Understanding Virial theorem

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Abstract

In this article, we differentiate between the Virial Theorem and the Virial Relation, and obtain the virial relations for simple, additive, and polynomial-type potentials. We also stress the need to introduce the Virial Theorem in detail in undergraduate studies.

1 Introduction

In mechanics classes, many theorems are taught, and among them, the virial theorem often receives little prominence despite its great usefulness [1, 2, 3, 4]. In practice, the virial theorem is widely used in many branches of physics, such as astrophysics and statistical mechanics [5, 6]. In fact, the virial theorem can be used to introduce the famous "Particle in a Box" problem in quantum mechanics, with the help of Cauchy's boundary conditions [7]. Frank Rioux, in his paper [8], presented the use of the virial theorem in an introductory chemistry undergraduate classroom to study chemical bonding in molecules. Thus, introducing the virial theorem in a clear and concise manner in undergraduate classrooms is essential [9]. Instead of using conventional examples like oscillators, developing the virial theorem for nonlinear oscillators is also useful and simple, which will later help students tackle problems in quantum mechanics [10]. Let us first introduce the virial theorem in the next section.

2 Virial Theorem- A Recap

The virial theorem [VT], derived by Clausius, gives the relation between the average kinetic energy and the virial of a system. First, we will have a recap of the virial theorem. Let

$$G = \sum_i \vec{p}_i \cdot \vec{r}_i \tag{1}$$

where G is the product of the momentum and the position of the particle in a bounded system [11]. Taking the time derivative,

$$\frac{dG}{dt} = \sum_i \left[\frac{d\vec{p}_i}{dt} \cdot \vec{r}_i + \vec{p}_i \cdot \frac{d\vec{r}_i}{dt} \right] \quad (2)$$

Here, the first term on the right side is

$$\sum_i \vec{F}_i \cdot \vec{r}_i$$

where $\vec{p}_i = \vec{F}_i$. The second term

$$\sum_i \vec{p}_i \cdot \frac{d\vec{r}_i}{dt} = \sum_i (m\dot{\vec{r}}_i) \cdot \dot{\vec{r}}_i = m(\dot{\vec{r}}_i)^2 = 2K$$

So Eq. 2 becomes

$$\frac{dG}{dt} = \sum_i \vec{F}_i \cdot \vec{r}_i + 2K \quad (3)$$

If the quantity G is bounded [12] in a time interval, then

$$\frac{1}{\tau} \int_0^\tau \frac{dG}{dt} dt = \frac{1}{\tau}(G(\tau) - G(0)) = 0 \quad (4)$$

The gravitational system of planets is an example of a bounded system. The planets of the gravitational system go in regular orbits, and G, any periodic function, will vary between two finite values. The positions and velocities of particles will have upper and lower limits. Then, the time average goes to zero for a large value of τ. A harmonic oscillator bounded by an elastic force and a hydrogen atom bounded by an electrostatic force are other examples where G is bounded. So, for a bounded system, from Eqs. 3 and 4 , we have

$$2\langle K \rangle = -\sum_i \langle F_i \cdot r_i \rangle \quad (5)$$

The symbol $\langle \ \rangle$ represents the time average. Let

$$\mathcal{V} = \sum_i \langle F_i \cdot r_i \rangle \quad (6)$$

where $\mathcal{V}$ is called the virial. Then

$$2\langle K \rangle = -\mathcal{V}$$

Eq. 6 is the virial theorem (VT) in classical mechanics. Note that the kinetic energy considered here is $\frac{1}{2}m\dot{r}^2$, which is for non-relativistic particles.

3 Virial Relation

For any conservative force $\vec{F}$, we can write

$$\vec{F} = -\nabla V$$

where V is the potential energy (PE). All bounded forces are conservative forces. Then, Eq.5 for all particles can be written as

$$2\langle K \rangle = \langle \nabla V \cdot \vec{r} \rangle \quad (7)$$

where V is the PE of the system. For example, if the PE for a system is $V = K' r^a$, where K' is the force constant, we get

$$2\langle K \rangle = a\langle V \rangle \quad (8)$$

where a is a constant. Similarly, for any system, if the Hamiltonian is given, we can find the relation between the average kinetic energy (KE) and the average potential energy (PE), and such a relation is called the Virial relation (VR). Thus, the relation between kinetic energy and the *virial* is called the Virial theorem, and the relation between kinetic energy and potential energy obtained from the Virial theorem is called the Virial relation.

3.1 Some examples for VR

1. In the case of a linear harmonic oscillator, $V = \frac{1}{2}K'r^2$ where K' is the force constant. Then

$$\langle \nabla V \cdot \vec{r} \rangle = 2\langle V \rangle$$

$$2\langle K \rangle = 2\langle V \rangle$$

or the virial relation is

$$\langle K \rangle = \langle V \rangle$$

2. In the gravitational problems $V = \frac{-GMm}{r}$. Then

$$\langle \nabla V.\vec{r} \rangle = -\langle V \rangle$$

The VR is

$$2\langle K \rangle = -\langle V \rangle$$

3. For a pure quartic oscillator, $V = \frac{1}{4}K'r^4$. Then

$$\langle \nabla V.\vec{r} \rangle = 4\langle V \rangle$$

$$2\langle K \rangle = 4\langle V \rangle$$

or VR is

$$\langle K \rangle = 2\langle V \rangle$$

From the virial relation, we can find some unknown parameters of the system by finding KE and PE[8, 9]. We give a simple example of finding the average radius of a hydrogen atom[13]. The PE of hydrogen atom is $\frac{-e^2}{4\pi\epsilon_0 r}$ and the virial relation is

$$2\langle K \rangle = -\langle V \rangle$$

The total energy

$$\langle E \rangle = \langle K \rangle + \langle V \rangle = \frac{\langle V \rangle}{2} = -\frac{1}{2}\langle \frac{e^2}{4\pi\epsilon_0 r} \rangle$$

But we know that the energy of the n^{th} state is

$$E_n = \frac{-2m\pi^2}{h^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{n^2}$$

Comparing we get the average radius of the atom as

$$\langle \frac{1}{r} \rangle_n = \frac{1}{a_0 n^2}$$

where $a_0 = 5.29 \times 10^{-11} m$ is the Bohr radius. For the first orbit the radius of the hydrogen atom is $5.29 \times 10^{-11} m$ and for the second orbit it is $21.16 \times 10^{-11} m$ which matches with the results earlier obtained.

4 VR for more potential energies

All the systems we dealt with have potential energy (PE) in a simple and familiar form. In some systems, PE contains terms with more than one variable, like $V = x^2y^2$ (polynomial type), and in some other systems, PE consists of several terms like $V = x^2 + y^2$ (additive type). In all these cases, the method to derive the virial relation is not the same as mentioned earlier.

For example, in the case of a coupled quartic oscillator, the PE for the N=2 model is

$$V(x, y) = \frac{(1-\alpha)}{12}(x^4 + y^4) + \frac{1}{2}x^2y^2$$

where α is a constant [14]. This potential energy is of the form

$$V(x,y) = A(x^4 + y^4) + Bx^2y^2$$

It contains a polynomial term and also is an additive potential. Many similar potentials are available for oscillators, such as the Henon-Heiles oscillator [15], the Van der Pol oscillator [16], and the Duffing oscillator [17].

In the next two subsections, we will apply the virial theorem (VT) for additive and polynomial-type potential energies and find the virial relation (VR).

4.1 VR for Polynomial-Type Potential Energies

Let

$$V = {q_1}^{n_1}{q_2}^{n_2}{q_3}^{n_3}$$

Then

$$\nabla V \cdot \vec{r} = (n_1{q_1}^{n_1}{q_2}^{n_2}{q_3}^{n_3}$$

$$+n_2{q_1}^{n_1}{q_2}^{n_2}{q_3}^{n_3} + n_3{q_1}^{n_1}{q_2}^{n_2}{q_3}^{n_3})$$

$$\nabla V \cdot \vec{r} = (n_1 + n_2 + n_3)V$$

So for $V = {q_1}^{n_1}{q_2}^{n_2}.....{q_m}^{n_m}$

$$\nabla V \cdot \vec{r} = \sum_{i=1}^{m} n_i V \tag{9}$$

Here, we can write $\langle \nabla V.\vec{r} \rangle = a\langle V \rangle$, since $\sum_{i=1}^{m} n_i$ will be a number. So, the VR for polynomial-type potential energies is

$$2\langle K \rangle = \left(\sum_{i=1}^{m} n_i\right) \langle V \rangle \tag{10}$$

Example
Let

$$V = x^2y^2$$

$$\nabla V \cdot \vec{r} = 2x^2y^2 + 2x^2y^2 = 4V$$

$$\nabla V \cdot \vec{r} = (n_1 + n_2)V$$

where $n_1 = 2$ and $n_2 = 2$. Hence, the VR is

$$\langle K \rangle = 2\langle V \rangle$$

4.2 VR for additive potential energies

Let

$$V = V_1 + V_2 = {q_1}^{n_1} + {q_2}^{n_2}$$

$$\nabla V \cdot \vec{r} = n_1{q_1}^{n_1} + n_2{q_2}^{n_2} = n_1V_1 + n_2V_2$$

In general if

$$V = \sum_{i=1}^{m} {q_i}^{n_i} \tag{11}$$

$$2\langle K \rangle = \langle \sum_{i=1}^{m} n_i V_i \rangle \tag{12}$$

If $n_i's$ are same $(n_i = n)$ then we can write $\langle \nabla V.\vec{r} \rangle = a\langle V \rangle$.

5 Conclusions

Unknown secrets about matter in the universe were revealed by the introduction of dark matter, and its initial studies were conducted with the help of the virial theorem. Such studies motivated many to undertake research on the virial theorem in a more comprehensive way. However, in many courses, the virial theorem is not given sufficient importance, one reason being that many popular textbooks do not adequately cover it. We suggest that the various applications of the virial theorem and its immense scope must be introduced in all undergraduate physics studies. This work, we hope, may serve as a catalyst for this purpose

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