

# A GENERAL EXPRESSION FOR EQUIPARTITION OF ENERGY

## UNA EXPRESIÓN GENERAL PARA LA EQUIPARTICIÓN DE LA ENERGÍA

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### I. INTRODUCTION

Equipartition theorem (EPT) is a very useful result obtained in thermodynamics. There were many physicists behind the development of this great concept. Rief [1], a famous author of the statistical physics book “Fundamentals of Statistical and Thermal Physics” wrote about the equipartition theorem as “If a system described by classical statistical mechanics is in equilibrium at the absolute temperature T, every independent quadratic term in its energy has a mean value equal to  $\frac{1}{2}kT$ .” It was John James Waterston [2] who proposed the equipartition of energy first. Maxwell [3] and Boltzmann had also contributed to the theorem of equipartition. In order to find the energy distribution in black body radiation, Lord Rayleigh [4] used equipartition theorem. Those phenomena which were not in accordance with the EPT were later solved by the quantum theory [5,6]. Just like Rief many other authors considered systems with quadratic Hamiltonian, while non quadratic systems were not analyzed in their respective publications [1,7–10]. Recently using Tolman’s theorem [11] we [12] developed a general expression for the EPT which is applicable to non quadratic Hamiltonian also, which is given below.

$$\langle E \rangle = \frac{DNkT}{l}, \tag{1}$$

where  $l$  is the power of energy function,  $N$  is the number of particles,  $k$  is the Boltzmann constant,  $T$  is the absolute temperature and  $D$  is the dimension. In the above mentioned paper we used only simple non quadratic Hamiltonian. But in this paper we develop a general expression for any type of Hamiltonian that can be expressed in polynomial form. Finally we applied the general equation to two nonlinear Hamiltonians which contain all possible combinations of position and momentum to find the internal energy.

### II. FINDING AVERAGE ENERGY

In this paper our aim is not to redefine the EPT, but to find an expression for average energy for some Hamiltonian’s in the polynomial form. We will do this only for one dimensional Hamiltonian, which can be extended to  $D$  dimension. Usually

we apply the EPT for systems with Hamiltonian having one or several terms with each term of the form  $q^l$  where  $q$  is momentum or position variable and  $l$  is the power of that variable and we get the average energy using Tolman’s theorem given by the equation

$$\left\langle q \frac{\partial H}{\partial q} \right\rangle = kT. \tag{2}$$

But if we have a Hamiltonian containing terms like  $q_1q_2$  (product of two variables) or  $q_1^2q_2$ , we cannot apply the above method to find the average energy. Hence, we find the average energy using Statistical Mechanics and then formulate a general expression. First we find the partition function and then we separate the partition function into temperature dependent and independent terms and then find the average energy.

### III. GENERAL EXPRESSION FOR THE EQUIPARTITION OF ENERGY

If we have a Hamiltonian with  $n$  variables  $q_1, q_2, q_3, \dots, q_n$  with powers  $l_1, l_2, l_3, \dots, l_n$  like

$$H = \prod_i a_i q_i^{l_i},$$

where  $i$  is from 1 to  $n$  and  $a_i$ ’s are constants.

This will contribute

$$\langle E \rangle = \frac{nkT}{\sum_{i=1}^n l_i},$$

towards the internal energy where  $\sum_{i=1}^n l_i$  should not be zero.

Hamiltonian

$$H = a_1 q_1^{l_1} a_2 q_2^{l_2} a_3 q_3^{l_3} \dots a_n q_n^{l_n} = \prod_i a_i q_i^{l_i}.$$

Single particle partition function

$$Q = C_1 \int_a^b dq_1 dq_2 dq_3 \dots dq_n e^{-\frac{1}{kT} \left( \prod_i a_i q_i^{l_i} \right)},$$

where  $C_1$  is a constant.

$$Q = C_1 \int_a^b dq_1 dq_2 dq_3 \dots dq_n e^{-\frac{\prod_i a_i}{k} \left( \frac{q_1^{l_1} q_2^{l_2} \dots q_n^{l_n}}{T} \right)}$$

Now we will separate the partition function into temperature dependent and independent terms by the change of variables. We know from the EPT for a single variable that for any arbitrary variable  $q^n$ , average energy is  $\frac{DkT}{n}$ . Thus the contribution from each  $q$  will depend on its power. If  $q_i$ 's have the same power then they contribute equally to the energy. Then we will divide  $T$  equally to all the  $q_i$ 's. If  $q_i$ 's have different power then we have to find the ratio of the powers and then divide  $T$  in that ratio. That is each  $q_i^{l_i}$  will

be divided by  $T^{\frac{l_i}{\sum_i l_i}}$ .

$$Q = C_1 \int_a^b dq_1 dq_2 \dots dq_n e^{-\frac{\prod_i a_i}{k} \left( \frac{q_1^{l_1}}{T^{\frac{l_1}{\sum_i l_i}}} \frac{q_2^{l_2}}{T^{\frac{l_2}{\sum_i l_i}}} \dots \frac{q_n^{l_n}}{T^{\frac{l_n}{\sum_i l_i}}} \right)}$$

Putting  $\frac{q_1}{T^{\frac{l_1}{\sum_i l_i}}} = q_1'$ ,  $\frac{q_2}{T^{\frac{l_2}{\sum_i l_i}}} = q_2'$ , ...,  $\frac{q_n}{T^{\frac{l_n}{\sum_i l_i}}} = q_n'$  we get the partition function as

$$Q = CT^{\frac{n}{\sum_{i=1}^n l_i}},$$

where  $C$  is independent of temperature. Then the average energy

$$U = \frac{nkT}{\sum_{i=1}^n l_i}.$$

### III.1. Note 1

If  $\sum_{i=1}^n l_i = 0$  like  $l_2 = -l_1$  or  $l_3 = -(l_1 + l_2)$  we get zero in the denominator. Such cases cannot occur because, then their contribution to the energy will be zero and we cannot have a formula like this.

### III.2. Note 2

We took the limits of the integral as  $a$  to  $b$ . In case of potentials with even exponents the limits are from  $-\infty$  to  $\infty$ . Here if the  $l_i$ 's are odd we take the modulus of  $q_i$  or we have to take the limit from 0 to infinity. Such issues usually occur in statistical mechanics. For example if we are taking the gravitation potential  $V = mgz$ ,  $z$  is the height from the earth and we can take the limit only from 0 to  $\infty$ .

## IV. EXAMPLES

We will work out one example using the same procedure as above. After confirming that our general formula will work we will apply for other Hamiltonian forms.

### IV.1. Two different position variables with same power

1. Consider a potential of the form  $V = Kxy$ . Then let the Hamiltonian be

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + Kxy.$$

Here we already know the contribution from first two terms ( $\frac{kT}{2}$  each) which contains only one variable. We have to find out the contribution by the term  $Kxy$  towards average energy. For that we will find the average energy by the whole Hamiltonian and then subtract the contribution by the first two terms. Single particle partition function is

$$Q_1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dp_x dp_y dx dy}{h^2} e^{-\frac{1}{kT} \left( \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + Kxy \right)},$$

Putting  $\frac{p_x}{T^{\frac{1}{2}}} = p_x'$ ,  $\frac{p_y}{T^{\frac{1}{2}}} = p_y'$ ,  $\frac{x}{T^{\frac{1}{2}}} = x'$ ,  $\frac{y}{T^{\frac{1}{2}}} = y'$

$$Q_1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{T^{\frac{1}{2}} dp_x' T^{\frac{1}{2}} dp_y' T^{\frac{1}{2}} dx' T^{\frac{1}{2}} dy'}{h^2} e^{-\frac{1}{k} \left( \frac{p_x'^2}{2m} + \frac{p_y'^2}{2m} + Kx'y' \right)}.$$

We get  $Q_1 = CT^2$  where  $C$  is independent of  $T$ .

$$U = kT^2 \frac{\partial \ln CT^2}{\partial T} = 2kT.$$

We can see that potential energy  $V = Kxy$  alone contributes  $kT$  towards internal energy, since the 2 dimensional kinetic energy contributes  $kT$ . Now we can find the same by using our general expression. We have

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{1+1} = kT.$$

2. Take another potential  $V = Kx^2y^2 = K(xy)^2$

Here  $n = 2$ ,  $l_1 = 2$  and  $l_2 = 2$ .

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{2+2} = \frac{kT}{2}.$$

Similarly we can show that  $V = K(xy)^3$  contributes  $\frac{1}{3}kT$ ,  $V = K(xy)^4$  contributes  $\frac{1}{4}kT$  towards internal energy.

### IV.2. Two position variables with same power with $l$ negative

1.  $V = \frac{K}{xy}$

Here  $n = 2$ ,  $l_1 = -1$  and  $l_2 = -1$ . So

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{-1-1} = \frac{kT}{-1}.$$

2.  $V = \frac{K}{x^2y^2} = \frac{K}{(xy)^2}$

Here  $n = 2$ ,  $l_1 = -2$  and  $l_2 = -2$ .

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{-2-2} = \frac{kT}{-2}.$$

Similarly we can show that  $V = \frac{K}{(xy)^3}$  contributes  $\frac{kT}{-3}$ , and  $V = \frac{K}{(xy)^4}$  contributes  $\frac{kT}{-4}$  towards internal energy.

#### IV.3. Two position variables with different powers

1. For a potential  $V = Kx y^2$

$n = 2, l_1 = 1$  and  $l_2 = 2$ .

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{1+2} = \frac{2kT}{3}.$$

So  $V = Kx y^2$  contributes  $\frac{2}{3}kT$  towards internal energy.

2.  $V = Kx y^3$

Here  $n = 2, l_1 = 1$  and  $l_2 = 3$ .

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{1+3} = \frac{kT}{2}.$$

#### IV.4. Two position variables with different powers with $l_1$ and $l_2$ negative

$$V = \frac{K}{xy^2}$$

Here  $n = 2, l_1 = -1$  and  $l_2 = -2$ . By using our general expression

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{-1-2} = \frac{-2kT}{3}.$$

#### IV.5. Position and momentum variables with same and different powers

1.  $H = xp_x$

Here  $n = 2, l_1 = 1$  and  $l_2 = 1$ .

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{1+1} = kT.$$

2.  $H = x^2 p_x$

Here  $n = 2, l_1 = 2$  and  $l_2 = 1$ .

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{2kT}{2+1} = \frac{2kT}{3}.$$

3.  $H = x^2 y^4 p_x p_y^2$

Here  $n = 4, l_1 = 2, l_2 = 3, l_3 = 1$  and  $l_4 = 2$ . So

$$U = \frac{nkT}{\sum_{i=1}^n l_i} = \frac{4kT}{2+4+1+2} = \frac{4kT}{9}.$$

### V. TWO NONLINEAR OSCILLATORS

#### V.1. Henon Heiles oscillator

In 1964 Michel Henon and Carl Heiles published an article titled "The applicability of the third integral of motion: Some numerical experiments" [13]. Their idea was to find a third integral of motion in a galactic dynamics. For that purpose they took a simplified two dimensional nonlinear

axi-symmetric potential. They showed that this potential is equivalent to the problem of the motion a particle in a plane in an arbitrary potential. After several trials they took the following potential for study

$$V(x, y) = \frac{1}{2}x^2 + \frac{1}{2}y^2 - \frac{1}{3}y^3 + x^2 y.$$

The Hamiltonian of a Henon Heiles oscillator is

$$H = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \frac{1}{2}x^2 + \frac{1}{2}y^2 - \frac{1}{3}y^3 + x^2 y.$$

In this Hamiltonian we have both  $x$  and  $y$  coordinates coming together. We had avoided constants with each component necessary for dimensional balance, which are not required for our purpose.

#### V.2. Van der pol oscillator

The Van der pol oscillator is an oscillator with non-linear damping obtained by Balthazar Van der pol, a Dutch electrical engineer who initiated modern experimental dynamics in the laboratory during the 1920's and 1930's. He first introduced this oscillator [14] in order to describe triode oscillations in electrical circuits. The Hamiltonian of Van der Pol oscillator [15] is

$$H = p_x p_y + xy - \mu(1 - x^2) y p_y.$$

In this Hamiltonian we have different combinations of position and momentum coordinates. Thus we had two different types of Hamiltonian which contain different combinations of position and momentum so that can apply the general equation for the EPT.

### VI. APPLICATION OF THE GENERAL EQUATION

We will now apply our new expression to find the average energy of HHO and VPO oscillators. Based on the above Hamiltonian, the internal energy of a Henon Heiles oscillator is

$$U = \frac{kT}{2} + \frac{kT}{2} + \frac{kT}{2} + \frac{kT}{2} + \frac{kT}{3} + \frac{2}{3}kT = 3kT.$$

For a Vander pol oscillator we get

$$U = kT + kT + \frac{3}{4}kT + kT = \frac{15}{4}kT.$$

We had shown that it is very easy to find the internal energy of any complicated Hamiltonian using our expression. Otherwise using statistical mechanics to obtain internal energy would be very difficult [16].

### VII. CONCLUSION

We developed a general expression for the equipartition theorem, which is applicable for all types of Hamiltonian appearing in the form of a polynomial. Using this general EPT we obtained the average energy of Henon Heiles and Van der Pol oscillators very easily.

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