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THE FRACTIONAL VIRIAL THEOREM

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Abstract. Fractional calculus is an emerging field and its has many applications in several fields of science and engineering. One of the major issue in this field is to apply this type of calculus to the real world applications. In this paper the fractional generalization of the classical virial theorem is presented.

1. Introduction

During the last decades the fractional calculus, which deals with fractional derivatives and integrals of any order, started to be applied intensively in various fields of science and engineering [30, 28, 39, 20, 32, 44, 23, 27, 19, 46, 31, 43, 22]. Based on some examples from the field of viscoelasticity Heymans and Podlubny have proved that it is possible to attribute some physical meaning to initial conditions expressed in terms of Riemann-Liouville fractional derivatives [21].

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. 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 [37, 38, 26, 24, 45, 25, 42, 29]. 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. Recently, the fractional variational principles started to play an important role in physics and in the control theory [8, 29, 5, 41, 33, 34, 35, 18, 1, 2, 3, 36, 4, 6, 7, 40, 14, 17, 15]. Fractional Nambu mechanics has been obtained [9]. The generalized Newtonian law and fractional Langevin equation and potentials corresponding to different kinds of forces involving both the right and the left fractional derivatives has been introduced [10]. The fractional multi time Lagrangian equations for dynamical systems within Riemann-Liouville derivatives and fractional multi time constant of motion are discussed in [13]. The classical constraint Hamiltonian formulation using Dirac brackets successfully leads the equations is obtained from fractional Euler-Lagrange equations [16]. The generalized Newtonian equations with memory and presented a physical model for application has been

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obtained [11]. Using the fractional differential forms, the classical electromagnetic equations involving the fractional derivatives have been worked out [12].
As it is known in mechanics, the virial theorem provides a general equation which connects the average over time of the total kinetic energy of a stable system, bounded by potential forces. The range of the applicability of the virial theorem is very diverse. It is applicable to dynamical and thermodynamical systems, systems with velocity dependent forces, viscous systems, systems exhibiting macroscopic motions such as rotation, systems with magnetic fields and even some systems which require general relativity for their description. Actually the theorem represents a basic structural relationship that the system must obey. However,this theorem it is difficult to be applied in some practical applications because the conditions of their fulfillment are too strict to be easily fulfilled.

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. Section 5 is dedicated to our conclusions.

2. Basic definitions

In the following we present briefly several basic definitions concerning fractional calculus.

If $f(x) \in C[a,b]$ and $\alpha > 0$ then

$$ {}_a\mathbf{I}_x^\alpha f(x) := \frac{1}{\Gamma(\alpha)} \int_a^x \frac{f(t)}{(x-t)^{1-\alpha}} dt, \qquad x > a, $$

and

$$ {}_x\mathbf{I}_b^\alpha f(x) := \frac{1}{\Gamma(\alpha)} \int_x^b \frac{f(t)}{(x-t)^{1-\alpha}} dt, \qquad x < b, $$

are called the left-sided and right-sided Riemann-Liouville fractional integral of order α, respectively.

The left Riemann-Liouville (RL) fractional derivative has the form

$$ {}_a\mathbf{D}_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dt}\right)^n \int_a^t (\tau - t)^{n-\alpha-1} f(\tau) d\tau, \tag{2.1} $$

and the right RL fractional derivative is given below

$$ {}_t\mathbf{D}_b^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \left(-\frac{d}{dt}\right)^n \int_t^b (\tau - t)^{n-\alpha-1} f(\tau) d\tau. \tag{2.2} $$

The order α satisfies $n-1 \leqslant \alpha < n$ and Γ denotes the Euler's gamma function.

As it can be seen from (2.1), the RL derivative of a constant is not zero and its expression is given below

$$ {}_a\mathbf{D}_t^{\alpha} C = C \frac{(t-a)^{-\alpha}}{\Gamma(1-\alpha)}. \tag{2.3}$$

However, the RL derivative of a power has the form

$$ {}_a\mathbf{D}_t^{\alpha} t^{\beta} = \frac{\Gamma(\alpha+1)(t-a)^{\beta-\alpha}}{\Gamma(\beta-\alpha+1)}, \tag{2.4}$$

for $\alpha > -1, \beta \geqslant 0$. The composite of fractional derivatives is crucial in various applications and it presented below

$$\begin{aligned} {}_a\mathbf{D}_t^{\alpha}\, {}_a\mathbf{D}_t^{\sigma} f(t) &= {}_a\mathbf{D}_t^{\alpha+\sigma} f(t) \\ &\quad - \sum_{j=1}^{k} {}_a\mathbf{D}_t^{\sigma-j} f(t)|_{t=a} \frac{(t-a)^{-\alpha-j}}{\Gamma(1-\beta-j)}, \end{aligned} \tag{2.5}$$

Here $0 \leqslant k-1 \leqslant q \leqslant k$, $p \geqslant 0$ and k is an integer number. The fractional product rule has the form

$$ {}_a\mathbf{D}_t^{\alpha}(fg) = \sum_{j=0}^{\infty} \binom{\alpha}{j} \left({}_a\mathbf{D}_t^{\alpha-j} f\right) \left(\frac{\partial^j g}{\partial t^j}\right), \tag{2.6}$$

where the binomial coefficient has the form $\binom{\alpha}{j} = \frac{\Gamma(\alpha+1)}{j!\Gamma(\alpha-j+1)}, j \in N_0$.

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

$$ {}_a\mathbf{D}_t^{p} \phi(t) = \sum_{k=0}^{\infty} \binom{p}{k} \phi^{(k)}(t) {}_a\mathbf{D}_t^{p-k} H(t-a). \tag{2.7}$$

Finally, replacing the fractional derivative of $H(t-a)$ we obtain

$$ {}_a\mathbf{D}_t^{p} \phi(t) = \frac{(t-a)^{-p}}{\Gamma(1-p)}\phi(t) + \sum_{k=1}^{\infty} \binom{p}{k} \frac{(t-a)^{k-p}}{\Gamma(k-p+1)} \phi^{(k)}(t) \tag{2.8}$$

under the assumption $t > a$.

We observe that when α becomes an integer we obtain

$$ {}_a\mathbf{D}_t^{\alpha} f(t) = \left(\frac{df(t)}{dt}\right)^{\alpha}, \; {}_t\mathbf{D}_b^{\alpha} f(t) = \left(-\frac{df(t)}{dt}\right)^{\alpha}. \tag{2.9}$$

In the following we define the left and the right Caputo derivatives. Namely, the left Caputo fractional derivative has the form

$$ {}_a^C\mathbf{D}_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-\tau)^{n-\alpha-1} \left(\frac{d}{d\tau}\right)^n f(\tau) d\tau, \tag{2.10}$$

and the right Caputo fractional derivative is given by

$$ {}_{a}^{C}\mathbf{D}_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \int_t^b (\tau - t)^{n-\alpha-1} \left(-\frac{d}{d\tau}\right)^n f(\tau) d\tau, \tag{2.11} $$

where $n-1 < \alpha < n$. In the following we briefly present some properties of fractional derivatives and integrals:

$$ {}_{a}^{C}\mathbf{D}_t^{\alpha}(f(t)+g(t)) = {}_{a}^{C}\mathbf{D}_t^{\alpha} f(t) + {}_{a}^{C}\mathbf{D}_t^{\alpha} g(t), \tag{2.12} $$

$$ {}_{a}^{C}\mathbf{D}_t^{\alpha} c = 0, \quad c \quad \text{is constant.} \tag{2.13} $$

As it can be seen from above mentioned formulas, in the Caputo 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.

The fractional integration by parts formula is given below

$$ \int_a^b f(t)[{}_a\mathbf{D}_t^{\alpha} g(t)]dt = \int_a^b g(t)[{}_t\mathbf{D}_b^{\alpha} f(t)]dt. \tag{2.14} $$

We mention that (2.14) is valid under the assumption that $f(t) \in {}_tI_b^{\alpha}(L_p)$, $g(t) \in {}_aI_t^{\alpha}(L_p)$, $\frac{1}{p}+\frac{1}{q} \leqslant 1+\alpha$. In the following we enlist some other basic formulas of fractional integrals and derivatives, namely

$$ {}_a\mathbf{D}_t^{\alpha}(t-a)^{\beta} = \frac{\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha)}(t-a)^{\beta-\alpha} \quad (\beta > \alpha), \tag{2.15} $$

$$ {}_a\mathbf{I}_t^{\alpha}(t-a)^{\beta} = \frac{\Gamma(\beta+1)}{\Gamma(\beta+1+\alpha)}(t-a)^{\beta+\alpha}, \tag{2.16} $$

$$ {}_a\mathbf{I}_t^{\alpha}\, {}_a\mathbf{D}_t^{\alpha} x(t) = x(t) - \sum_{j=1}^{n} \frac{({}_a\mathbf{D}_t^{\alpha-j}x)(a)}{\Gamma(\alpha+1-j)}(t-a)^{\alpha-j}, \tag{2.17} $$

$$ {}_t\mathbf{I}_b^{\alpha}\, {}_t\mathbf{D}_b^{\alpha} x(t) = x(t) - \sum_{j=1}^{n} \frac{({}_t\mathbf{D}_b^{\alpha-j}x)(b)}{\Gamma(\alpha+1-j)}(b-t)^{\alpha-j}, \tag{2.18} $$

$$ {}_a\mathbf{I}_t^{\alpha}\, {}_a^{C}\mathbf{D}_t^{\alpha} x(t) = x(t) - \sum_{j=0}^{n-1} \frac{(D^j x)(a)}{\Gamma(j+1)}(t-a)^{j}, \tag{2.19} $$

$$ {}_t\mathbf{I}_b^{\alpha}\, {}_t^{C}\mathbf{D}_b^{\alpha} x(t) = x(t) - \sum_{j=0}^{n-1} \frac{((-D)^j x)(b)}{\Gamma(j+1)}(b-t)^{j}. \tag{2.20} $$

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 $\overrightarrow{\dot{p}_i} = \overrightarrow{F_i}$, where $\overrightarrow{p_i}$ denotes the canonical momenta, $\overrightarrow{r_i}$ are the position vectors and $\overrightarrow{F_i}$ are the external forces. Here $i = 1, \cdots n$.

The total time derivative of the following quantity $G = \sum_{i=1}^{n} \overrightarrow{p_i} \cdot \overrightarrow{r_i}, i = 1, \cdots, n$ has the form

$$\frac{dG}{dt} = \sum_{i=1}^{n} \overrightarrow{\dot{r}_i} \cdot \overrightarrow{p_i} + \sum_{i=1}^{n} \overrightarrow{\dot{p}_i} \cdot \overrightarrow{r_i}. \tag{3.1}$$

We mention that the dot represents the inner product between two vectors. We notice that the first term of (3.1) can be written as

$$\sum_{i=1}^{n} \overrightarrow{\dot{r}_i} \cdot \overrightarrow{p_i} = \sum_{i=1}^{n} m_i v_i^2 = 2T, \tag{3.2}$$

where T denotes the kinetic energy and v_i denotes the velocity.

By inspection we observe that the second term in (3.1) becomes

$$\sum_{i=1}^{n} \overrightarrow{\dot{p}_i} \cdot \overrightarrow{r_i} = \sum_{i=1}^{n} \overrightarrow{F_i} \cdot \overrightarrow{r_i}. \tag{3.3}$$

As a result the total time derivative of G is given by

$$\frac{dG}{dt} = 2T + \sum_{i=1}^{n} \overrightarrow{F_i} \cdot \overrightarrow{r_i}. \tag{3.4}$$

Finally, if we take the time average of (3.1) between 0 and τ we obtain

$$2\overline{T} + \sum_{i=1}^{n} \overline{\overrightarrow{F_i} \cdot \overrightarrow{r_i}} = \frac{1}{\tau}[G(\tau) - G(0)]. \tag{3.5}$$

By considering τ sufficiently long we finally obtain

$$\bar{T} = -\frac{1}{2} \sum_{i=1}^{n} \overline{\overrightarrow{F_i} \cdot \overrightarrow{r_i}}. \tag{3.6}$$

4. The virial theorem – fractional generalization

In the following we consider the fractional generalization of Newton's second law as given below

$${}_a\mathbf{D}_t^{\alpha} \overrightarrow{p_i^f} = \overrightarrow{F_i}, \tag{4.1}$$

where $\overrightarrow{p_i^f}$ denotes the fractional canonical momenta. In the following the superscript f of a quantity denotes the fact that it is a fractional generalization of a corresponding classical one.As a consequence of this we define the following fractional quantity

$$G^f = \sum_{i=1}^{n} \overrightarrow{p_i^f} \cdot \overrightarrow{r_i}. \tag{4.2}$$

The next step is to take the fractional Riemann-Liouville derivative of (4.2). As a result we obtain the following expression

$$\begin{aligned} {}_a\mathbf{D}_t^\alpha G^f &= \sum_{i=1}^{n}\sum_{j=1}^{3} {}_a\mathbf{D}_t^\alpha (p_i{}^{fj} r_j^i) \\ &= \sum_{k=3}^{\infty}\sum_{i=1}^{n}\sum_{j=1}^{3} \binom{\alpha}{k} p_i^{fj} ({}_a\mathbf{D}_t^{\alpha-k} r_j^i) \\ &\quad + \sum_{i=1}^{n}\sum_{j=1}^{3} p_i^{fj} {}_a\mathbf{D}_t^\alpha r_j^i \\ &\quad + \sum_{i=1}^{n}\sum_{j=1}^{3} \alpha \frac{dp_i^{fj}}{dt} {}_a\mathbf{D}_t^{\alpha-1} r_j^i. \end{aligned} \tag{4.3}$$

Taking into account that the fractional momenta has the from

$$p_i^f = m_{i\,a}\mathbf{D}_t^\alpha r_i \tag{4.4}$$

we define the fractional kinetic energy as

$$T^f = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{3} p_i^{fj} {}_a\mathbf{D}_t^\alpha r_j^i. \tag{4.5}$$

By inspection we observe that

$$\begin{aligned} 2T^f &+ \sum_{i=1}^{n}\sum_{j=1}^{3} \alpha \frac{dp_i^{fj}}{dt} {}_a\mathbf{D}_t^{\alpha-1} r_j^i \\ &+ \sum_{k=3}^{\infty}\sum_{i=1}^{n}\sum_{j=1}^{3} \binom{\alpha}{k} p_i^{fj} ({}_a\mathbf{D}_t^{\alpha-k} r_j^i) = {}_a\mathbf{D}_t^\alpha G^f, \end{aligned} \tag{4.6}$$

which implies that

$$\begin{aligned} 2T^f &= -\sum_{i=1}^{n}\sum_{j=1}^{3} \alpha \frac{dp_i^{fj}}{dt} {}_a\mathbf{D}_t^{\alpha-1} r_j^i \\ &\quad - \sum_{k=3}^{\infty}\sum_{i=1}^{n}\sum_{j=1}^{3} \binom{\alpha}{k} p_i^{fj} ({}_a\mathbf{D}_t^{\alpha-k} r_j^i) + {}_a\mathbf{D}_t^\alpha G^f \end{aligned} \tag{4.7}$$

Finally, taking the time average we obtain

$$2\overline{T^f} = -\sum_{i=1}^{n}\sum_{j=1}^{3}\overline{\alpha\frac{dp_i^{fj}}{dt}{}_a\mathbf{D}_t^{\alpha-1}r_j^i} - \sum_{k=3}^{\infty}\sum_{i=1}^{n}\sum_{j=1}^{3}\binom{\alpha}{k}\overline{p_i^{fj}({}_a\mathbf{D}_t^{\alpha-k}r_j^i)} + \overline{{}_a\mathbf{D}_t^{\alpha}G^f}, \tag{4.8}$$

which is a fractional generalization of the classical virial theorem. At this stage we observe that besides the classical expected generalization term we have two more terms which are coming due to the non-locality of the fractional differential operator.

5. Conclusions

The virial theorem was generalized to the fractional case.The form of the fractional virial theorem illustrates that the classical virial theorem is recovered when $\alpha \longmapsto 1$. The main open problem is to find the correct generalization of the fractional Newton equation. In this present paper we suppose that we can fractionalize the Newton equation by replacing the classical derivative with Riemann-Liouville fractional derivative. The obtained theorem permits to define explicitly the terms causing deviations from the ideal virial form. The obtained results show that the fractional virial theorem can be applicable for the characterization of the complex systems.

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