Conservation theorems and ergodicity

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(Received 12 October 2015, accepted 18 February 2016)

Abstract

Definitions of average speed, average acceleration, momentum and strength, along with the conservation theorems: impulse-momentum and work-energy a representative expression of the ergodic hypothesis for a particle, which is considered in statistical mechanics is obtained very regularly, this expression indicates that the spatial averages are equivalent to temporal averages, the validity of this expression for three cases is considered 1) rotational movement, i.e. working with the rotational analog of expression found where involving the torca concept in the rotational case, is also considered 2) a motion with acceleration time dependent, which is obtained as the product of kinetic energy by the change in time is exactly equal to the product of the change in momentum by displacement amounts in some way involving the necessary properties to establish the ergodic hypothesis, 3) finally we consider the behavior of a particle in a gravitational field, with these ideas in mind, the kinematics of a particle is solved. This proposal helps clarify the concepts surrounding the ergodic hypothesis used in statistical mechanics from first principles of physics with other basic concepts.

Keywords: Ergodic Hypothesis, Conservations Theorems, Fundamentals Concepts in Physics Education.

Resumen

A partir de las definiciones de velocidad media, aceleración media, momento y fuerza, junto con los teoremas de conservación: impulso-momento y trabajo-energía presentamos una expresión representativa de la hipótesis ergódica para una partícula, que es considerada en la mecánica estadística con mucha regularidad, esta hipótesis indica que los promedios espaciales son equivalentes a los promedios temporales, mostramos la validez de nuestra expresión para tres casos a considerar 1) movimiento rotacional, es decir, trabajamos con el análogo de la fuerza para la rotación es decir la torca, también se considera 2) una movimiento con aceleración dependiente del tiempo, se muestra como el producto de la energía cinética por el cambio en el tiempo es exactamente igual al producto de la variación del impulso por cantidades de desplazamiento de algún modo relacionadas con las propiedades necesarias para establecer la hipótesis ergódica, finalmente tenemos 3) el comportamiento de una partícula en un campo gravitatorio. Con estas ideas en mente, la cinemática de una partícula se resuelve. Esta propuesta ayuda a aclarar los conceptos que rodean la hipótesis ergódica utilizada en la mecánica estadística desde los primeros principios de la física con otros conceptos básicos.

Palabras clave: Hipótesis ergódica, Teoremas de conservación, Conceptos fundamentales de Educación en Física.

PACS: 01.40.gb, 01.40.gf, 01.55.+b, 01.30.Os **ISSN 1870-9095**

I. INTRODUCCIÓN

The ergodic hypothesis was introduced by Boltzmann to introduce the distribution function of a particle system to take the limit when the number of particles tends to infinity (limit $N \rightarrow \infty$).

The momentum of a particle in a conservative system satisfies the distribution that of statistical mechanics courses we have been presented as Maxwell-Boltzmann distribution.

Boltzmann showed that the probability that a particle have a moment $p \pm dp$, implies that the function in the limit of many particles approaches such distribution.

$$f(p \pm dp)=Exp[-\beta|p|^2]\, dp. \quad (1)$$

There is an important assumption behind the result of Boltzmann, this assumption is known as the ergodic hypothesis, which states that in statistical mechanics the relationship between theory and experiment is entirely consistent.

This Boltzmann ergodic hypothesis holds that "the temporal averages and ensemble averages must coincide in the limit of very long time" [1]. In other words: the temporal averages are equal to spatial averages for times very large.

With this hypothesis, those researchers working on molecular simulation can use two tools to study the behavior of particles: Molecular Dynamics simulation (MD) that solves the equations of motion for all particles in time and Monte Carlo simulation (MC) which moves in configuration space the positions of all the particles. However, to comparing specific properties of the system, both simulations lead to the same results [2].

In the elementary courses of classical mechanics are the concepts of position, mass and time as fundamental physical quantities, since they yield derived physical properties such as velocity, acceleration, force, and many others.

Based on these latter properties, it is possible to study and understand the movement, both its causes, such as how objects move.

By taking differences of time and position is dined the concept of average velocity. Then to take infinitesimal elements for the time and consequently to the position the instantaneous velocity is obtained.

The same applies to the concept of average acceleration, which corresponds to differences for the time and velocity in the velocity and time space, in the process limit as time approaches zero, the average acceleration becomes instantaneous acceleration.

Similarly one can define the concept of average force and the concept of instantaneous force; although it is true in physics textbooks [3] and calculus [4] are not presented as well.

On the other hand, in the regular courses in physics are two conservation theorems that are of paramount importance, the work-energy theorem which relates the kinetic and potential energy with the work done over to particle and the impulse-momentum theorem, which relates force for the change in momentum.

Generally these two theorems are presented in textbooks as independent theorems, although in both theorems the force is involved, while the first one are said to be external forces that produce the work, the second one says that they are impulsive forces *i.e.* those that produce a change in momentum, which act in extremely short times.

But what happens when a force compliance with these two features? That is, while is external is impulsive too, then when this happens we tie the two theorems and a result we obtain an expression that can be the source of the ergodic hypothesis.

Statistical mechanics is a branch of physics that in its simplest definition [2] provides a bridge between microscopic and microscopic properties of a system, it is then necessary to understand the macroscopic properties can be estimated as an average of the collective properties the system. And this is where the definitions and concepts of the fundamental physics of movement occupy a place of importance and superiority.

In this paper, from basic results of properties and theorems of classical mechanics, we have obtained an expression that allows us to understand the ergodic hypothesis, which we believe is based on two fundamental theorems of physics to conservative systems: the impulse-momentum theorem and the work-energy theorem.

Such theorems have been presented in textbooks as independent; however in this paper we establish their mutual relationship.

The paper proceeds as follows: Section 1 presents the basic physical concepts we need for the deduction, in section 2 we present the derivation of the expression for a particle, in section 3 we discuss the results and present some examples, finally section 4, we present our conclusions.

II. THEORY

A. Fundamental concepts

In the vector space for the position, physically the average velocity of a particle is defined as the rate of change of position per unit time:

$$\langle \boldsymbol{v} \rangle = \frac{\Delta \boldsymbol{r}}{\Delta t}. \tag{2}$$

Where Δr is the change of position: $\Delta r = r_f - r_o$ and Δt is the change in time $t = t_f - t_o$. Arithmetically the average velocity is the mean speed. In the simplest case we consider the simple average is:

$$\langle \boldsymbol{v} \rangle = \frac{1}{2}(\boldsymbol{v}_1 + \boldsymbol{v}_2). \tag{3}$$

Alternative expression for the average velocity. By dividing time into infinitesimal elements and consider the limit when approaching tf $\rightarrow$t0, the expression (1) becomes the instantaneous velocity. In terms of instantaneous velocity is defined the moment of the particle.

$$\boldsymbol{P} = m\boldsymbol{v}. \tag{4}$$

In the velocity space defined average acceleration of the particle as the rate of change of velocity per unit of time.

$$\langle \boldsymbol{a} \rangle = \frac{\Delta \boldsymbol{v}}{\Delta t}. \tag{5}$$

Newton's second law is:

$$\boldsymbol{F} = m\boldsymbol{a}. \tag{6}$$

The force (6) is the rate of change of the moment per unit time, which in terms of equations (2 and 5) the average force is defined as:

$$\boldsymbol{F} = \frac{\Delta \boldsymbol{P}}{\Delta t} = \frac{m\Delta \boldsymbol{v}}{\Delta t} = m\langle \boldsymbol{a} \rangle. \tag{7}$$

That in the limit as the time interval is infinitesimal we obtain the instantaneous force:

$$\boldsymbol{F} = \lim_{\Delta t \to \infty} \frac{\Delta \boldsymbol{P}}{\Delta t} = \frac{d\boldsymbol{P}}{dt}. \tag{8}$$

The expression (10) indicates that the force felt by the particle can be expressed as the rate of change of the moment, about the time it takes to make these changes.

B. Conservation theorems

The physical definition of work is the integral of the scalar product between the force and displacement:

$$W = \pm\int_{r_i}^{r} \boldsymbol{F} \cdot d\boldsymbol{r}. \tag{9}$$

For a particle of mass *m* moving with constant acceleration, and that both the acceleration vector as the displacement vector maintain the same direction, it is possible to demonstrate that expression of the work takes the following form:

$$W = \frac{1}{2} m\left(v_f^2 - v_0^2\right). \tag{10}$$

The translational kinetic energy[1] of the particle is also defined in terms of mass and velocity squared:

$$K = \frac{1}{2} m v^2. \tag{11}$$

If the particle is in an external field, *e.g.*, a gravitational field, it provides a contribution to the total energy of the particle, called energy potential [4] and it is denoted by (U ≈ energy potential.)

If we think in a gravitational field and calculate the work to move a particle from one position to another, either closer to the source of the field or away from it, is obtained the following result:

$$U = mg(\boldsymbol{r}_f - \boldsymbol{r}_o). \tag{12}$$

Where ($\boldsymbol{r}_f$ - $\boldsymbol{r}_0$) represents the change of position respect to the reference system.

Then as the system is conservative and based on the expressions shown for employment contributions for a single particle, equations (10) and (12), is presented the work-energy theorem:

$$\Delta K = W$$
$$\Delta U = -W. \tag{13}$$

That together giving rise to principle of conservation of total energy.

By integrating with respect to time the expression (8) is possible to find the impulse-momentum theorem:

$$\int_{t_0}^{t} \frac{d\boldsymbol{P}}{dt} \cdot dt = \int_{t_0}^{t} \boldsymbol{F} \cdot dt. \tag{14}$$

The left member of equality is resolved using the fundamental theorem of calculus, which indicates that the integral is evaluated in the variable, the corresponding limits of integration, that is:

$$\varDelta\boldsymbol{P} = \int_{t_0}^{t} \boldsymbol{F} \cdot dt = \boldsymbol{J}. \tag{15}$$

Where we have defined a new vector quantity J, called as the impulse. This result is deduced from Newton's second law, and thus represents a general result.

This result is presented in textbooks only in the case of impulsive forces acting in a very short time, such as a collision between two particles, for example.

It is said that the force should appear in the integral is an impulsive force, and the integration time is the time it takes for the collision to occur.

III. MODEL

If we start from the first equality of equation (13) and combine with equation (11) gives the equation (10) which can be written as follows:

$$\int_{r_0}^{r} \boldsymbol{F} \cdot d\boldsymbol{r} = \frac{1}{2} m\left(v_f^2 - v_0^2\right). \tag{16}$$

The equation (20) is correct because both sides of the equation are scalar quantities. It decomposes the difference of squares and the following is obtained:

$$\int_{r_0}^{r} \boldsymbol{F} \cdot d\boldsymbol{r} = \frac{1}{2} m\left(v_f - v_0\right)\left(v_f + v_0\right). \tag{17}$$

With use of the expression (3) can be written as:

$$\int_{r_0}^{r} \boldsymbol{F} \cdot d\boldsymbol{r} = m\langle v\rangle\left(v_f - v_0\right). \tag{18}$$

Or similarly

$$\int_{r_0}^{r} \boldsymbol{F} \cdot d\boldsymbol{r} = \langle \boldsymbol{v}\rangle \cdot \varDelta\boldsymbol{P}, \tag{19}$$

that use of the expression (17) can be written as:

$$\int_{r_0}^{r} \boldsymbol{F} \cdot d\boldsymbol{r} = \langle \boldsymbol{v}\rangle \cdot \int_{t_0}^{t} \boldsymbol{F} dt. \tag{20}$$

Now with the help of (2) we have:

$$\int_{r_0}^{r_f} \boldsymbol{F} \cdot d\boldsymbol{r} = \frac{\varDelta\boldsymbol{r}}{\varDelta t} \cdot \int_{t_0}^{t_f} \boldsymbol{F} dt \tag{21}$$

The angle between $\boldsymbol{F}$ and $\boldsymbol{r}$ on both sides of the equation (20) is the same, so we can write only in magnitude and multiplying the expression by the factor $1/\varDelta r$, to obtain:

$$\frac{1}{\varDelta r}\int_{r_0}^{r} F dr = \frac{1}{\varDelta t}\int_{t_0}^{t} F dt. \tag{22}$$

The expression (22) can be interpreted as follows:

For a single particle, the average force in the space of positions is equal to the average force over time. This seems to be the expression of the ergodic hypothesis used in statistical mechanics.

However, Boltzmann states the ergodic hypothesis is valid for large times.

IV. DISCUSSION

The result given in equation (22) has some implications. Note first that the fundamental representation of this expression is based on products of differences of two quantities. The left

[1] Of course there are different contributions to the kinetic energy, it is presented here is the translational contribution.

member is actually the kinetic energy change divided by the spatial change, while the right side is represented by the change in momentum divided by the temporary change.

$$\Delta K\,\Delta t = \Delta P \Delta r. \quad (23)$$

The change of kinetic energy time's change of time is equal to the change of momentum time's change of position. This latest product, viewed from a quantum perspective corresponds to the uncertainty principle Heisenberg[2].

When performing a dimensional analysis for both expressions, we note that both sides of equality units are units of energy per unit of time [E] [T]. In the International System would Js.

To verify the accuracy of this result and thus the above is an example here.

A. Example 1 free falling

Suppose a particle of mass m, is located within a gravitational field. The particle is drawn from a height H, to the ground.

Obviously this example can be solved through energy conservation theorems or using the kinematic equations for motion uniformly accelerated. Consider that the starting point where the movement is at the height H and the end point at the origin of the coordinate system[3], then we define energy: kinetic, potential and total as follows:

TABLE I. Different contribution of energy to free falling.

	K	*U*	*E*
start	*0*	*mgH*	*mgH*
finish	$mv_f^2/2$	*0*	$mv_f^2/2$
Δ	$mv_f^2/2$	*mgH*	*0*

As shown in the table, the total energy the beginning and the end is the same, we can equate these contributions and obtain the value of the velocity at the final point.

$$v = \sqrt{2gH}. \quad (24)$$

Using the kinematics equations, we calculate the time it takes the fall Δt of the particle. The equations of motion for this case are as follows:

$$\Delta y = y_f - y_0 = -\tfrac{1}{2} g \Delta t^2$$
$$\Delta v = v_f - v_0 = -g\Delta t. \quad (25)$$

Of course both y_f as well as v_0 are zero according to the reference system, using the results in Table I we obtain:

$$\Delta y = y_f - y_0 = -H$$
$$\Delta v = v_f - v_0 = -\sqrt{2gH}. \quad (26)$$

That based on the equations (24-26), we can verify the expression (22)

$$\Delta K \Delta t = \Delta P \Delta r$$
$$\tfrac{1}{2} 2mgH\left(\tfrac{\sqrt{2gH}}{g}\right) = -m\sqrt{2gH}(-H) \quad (27)$$
$$mH\left(\sqrt{2gH}\right) = m\sqrt{2gH}(H).$$

Of course, it is clear that for all the movements relation MUA and MRU (29) is true, so it is important to see a more complete kind of movement and verify validity.

B. Example 2 Rotational Motion

Suppose a rigid system with moment of inertia I, rotating about a fixed axis, with radius R, and moves at an angle φ, from an initial angle φ_0.

For the rotational case is evident that they must change the expression (21-23) which rewrite as follows:

$$\frac{1}{\Delta\phi}\int_{\phi_i}^{\phi} \tau\, d\phi = \frac{1}{\Delta t}\int_{t_i}^{t} \tau\, dt. \quad (28)$$

That satisfies the relation:

$$\Delta K_r \Delta t = \Delta L \Delta\phi. \quad (29)$$

Where K_R is the rotational kinetic energy, L is the angular momentum of the system. In this case, the system rotates without moving, the contribution of potential energy is the same before and after the rotate, we know that under the following relationships:

$$\Delta K_r = \tfrac{1}{2}\left(w_f^2 - w_0^2\right)$$
$$\Delta L = I\left(w_f - w_0\right). \quad (30)$$

According to the equations of rotational kinematics we know that:

$$\Delta\phi = \tfrac{1}{2}\left(w_f + w_0\right)\Delta t. \quad (31)$$

That substituting the expressions (37-39) in (36) we obtain the following expressions:

$$\tfrac{1}{2} I\left(w_f^2 - w_0^2\right)\Delta t = I\left(w_f - w_0\right)\tfrac{1}{2}\left(w_f + w_0\right)\Delta t. \quad (32)$$

Where again is obtained the equal results.

[2] We're not saying that this expression is the equivalent of the uncertainty principle in its classical treatment, only commented that the product of the change in time and change in the position are known.

[3] We locate the origin of the coordinate system on the ground, where the potential energy is set to zero.

C. Example 3 Motion with time-dependent acceleration

Suppose now that the position, velocity and acceleration are time dependent functions, an example is the mass-spring system that leads to simple harmonic motion for small oscillations.

If we proceed as for average velocity and acceleration, where infinitesimal elements are taken for the time we know that $\Delta t \rightarrow 0$ and $\Delta r \rightarrow 0$, therefore we obtain the spatial and temporal derivative in equations (2 and 5). Then we take infinitesimal elements of time and write the equation (23) in terms of derivatives.

$$\frac{dK}{dr} = \frac{dP}{dt}. \quad (33)$$

The right-we know because we know that is the force acting on the particle, the left side seems a fallacy. Since we know that kinetic energy is a function of velocity squared, therefore, claimed as a dependent of the position is unheard of, I even read it produce itching. However, by applying the chain rule gives the following:

$$\frac{dK}{dr} = \frac{dK}{dv} \cdot \frac{dv}{dt} \cdot \frac{dt}{dr}. \quad (34)$$

Since the translational kinetic energy is defined by (11), then the first derivative is given by:

$$\frac{dK}{dv} = \frac{1}{2} m \frac{dv^2}{dv} = mv. \quad (35)$$

The second derivative in (34) is just the acceleration, and the third derivative yields the reciprocal of the velocity, so we have as a result:

$$\frac{dK}{dr} = \frac{mva}{v} = ma. \quad (36)$$

After all, this result is known from the work-energy theorem equation (13), that integrating this expression with respect to the position on both sides of the equation, it retrieves the theorem. Then, we known three expressions for the force experienced by a particle, namely:

$$F = \frac{dK}{dr} = -\frac{dU}{dr} = \frac{dP}{dt}. \quad (37)$$

In considering the following equality

$$F = \frac{dK}{dr} = \frac{dP}{dt}. \quad (38)$$

We can write as follows:

$$\frac{dK}{dr} - \frac{dP}{dt} = 0. \quad (40)$$

that applying the chain rule we obtain the first member:

$$\frac{dK}{dr} = \frac{dK}{dt} \cdot \frac{dt}{dr} = \frac{1}{v} \frac{dK}{dt}. \quad (41)$$

that substituting the expression (41) in (40) is possible to write as:

$$\frac{1}{v} \frac{dK}{dt} - \frac{dP}{dt} = 0$$

$$\frac{1}{v}\left[\frac{dK}{dt} - v \frac{dP}{dt} \right] = 0. \quad (42)$$

What follows the expression of power, defined as the rate of change of kinetic energy with respect to time, in another way: as the product of force and velocity.

But perhaps the most improbable given to making equality between the first two members of the right side of the expression (37).

$$\frac{dK}{dr} + \frac{dU}{dr} = 0. \quad (43)$$

Implies that:

$$\frac{d}{dr}[K + U] = \frac{d}{dr}[E] = 0. \quad (44)$$

Indicates that for a conservative system, the derivative of the total energy with respect to the position is constant, which is then the key point in this discussion, because if on the one hand we have the energy change with time is constant and other side is that we establish that the change of energy with respect to the position is also constant, then it makes much sense to say that spatial averages are also equivalent to the average time for a conservative system.

VI. CONCLUSIONS

We presented that the ergodic hypothesis is satisfied for a single particle, where an average of the force that drives the particle to get moving, held in position space is exactly equal to an average of this same force in time.

This result implies a ratio of products changes only apply to cases where the acceleration is constant, where translational and rotational acceleration variable systems are not out of this result.

We are extending this result to a system of many particles, where the sum of the internal forces produce no movement of displacement for the center of mass of the system, however, each particle receives the effects of other particles in the system, and the effect of is that within the particles are moving, as is the case of the intermolecular interaction force that is present in a fluid system, where his statistical study of the ergodic hypothesis requires.

ACKNOWLEDGEMENTS

The authors wish to express our gratitude to the Universidad Autónoma Metropolitana and particularly the area of Molecular Atomic Applied Physics (FAMA), for the facilities provided for the preparation of this work.

REFERENCES

[1] Tolman, R. C., *The principles of Statistical Mechanics*, (Dover Publications, New York, 1979).
[2] McQuarrie, D. A., *Statistical thermodynamics*, (Harper and Row, New York, 1973).
[3] Resnick, R., Halliday, D., Krane, K., *Physics Vol. 1*, 5th Ed., (John Wiley &Sons, 2002).
[4] Sokowsky, E. W., *Cálculo con geometría analítica*, 2ª Ed., (Grupo Editorial Iberoamericana, México, 1989).