machado (2003); Mainardi et al (2001); Liang et al (2006); Diethelm, Ford (2002); Lorenzo (2004); Luchko and Gorenflo (1999); Momani, Odibat (2008); Frederico, Torres (2007); Trujillo (1999); Atanackovic, Stankovic (2008); Maaraba et al. (2008); Magin et al (2008)). Based of some examples from the field of viscoelasticity Heymans and Podlubny have proved that it is possible to attribute physical meaning to initial conditions expressed in terms of Riemann-Liouville fractional derivatives (Heymans, Podlubny (2006)).

An interesting and recent direction in fractional calculus area is the field of the fractional variational principles. As a result several formulations of the fractional Euler-Lagrange equations have been reported in the literature and applied to several important dynamical systems (Riewe (1996); Klimek (2001); Agrawal (2002); Baleanu, Avkar (2004a); Baleanu (2004b,c); Muslih, Baleanu (2005); Agrawal (2006); Tarasov, (2006); Agrawal (2007); Atanackovic et al (2008); Cresson (2007); El-Nabulsi and Torres (2007); Baleanu, Trujillo (2008)).

The next step was to obtain the fractional Hamilton equations. There are several ways to define the fractional Hamiltonian and all of them coincide in the classical limits with the classical results Riewe (1997); Klimek (2002); Baleanu et al (2006a); Baleanu, Agrawal (2006b); Baleanu et al (2008a); Baleanu (2008b); Baleanu, Muslih (2008d); Tarasov, Zaslavsky (2008); Rabei et al. (2008). Recently, the fractional variational principles started to play an important role in physics and in the control theory.

The non-locality is a major characteristic of the fractional differential operators, therefore some techniques should be used or developed in order to deal with theories involving such kind of operators.

The aim of this paper is to investigate the fractional generalization of the classical virial theorem.

The plan of the paper is as follows:

In Section 2 we briefly present some basic definitions and properties of the Riemann-Liouville (RL) and Caputo derivatives. In Section 3 we present briefly the classical virial theorem. Section 4 deals with the fractional generalization of the classical virial theorem.

2. BASIC DEFINITIONS

In the following we present briefly several basic definitions of the fractional calculus. The left Riemann-Liouville (RL) derivative has the form

\[ aD^\alpha_t f(t) = \frac{1}{\Gamma(n-\alpha)} \left( \frac{d}{dt} \right)^n \int_a^t (t-\tau)^{n-\alpha-1} f(\tau) d\tau, \]  

(1)

and the right RL fractional derivative is given below

\[ bD^\alpha_t f(t) = \frac{1}{\Gamma(n-\alpha)} \left(-\frac{d}{dt}\right)^n \int_t^b (\tau-t)^{n-\alpha-1} f(\tau) d\tau. \]  

(2)

The order \( \alpha \) satisfies \( n-1 \leq \alpha < n \) and \( \Gamma \) denotes the Euler’s gamma function.

As it can be seen from (1), the RL derivative of a constant is not zero and its expression is given below

\[ aD^\alpha_t C = C \frac{(t-a)^{-\alpha}}{\Gamma(1-\alpha)}. \]  

(3)

However, the RL derivative of a power has the form

\[ aD^\alpha_t t^\beta = \frac{\Gamma(\alpha+1) t^{\beta-\alpha}}{\Gamma(\beta-\alpha+1)}, \]  

(4)

for \( \alpha > -1, \beta \geq 0 \). The composite of fractional derivatives is crucial in various applications and it presented below.
\[ aD_t^\alpha aD_t^\sigma f(t) = aD_t^{\alpha+\sigma} f(t) \]
\[ = \sum_{j=1}^{k} aD_t^{\alpha-j} f(t) |_{t=a} \frac{(t-a)^{-\alpha-j}}{\Gamma(1-\beta-j)}. \] 
Here \( 0 \leq k-1 \leq q \leq k, p \geq 0 \) and \( k \) is an integer number. The fractional product rule has the form
\[ aD_t^\alpha (fg) = \sum_{j=0}^{\infty} \binom{\alpha}{j} aD_t^{\alpha-j} f \left( \frac{\partial^j g}{\partial t^j} \right). \]

Let us consider an analytic function \( \phi(t) \) and \( f(t) = H(t-a) \), where \( H(t) \) denotes the Heaviside function. By making use the Leibniz rule together with the formula for the fractional differentiation of the Heaviside function we obtain the following result
\[ aD_t^\alpha \phi(t) = \sum_{k=0}^{\infty} \binom{\alpha}{k} \phi^{(k)}(t) aD_t^{\alpha-k} H(t-a). \]
Finally, replacing the fractional derivative of \( H(t-a) \) we obtain
\[ aD_t^\alpha \phi(t) = \frac{(t-a)^{-\alpha}}{\Gamma(1-\alpha)} \phi(t) + \sum_{k=1}^{\infty} \binom{\alpha}{k} \frac{(t-a)^{-\alpha-k}}{\Gamma(k+1)} \phi^{(k)}(t) \]
under the assumption \( t > a \).

We observe that when \( \alpha \) becomes an integer we obtain
\[ aD_t^\alpha f(t) = \left( \frac{df(t)}{dt} \right)^\alpha, \quad aD_t^\alpha f(t) = \left( -\frac{df(t)}{dt} \right)^\alpha. \]
In the following we define the left and the right Caputo derivatives. Namely, the left Caputo fractional derivative has the form
\[ C^\alpha aD_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-\tau)^{n-\alpha-1} \frac{df(\tau)}{d\tau} d\tau, \]
and the right Caputo fractional derivative is given by
\[ C^\alpha aD_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_t^b (\tau-t)^{n-\alpha-1} \frac{df(\tau)}{d\tau} d\tau, \]
where \( n-1 < \alpha < n \).

In this case the derivative of a constant is zero and we can define properly the initial conditions for the fractional differential equations which can be handle by using an analogy with the classical case.

3. THE VIRIAL THEOREM-CLASSICAL CASE

In this section we give briefly the classical virial theorem.

Let us consider that the Newton’s second law \( \vec{F}_i = m_i a_i \) \( i = 1, \ldots, n \).

The total time derivative of the following quantity \( G = \sum_i \vec{p}_i \cdot \vec{r}_i, i = 1, \ldots, n \) has the form
\[ \frac{dG}{dt} = \sum_i \vec{p}_i \cdot \vec{r}_i + \sum_i \vec{p}_i \cdot \vec{r}_i. \] 

The first term of (12) can be written as
\[ \sum_i \vec{p}_i \cdot \vec{p}_i = \sum_i m_i V_i^2 = 2T. \]

The second term in (12) becomes
\[ \sum_i \vec{p}_i \cdot \vec{r}_i = \sum_i \vec{F}_i \cdot \vec{r}_i. \]

As a result the total time derivative of \( G \) becomes
\[ \frac{dG}{dt} = 2T + \sum_i \vec{F}_i \cdot \vec{r}_i. \]

If we take the time average of (12) between 0 and \( \tau \) we obtain
\[ 2T + \sum_i \vec{F}_i \cdot \vec{r}_i = \frac{1}{\tau} [G(\tau) - G(0)]. \]

By making use of \( \tau \) sufficiently long we obtain
\[ \bar{T} = \frac{1}{2} \sum_i \vec{F}_i \cdot \vec{r}_i. \]

4. THE VIRIAL THEOREM-FRACTIONAL GENERALIZATION

The fractional generalization of Newton’s second law is given below
\[ aD_t^\alpha \vec{p}_i = \vec{F}_i. \]

We define the following fractional quantity
\[ G^\alpha = \sum_i \vec{p}_i \cdot \vec{r}_i \]

The next step is to take the fractional Riemann-Liouville derivative of (19).

As a result we obtain the following
\[ aD_t^\alpha G^\alpha = \sum_{i,j=1}^{n} aD_t^\alpha (p_i f_j r_j) \]
\[ = \sum_{k=1}^{\infty} \sum_{i,j=1}^{n} \binom{\alpha}{k} p_i f_j (aD_t^{\alpha-k} r_j) \]
\[ + \sum_{i=1}^{n} p_i f_j aD_t^{\alpha} r_j \]
\[ + \sum_{i=1}^{n} \sum_{i=1}^{n} \alpha aD_t^{\alpha} r_j. \]

Taking into account that
\[ p_i f_j = m_{ia} a_i \]
and define the fractional kinetic energy as
\[ T^\alpha = \frac{1}{2} \sum_{i,j=1}^{n} p_i f_j aD_t^{\alpha} r_j \]
we obtain that
\[ 2T^f + \sum_{j=1}^{n} \sum_{i=1}^{m} \alpha \frac{dp_{ij}}{dt} aD^{\alpha-1}r_j \]
\[ + \sum_{k=1}^{\infty} \sum_{i=1}^{m} \left( \frac{1}{k} \right) p_{ij}^{(k)} (aD^{\alpha-k}r_j) = aD^{\alpha}G^f \]  
(23)

or
\[ 2T^f = \sum_{j=1}^{n} \sum_{i=1}^{m} \alpha \frac{dp_{ij}}{dt} aD^{\alpha-1}r_j \]
\[ - \sum_{k=1}^{\infty} \sum_{i=1}^{m} \left( \frac{1}{k} \right) p_{ij}^{(k)} (aD^{\alpha-k}r_j) + aD^{\alpha}G^f \]  
(24)

Finally, taking the time average we obtain
\[ \overline{2T^f} = \sum_{j=1}^{n} \sum_{i=1}^{m} \alpha \frac{dp_{ij}}{dt} aD^{\alpha-1}r_j \]
\[ - \sum_{k=1}^{\infty} \sum_{i=1}^{m} \left( \frac{1}{k} \right) p_{ij}^{(k)} (aD^{\alpha-k}r_j) + aD^{\alpha}G^f, \]  
(25)

which is a fractional generalization of the classical virial theorem.

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