

Exact calculation of the number of degrees of freedom of a rigid body composed of n particles

J. Bernal, R. Flowers-Cano, and A. Carbajal-Dominguez

Universidad Juárez Autónoma de Tabasco,

km. 1 Carretera Cunduacán-Jalpa, Cunduacán, Tabasco, 86690, México,

e-mail: jorge.bernal@dacb.ujat.mx, flowerscano@hotmail.com,

adrian.carbajal@dacb.ujat.mx

Recibido el 14 de agosto de 2009; aceptado el 10 de septiembre de 2009

In this work we correct a calculation made by Albert Einstein that appears in his book titled *The Meaning of Relativity* (Princeton, 1953), and by means of which he tries to obtain the number of degrees of freedom of a system composed of n particles with fixed relative distances and which are immersed in a three-dimensional space. As a result of our analysis, we develop expressions which yield the number of degrees of freedom of an analogous system, not only in three, but in any arbitrary number D of dimensions.

Keywords: Degrees of freedom; rigid body; ideal gas; heat capacity.

En este trabajo se corrige el cálculo hecho por Einstein que aparece en su libro titulado “The meaning of Relativity” (Princeton, 1953), por medio del cual él trata de obtener el número de grados de libertad para un sistema constituido por n partículas, cuyas distancias se mantienen fijas y que se encuentran en un espacio tridimensional. Como resultado del presente análisis, se desarrollan expresiones que permiten hallar el número correcto de grados de libertad de sistemas como el descrito, además de las correspondientes generalizaciones para un espacio de dimensión arbitraria D .

Descriptores: Grados de libertad; cuerpo rígido; gas ideal; calores específicos.

PACS: 45.05.+x; 45.40.-f; 45.50.-j

The number of independent coordinate variables needed to simultaneously determine the position of every particle in a dynamical system is called the number of degrees of freedom of that system. So a system of n free particles in a three-dimensional space has $3n$ degrees of freedom, because three coordinates are needed to specify the location of the center of mass of each particle. However, if the particles are no longer all free, but there are restrictions imposed on the system, the number of degrees of freedom will be less than $3n$; $3n$ coordinates are still needed to locate the centers of mass, but less than $3n$ values are assignable at will to the coordinate variables [1]. Specifically, we are interested in the system made up of n particles in three-dimensional space, which hold fixed distances between them. For the sake of clarity, this system will be referred to from now on as S_3 , and the number of its degrees of freedom will be referred to as N_3 .

Usually, N_3 is calculated by giving S_3 the treatment of a rigid body. Mechanics recognizes two types of rigid bodies: those made up of a continuous distribution of mass; and those formed by n mass points joined by rigid links [2]. Thus, S_3 is equivalent to a rigid body of the second type.

It is not difficult to calculate the number of degrees of freedom of a rigid body of continuous mass. For most cases, the number of degrees of freedom is six, as three coordinates are needed to locate the body’s center of mass and three more to describe its orientation [1, 2]. But if the mass is all distributed along a single line, then it will be impossible for the body to rotate about that line, and therefore, such a body has only five degrees of freedom [2, 3]. A similar reasoning is used to calculate N_3 , after assuming that S_3 may be viewed

as a sole body instead of a collection of particles. Hence, N_3 is five when $n = 2$, since the mass points lie all along the same line, and is six when $n > 2$ [4]. The case in which $n > 2$ particles all lie on the same line will not be considered in this work.

These same results should be attainable through individual consideration of the particles which make up S_3 . Counting the number of degrees of freedom of S_3 is fairly easy when n is equal to two: six coordinates are needed to locate the centers of mass of the particles, but there is one restriction (one rigid link), so the number of degrees of freedom of S_3 is five. It is not hard either to calculate the number of degrees of freedom of S_3 when $n = 3$. Thus, nine coordinates are needed to specify the positions of the particles’ centers of mass; but since there are three restrictions, the number of degrees of freedom is six. That is, if the triad does not lie all along the same line; if that is so, there are four restrictions and the number of degrees of freedom of the system is again five.

The operation of calculating N_3 by consideration of the individual particles would be much easier if an expression were developed that would yield the number of degrees of freedom of S_3 for any given value of n . Albert Einstein figures among those who tried to develop just such an expression. Einstein dealt with this problem in one of his books [5], using it as an example of the importance that geometrical concepts have a correspondence with real objects. He reasoned more or less along the following lines:

If one particle (let this particle be called particle 1) is arbitrarily chosen from among the n that compose S_3 , $n-1$ equa-

tions are needed to express the fact that this particle holds fixed distances with the rest

$$(x_j - x_1)^2 + (y_j - y_1)^2 + (z_j - z_1)^2 = d \quad (1)$$

where d is a constant and $j = 1, 2, 3, \dots, n$

But when a second particle is taken into consideration, to express that the distances between this and the other particles remain constant, only $n - 2$ equations are needed, because the equation that shows that the distance between particles 1 and 2 is constant is already included in (1). If a third particle is considered, there would be $n - 3$ equations more; for a fourth particle, there would be $n - 4$ equations more, and so on. In total, there are $n(n - 1)/2$ different equations. These equations represent the system's restrictions; they are the constraint equations of the system.

Einstein must have thought that he would obtain the number of degrees of freedom of S_3 merely by subtracting the number of constraint equations from $3n$:

$$N_3 = 3n - \frac{n(n-1)}{2} \quad (2)$$

If (2) is solved for $n > 4$, it will be seen that the values of N_3 differ from those obtained when S_3 was viewed as a single body. Why does this happen? Maybe because it is not appropriate to consider the collection of particles with rigid links as one body. Or more likely, because the count of the degrees of freedom of S_3 by consideration of the individual particles was not done correctly. Which ever the reason may be, we will soon find out.

As it turns out, there is something definitely wrong with (2), and it is that

$$3n - \frac{n(n-1)}{2} \approx -\frac{n^2}{2} < 0, \quad (3)$$

for $n \gg 1$, which is absurd.

Einstein did notice this flaw, because in his book, instead of (2) he has:

$$N_3 = \frac{n(n-1)}{2} - 3n \quad (4)$$

We cannot think of any physical or mathematical justification for this change of signs, and although it removes the problem of getting a negative value of N_3 when $n \gg 1$, it brings up a new problem.

In the limit when n tends to infinity, the system S_3 is equivalent to a rigid body of continuous mass. So it would be expected that if the limit of N_3 is taken when n tends to infinity, this limit should be equal to six. But this does not hold true for N_3 as defined in (4); the limit when n tends to infinity diverges.

Einstein introduced, as a footnote, the following correction:

$$N_3 = \frac{n(n-1)}{2} - 3n + 6 \quad (5)$$

Nonetheless, the limit when n tends to infinity of the modified N_3 is still undefined, so (5) cannot be the correct expression for N_3 either.

When we took up the task of developing an accurate expression for N_3 , we did not take up the problem from where Einstein left off, but instead, we directed our attention back to (2), which is the expression that Einstein must have come up with originally, in spite of the fact that it doesn't appear in his book. We did so because, as incorrect as it may be, there is a consistent line of thinking behind expression (2), which there is not behind expressions (4) or (5).

Expression (3) gave us a hint of where the flaw in (2) may be. Not in the signs, but rather, in the lack of a term. A term that shouldn't be a constant, but dependent on n . A term that added up to the other two would not only make N_3 positive for $n \gg 1$, but would actually make it equal to six. So there must be an additional source of degrees of freedom which Einstein failed to consider. If we could identify where this source of degrees of freedom was, we would have our problem solved.

A group of n particles may rotate in space without dissatisfying the condition that the distances between the particles remain constant. However, it is meaningless to talk about rotations without first establishing an adequate reference frame. To do so we arbitrarily selected three particles from S_3 ; the points where the centers of mass of these particles are located generate a plane P in three-dimensional space. And the vector \mathbf{v} , which is orthogonal to P , designates an arbitrary direction in space. We must point out that we are defining \mathbf{v} as a fixed vector, and that it is perpendicular to P in its original position, but as S_3 rotates, this perpendicularity relation will be lost. Therefore, it is convenient to make a copy of P , which we will call P' , and hold this copy fixed in the original position of P . Thus \mathbf{v} will all ways be orthogonal to P' . By considering the plane P' and its normal vector, we are defining a three-dimensional coordinate system.

Now, if we choose two particles, different from the ones used to generate the plane, the line that joins their centers of mass is a possible rotation axis for S_3 . And since the number of ways in which pairs may be chosen from a set of $n - 3$ particles is

$$C_{n-3}^2 = \frac{(n-3)!}{2!(n-5)!} = \frac{(n-3)(n-4)}{2}, \quad (6)$$

for $n \geq 3$, there will be an equal number of such axes. Each of these axes forms, with the direction of the vector \mathbf{v} , an angle φ_i which is a function of time and determines a possible rotation of the system. In general, the different φ_i will not hold relations of linear independence.

We believe that the number of φ_i allowed to S_3 for a given value of n is the term missing in Einstein's calculation, and we propose that the number of degrees of freedom for the system S_3 be given by:

$$N_3 = 3n - \frac{n(n-1)}{2} + \frac{(n-3)(n-4)}{2} = 6, \quad (7)$$

when $n \geq 3$.

However, (2) seems to be the correct expression for $n = 2$. It also works for $n = 3$ and $n = 4$, which is not

surprising, since for this value of n the last term in expression (7) is equal to zero, so (7) and (2) are equivalent.

Once we had developed these expressions, we were curious as to whether, by following the same line of reasoning, we could calculate the number of degrees of freedom of S_4 , that is, of the system made up of n particles with fixed relative distances, but which is, unlike S_3 , immersed in a four-dimensional space.

In this four-dimensional case, four coordinates are needed to locate the center of mass of each particle, which makes $4n$ coordinates for the set of n particles. And the number of constraint equations is the same as for S_3 .

In principle, the number of degrees of freedom should be the same as for a tetra-dimensional rigid body. And in four dimensions there are ten degrees of freedom for the rigid body: four coordinates are needed to locate its center of mass and

there are six possible rotation angles. Now, in the case of the n particles with fixed distances, we need $4n$ coordinates to locate the particles' centers of mass, while the number of distances is still $n(n-1)/2$. And the number of possible rotation angles is obtained by observing that a "hyperplane" can be defined with four points and that the number of different ways in which pairs may be chosen from a group of $n-4$ particles is given by:

$$C_{n-4}^2 = \frac{(n-4)!}{2!(n-6)!} = \frac{(n-4)(n-5)}{2}, \quad (8)$$

for $n \geq 4$.

Then, the number of degrees of freedom of S_4 is

$$N_4 = 4n - \frac{n(n-1)}{2} + \frac{(n-4)(n-5)}{2} = 10, \quad (9)$$

when $n \geq 4$, and

$$N_4 = 4n - \frac{n(n-1)}{2}, \quad (10)$$

when $2 \leq n \leq 5$, since the number of possible φ_i is equal to zero for these values of n .

That N_4 is equal to ten for any value of n less than or equal to four is consistent with the fact that ten is also the number of degrees of freedom of a rigid body in four-dimensional space (four coordinates are needed to locate the center of mass, and six more to describe the orientation of the body). Indeed, our procedure works for the four-dimensional as it does for the three-dimensional case. Moreover, we believe that it works for the general case. We propose that for a system of n particles with fixed relative distances, immersed in a space of D dimensions, the number of degrees of freedom is given by:

$$\begin{aligned} N_D &= Dn - \frac{n(n-1)}{2} + \frac{(n-D)(n-D-1)}{2} \\ &= \frac{D(D+1)}{2}, \end{aligned} \quad (11)$$

when $n \geq D$, and by:

$$N_D = Dn - \frac{n(n-1)}{2}, \quad (12)$$

when $2 \leq n \leq D+1$.

These results coincide entirely with those which would have been obtained by viewing S_D as a single body.

Counting the number of degrees of freedom of S_D by considering the individual particles is something which had never been done before. Just the three-dimensional case proved to be complicated enough, even for Albert Einstein, who was never able to write the correct expressions for the number of degrees of freedom of S_3 in Ref. 5, in spite of several revisions he made of this book.

There seemed to be contradictions between the values of N_3 obtained viewing S_3 as a sole body and those reached by considering the individual particles. This was only because the count of the degrees of freedom of S_3 from the

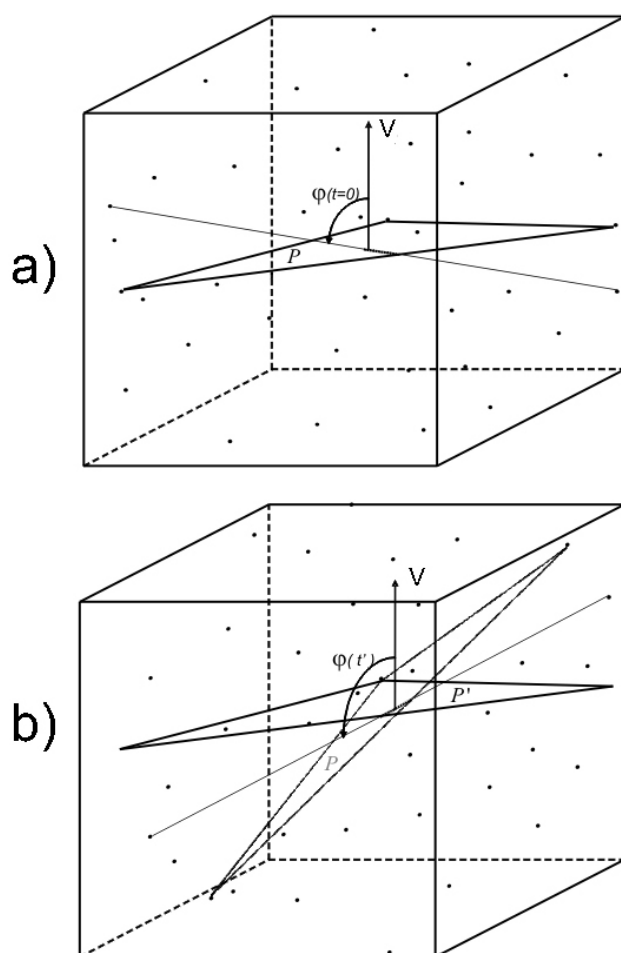


FIGURE 1. At instant $t = 0$ (a) the system is in its initial position. The line that connects the centers of mass of two arbitrary particles forms an angle $\varphi(t = 0)$ with the direction of the vector \mathbf{v} orthogonal to the reference plane P . At a future instant $t = t'$ (b) the system has rotated with respect to its original position. The plane P has moved, but a copy P' remains in the original position of P , so now \mathbf{v} is perpendicular to P' and the line that joins the centers of mass of the particles we had considered forms an angle $\varphi(t')$ with the direction of \mathbf{v} .

latter standpoint was never done properly. In this paper, we prove that both methods are equivalent, not only in three, but in any number D of dimensions.

This may be of interest for those who study the Kinetic Theory of Gases. In the Kinetic Theory of Gases and more specifically, in the Ideal Gas Model, the internal energy and the heat capacities at constant volume and constant pressure of an ideal gas are calculated as functions of the degrees of freedom of the gas, which are counted per molecule. And for molecules consisting of more than one atom, the number of degrees of freedom is calculated treating the molecules as rigid bodies. Thus, a diatomic molecule has five degrees of freedom and a polyatomic molecule has six. According to the Equipartition of Energy Theorem, each of these degrees of freedom is associated with an energy of quantity $1/2kT$. Hence, the internal energy U of a diatomic molecule is $U = 5/2kT$ and that of a polyatomic molecule is $U = 3kT$. Multiplying these results by Avogadro's number, $N_A = 6 \times 10^{23}$, gives the internal energy of an ideal gas, which is $U = 5/2N_AkT = 5/2RT$ and $U = 3N_AkT = 3RT$ for diatomic and polyatomic gases, respectively [6, 7].

The heat capacity at constant volume C_v is related to the internal energy by the expression $C_v = (\partial U / \partial T)$; thus $C_v = 5/2R$ for diatomic gases and $C_v = 3R$ for polyatomic ones. The heat capacity at constant pressure C_p is given by $C_p = C_v + R$.

The values of the heat capacities predicted using the Ideal Gas Model agree very well with the values obtained experimentally in the case of diatomic gases, but fall rather short for polyatomic gases [6], [7]. This is due to the fact that besides the energies associated with the translational and rotational degrees of freedom, there is also vibrational energy. This vibrational energy is quantized, which means that it does not spread over a continuous spectrum of values, but is distributed in discrete states [7, 8].

In the case of most diatomic molecules, the difference between the state of lowest energy (the ground state) and the state that follows is such that the leap from the ground state to the next may only be achieved at temperatures of approximately 3500 K. Thus, at room temperatures, the vibrational energy will remain in the ground state and its contributions to the total internal energy of the molecule will be negligible. Something very different occurs with polyatomic gases, where the molecules have several independent vibration modes. For some of these modes, the spacing between energy states is considerably smaller than for diatomic molecules. Hence, the vibrational energy will make an im-

portant contribution to the total internal energy of a polyatomic molecule at room temperature, or even less. Once the vibrational energy is considered, the predicted heat capacities have a very good correspondence with experimental values [8, 9].

In any case, the additional consideration of this quantized vibrational energy does not modify the fact that the rotational and translational energies of a gas molecule are calculated by treating this molecule as a rigid body. Treating molecules as rigid bodies is correct, but it had never been formally justified. This work gives a formal justification to this procedure.

Furthermore, we believe that this paper clarifies the so-called "degree of freedom paradox". This paradox consists in the fact that, if we make a microscopical analysis of a system which if treated as a rigid body has a finite number of degree of freedom, it turns out that it has an infinite number of degrees of freedom and therefore, infinite heat capacities, which is absurd [10]. This contradiction was attributed to a flaw in classical mechanics. Our work suggests that rather, it is a result of not knowing how to count the number of degrees of freedom particle by particle.

This work may also imply that statements like the following are not correct. According to Herbert Goldstein, "a rigid body with N particles can at most have $3N$ degrees of freedom" as can be read in his *Classical Mechanics* textbook [3], in the chapter dealing with the kinematics of rigid body motion. However, our analysis shows that the maximum number of degrees of freedom for any rigid body in three-dimensional space is six.

In conclusion, we obtained expressions that yield the number of degrees of freedom of a rigid body constituted by n particles in a three-dimensional space and we extended our results to an arbitrary number D of spatial dimensions. The results for the three-dimensional case disagree with those obtained by Albert Einstein and which appear in [5]. We believe that with our analysis of the three-dimensional case we can justify, formally, the fact that a rigid non-linear polyatomic molecule all ways has six degrees of freedom, a situation that has not been sufficiently explained in the literature, in spite of its widespread use in the calculation of the internal energies and heat capacities of ideal polyatomic gases.

Acknowledgements

We thank Trinidad Cruz-Sánchez for his valuable contribution to the fulfillment of this work.

1. G.R. Fowles, *Analytical Mechanics* (Holt, Rinehart and Winston, New York, 1962).
2. F. Scheck, *Mechanics* (Springer - Verlag, Berlin, 1990).
3. H. Goldstein, C. Poole, and J. Safko, *Classical Mechanics* (Ad-

dison Wesley, San Francisco, 2003).

4. N.C. Barford, *Mechanics* (Editorial Reverté, Barcelona, 1976).
5. A. Einstein, *The Meaning of Relativity* (Princeton University Press, Princeton, 1953).

6. R. Resnick, D. Halliday, and K.S. Krane, *Física, Volumen 1* (CECSA, México, 1997).
7. G.W. Castellan, *Fisicoquímica* (Addison Wesley Longman, 1986).
8. F. Mandl, *Física Estadística* (Editorial Limusa, México, 1976).
9. T.L. Hill, *An Introduction to Statistical Thermodynamics* (Dover Publications, New York, 1976).
10. K. Huang, *Statistical Mechanics* (John Wiley & Sons, New York, 1963).