THE SOLUTION TO THE THREE-BODY PROBLEM
AND SOME APPLICATIONS

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Abstract. Here we provide and explain the coordinate transformation according to which every weighted quadratic form of the absolute Cartesian coordinates or velocities of three particles is separable into quadratic terms of the relative and centre-of-mass coordinates or velocities. This solution is applied to define a new set of weighted colour coordinates YJK in the colour space, and also to solve the dynamical system Sun-Earth-Moon. The weighted Laplacian and hence the quantum Hamiltonian operator for a system of three particles are also given in relative coordinates, and applied to calculate the vibrational energy levels of carbon dioxide and the electronic energy of the ground state of the hydrogen-molecule-ion and two-electron atomic systems like the helium atom.

Contents

1. Introduction

The systems of many particles are of fundamental interest in statistical mechanics, quantum physics and celestial mechanics. Since Lagrange submitted his prize memoir *Essai sur le Problème des Trois Corps* in 1772, many investigations on the three-body and the *N*-body problems have been carried out, especially related to celestial mechanics [40, p 319]. However, the *N*-body problem is not integrable in general as shown by Painlevé, and some techniques, like Laplace's perturbation theory and Poincaré's topological methods, have been developed to approximate the solutions [25, p 400]. On the other hand, the dynamics of N interacting bodies is not always stable and can become chaotic even for the three-body system [49]. According to the König theorem, the kinetic energy of a system of particles is the kinetic energy of the centre of mass plus the kinetic energy of the particles with respect to the centre of mass. From now on, the coordinates and velocities of particles with respect to any origin (even the centre of mass) will be called *absolute* coordinates and *absolute* velocities[1]. The differences of the absolute coordinates and absolute velocities of every pair of particles will be called *relative* coordinates and *relative* velocities respectively. The König theorem only provides a partial solution to the N-body problem because it yields the internal kinetic energy as a quadratic form of the absolute velocities with respect to the centre of mass. However, the potential energy is usually a function of the relative coordinates so that the latter do not adapt well to the former. The question is whether the kinetic energy of a system of three particles with respect to the centre of mass can be expressed as a quadratic form of the relative velocities. Since the derivation with respect to time is a linear operation, this question is equivalent to outlining the same problem with coordinates instead of velocities. If this expression exists, it should be invariant under the exchange of particles. In other words, it should contain all the relative coordinates in a symmetrical way. It will be shown that this symmetry is the key to find the answer to this question.

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[1]The velocities with respect to the centre of mass and the corresponding kinetic energy are usually called *internal* velocities and *internal* kinetic energy.

2. Antecedents

Firstly, let us review some geometric theorems related to the three-body problem. Leibniz's theorem [57, p 97] states that, if P is any point in the Euclidean plane and $\triangle ABC$ a triangle whose centroid is G, then the following identity is satisfied

$$PA^2 + PB^2 + PC^2 = \frac{1}{3}\left(AB^2 + BC^2 + CA^2\right) + 3PG^2 . \tag{1}$$

An alternative version equivalent to this theorem states that the geometric locus of the points P such that $PA^2 + PB^2 + PC^2 = k^2$ is a circle with centre G and radius

$$r = \|GP\| = \sqrt{\frac{k^2}{3} - \frac{AB^2 + BC^2 + CA^2}{9}} . \tag{2}$$

Apollonius' circle theorem states that, given two points A and B, the locus of the points P such that $\|PA\| = k\|PB\|$ is a generalized[2] circle having the centre O and radius r given by

$$O = \frac{A - k^2 B}{1 - k^2} , \qquad r = \|OP\| = \frac{k\|AB\|}{1 - k^2} . \tag{3}$$

For $k = 1$ the radius is infinite and the locus is the bisector of AB. Note that $\|PA\| = k\|PB\|$ implies $PA^2 - k^2 PB^2 = 0$, which is a special case of the geometric outlining of the two-body problem: *Given two points A and B, which is the geometric locus of the points P such that $a\, PA^2 + b\, PB^2 = k^2$?* The solution has been known since a long time ago: The points P lie on a circle centred at the centre of mass G

$$G = \frac{a\, A + b\, B}{a + b} , \qquad \|GP\| = \sqrt{\frac{k^2}{a + b} - \frac{a\, b}{(a + b)^2}AB^2} . \tag{4}$$

This geometric solution is equivalent to writing

$$a\, PA^2 + b\, PB^2 = (a + b)PG^2 + \frac{a\, b}{a + b}AB^2. \tag{5}$$

Defining the reduced mass of the binary system as $\mu = a\, b/(a + b)$ and denoting with $m = a + b$ the total mass of the system, we have the usual notation in physics

$$a\, PA^2 + b\, PB^2 = m\, PG^2 + \mu AB^2. \tag{6}$$

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[2]Also admitting circles with infinite radius, which are lines.

In reference [31, p 163] we find the following *Satz von Leibniz*: If $a + b + c = 1$, $G = a\,A + b\,B + c\,C$ and X is any point, then

$$a\,XA^2 + b\,XB^2 + c\,XC^2 - XG^2 = a\,GA^2 + b\,GB^2 + c\,GC^2 \qquad (7)$$

whose *Korollar C* is

$$a\,b\,AB^2 + b\,c\,BC^2 + c\,a\,CA^2 = \rho^2 - OG^2 \qquad (8)$$

where O is the circumcentre and ρ is the radius of the circumscribed circle. Finally, in [3, p 59] the *scalar function of Leibniz* $f(P)$ is defined as

$$f(P) = \sum_{i=1}^{k} a_i\,PA_i^2 \qquad (9)$$

and, assuming that $\sum a_i \neq 0$, then there exists a fixed vector v such that, for every point P' the equation

$$f(P') = f(P) + 2\,PP' \cdot v \qquad (10)$$

is satisfied.

3. Apollonius' Lost Theorem

An essential question of the classical three-body problem is the following: *How can the internal kinetic energy of a system of three particles be written with relative velocities*? The kinetic energy is a separable quadratic form of the absolute velocities of each particle. Since the derivative with respect to time is a linear operator and the relative velocities are differences of the absolute velocities, which are also linear equations, this problem is equivalent to writing $a\,A^2 + b\,B^2 + c\,C^2$ with relative and centre-of-mass coordinates, and concretely, to wondering whether an expression like (1) and (5) can exist for every three vertices A, B and C of a triangle having different weights.

Theorem 1 (Apollonius' Lost Theorem [20, p 57], [21, p 78]). *Let $\triangle ABC$ be a triangle in the Euclidean plane. The geometric locus of the points P such that $a\,PA^2 + b\,PB^2 + c\,PC^2 = k^2$ with a, b and $c \in \mathbb{R}$ such that $a + b + c \neq 0$ is a circle centred at the centre of mass $G = (aA + bB + cC)/(a + b + c)$.*

Proof: Without loss of generality, one can take $a + b + c = 1$ in order to remove denominators. After developing $PG^2 = [P - (a\,A + b\,B + c\,C)]^2$ by means of the scalar product and gathering terms, we arrive at

$$PG^2 = a\,PA^2 + b\,PB^2 + c\,PC^2 - a\,b\,AB^2 - b\,c\,BC^2 - c\,a\,CA^2 \qquad (11)$$

whence $\|PG\| = \sqrt{k^2 - (a\,b\,AB^2 + b\,c\,BC^2 + c\,a\,CA^2)}$ is constant, and P therefore lies on a circle centred at G.   ∎

Remark 2. *If* $a + b + c = m$ *instead of 1 and* $m \neq 0$*, the equation* (11) *then becomes*

$$a\,PA^2 + b\,PB^2 + c\,PC^2 = m\,PG^2 + \frac{a\,b}{m}\,AB^2 + \frac{b\,c}{m}\,BC^2 + \frac{c\,a}{m}\,CA^2 \,. \quad (12)$$

Remark 3. *If* a*,* b *and* c *are the masses of the particles centred at the points* A*,* B *and* C*,* m *is the mass of the system of three particles,* G *is their centre of mass, and* P *can be taken as the origin of coordinates. This is just a simultaneous generalization of the solution to the two-body problem* (5) *and Leibniz's theorem* (1)*.*

Remark 4. *The equation* (12)*, which was deduced for the plane, is also valid for every* N*-dimensional Euclidean space because of the addition of squares.*

4. Application to Colour Image Processing

The sensitivity of the human eye to light intensity follows a non-linear power law (*gamma law*). When an electric voltage is applied to a CRT (cathodic ray tube) monitor, the light power emitted by the electrons colliding with the screen phosphor also fits a non-linear law. Fortunately, both functions are almost coincident, so that the applied voltage can be considered proportional to the light sensitivity of human eye [47]. From now on, I will refer to lightness perceived by the human eye, which is quite proportional to applied voltages.

The RGB (red, green, blue) space is the most frequently used colour space, although a small part of colours perceived by the human eye falls out of it. The main question to deal with is the fact that the human eye has different sensitivities to the three colours, from green the highest to blue the lowest. This was taken into account when defining the YUV coordinates of the colour space used in the PAL TV format. The Y (*luma*) colour coordinate was defined as

$$Y = w_R\,R + w_G\,G + w_B\,B \,, \qquad\qquad RGB \in [0,1]^3 \,. \qquad (13)$$

The combination $R = G = B = 0$ corresponds to black, $R = G = B = 1$ to white, and grey is the addition of equal amounts of the three fundamental colours RGB. *Luma* is defined by the weights $w_R = 0.299$, $w_G = 0.587$ and $w_B = 0.114$ [48, p 7] satisfying $w_R + w_G + w_B = 1$, and it approximates to the lightness of

colours. On the other hand, the chrominance components U and V were defined as

$$U = \frac{B-Y}{1-w_B}U_{max} \approx 0.492(B-Y)\,, \qquad U_{max} = 0.436$$

$$V = \frac{R-Y}{1-w_R}V_{max} \approx 0.877(R-Y)\,, \qquad V_{max} = 0.615\,. \tag{14}$$

In the space $YPbPr$, the chromatic components are

$$P_B = 0.5\frac{B-Y}{1-w_B}\,, \qquad P_R = 0.5\frac{R-Y}{1-w_R}\,. \tag{15}$$

Its digital version $YCbCr$ uses integers such that $RGB \in [0,255]^3$ and then $Y \in [16,235]$ and $C_B,\ C_R \in [16,240]$. The JPEG image format enlarges these ranges of integers to $Y \in [0,255]$ and $C_B,\ C_R \in [0,255]$.

We propose using new chrominance components corresponding to relative coordinates defined in the following way

$$J = R - G \in [-1,1], \quad K = G - B \in [-1,1], \quad I = B - R \in [-1,1] \tag{16}$$

which are linear dependent since

$$I + J + K = 0\,. \tag{17}$$

Of course, two chrominance components are enough together with luma Y (13) to define a colour and, since green is the lightest colour of the three fundamental colours, it seems most suitable to take only J and K. Let us call this colour system *YJK*, whose conversion matrix from *RGB* is

$$\begin{pmatrix} Y \\ J \\ K \end{pmatrix} = \begin{pmatrix} w_R & w_G & w_B \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} R \\ G \\ B \end{pmatrix}\,. \tag{18}$$

If we consider the three fundamental colours as the coordinates of three masses lying on the segment [0, 1], then luma Y is the centre of mass and I, J and K are the relative coordinates, the distances between colours. From Apollonius' lost theorem (11), it seems natural to define a colour metric (colour norm) $\|c\|$ given by the scalar function of Leibniz [3, p 59]

$$\|c\|^2 = \|RGB\|^2 = w_R\,R^2 + w_G\,G^2 + w_B\,B^2\,. \tag{19}$$

Note that if $R = G = B$ then the colour is grey and the colour norm is the grey scale. Therefore, we define the square root of (19) as the grey level of every

colour. This grey scale definition takes into account the different lightness of the fundamental colours and is better than the rough definition of lightness as $(R + G + B)/3$ in the LHS model [32, p 53]. By means of (12), the norm $\|c\|$ (the grey level) can be obtained from the YJK coordinates as

$$\|c\|^2 = \|YJK\|^2 = Y^2 + w_R\, w_B\, I^2 + w_R\, w_G\, J^2 + w_G\, w_B\, K^2 \ . \qquad (20)$$

Moreover, this norm clearly defines a distance between two colours c_1 and c_2 in the colour space

$$d(c_1, c_2) = \|c_2 - c_1\| = \sqrt{w_R\,(R_2 - R_1)^2 + w_G\,(G_2 - G_1)^2 + w_B\,(B_2 - B_1)^2}$$
$$\qquad (21)$$
$$= \sqrt{(Y_2 - Y_1)^2 + w_R\, w_B\,(I_2 - I_1)^2 + w_R\, w_G\,(J_2 - J_1)^2 + w_G\, w_B\,(B_2 - B_1)^2}.$$

 Some properties of this distance are

   a) The distance between black and white is one.

   b) The distance from opposite fundamental colours is also one. For instance yellow $= (1, 1, 0)_{RGB}$ and blue $= (0, 0, 1)_{RGB}$ then d(yellow, blue) $= 1$. In the same way the distances between green and magenta, and between cyan and red are one.

   c) It satisfies the triangular inequality $d(c_1, c_3) \le d(c_1, c_2) + d(c_2, c_3)$.

The chrominance components of the colour coordinates YJK could be plotted in a plane with Cartesian coordinates J and K like it is usually done for the U and V coordinates. But if we wish to preserve the symmetry of the I, J and K chrominance components, another graph must be plotted. Let us consider three unitary vectors $\mathbf{e}_I$, $\mathbf{e}_J$ and $\mathbf{e}_K$ forming angles of $120°$ and defining the corresponding coordinate axes

$$\mathbf{e}_I = -\frac{\sqrt{3}}{2}\mathbf{e_1} - \frac{1}{2}\mathbf{e_2}\ , \qquad \mathbf{e}_J = \frac{\sqrt{3}}{2}\mathbf{e_1} - \frac{1}{2}\mathbf{e_2}\ , \qquad \mathbf{e}_K = \mathbf{e_2}\ . \qquad (22)$$

Then, the coordinates IJK of any point $\mathbf{P}(x\mathbf{e_1} + y\mathbf{e_2})$ in this plane are its orthogonal projections onto the axes, which are obtained through the scalar product

$$I = \mathbf{P}\cdot\mathbf{e}_I = (x\mathbf{e_1} + y\mathbf{e_2})\cdot(-\frac{\sqrt{3}}{2}\mathbf{e_1} - \frac{1}{2}\mathbf{e_2}) = -\frac{\sqrt{3}}{2}x - \frac{1}{2}y$$
$$J = \mathbf{P}\cdot\mathbf{e}_J = (x\mathbf{e_1} + y\mathbf{e_2})\cdot(\frac{\sqrt{3}}{2}\mathbf{e_1} - \frac{1}{2}\mathbf{e_2}) = \frac{\sqrt{3}}{2}x - \frac{1}{2}y \qquad (23)$$
$$K = \mathbf{P}\cdot\mathbf{e}_K = (x\mathbf{e_1} + y\mathbf{e_2})\cdot\mathbf{e_2} = y\ .$$
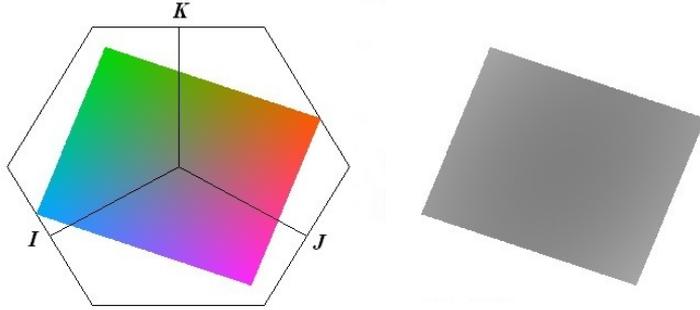
Figure 1. Left: Plot of IJK coordinates for all the possible values of RGB calculated for luma $Y = 0.5$. Right: Grey level of the same colours calculated according to (19).

The components IJK so obtained satisfy (17). Fig. 1 shows the coordinate plot. Since $-1 \leq I, J, K \leq 1$, all the possible values of I, J and K lie inside a hexagon. A point in the plane is obtained from IJK as

$$x \, \mathbf{e_1} + y \, \mathbf{e_2} = \frac{2}{3}(I \, \mathbf{e}_I + J \, \mathbf{e}_J + K \, \mathbf{e}_K) \,. \tag{24}$$

The main advantage of the YJK codification is the fact that the chrominance components J and K are only obtained from subtraction, which is a fast operation at the CPU level. It is also easy to implement an electric circuit to encode and to decode the YJK signal. On the other hand, the J and K signals can be applied directly as a voltage difference between adjacent pixels with different colours in a screen, which reduces to 1/3 the arithmetic operations to decode video signal. Since YJK have been defined as the linear combinations (18) of RGB, YJK also satisfy Grassmann's laws of additive colour mixtures [18, p 8].

5. Application to Classical Mechanics

Some known solutions to the classical three-body problem have been masterly explained by Hestenes [25, pp 398-418], and let us recall his treatment here keeping his own notation. The dynamics of three bodies located at the points $\mathbf{x_1}$, $\mathbf{x_2}$ and $\mathbf{x_3}$ in the Euclidean three-dimensional space under their mutual gravitational attraction can be written through the vector equations

$$\ddot{\mathbf{x}}_{\mathbf{1}} = -m_2 \frac{\mathbf{x_1} - \mathbf{x_2}}{\|\mathbf{x_1} - \mathbf{x_2}\|^3} - m_3 \frac{\mathbf{x_1} - \mathbf{x_3}}{\|\mathbf{x_1} - \mathbf{x_3}\|^3}$$

$$\ddot{\mathbf{x}}_{\mathbf{2}} = -m_3 \frac{\mathbf{x_2} - \mathbf{x_3}}{\|\mathbf{x_2} - \mathbf{x_3}\|^3} - m_1 \frac{\mathbf{x_2} - \mathbf{x_1}}{\|\mathbf{x_2} - \mathbf{x_1}\|^3} \tag{25}$$

$$\ddot{\mathbf{x}}_3 = -m_1 \frac{\mathbf{x}_3 - \mathbf{x}_1}{\|\mathbf{x}_3 - \mathbf{x}_1\|^3} - m_2 \frac{\mathbf{x}_3 - \mathbf{x}_2}{\|\mathbf{x}_3 - \mathbf{x}_2\|^3}$$

where he absorbs the gravitational constant into the definition of mass. Then, after the introduction of the relative coordinates

$$\mathbf{s}_1 = \mathbf{x}_3 - \mathbf{x}_2 , \qquad \mathbf{s}_2 = \mathbf{x}_1 - \mathbf{x}_3 , \qquad \mathbf{s}_3 = \mathbf{x}_2 - \mathbf{x}_1 \qquad (26)$$

he obtains the symmetric form of the dynamic equations[3]

$$\ddot{\mathbf{s}}_1 = -\frac{m\,\mathbf{s}_1}{\|\mathbf{s}_1\|^3} + m_1 \mathbf{G}, \quad \ddot{\mathbf{s}}_2 = -\frac{m\,\mathbf{s}_2}{\|\mathbf{s}_2\|^3} + m_2 \mathbf{G}, \quad \ddot{\mathbf{s}}_3 = -\frac{m\,\mathbf{s}_3}{\|\mathbf{s}_3\|^3} + m_3 \mathbf{G} \quad (27)$$

where $m = m_1 + m_2 + m_3$ and $\mathbf{G}$[4] is

$$\mathbf{G} = \frac{\mathbf{s}_1}{\|\mathbf{s}_1\|^3} + \frac{\mathbf{s}_2}{\|\mathbf{s}_2\|^3} + \frac{\mathbf{s}_3}{\|\mathbf{s}_3\|^3} \, . \qquad (28)$$

From this point, Hestenes deduces Lagrange's equilateral solution in one page (the deduction by Erich Kähler took fifteen pages [30]) and he finds other solutions very quickly, too. From now on, we leave Hestenes' deduction and return to our notation.

A theorem that is an extension of Apollonius' lost theorem (12) has an immediate application to the study of the dynamics of a system of three particles.

Theorem 5. *Let* $\mathbf{D} = \mathbf{B} - \mathbf{A}$*,* $\mathbf{E} = \mathbf{C} - \mathbf{B}$ *and* $\mathbf{F} = \mathbf{A} - \mathbf{C}$ *be the relative coordinates where* $\mathbf{A}$*,* $\mathbf{B}$ *and* $\mathbf{C}$ *are respectively the position vectors of the masses* a*,* b*,* c *in the three-Euclidean space, and let the relative velocities be*

$$\dot{\mathbf{D}} = \dot{\mathbf{B}} - \dot{\mathbf{A}}, \qquad \dot{\mathbf{E}} = \dot{\mathbf{C}} - \dot{\mathbf{B}} , \qquad \dot{\mathbf{F}} = \dot{\mathbf{A}} - \dot{\mathbf{C}} . \qquad (29)$$

Let $\mathbf{G}$ *be the position vector of the centre of mass and let* $\dot{\mathbf{G}}$ *be its velocity*

$$\mathbf{G} = \frac{a\mathbf{A} + b\mathbf{B} + c\,\mathbf{C}}{a + b + c} \qquad \Rightarrow \qquad \dot{\mathbf{G}} = \frac{a\dot{\mathbf{A}} + b\dot{\mathbf{B}} + c\,\dot{\mathbf{C}}}{a + b + c} \, . \qquad (30)$$

Since the absolute and relative velocities are linked by the same algebraic equations as those for coordinates, they also satisfy an identity analogous to (12)

$$a\,\dot{\mathbf{A}}^2 + b\,\dot{\mathbf{B}}^2 + c\,\dot{\mathbf{C}}^2 = m\dot{\mathbf{G}}^2 + \frac{a\,b}{m}\dot{\mathbf{D}}^2 + \frac{b\,c}{m}\dot{\mathbf{E}}^2 + \frac{c\,a}{m}\dot{\mathbf{F}}^2 \qquad (31)$$

where $m = a + b + c$*.*

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[3] According to Hestenes, the equations (27) were found by Broucke and Lass in 1973 [5].

[4] $\mathbf{G}$ is Hestenes' notation, not to be mistaken for the centre of mass in our notation.

Proof: By substitution of (29) and (30) into the *rhs* of (31) we find

$$
m\dot{\mathbf{G}}^2 + \frac{a\,b}{m}\dot{\mathbf{D}}^2 + \frac{b\,c}{m}\dot{\mathbf{E}}^2 + \frac{c\,a}{m}\dot{\mathbf{F}}^2
$$
$$
= \frac{1}{m}\left[(a\dot{\mathbf{A}} + b\dot{\mathbf{B}} + c\dot{\mathbf{C}})^2 + a\,b(\dot{\mathbf{B}} - \dot{\mathbf{A}})^2 + b\,c(\dot{\mathbf{C}} - \dot{\mathbf{B}})^2 + c\,a(\dot{\mathbf{A}} - \dot{\mathbf{C}})^2\right]
$$
$$
= \frac{1}{m}\left[a(a+b+c)\dot{\mathbf{A}}^2 + b(a+b+c)\dot{\mathbf{B}}^2 + c(a+b+c)\dot{\mathbf{C}}^2\right]
$$
$$
= a\,\dot{\mathbf{A}}^2 + b\,\dot{\mathbf{B}}^2 + c\,\dot{\mathbf{C}}^2. \qquad\blacksquare
$$

Therefore, the kinetic energy of a system of three particles with respect to an inertial reference frame is equal to the kinetic energy of the centre of mass with respect to the same frame plus a linear combination of the squares of the relative velocities. The Lagrange function $\mathcal{L}$ of a system of three bodies interacting gravitationally and having masses a, b and c is then obtained from (31)

$$
\mathcal{L} = \frac{m}{2}\dot{\mathbf{G}}^2 + \frac{a\,b}{2m}\dot{\mathbf{D}}^2 + \frac{b\,c}{2m}\dot{\mathbf{E}}^2 + \frac{c\,a}{2m}\dot{\mathbf{F}}^2 + k\left(\frac{a\,b}{\|\mathbf{D}\|} + \frac{b\,c}{\|\mathbf{E}\|} + \frac{c\,a}{\|\mathbf{F}\|}\right)
$$
$$
+ \boldsymbol{\lambda}\cdot(\mathbf{D} + \mathbf{E} + \mathbf{F}). \quad (32)
$$

Here k is the gravitational constant, and the holonomic constraint $\mathbf{D} + \mathbf{E} + \mathbf{F} = 0$ has been added through scalar multiplication by a Lagrange multiplier vector $\boldsymbol{\lambda}$ [5]. The linear dependence of relative coordinates can always be introduced into the Lagrange equations of motion by means of Lagrange multipliers [38, p 60]. In this way, the three relative coordinates become linearly independent, and Lagrange equations $\mathrm{d}\mathcal{L}/\mathrm{d}q_i = \mathrm{d}(\mathrm{d}\mathcal{L}/\mathrm{d}\dot{q}_i)/\mathrm{d}t$ can be applied to each of them obtaining the same equations as (27)

$$
\ddot{\mathbf{D}} = -\frac{k\,m}{\|\mathbf{D}\|^3}\mathbf{D} + \frac{m}{a\,b}\boldsymbol{\lambda}, \quad \ddot{\mathbf{E}} = -\frac{k\,m}{\|\mathbf{E}\|^3}\mathbf{E} + \frac{m}{b\,c}\boldsymbol{\lambda}, \quad \ddot{\mathbf{F}} = -\frac{k\,m}{\|\mathbf{F}\|^3}\mathbf{F} + \frac{m}{c\,a}\boldsymbol{\lambda} \quad (33)
$$

where we now see that Hestenes' $\mathbf{G}$ in (27) is in fact a Lagrange multiplier proportional to $\boldsymbol{\lambda}$. In order to see its meaning, add the three equations (33)

$$
\ddot{\mathbf{D}} + \ddot{\mathbf{E}} + \ddot{\mathbf{F}} = -k\,m\left(\frac{\mathbf{D}}{\|\mathbf{D}\|^3} + \frac{\mathbf{E}}{\|\mathbf{E}\|^3} + \frac{\mathbf{F}}{\|\mathbf{F}\|^3}\right) + \left(\frac{m}{a\,b} + \frac{m}{b\,c} + \frac{m}{c\,a}\right)\boldsymbol{\lambda} = 0
$$

to find

$$
\boldsymbol{\lambda} = \frac{a\,b\,c\,k}{m}\left(\frac{\mathbf{D}}{\|\mathbf{D}\|^3} + \frac{\mathbf{E}}{\|\mathbf{E}\|^3} + \frac{\mathbf{F}}{\|\mathbf{F}\|^3}\right). \qquad (34)
$$

Let us apply these equations to the system Sun-Earth-Moon.
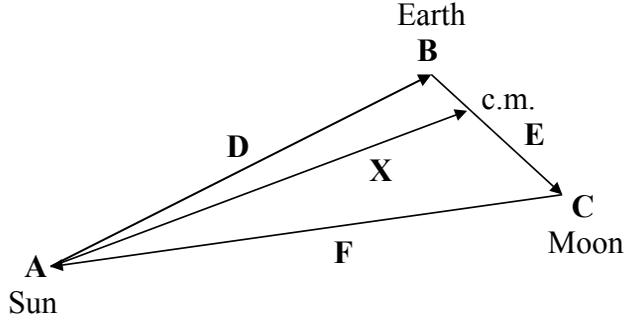
Figure 2. Sketch of the system Sun-Earth-Moon. The centre of mass of the system Earth-Moon is indicated by "c.m.".

5.1. The Dynamic System Sun-Earth-Moon

We will only consider the gravitational interaction of the Sun, Earth and the Moon taken as punctual masses. This problem was called the *main problem* of lunar theory by Brown [4, p 298] [6, p 308]. Hill developed the theory of lunar motion, whose modern treatment can be found at [10, p 180], and Brown worked on lunar tables based on Hill's theory. We show below that the Lagrangian (32) provides an easier and clearer treatment of the lunar theory that permits the calculation of all the perturbations to Moon's Keplerian motion.

Let us assign the position $\mathbf{A}$ to the Sun, the position $\mathbf{B}$ to Earth and the position $\mathbf{C}$ to the Moon as displayed in Fig. 2. If we build the linear combination

$$b\,\ddot{\mathbf{D}} - c\,\ddot{\mathbf{F}} = -k\,m\,b\frac{\mathbf{D}}{\|\mathbf{D}\|^3} + k\,m\,c\frac{\mathbf{F}}{\|\mathbf{F}\|^3} \qquad (35)$$

the Lagrange multiplier $\boldsymbol{\lambda}$ is removed. Let us introduce the Jacobi coordinate $\mathbf{X}$ (see Fig. 2) as the vector going from the Sun to the centre of mass of the system Earth-Moon

$$\mathbf{X} = \frac{b\mathbf{D} - c\mathbf{F}}{b + c}. \qquad (36)$$

Notice that $\mathbf{D} \cong -\mathbf{F} \cong \mathbf{X}$, because $\|\mathbf{E}\|/\|\mathbf{D}\| \leq 2.56{\cdot}10^{-3}$ according to the astronomical data. Development in power series of $\|\mathbf{E}\|/\|\mathbf{X}\|$ will give approximations of different orders.

5.1.1. Zero-Order Approximation

In this approximation, all the powers of $\|\mathbf{E}\|/\|\mathbf{X}\|$ are disregarded. It does not have enough precision to be compared with astronomical data but it provides a very interesting and clear physical image of the Sun-Earth-Moon dynamical system. With this approximation the equation (35) becomes

$$\ddot{\mathbf{X}} = \frac{b\ddot{\mathbf{D}} - c\ddot{\mathbf{F}}}{b+c} \cong -k\,m\frac{\mathbf{X}}{\|\mathbf{X}\|^3} \tag{37}$$

or equivalently

$$\frac{a(b+c)}{m}\ddot{\mathbf{X}} \cong -k\,a(b+c)\frac{\mathbf{X}}{\|\mathbf{X}\|^3}. \tag{38}$$

On the left we can find the reduced mass of a two-body system formed by the mass a of the Sun and the mass $b+c$ of the system Earth-Moon times their mutual acceleration. On the right we find their gravitational interaction. This is the equation of the very well known and solved problem of two bodies interacting gravitationally, which is integrable. It tells us that the orbit of the centre of mass of Earth and the Moon is an ellipse with the Sun at one focus. The former approximation $\|\mathbf{E}\| \ll \|\mathbf{D}\| \cong \|\mathbf{F}\| \cong \|\mathbf{X}\|$ reduces the Lagrange multiplier $\boldsymbol{\lambda}$ (34) of the system Sun-Earth-Moon to

$$\boldsymbol{\lambda} \cong \frac{a\,b\,c\,k}{m}\frac{\mathbf{E}}{\|\mathbf{E}\|^3}. \tag{39}$$

Then, the equation of the relative motion Earth-Moon (second of (33)) is

$$\ddot{\mathbf{E}} = -k\,m\frac{\mathbf{E}}{\|\mathbf{E}\|^3} + \frac{m}{b\,c}\boldsymbol{\lambda} \cong -k(b+c)\frac{\mathbf{E}}{\|\mathbf{E}\|^3} \tag{40}$$

or in a more recognizable form

$$\frac{b\,c}{b+c}\ddot{\mathbf{E}} \cong -k\,b\,c\frac{\mathbf{E}}{\|\mathbf{E}\|^3}. \tag{41}$$

On the left we can find the reduced mass of Earth and the Moon times their relative acceleration, and on the right we recognize the force of gravitation between Earth and the Moon according to Newton's law. Therefore, the system Earth-Moon is also integrable as a two-body problem. Notice that no fixed plane of the motion of the whole system is assumed. This decomposition only says that Earth and the Moon are moving in a plane, and that the centre of mass of Earth and the Moon is moving around the Sun in another plane, the ecliptic. Both planes are not

coincident but form an angle of about $5°$. The orbit of the Moon is then an ellipse with the centre of mass of Earth and the Moon at one focus, which lies inside Earth. This centre of mass follows another ellipse with the centre of the Sun at one focus. Since the approximation $\|\mathbf{E}\| \ll \|\mathbf{X}\|$ is very good, corrections to these motions are small. The scalar multiplication by $\dot{\mathbf{E}}$ in (40) and integration with respect to time yield

$$\frac{\dot{\mathbf{E}}^2}{2} \cong \frac{k(b+c)}{\|\mathbf{E}\|} - K, \qquad K > 0. \tag{42}$$

By introducing polar coordinates we have

$$\dot{r}^2 + r^2\dot{\theta}^2 \cong \frac{2k(b+c)}{r} - 2K \tag{43}$$

where $r = \|\mathbf{E}\|$ is the radius of Moon's orbit around Earth. Since the force is central, the angular momentum of the system Earth-Moon is a constant of the motion. We introduce the constant $K' = r^2\dot{\theta}$, which is proportional to the angular momentum[5], in order to replace $\dot{\theta}$

$$\dot{r}^2 \cong -\frac{(K')^2}{r^2} + \frac{2k(b+c)}{r} - 2K. \tag{44}$$

By dividing by the square of $\dot{\theta} = K'/r^2$, one finds the differential equation of the orbit

$$\left(\frac{\dot{r}}{\dot{\theta}}\right)^2 = \left(\frac{\mathrm{d}r}{\mathrm{d}\theta}\right)^2 \cong r^4\left(-\frac{1}{r^2} + \frac{2k(b+c)}{r(K')^2} - \frac{2K}{(K')^2}\right). \tag{45}$$

Now we introduce the variable $s = 1/r$

$$\left(\frac{\mathrm{d}s}{\mathrm{d}\theta}\right)^2 \cong -s^2 + \frac{2k(b+c)s}{(K')^2} - \frac{2K}{(K')^2}. \tag{46}$$

Derivation with respect to θ and simplification yields

$$\frac{\mathrm{d}^2s}{\mathrm{d}\theta^2} + s \cong \frac{k(b+c)}{(K')^2} \tag{47}$$

whose general solution is a linear combination of a sine and a cosine plus the constant on the *rhs*. If we want r and s to reach respectively the minimal and maximal values at $\theta = 0$, then the solution must come from the cosine

$$s = \frac{k(b+c)}{(K')^2}(1 + \epsilon\cos\theta) \qquad \Rightarrow \qquad r = \frac{\frac{(K')^2}{k(b+c)}}{1 + \epsilon\cos\theta} = \frac{r_0(1 - \epsilon^2)}{1 + \epsilon\cos\theta}. \tag{48}$$

---

[5]The constancy of $r^2\dot{\theta}$ is also deduced from Kepler's second law: The radius vector $\mathbf{E}$ from Earth to the Moon sweeps out equal areas during equal intervals of time.

This is the polar equation of a conic with eccentricity $\epsilon < 1$ (an ellipse) and semi-major axis r_0, whence it follows that

$$\frac{(K')^2}{k(b+c)} = r_0(1 - \epsilon^2). \tag{49}$$

Hence, the total mass of the system Earth-Moon is calculated from

$$b + c = \frac{(K')^2}{kr_0(1 - \epsilon^2)}. \tag{50}$$

The constant $K' = r^2\dot{\theta}$ is determined from the orbital period T because

$$K' \int_0^T \mathrm{d}t = \int_0^{2\pi} r^2 \mathrm{d}\theta = 2\pi r_0^2 \sqrt{1 - \epsilon^2} \quad \Rightarrow \quad K' = \frac{2\pi r_0^2}{T}\sqrt{1 - \epsilon^2} \tag{51}$$

owing to the fact that this integral is twice the area of the ellipse. Substitution into equation (50) yields

$$b + c = \frac{4\pi^2 r_0^3}{kT^2} \tag{52}$$

expressed by Kepler's third law. It permits finding the mass $b + c$ of the system Earth-Moon provided the gravitational constant k is known with enough accuracy. The observed values are $T = 27.321661$ days (sidereal month) and $r_0 = 384,400$ km. Taking a value of $k = 6.67408 \cdot 10^{-11}$ N·m^{2}kg^{-2} for the gravitational constant [53, p 1-1], one finds $b + c = 6.02944 \cdot 10^{24}$ kg. For the known ratio 81.3:1 of the masses of Earth and the Moon, one finally finds their values: $5.95618 \cdot 10^{24}$ and $7.3262 \cdot 10^{22}$ kg respectively, somewhat lower than the accepted values of $5.9736 \cdot 10^{24}$ [53, p 14-2] and $7.3483 \cdot 10^{22}$ kg [53, p 14-4]. Approximations of higher orders of $\|\mathbf{E}\|/\|\mathbf{X}\|$ imply corrections to the equation of motion and also to the masses of Earth and the Moon, which are calculated from the orbital parameters.

The parameter K is obtained from the differential equation (44), for which the radial velocity vanishes at the maximum and minimum of r

$$\frac{(K')^2}{r_0^2(1 - \epsilon)^2} - \frac{2k(b+c)}{r_0(1 - \epsilon)} + 2K = 0\,, \qquad \frac{(K')^2}{r_0^2(1 + \epsilon)^2} - \frac{2k(b+c)}{r_0(1 + \epsilon)} + 2K = 0. \tag{53}$$

The arithmetic mean of both equations yields

$$\frac{(K')^2(1 + \epsilon^2)}{r_0^2(1 - \epsilon^2)^2} - \frac{2k(b+c)}{r_0(1 - \epsilon^2)} + 2K = 0. \tag{54}$$

The introduction of equation (50) into (54) finally gives

$$K = \frac{(K')^2}{2r_0^2(1 - \epsilon^2)} = \frac{k(b+c)}{2r_0} = \frac{2\pi^2 r_0^2}{T^2} \tag{55}$$

with the help of (52) in the last step. The last fraction in (55) allows us to calculate the constant K from the orbital parameters. From (48) and from the constancy of the angular momentum we have

$$\dot{\theta} = \frac{K'}{r^2} = \frac{K'(1 + \epsilon \cos \theta)^2}{r_0^2(1 - \epsilon^2)^2} = \frac{2\pi(1 + \epsilon \cos \theta)^2}{T(1 - \epsilon^2)^{3/2}} \tag{56}$$

after applying (51). Although this differential equation is separable, we want θ as a function of time. Therefore, we develop in power series of ϵ

$$\dot{\theta} = \frac{2\pi}{T} \left(1 + 2\epsilon \cos \theta + O(\epsilon^2)\right). \tag{57}$$

The zero-order approximation to its solution is $\theta = 2\pi t/T$, which we introduce into this differential equation up to the first power of ϵ

$$\dot{\theta} \cong \frac{2\pi}{T} \left(1 + 2\epsilon \cos \frac{2\pi t}{T}\right) \tag{58}$$

in order to find by integration the first-order approximation to the solution

$$\theta \cong \frac{2\pi t}{T} + 2\epsilon \sin \frac{2\pi t}{T}. \tag{59}$$

Let us now approximate r as a function of time

$$r = \frac{r_0(1 - \epsilon^2)}{1 + \epsilon \cos \theta} = r_0 \left(1 - \epsilon \cos \theta + O(\epsilon^2)\right). \tag{60}$$

Since $\cos(2\epsilon \sin(2\pi t/T)) = 1 + O(\epsilon^2)$ and $\sin(2\epsilon \sin(2\pi t/T)) = 2\epsilon \sin(2\pi t/T) + O(\epsilon^3)$, we have

$$\cos \theta = \cos \left(\frac{2\pi t}{T} + 2\epsilon \sin \frac{2\pi t}{T}\right) = \cos \frac{2\pi t}{T} - 2\epsilon \sin^2 \frac{2\pi t}{T} + O(\epsilon^2) \tag{61}$$

whence

$$r = r_0 \left(1 - \epsilon \cos \frac{2\pi t}{T} + O(\epsilon^2)\right). \tag{62}$$

We judge this approximation as very simple and at the same time good enough for the purposes that follow.

5.1.2. First-Order Approximation

Let us go one step further by taking into account terms involving the first power of $\|\mathbf{E}\|/\|\mathbf{X}\|$ that we disregarded in the zero-order approximation. The Jacobi coordinate $\mathbf{X}$ satisfies

$$\mathbf{X} = \frac{b\mathbf{D} - c\mathbf{F}}{b + c} = \mathbf{D} + \frac{c}{b + c}\mathbf{E} = -\mathbf{F} - \frac{b}{b + c}\mathbf{E} \qquad (63)$$

whence

$$\mathbf{D}^2 = \mathbf{X}^2 - \frac{2c}{b + c}\mathbf{X} \cdot \mathbf{E} + \frac{c^2}{(b + c)^2}\mathbf{E}^2$$

$$\mathbf{F}^2 = \mathbf{X}^2 + \frac{2b}{b + c}\mathbf{X} \cdot \mathbf{E} + \frac{b^2}{(b + c)^2}\mathbf{E}^2. \qquad (64)$$

We disregard the last term because it is of second order. Hence

$$\frac{1}{\|\mathbf{D}\|^3} \cong \frac{1}{\|\mathbf{X}\|^3}\left(1 - \frac{2c}{b + c}\frac{\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^2}\right)^{-\frac{3}{2}} \cong \frac{1}{\|\mathbf{X}\|^3}\left(1 + \frac{3c}{b + c}\frac{\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^2}\right)$$

$$\frac{1}{\|\mathbf{F}\|^3} \cong \frac{1}{\|\mathbf{X}\|^3}\left(1 + \frac{2b}{b + c}\frac{\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^2}\right)^{-\frac{3}{2}} \cong \frac{1}{\|\mathbf{X}\|^3}\left(1 - \frac{3b}{b + c}\frac{\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^2}\right). \qquad (65)$$

Substitution of these approximations into the Lagrange multiplier (34) yields

$$\boldsymbol{\lambda} \cong \frac{a\,b\,c\,k}{m}\left(\frac{\mathbf{D}}{\|\mathbf{X}\|^3} + \frac{\mathbf{E}}{\|\mathbf{E}\|^3} + \frac{\mathbf{F}}{\|\mathbf{X}\|^3} + \frac{3\,\mathbf{X} \cdot \mathbf{E}}{(b + c)\|\mathbf{X}\|^5}(c\mathbf{D} - b\mathbf{F})\right)$$

$$= \frac{a\,b\,c\,k}{m}\left(\frac{\mathbf{E}}{\|\mathbf{E}\|^3} - \frac{\mathbf{E}}{\|\mathbf{X}\|^3} + \frac{3\,\mathbf{X} \cdot \mathbf{E}}{(b + c)\|\mathbf{X}\|^5}(c\mathbf{D} - b\mathbf{F})\right). \qquad (66)$$
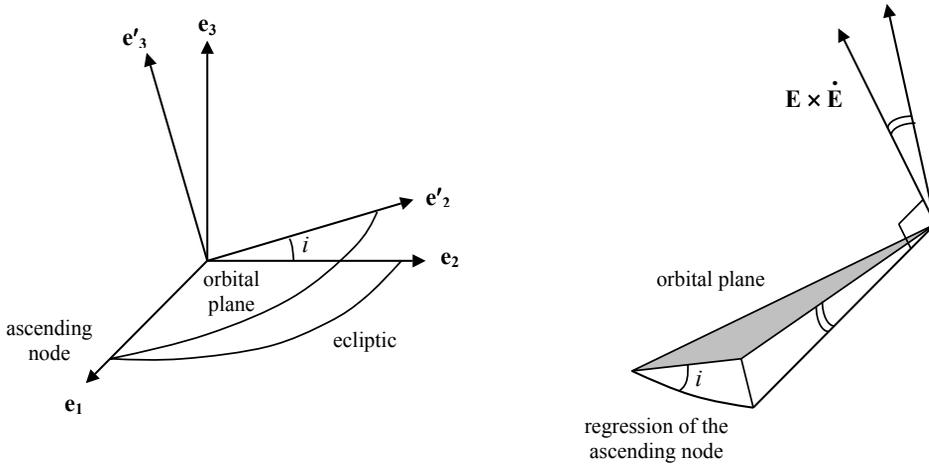
From (63) we find

$$\frac{c\mathbf{D} - b\mathbf{F}}{b + c} = \mathbf{X} + \frac{b - c}{b + c}\mathbf{E} \qquad (67)$$

and

$$\boldsymbol{\lambda} \cong \frac{a\,b\,c\,k}{m}\left(\frac{\mathbf{E}}{\|\mathbf{E}\|^3} - \frac{\mathbf{E}}{\|\mathbf{X}\|^3} + \frac{3\,\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^5}\left(\mathbf{X} + \frac{b - c}{b + c}\mathbf{E}\right)\right)$$

$$\cong \frac{a\,b\,c\,k}{m}\left(\frac{\mathbf{E}}{\|\mathbf{E}\|^3} - \frac{\mathbf{E}}{\|\mathbf{X}\|^3} + \frac{3\,\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^5}\mathbf{X}\right). \qquad (68)$$

because we limit the approximation to first-degree powers of $\|\mathbf{E}\|/\|\mathbf{X}\|$. Then, the equation of the relative motion Earth-Moon (second of (33)) is

$$\ddot{\mathbf{E}} = -k\,m\frac{\mathbf{E}}{\|\mathbf{E}\|^3} + \frac{m}{b\,c}\boldsymbol{\lambda} \cong -k\left(\frac{(b + c)}{\|\mathbf{E}\|^3} + \frac{a}{\|\mathbf{X}\|^3}\right)\mathbf{E} + \frac{3ka\,\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^5}\mathbf{X}. \qquad (69)$$

Figure 3. On the left, sketch of the orbital plane of the Moon and the ecliptic. Their intersection is the line joining the ascending and descending nodes. The right figure shows why the regression of the ascending node is obtained from the division of the x-component of the variation of $\mathbf{E} \times \dot{\mathbf{E}}$ by $\sin i$.

Notice that, without the last term, the vectors $\mathbf{E}$, $\dot{\mathbf{E}}$ and $\ddot{\mathbf{E}}$ would lie in the same plane (the orbital plane of the Moon), and this plane would be kept constant. However, owing to the inclination of the orbital plane of the Moon with respect to the ecliptic, $\mathbf{X}$ does not lie in this plane, which means an oblique acceleration of the Moon. Therefore, the last term changes the orbital plane of the Moon.

Variation of the Angular Momentum of the Moon

From (69) we find that the variation of the angular momentum with time is proportional to

$$\frac{\mathrm{d}(\mathbf{E} \times \dot{\mathbf{E}})}{\mathrm{d}t} = \mathbf{E} \times \ddot{\mathbf{E}} \cong \frac{3ka\,\mathbf{X} \cdot \mathbf{E}}{\|\mathbf{X}\|^5}\,\mathbf{E} \times \mathbf{X}. \qquad (70)$$

Let us take a frame whose xy plane is the ecliptic. The vector $\mathbf{e_1}$ will be the unitary vector with the direction of the ascending node, that is, the intersection of the ecliptic with the orbital plane of the Moon when it goes over the ecliptic, and $\mathbf{e_2}$ will be the perpendicular vector in the ecliptic rotated 90° anticlockwise, that is, in the direction of Earth motion (Fig. 3). According to the zero-order approximation, the orbital plane of the Moon is invariant and both vectors are constant, but this statement is not exact. Owing to the regression of the nodes, $\mathbf{e_1}$ and $\mathbf{e_2}$ really form

a slowly rotating frame. The orbital motion of Earth (more exactly the motion of the centre of mass Earth-Moon) is expressed by the rotation of the vector $\mathbf{X}$, just like the orbital motion of the Moon is also expressed by the rotation of the vector $\mathbf{E}$. The times taken for Earth and the Moon to complete one revolution with respect to the ascending node are defined as the draconic year (346.62008 days) and draconic month (27.21222 days). The regression of the nodes causes them to differ from the sidereal year (365.25636 days) and sidereal month (27.32166 days), and it will be calculated below.

Let r, θ be the polar coordinates of the orbit of the Moon, and R, ϕ be the polar coordinates of the orbit of Earth in the ecliptic. Then

$$\mathbf{E} = r(\cos\theta\,\mathbf{e_1} + \sin\theta\,(\cos i\,\mathbf{e_2} + \sin i\,\mathbf{e_3})) \tag{71}$$
$$\mathbf{X} = R(\cos\phi\,\mathbf{e_1} + \sin\phi\,\mathbf{e_2})$$

where $\mathbf{e_3}$ is the unitary vector perpendicular to the ecliptic, and i is the inclination of the orbital plane of the Moon, that is, the angle it forms with the ecliptic. Then

$$\mathbf{E} \cdot \mathbf{X} = Rr(\cos\theta\cos\phi + \cos i\sin\theta\sin\phi)$$
$$\mathbf{E} \times \mathbf{X} = Rr[-\sin i\sin\theta\sin\phi\,\mathbf{e_1} + \sin i\sin\theta\cos\phi\,\mathbf{e_2} \tag{72}$$
$$+(\cos\theta\sin\phi - \cos i\sin\theta\cos\phi)\,\mathbf{e_3}].$$

By introducing the unitary vectors $\mathbf{e_2'} = \cos i\,\mathbf{e_2} + \sin i\,\mathbf{e_3}$ and $\mathbf{e_3'} = -\sin i\,\mathbf{e_2} + \cos i\,\mathbf{e_3}$, which are respectively coplanar and perpendicular to the orbital plane of the Moon (Fig. 3 left), we can write

$$\mathbf{E} \times \mathbf{X} = Rr\left[\sin i\sin\phi\,(-\sin\theta\,\mathbf{e_1} + \cos\theta\,\mathbf{e_2'})\right.$$
$$\left. +(-\sin\theta\cos\phi + \cos i\cos\theta\sin\phi)\,\mathbf{e_3'}\right]. \tag{73}$$

From (71) we also have

$$\mathbf{E} = r\left(\cos\theta\,\mathbf{e_1} + \sin\theta\,\mathbf{e_2'}\right). \tag{74}$$

By derivation

$$\dot{\mathbf{E}} = \dot{r}(\cos\theta\,\mathbf{e_1} + \sin\theta\,\mathbf{e_2'}) + r\dot{\theta}\,(-\sin\theta\,\mathbf{e_1} + \cos\theta\,\mathbf{e_2'}) \tag{75}$$

whence

$$\mathbf{E} \times \dot{\mathbf{E}} = r^2\dot{\theta}\,\mathbf{e_3'} \qquad \Rightarrow \qquad \|\mathbf{E} \times \dot{\mathbf{E}}\| = r^2\dot{\theta} = K'. \tag{76}$$

Then, from equations (70), (72) and (73) we finally obtain

$$\frac{1}{\|\mathbf{E} \times \dot{\mathbf{E}}\|}\frac{\mathrm{d}(\mathbf{E} \times \dot{\mathbf{E}})}{\mathrm{d}t} \approx \frac{3kar^2}{K'R^3}(\cos\theta\cos\phi + \cos i\sin\theta\sin\phi)$$
$$\times\left[\sin\phi\sin i(-\sin\theta\mathbf{e_1} + \cos\theta\mathbf{e_2'}) + (-\sin\theta\cos\phi + \cos i\cos\theta\sin\phi)\mathbf{e_3'}\right]. \tag{77}$$

Since $i \approx 5.15° = 0.045 \ll 1$, we apply the approximation $\cos i = 0.99898 \approx 1$. We also change time t for θ taking into account that $\dot{\theta} = K'/r^2$

$$\frac{1}{\|\mathbf{E} \times \dot{\mathbf{E}}\|} \frac{\mathrm{d}(\mathbf{E} \times \dot{\mathbf{E}})}{\mathrm{d}\theta} \approx \frac{3kar^4}{(K')^2 R^3} \cos(\theta - \phi) \cdot [-\sin\theta \sin\phi \sin i \mathbf{e_1} \\ + \cos\theta \sin\phi \sin i \mathbf{e_2'} - \sin(\theta - \phi)\mathbf{e_3'}] . \tag{78}$$

The component in the direction of $\mathbf{e_1}$ implies regression of the nodes. The component in the direction $\mathbf{e_2'}$ implies a change of the inclination of the orbit, and the component in the direction of $\mathbf{e_3'}$ implies raising or lowering the norm of the angular momentum. Let us consider each component separately.

The rate of increase in the ecliptic longitude l of the ascending node is obtained from division of the first component by $\sin i$ (Fig. 3 right)

$$\frac{\mathrm{d}l}{\mathrm{d}\theta} = -\frac{3kar^4}{(K')^2 R^3} \cos(\theta - \phi) \sin\theta \sin\phi \\ = -\frac{3kar^4}{4(K')^2 R^3} \left[1 + \cos(2\theta - 2\phi) - \cos 2\theta - \cos 2\phi\right] . \tag{79}$$

K' is obtained from (50) in the zero-order approximation

$$(K')^2 = k(b+c)r_0(1 - \epsilon^2) \tag{80}$$

so that we find

$$\frac{\mathrm{d}l}{\mathrm{d}\theta} = -\frac{3ar^4}{4(b+c)r_0(1 - \epsilon^2)R^3} \left[1 + \cos(2\theta - 2\phi) - \cos 2\theta - \cos 2\phi\right] . \tag{81}$$

The oscillations on the right satisfy the inequality

$$-\frac{1}{2} \le 1 + \cos(2\theta - 2\phi) - \cos 2\theta - \cos 2\phi \le 4 \tag{82}$$

whence

$$-\frac{3ar^4}{(b+c)r_0(1 - \epsilon^2)R^3} \le \frac{\mathrm{d}l}{\mathrm{d}\theta} \le \frac{3ar^4}{8(b+c)r_0(1 - \epsilon^2)R^3} . \tag{83}$$

The maximum regression rate takes place for $\theta = 90°$ or $270°$ and $\phi = 90°$ or $270°$, while the maximum of slight advance rate (opposite to the mean rate) takes place for $\theta = 30°$ or $210°$ and $\phi = 150°$ or $330°$, or the other way round since the expression is symmetric with respect to the exchange of θ and ϕ. The actual extremes can differ somewhat from these values because r is not constant but depends on θ.

Now we introduce r given by the Keplerian elliptic orbit (60) into (81)

$$\frac{\mathrm{d}l}{\mathrm{d}\theta} = -\frac{3ar_0^3(1-\epsilon^2)^3(1+\cos(2\theta-2\phi)-\cos 2\theta-\cos 2\phi)}{4(b+c)R^3(1+\epsilon\cos\omega\theta)^4} \;. \qquad (84)$$

In the zero-order approximation of the orbit (60) $\omega = 1$, but the nodal regression causes ω to differ slightly from this value. We define the constant

$$\lambda = \frac{ar_0^3(1-\epsilon^2)^3}{2(b+c)R^3} = 2.764188 \cdot 10^{-3} \qquad (85)$$

calculated from the usually admitted masses of the Sun, Earth and the Moon, $a = 1.9884 \cdot 10^{30}$, $b = 5.9736 \cdot 10^{24}$ and $c = 7.3483 \cdot 10^{22}$ kg [53, pp 14-2 and 14-4], mean semimajor axes of the orbits of Earth and the Moon, $R = 149,598,023$ km and $r_0 = 384,400$ km, and mean eccentricity $\epsilon = 0.0549$. By linearisation of the denominator we have

$$\frac{\mathrm{d}l}{\mathrm{d}\theta} = -\frac{3\lambda}{2}(1-4\epsilon\cos\omega\theta)(1+\cos(2\theta-2\phi)-\cos 2\theta-\cos 2\phi) \;. \qquad (86)$$

If we suppose that ϕ changes uniformly with time (circular motion of Earth) but θ is given by (59) obtained from the Keplerian elliptic orbit of the Moon in the zero-order approximation then

$$\phi \cong \alpha(\theta - 2\epsilon\sin\omega\theta) \qquad (87)$$

where $\alpha = 27.21222/346.6201 = 0.07850734$ is the quotient of the draconic month and year, and $\omega \cong 1$. The fact that $\epsilon \ll 1$ allows us to approximate

$$\cos 2\phi \cong \cos 2\alpha\theta + 4\alpha\epsilon\sin 2\alpha\theta\sin\omega\theta \qquad (88)$$

$$\begin{aligned} \cos(2\theta-2\phi) &= \cos(2\theta-2\alpha\theta+4\alpha\epsilon\sin\omega\theta) \\ &\cong \cos\eta\theta - 4\alpha\epsilon\sin\eta\theta\sin\omega\theta \end{aligned} \qquad (89)$$

where $\eta = 2 - 2\alpha = 1.84298532$ is introduced in order of brevity. In the same way

$$\sin(2\theta-2\phi) \cong \sin\eta\theta + 4\alpha\epsilon\cos\eta\theta\sin\omega\theta \;. \qquad (90)$$

Since $4\alpha\epsilon = 0.017 \ll 1$ we can go further in this approximation

$$\cos 2\phi \cong \cos 2\alpha\theta, \qquad \sin(2\theta-2\phi) \cong \sin\eta\theta, \qquad \cos(2\theta-2\phi) \cong \cos\eta\theta \quad (91)$$

which is good enough for many purposes. The introduction of this approximation into (86) gives

$$\begin{aligned}
\frac{\mathrm{d}l}{\mathrm{d}\theta} &\approx -\frac{3\lambda}{2}(1 - 4\epsilon\cos\omega\theta)(1 + \cos\eta\theta - \cos 2\theta - \cos 2\alpha\theta) \\
&= -\frac{3\lambda}{2}[1 + \cos\eta\theta - \cos 2\theta - \cos 2\alpha\theta - 2\epsilon(2\cos\omega\theta \\
&\quad + \cos(\eta\theta - \omega\theta) + \cos(\eta\theta + \omega\theta) - \cos(2\theta - \omega\theta) \\
&\quad - \cos(2\theta + \omega\theta) - \cos(\omega\theta - 2\alpha\theta) - \cos(\omega\theta + 2\alpha\theta))]
\end{aligned} \tag{92}$$

after transforming products of trigonometric functions into additions. The mean value is then

$$\overline{\frac{\mathrm{d}l}{\mathrm{d}\theta}} = -\frac{3\lambda}{2} = -\frac{3ar_0^3(1 - \epsilon^2)^3}{4(b + c)R^3} \tag{93}$$

which exhibits the regression of the ascending node. This expression is slightly different from that obtained in [19, p 61] through a process of integration that is absent here. In each orbital revolution of the Moon, the longitude of the ascending node should decrease in the mean by

$$|\overline{\Delta l}| = -2\pi\overline{\frac{\mathrm{d}l}{\mathrm{d}\theta}} = \frac{3\pi ar_0^3(1 - \epsilon^2)^3}{2(b + c)R^3} = 0.026052 = 1°29'34''. \tag{94}$$

The nodes would turn 2π rad after 241.11 draconic months, that is, 6561 days or 17.96 years. The observed value is a decrease in the ecliptic longitude of the nodes by $1°26'27''$ and a returning period of 18.61 years. This discordance seems to suggest that the masses of Earth and the Moon are 3.6% higher than the accepted values. The regression of the nodes means that $\mathbf{e_1}$ and $\mathbf{e_2}$ are not constant vectors but that they slowly rotate. In this way, the Moon and Earth find again the ascending node in a draconic month (27.21222 days) and year (346.62 days), which are shorter than a sidereal month and year. The perigee of the Keplerian orbit found in the zero-order approximation has constant ecliptic longitude, while the ascending node has retrograde motion. Since θ and ϕ are the angles with respect to the ascending node, the Keplerian orbit now becomes

$$r = \frac{r_0(1 - \epsilon^2)}{1 + \epsilon\cos\omega\theta}, \qquad \omega = 1 - \frac{3\lambda}{2} = 0.99585372. \tag{95}$$

Integration of (92) yields

$$\begin{aligned}
l(\theta) = -\frac{3\lambda}{2}\Bigg[&\theta + \frac{\sin\eta\theta}{\eta} - \frac{\sin 2\theta}{2} - \frac{\sin 2\alpha\theta}{2\alpha} - 2\epsilon\bigg(\frac{2\sin\omega\theta}{\omega} \\
&+ \frac{\sin(\eta\theta - \omega\theta)}{\eta - \omega} + \frac{\sin(\eta\theta + \omega\theta)}{\eta + \omega} - \frac{\sin(2\theta - \omega\theta)}{2 - \omega} \\
&- \frac{\sin(2\theta + \omega\theta)}{2 + \omega} - \frac{\sin(\omega\theta - 2\alpha\theta)}{\omega - 2\alpha} - \frac{\sin(\omega\theta + 2\alpha\theta)}{\omega + 2\alpha}\bigg)\Bigg].
\end{aligned} \tag{96}$$

When the Moon crosses the ecliptic at the ascending node, $\theta = 2\pi n$ with $n \in \mathbb{Z}$ and

$$l_n = l(2\pi n) = -\frac{3\lambda}{2}\left[2\pi n - \frac{\sin 4\alpha\pi n}{\alpha\eta} - 2\epsilon\left(\frac{8\sin 2\omega\pi n}{\omega(4 - \omega^2)}\right.\right.$$
$$\left.\left. -\frac{2\sin(4\alpha\pi n + 2\omega\pi n)}{(\eta - \omega)(\omega + 2\alpha)} + \frac{2\sin(4\alpha\pi n - 2\omega\pi n)}{(\eta + \omega)(\omega - 2\alpha)}\right)\right] \tag{97}$$

where we have taken into account that $\eta = 2 - 2\alpha$. Discarding the last three terms, the increase of the ecliptic longitude between two successive passages of the Moon through the ascending node is

$$l_{n+1} - l_n \cong -\frac{3\lambda}{2}\left(2\pi - \frac{\sin 4\alpha\pi(n+1) - \sin 4\alpha\pi n}{\alpha\eta}\right). \tag{98}$$

The discarded terms only contribute to the final result by at most 1.8% so that we omit their calculation. By transforming differences of trigonometric functions into their products, we find

$$l_{n+1} - l_n \cong -3\lambda\pi + \frac{3\lambda\sin 2\alpha\pi}{\alpha\eta}\cos(2\alpha\pi(2n+1)) . \tag{99}$$

In order to repeat the same value of $\cos(2\alpha\pi(2n+1))$, the argument of the cosine must increase by 2π, meaning $n = 1/2\alpha$ draconic months, which is half a draconic year (173.31 days), just the observed period of the oscillation of the draconic month [15]. The amplitude of this oscillation is

$$\left|l_{n+1} - l_n + 3\lambda\pi\right| \leq \frac{3\lambda\sin 2\alpha\pi}{\alpha\eta} = 0.027139 = 1°33'18''. \tag{100}$$

That is, sometimes the node does not advance between two successive Moon's passages and others the node has retrograde motion at about twice the rate. From $\theta = 2\pi(n + 1/2)$, it follows $2\phi = 2\alpha\pi(2n + 1)$, so that there is not any nodal regression for $\phi = \pi k$, $k \in \mathbb{Z}$ (syzygies), and their regression is maximum for $\phi = \pi(k + 1/2)$ (quadratures) as already deduced by Newton [41, p 463] with the approximation of circular orbit.

The component of $\mathbf{e}_2'$ in (78) provides how the inclination of Moon's orbital plane varies with θ. If the former is positive the latter decreases, whence

$$\frac{\mathrm{d}i}{\mathrm{d}\theta} = -\frac{3kar^4}{(K')^2R^3}\cos(\theta - \phi)\cos\theta\sin\phi\sin i$$
$$= -\frac{3kar^4\sin i}{4(K')^2R^3}\left[-\sin(2\theta - 2\phi) + \sin 2\phi + \sin 2\theta\right]. \tag{101}$$

Under the approximation (91), and after introducing the Keplerian elliptic orbit and K' given by (80), we find

$$\frac{\mathrm{d}i}{\mathrm{d}\theta} \approx -\frac{3ar_0^3 \sin i}{4(b+c)(1-\epsilon^2)R^3}(1 - 4\epsilon \cos \omega\theta)[-\sin \eta\theta + \sin 2\alpha\theta + \sin 2\theta]$$

$$\begin{aligned} =& -\frac{3\lambda \sin i}{2}[-\sin \eta\theta + \sin 2\alpha\theta + \sin 2\theta + 2\epsilon \sin(\eta\theta - \omega\theta) \\ &+ 2\epsilon \sin(\eta\theta + \omega\theta) + 2\epsilon \sin(\omega\theta - 2\alpha\theta) - 2\epsilon \sin(2\alpha\theta + \omega\theta) \\ &- 2\epsilon \sin(2\theta - \omega\theta) - 2\epsilon \sin(2\theta + \omega\theta)] \end{aligned} \qquad (102)$$

after transforming products of trigonometric functions into additions. Its integration for a small variation of i yields

$$\begin{aligned} i - \bar{i} \approx &\frac{3\lambda \sin \bar{i}}{2}\left(-\frac{\cos \eta\theta}{\eta} + \frac{\cos 2\alpha\theta}{2\alpha} + \frac{\cos 2\theta}{2} + \frac{2\epsilon \cos(\eta\theta - \omega\theta)}{\eta - \omega}\right. \\ &+ \frac{2\epsilon \cos(\eta\theta + \omega\theta)}{\eta + \omega} + \frac{2\epsilon \cos(\omega\theta - 2\alpha\theta)}{\omega - 2\alpha} - \frac{2\epsilon \cos(\omega\theta + 2\alpha\theta)}{\omega + 2\alpha} \\ &\left.- \frac{2\epsilon \cos(2\theta - \omega\theta)}{2 - \omega} - \frac{2\epsilon \cos(2\theta + \omega\theta)}{2 + \omega}\right). \end{aligned} \qquad (103)$$

Leaving aside the initial factor, the amplitudes of each oscillation are 0.5426 : 6.3688 : 0.50 : 0.1296 : 0.0387 : 0.1309 : 0.0952 : 0.1093 : 0.0367. Therefore, the first three terms are the main terms, while the fourth, sixth, seventh and eighth are a minor correction (not more than 6%), and the fifth and ninth can be discarded (not more than 1%). The largest term is the second term, with a relative amplitude of 80%. Its period is $1/(2\alpha) = 6.36882$ mean draconic months or 173.31 days, half a mean draconic year (346.62 days), which is just the observed main frequency. Since the first three terms are the main ones, we can use the approximated expression

$$i - \bar{i} \approx \frac{3\lambda \sin \bar{i}}{2}\left(-\frac{\cos \eta\theta}{\eta} + \frac{\cos 2\alpha\theta}{2\alpha} + \frac{\cos 2\theta}{2}\right). \qquad (104)$$

The mean value of the inclination of the orbit of the Moon is $\bar{i} = 5.145°$ for the three-year period 2008-2010 [15]. With this value, the inclination calculated from (104) has been plotted in Fig. 4 as a function of time $t = \theta\, T/(2\pi)$. If one calculates the inclination from the full expression (103), no significant change on the graph can be appreciated at a glance. Small differences can only be noticed by the superposition of both graphs, which are mostly coincident. Anyway, the agreement of the inclination (104) with observation is so good that the calculated
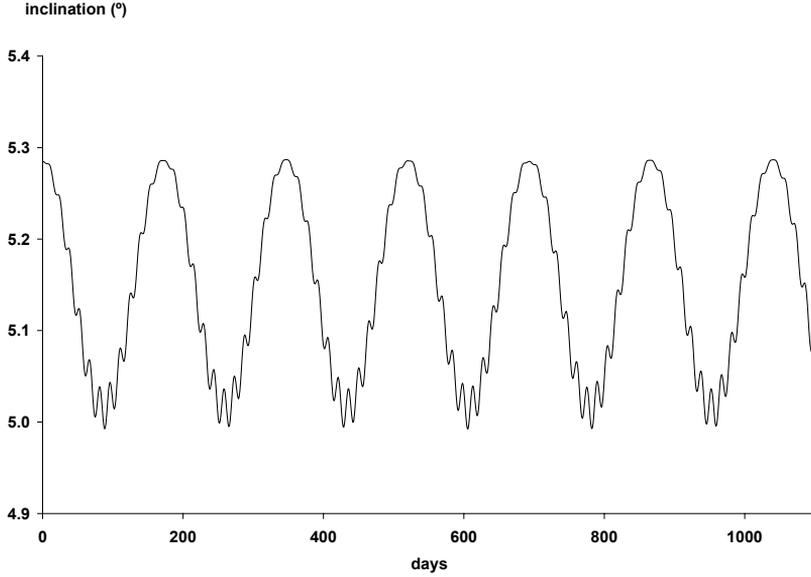
Figure 4. Inclination of Moon's orbit as a function of time calculated by means of (104) for a period of three years. Maximums occur when the ecliptic longitudes of the Sun and the ascending node are equal or differ by 180°, so that the main period is half a draconic year (173.31 days).

graph in Fig. 4 is indistinguishable from the plot of experimental data [15, Figs. 4-10].

The amplitude of oscillation could be obtained as

$$|i - \bar{i}| \leq \frac{3\lambda \sin \bar{i}}{2} \left(\frac{1}{1 - \alpha} + \frac{1}{\alpha} + 1 + \frac{2\epsilon}{\eta - \omega} \right) = 9'29''. \qquad (105)$$

However, the frequencies are not independent because $\eta + 2\alpha = 2$ and therefore the amplitude of the variation of the calculated inclination shown by Fig. 4 is somewhat less, $0.15° = 9'$, which is identical to the observed value [15].

The component of $\mathbf{e'_3}$ in (78) reports the relative variation of the norm of the angular momentum

$$\frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta} = -\frac{3kar^4}{(K')^2 R^3} \cos(\theta - \phi) \sin(\theta - \phi) = -\frac{3kar^4}{2(K')^2 R^3} \sin(2\theta - 2\phi). \quad (106)$$

We now apply the approximation (91) and introduce the Keplerian elliptic orbit (95) corrected for the nodal regression

$$\frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta} \approxeq -\frac{3kar_0^4(1 - 4\epsilon \cos \omega\theta)}{2K'^2 R^3} \sin \eta\theta \qquad (107)$$

whence

$$
\begin{aligned}
\frac{\mathrm{d}K'^2}{\mathrm{d}\theta} &\approx -\frac{3kar_0^4}{R^3}\left(\sin\eta\theta - 4\epsilon\cos\omega\theta\sin\eta\theta\right) \\
&= -\frac{3kar_0^4}{R^3}\left[\sin\eta\theta - 2\epsilon\sin(\eta\theta - \omega\theta) - 2\epsilon\sin(\eta\theta + \omega\theta)\right].
\end{aligned}
\tag{108}
$$

Integration yields

$$
\frac{K'^2}{\overline{K'^2}} \approx 1 + \frac{6\lambda}{(1-\epsilon^2)^4}\left[\frac{\cos\eta\theta}{\eta} - \frac{2\epsilon\cos(\eta\theta - \omega\theta)}{\eta - \omega} - \frac{2\epsilon\cos(\eta\theta + \omega\theta)}{\eta + \omega}\right] \tag{109}
$$

after taking as the mean value $\overline{K'^2} = k(b+c)r_0(1-\epsilon^2)$ given by (80) obtained in the zero-order approximation, and also considering the constant λ (85). In the mean, the norm of the angular momentum does not change, but its perturbation is a superposition of sinusoidal oscillations. The variation of the norm of the angular momentum is obtained from linearisation of the square root

$$
\frac{K'}{\overline{K'}} \approx 1 + \frac{3\lambda}{(1-\epsilon^2)^4}\left[\frac{\cos\eta\theta}{\eta} - \frac{2\epsilon\cos(\eta\theta - \omega\theta)}{\eta - \omega} - \frac{2\epsilon\cos(\eta\theta + \omega\theta)}{\eta + \omega}\right] \tag{110}
$$

whence $\overline{K'} \approx \sqrt{\overline{K'^2}}$. Its relative amplitude satisfies

$$
\frac{|\Delta K'|}{\overline{K'}} \leq \frac{3\lambda}{(1-\epsilon^2)^4}\left(\frac{1}{\eta} + \frac{2\epsilon}{\eta - \omega} + \frac{2\epsilon}{\eta + \omega}\right) = 5.97 \cdot 10^{-3} \tag{111}
$$

The amplitudes of the three oscillations are in the ratio 0.54:0.13:0.04. The period of the main oscillation is $T/\eta = T/(2-2\alpha) = 14.765$ days, half a synodic month (29.53 days).

The Orbit of the Moon

From (69) we find

$$
\mathbf{E} \cdot \ddot{\mathbf{E}} \approx -k\left(\frac{(b+c)}{\|\mathbf{E}\|} + \frac{a\|\mathbf{E}\|^2}{\|\mathbf{X}\|^3}\right) + \frac{3ka\,(\mathbf{X} \cdot \mathbf{E})^2}{\|\mathbf{X}\|^5}. \tag{112}
$$

By derivation of $r^2 = \mathbf{E}^2$ with respect to time, one finds $r\,\dot{r} = \mathbf{E} \cdot \dot{\mathbf{E}}$, and a new derivation yields

$$
\dot{r}^2 + r\,\ddot{r} = \dot{\mathbf{E}}^2 + \mathbf{E} \cdot \ddot{\mathbf{E}}. \tag{113}
$$

Since $\dot{\mathbf{E}}^2 = \dot{r}^2 + r^2\dot{\theta}^2$, which can be checked by derivation of (71), it follows

$$
r\,\ddot{r} = r^2\dot{\theta}^2 + \mathbf{E} \cdot \ddot{\mathbf{E}}. \tag{114}
$$

The introduction of (112) into (114) yields

$$r\,\ddot{r} = r^2\dot{\theta}^2 - k\left(\frac{(b+c)}{\|\mathbf{E}\|} + \frac{a\|\mathbf{E}\|^2}{\|\mathbf{X}\|^3}\right) + \frac{3ka\,(\mathbf{X}\cdot\mathbf{E})^2}{\|\mathbf{X}\|^5} \tag{115}$$

and the substitution of (72) with the approximation $\cos i \cong 1$ gives

$$r\,\ddot{r} = r^2\dot{\theta}^2 - k\left(\frac{(b+c)}{r} + \frac{ar^2}{R^3} - \frac{3ar^2\cos^2(\theta-\phi)}{R^3}\right)\cdot \tag{116}$$

By introducing the double angle, and extracting common factor, we obtain

$$\ddot{r} = r\dot{\theta}^2 - \frac{k(b+c)}{r^2}\left(1 - \frac{ar^3}{2(b+c)R^3} - \frac{3ar^3\cos(2\theta-2\phi)}{2(b+c)R^3}\right)\cdot \tag{117}$$

Now, taking into account that

$$\dot{r} = \frac{\mathrm{d}r}{\mathrm{d}\theta}\dot{\theta} \qquad \Rightarrow \qquad \ddot{r} = \frac{\mathrm{d}^2r}{\mathrm{d}\theta^2}\dot{\theta}^2 + \frac{\mathrm{d}r}{\mathrm{d}\theta}\ddot{\theta} \tag{118}$$

and that $\ddot{\theta}$ can be calculated by derivation of $K' = r^2\dot{\theta}$

$$\ddot{\theta} = \left[\frac{1}{r^2}\frac{\mathrm{d}K'}{\mathrm{d}\theta} - \frac{2K'}{r^3}\frac{\mathrm{d}r}{\mathrm{d}\theta}\right]\dot{\theta} = \left[\frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta} - \frac{2}{r}\frac{\mathrm{d}r}{\mathrm{d}\theta}\right]\dot{\theta}^2 \tag{119}$$

we finally have

$$\ddot{r} = \left[\frac{\mathrm{d}^2r}{\mathrm{d}\theta^2} - \frac{2}{r}\left(\frac{\mathrm{d}r}{\mathrm{d}\theta}\right)^2 + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}r}{\mathrm{d}\theta}\right]\dot{\theta}^2 \tag{120}$$

and the substitution into equation (117) yields

$$\frac{\mathrm{d}^2r}{\mathrm{d}\theta^2} - \frac{2}{r}\left(\frac{\mathrm{d}r}{\mathrm{d}\theta}\right)^2 + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}r}{\mathrm{d}\theta} = r - \frac{k(b+c)}{r^2\dot{\theta}^2}\left(1 - \frac{ar^3}{2(b+c)R^3}\right.$$
$$\left. - \frac{3ar^3\cos(2\theta-2\phi)}{2(b+c)R^3}\right)\cdot \tag{121}$$

We introduce the variable $s = 1/r$ whence

$$\frac{\mathrm{d}^2s}{\mathrm{d}\theta^2} + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}s}{\mathrm{d}\theta} + s = \frac{k(b+c)}{K'^2}\left(1 - \frac{a}{2(b+c)R^3s^3} - \frac{3a\cos(2\theta-2\phi)}{2(b+c)R^3s^3}\right)\cdot$$
$$\tag{122}$$

The substitution of the square of the angular momentum (109) yields, for the coefficient of the parenthesis in (122), the approximation

$$\frac{k(b+c)}{K'^2} \approx \frac{1}{r_0(1-\epsilon^2)}\left(1 - 6\lambda\left[\frac{\cos\eta\theta}{\eta} - \frac{2\epsilon\cos(\eta\theta-\omega\theta)}{\eta-\omega} - \frac{2\epsilon\cos(\eta\theta+\omega\theta)}{\eta+\omega}\right]\right)$$

that we have introduced together with the variable $u = r_0(1-\epsilon^2)s$ into (122) to give

$$\frac{\mathrm{d}^2u}{\mathrm{d}\theta^2} + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}u}{\mathrm{d}\theta} + u \approx \left(1 - 6\lambda\left[\frac{\cos\eta\theta}{\eta} - \frac{2\epsilon\cos(\eta\theta-\omega\theta)}{\eta-\omega}\right.\right.$$
$$\left.\left. - \frac{2\epsilon\cos(\eta\theta+\omega\theta)}{\eta+\omega}\right]\right) \times \left(1 - \frac{ar_0^3(1-\epsilon^2)^3}{2(b+c)R^3u^3} - \frac{3ar_0^3(1-\epsilon^2)^3\cos(2\theta-2\phi)}{2(b+c)R^3u^3}\right). \tag{123}$$

With the help of the constant λ (85), we rewrite this differential equation

$$\frac{\mathrm{d}^2u}{\mathrm{d}\theta^2} + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}u}{\mathrm{d}\theta} + u \approx \left(1 - 6\lambda\left[\frac{\cos\eta\theta}{\eta} - \frac{2\epsilon\cos(\eta\theta-\omega\theta)}{\eta-\omega}\right.\right.$$
$$\left.\left. - \frac{2\epsilon\cos(\eta\theta+\omega\theta)}{\eta+\omega}\right]\right) \times \left(1 - \frac{\lambda}{u^3} - \frac{3\lambda\cos(2\theta-2\phi)}{u^3}\right). \tag{124}$$

After applying the distributive property and also discarding terms in λ^2 because $\lambda \ll 1$, we find

$$\frac{\mathrm{d}^2u}{\mathrm{d}\theta^2} + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}u}{\mathrm{d}\theta} + u \approx 1 - \frac{\lambda}{u^3} - \frac{3\lambda}{u^3}\cos(2\theta-2\phi)$$
$$- \frac{6\lambda}{\eta}\cos\eta\theta + \frac{12\lambda\epsilon}{\eta-\omega}\cos(\eta\theta-\omega\theta) + \frac{12\lambda\epsilon}{\eta+\omega}\cos(\eta\theta+\omega\theta). \tag{125}$$

By introducing $v = u - 1 \ll 1$ we have

$$\frac{\mathrm{d}^2v}{\mathrm{d}\theta^2} + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}v}{\mathrm{d}\theta} + v = -\frac{\lambda}{(1+v)^3} - \frac{3\lambda\cos(2\theta-2\phi)}{(1+v)^3}$$
$$- \frac{6\lambda}{\eta}\cos\eta\theta + \frac{12\lambda\epsilon}{\eta-\omega}\cos(\eta\theta-\omega\theta) + \frac{12\lambda\epsilon}{\eta+\omega}\cos(\eta\theta+\omega\theta) \tag{126}$$

and the linear approximation yields

$$\frac{\mathrm{d}^2v}{\mathrm{d}\theta^2} + \frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta}\frac{\mathrm{d}v}{\mathrm{d}\theta} + (1-3\lambda)v \approx -\lambda - 3\lambda(1-3v)\cos(2\theta-2\phi)$$
$$- \frac{6\lambda}{\eta}\cos\eta\theta + \frac{12\lambda\epsilon}{\eta-\omega}\cos(\eta\theta-\omega\theta) + \frac{12\lambda\epsilon}{\eta+\omega}\cos(\eta\theta+\omega\theta). \tag{127}$$

With (80) and (85), the relative variation of the angular momentum (107) is

$$\frac{1}{K'}\frac{\mathrm{d}K'}{\mathrm{d}\theta} \cong -3\lambda(\sin\eta\theta - 4\epsilon\cos\omega\theta\sin\eta\theta) \tag{128}$$

while the substitution into (127) yields

$$\frac{\mathrm{d}^2v}{\mathrm{d}\theta^2} + (1-3\lambda)v = \lambda\left[-1 + 3(\sin\eta\theta - 4\epsilon\cos\omega\theta\sin\eta\theta)\frac{\mathrm{d}v}{\mathrm{d}\theta} - \frac{6}{\eta}\cos\eta\theta\right.$$
$$\left. -3(1-3v)\cos(2\theta-2\phi) + \frac{12\epsilon\cos(\eta\theta-\omega\theta)}{\eta-1} + \frac{12\epsilon\cos(\eta\theta+\omega\theta)}{\eta+1}\right]. \tag{129}$$

The solution to its homogeneous differential equation $\dfrac{\mathrm{d}^2v}{\mathrm{d}\theta^2} + (1-3\lambda)v = 0$ is

$$v = \epsilon\cos\omega\theta, \qquad \omega = \sqrt{1-3\lambda}. \tag{130}$$

Since $\lambda \ll \epsilon$, this approximated solution can be introduced into the *rhs* of (129) in order to find a better approximation
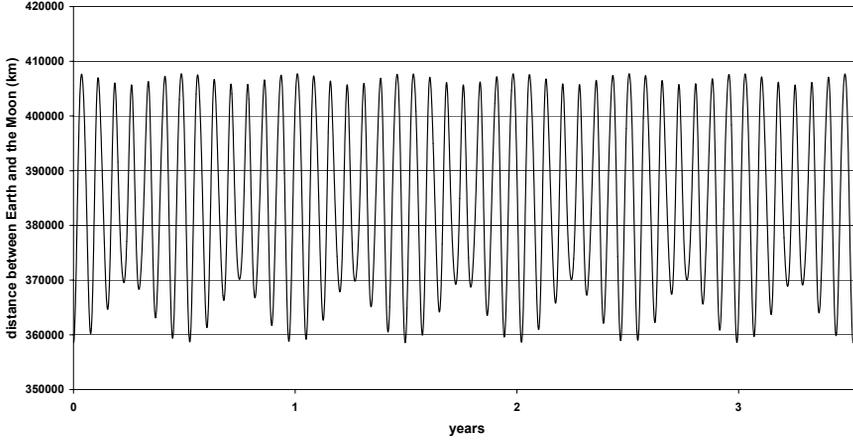
$$\frac{\mathrm{d}^2v}{\mathrm{d}\theta^2} + \omega^2v = \lambda\left[-1 - 3\epsilon\omega\sin\eta\theta\sin\omega\theta + (9\epsilon\cos\omega\theta - 3)\cos(2\theta - 2\phi)\right.$$
$$\left. -\frac{6}{\eta}\cos\eta\theta + \frac{12\epsilon}{\eta-\omega}\cos(\eta\theta-\omega\theta) + \frac{12\epsilon}{\eta+\omega}\cos(\eta\theta+\omega\theta)\right] \tag{131}$$

where we have discarded the terms with ϵ^2. In the first amplitude, we can use the approximation $\omega = 0.99584 \cong 1$. The introduction of this approximation into the differential equation gives

$$\frac{\mathrm{d}^2v}{\mathrm{d}\theta^2} + \omega^2v = \lambda\left[-1 + (12\alpha - 3)\epsilon\sin\eta\theta\sin\omega\theta + 9\epsilon\cos\eta\theta\cos\omega\theta\right.$$
$$\left. -\left(\frac{6}{\eta}+3\right)\cos\eta\theta + \frac{12\epsilon}{\eta-\omega}\cos(\eta\theta-\omega\theta) + \frac{12\epsilon}{\eta+\omega}\cos(\eta\theta+\omega\theta)\right] \tag{132}$$

where we have discarded again all terms containing ϵ^2. Transforming the products of trigonometric functions into their additions we find

$$\frac{\mathrm{d}^2v}{\mathrm{d}\theta^2} + \omega^2v = \lambda\left[-1 + \left(6\alpha + 3 + \frac{12}{\eta-\omega}\right)\epsilon\cos(\eta\theta - \omega\theta)\right.$$
$$\left. + \left(6 - 6\alpha + \frac{12}{\eta+\omega}\right)\epsilon\cos(\eta\theta+\omega\theta) - \left(\frac{6}{\eta}+3\right)\cos\eta\theta\right] \tag{133}$$

Figure 5. Distance between Earth and the Moon as a function of time calculated from (136) with $\omega = \sqrt{1 - 3\lambda} = 0.995845086$ (the perigee advances at $1°29'45''$ per draconic month with respect to the ascending node and has almost a constant ecliptic longitude).

and its solution according to Appendix 1, is

$$
\begin{aligned}
v(\theta) = \epsilon \cos \omega \theta + \lambda \Bigg[&-\frac{1}{\omega^2} + \left(6\alpha + 3 + \frac{12}{\eta - \omega} \right) \frac{\epsilon \cos(\eta\theta - \omega\theta)}{\omega^2 - (\eta - \omega)^2} \\
&+ \left(6 - 6\alpha + \frac{12}{\eta + \omega} \right) \frac{\epsilon \cos(\eta\theta + \omega\theta)}{\omega^2 - (\eta + \omega)^2} - \left(\frac{6}{\eta} + 3 \right) \frac{\cos \eta\theta}{\omega^2 - \eta^2} \Bigg].
\end{aligned}
\tag{134}
$$

By introducing the numerical values $\epsilon = 0.0549$, $\lambda = 2.764 \cdot 10^{-3}$, $\eta = 1.8430$, $\alpha = 0.078507$, $\omega = 0.99585$, we obtain

$$
v(\theta) = \epsilon \cos \omega \theta + A \cos(\eta\theta - \omega\theta) + B \cos(\eta\theta + \omega\theta) + C \cos \eta\theta + D \tag{135}
$$

where $A = 9.77 \cdot 10^{-3}$, $B = -2.1 \cdot 10^{-4}$, $C = 7.19 \cdot 10^{-3}$, $D = -2.75 \cdot 10^{-3}$. Then, the orbital equation becomes

$$
r = \frac{r_0(1 - \epsilon^2)}{1 + \epsilon \cos \omega \theta + A \cos(\eta\theta - \omega\theta) + B \cos(\eta\theta + \omega\theta) + C \cos \eta\theta + D} \cdot \tag{136}
$$

The distance between the Earth and the Moon calculated from (136) is plotted in Fig. 5 as a function of time $t = T\,\theta/(2\pi)$, where T is the draconic month. It has the same shape as that of Figs. 4-7 in [15]. The calculated apogee distance oscillates from 405,000 to 407,100 km, while the perigee distance oscillates from

359,000 to 370,800 km, which is close to the observed values: the observed apogee distance ranges from 404,168 to 406,602 km while the observed perigee distance ranges from 356,568 to 370,216 km [15]. The calculated apogee and perigee are synchronized with sidereal months. This is due to the fact that the frequency of the main oscillation of the orbit is the same as that obtained from the regression of the nodes

$$\omega = \sqrt{1 - 3\lambda} \cong 1 - \frac{3\lambda}{2} \tag{137}$$

within the experimental error. That is, the calculated advance of the perigee and the nodal regression compensate each other. However, we know that the perigee actually advances $3°$ in the mean with respect to stars in each anomalistic month. There is also disagreement in the modulation of the orbital oscillation. According to our calculations (Fig. 5), the period of modulation should be half a year, but actually it is longer: half the time it takes for the angle between the perigee and the Sun[6] to complete one revolution, which is 205.9 days[7]. When one takes $\omega = .987577$, which accounts for the actual advance of the perigee, instead of (137), a much better agreement is then obtained.

Variation of the Draconic Month

The equation (110) for the angular momentum can be written as

$$K' = \overline{K}' \left[1 + E \cos \eta\theta + F \cos(\eta\theta - \omega\theta) + G \cos(\eta\theta + \omega\theta)\right] \tag{138}$$

where $E = 4.55 \cdot 10^{-3}$, $F = -1.09 \cdot 10^{-3}$ and $G = -3.2 \cdot 10^{-4}$. Since $K' = r^2 \dot{\theta}$, the draconic month T is

$$T = \int_{2\pi n}^{2\pi(n+1)} \frac{r^2}{K'} \mathrm{d}\theta \,, \qquad n \in \mathbb{Z} \,.$$

From linearization of the square of (136) and the inverse of (138), we find

$$T \cong \frac{r_0^2 (1 - \epsilon^2)^2}{\overline{K}'} \int_{2\pi n}^{2\pi(n+1)} [1 - 2\epsilon \cos \omega\theta - (2A + F) \cos(\eta\theta - \omega\theta)$$
$$- (2B + G) \cos(\eta\theta + \omega\theta) - (2C + E) \cos \eta\theta - 2D] \, \mathrm{d}\theta$$

---

[6]The ecliptic longitude ϕ of $\mathbf{X}$, the vector going from the centre of the Sun to the centre of mass of the system Earth-Moon, which lies inside Earth, differs by $180°$ from the ecliptic longitude of the Sun observed from Earth.

[7]The longitudes of the perigee and the Sun advance $0.11140°$ and $0.98561°$ per day respectively [15], whence their difference increases by $0.87421°$ per day and completes one revolution in 411.80 days.

$$
\begin{aligned}
= \frac{r_0^2(1-\epsilon^2)^2}{K'} & \left[(1-2D)2\pi - \frac{2\epsilon}{\omega}[\sin(\omega 2\pi(n+1)) - \sin(\omega 2\pi n)] \right. \\
& - \frac{2A+F}{\eta-\omega}[\sin((\eta-\omega)2\pi(n+1)) - \sin((\eta-\omega)2\pi n)] \\
& - \frac{2B+G}{\eta+\omega}[\sin((\eta+\omega)2\pi(n+1)) - \sin((\eta+\omega)2\pi n)] \\
& \left. - \frac{2C+E}{\eta}[\sin(\eta 2\pi(n+1)) - \sin(\eta 2\pi n)] \right] \cdot
\end{aligned}
\tag{139}
$$

The mean value is

$$
\overline{T} = \frac{r_0^2(1-\epsilon^2)^2}{K'}(1-2D)2\pi \ .
\tag{140}
$$

Transforming the differences of sine functions into products we have

$$
\begin{aligned}
\frac{\Delta T}{\overline{T}} = - \frac{1}{(1-2D)2\pi} & \left[\frac{4\epsilon \sin\omega\pi}{\omega} \cos(\omega\pi(2n+1)) \right. \\
& + \frac{(4A+2F)\sin(\eta-\omega)\pi}{\eta-\omega} \cos((\eta-\omega)\pi(2n+1)) \\
& + \frac{(4B+2G)\sin(\eta+\omega)\pi}{\eta+\omega} \cos((\eta+\omega)\pi(2n+1)) \\
& \left. + \frac{(4C+2E)\sin\eta\pi}{\eta} \cos(\eta\pi(2n+1)) \right] \cdot
\end{aligned}
\tag{141}
$$

The relative amplitudes of each term are 21.9%:53.2%:0.7%:24.4%, so that we discard the third term. We also use the approximation $1 - 2D \approx 1$

$$
\begin{aligned}
\frac{\Delta T}{\overline{T}} \approx - \frac{1}{2\pi} & \left[\frac{4\epsilon \sin\omega\pi}{\omega} \cos(\omega\pi(2n+1)) \right. \\
& + \frac{(4A+2F)\sin(\eta-\omega)\pi}{\eta-\omega} \cos((\eta-\omega)\pi(2n+1)) \\
& \left. + \frac{(4C+2E)\sin\eta\pi}{\eta} \cos(\eta\pi(2n+1)) \right] \cdot
\end{aligned}
\tag{142}
$$

Let us introduce also the approximation $\omega \approx 1$ into the amplitudes. If we take into account that $\eta = 2 - 2\alpha$, we have

$$
\begin{aligned}
\frac{\Delta T}{\overline{T}} \approx - \frac{1}{2\pi} & [4\epsilon \sin\omega\pi \cos(\omega\pi(2n+1)) \\
& - \frac{(4A+2F)\sin 2\alpha\pi}{1-2\alpha} \cos((2\alpha+\omega)\pi(2n+1)) \\
& - \frac{(4C+2E)\sin 2\alpha\pi}{2-2\alpha} \cos(2\alpha\pi(2n+1))] \ .
\end{aligned}
\tag{143}
$$
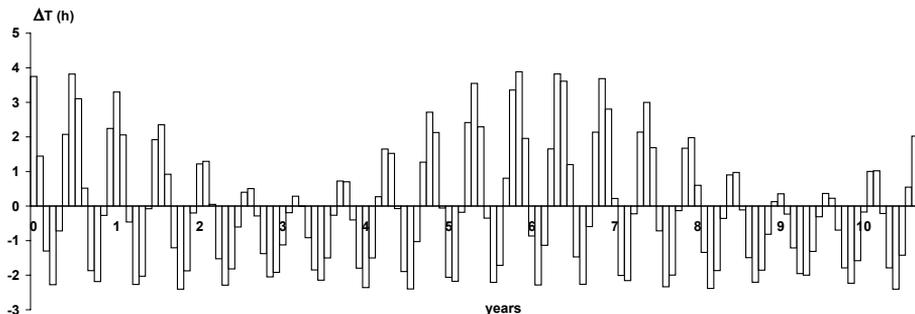
Figure 6. Variation of the draconic month T in hours as function of time in years calculated from (141) for $\omega = 0.987577$ (perigee separating by $4.4723°$ per month from the ascending node). Bars are draconic months, and numbers indicate years approximately. Graph begins at $n = 0$, where the angle between the perigee and the ascending node is zero.

Notice that these three frequencies are not independent. The main fast oscillation has the same period of half a draconic year (173.31 days) as the increment of the ecliptic longitude of the nodes (see comment to (99)). The amplitude of this oscillation is modulated by another long-range oscillation with frequency ω. According to our calculations, $\omega = 0.995845$ and the perigee would advance $1°30'$ with respect to the ascending node every month, so that it would take 240 draconic months=17.88 years to complete a revolution. Actually, the perigee advances about $4.5°$ with respect to the ascending node each month, which means that it takes 6 years for them to meet again [8]. This is just the observed period of the modulation in the oscillation of the draconic month. Its maximum relative amplitude is

$$\frac{\Delta T}{\overline{T}} \le \frac{1}{2\pi}\left(4\epsilon\sin\omega\pi + \frac{(4A+2F)\sin 2\alpha\pi}{1-2\alpha} + \frac{(4C+2E)\sin 2\alpha\pi}{2-2\alpha}\right) \quad (144)$$

which yields 3h 26min for $\omega = 0.995845$. For the actual value of $\omega = 0.987577$, the maximum amplitude would be 4h 9 min. In Fig. 6, the variation of the draconic month T calculated from (141) for $\omega = 0.987577$ (perigee progressing at $4.4723°$ per month with respect to the ascending node) is plotted as a function of time[9]. The comparison with [15, Figs. 4-11] shows that the actual draconic month can differ up to 6h from the mean value. The shape and periods of both figures

---

[8]The mean rates of the perigee and the ascending node are respectively $0.11140°$ east and $0.05295°$ west per day [15], that is, the perigee separates $0.16435°$ per day from the ascending node so that it takes 2190.45 days or 6 years for the angle between them to complete a revolution.

[9]For $\omega = 0.987577$, the orbital parameters of (136) are $A = 10.90 \cdot 10^{-3}$, $B = -2.1 \cdot 10^{-4}$ and $C = 7.14 \cdot 10^{-3}$, which slightly differ from those given above for $\omega = 0.995845$.

are similar although agreement is not complete. Fig. 6 also shows that oscillations reach the maximum and minimum amplitudes respectively when the perigee meets the ascending and descending nodes in concordance with observations. Calculation of ΔT for $\omega = 0.995845$ (perigee separating by $1.5°$ per month from the ascending node) yields a modulation of the amplitude with a period of 18 years that completely disagrees with observations and, therefore, it is not displayed here. Summarizing, the first-order approximation gives a good enough description of all the perturbations to Moon's motion except for the perigee advance. Although our lunar theory needs further refinement, it already permits identifying the amplitudes and frequencies of the main oscillations of the orbital parameters. Approximations of higher orders can be carried out, but the number of terms then arising would need much more space, so that a more refined lunar theory shall wait for a future paper exclusively devoted to it.

6. Application to Quantum Mechanics

Our interest in the N-body problem came from Hylleraas' treatment of the helium atom [26] [33, p 221], which seems unsatisfactory and suggested to us that the three-body problem should be reviewed, at least from a geometrical point of view, in order to find the corresponding Hamiltonian. On the other hand, molecular spectra (IR[10], ^{13}C-NMR and ^{1}H-NMR[11]) seem to indicate that some kind of solution to the N-body problem for quantum systems should exist. For instance, every functional group (such as carboxylic acid, ketone, amide, alcohol, anhydride, nitrile, etc.) has a characteristic absorption frequency in the IR spectra that is shifted in some degree by other neighbouring atoms and bonds in the molecules. Also, the main NMR frequencies of ^{1}H or ^{13}C are slightly shifted by neighbouring atoms. When outlining the Schrödinger equation for a system of many particles, the potential energy V is usually known as a function of the relative coordinates $x_{ij} = x_j - x_i$ while the kinetic energy operator $\hat{T}$ is a linear combination of the second partial derivatives with respect to the absolute coordinates x_i, and each operator does not adapt well to the other. We wondered whether an expression for $\hat{T}$ as a combination of derivatives of the relative coordinates x_{ij} exists or not. This transformation of coordinates has not been carried out before, except for the two-particle system or some special cases of more particles. Up to now, the Jacobi coordinates ξ_i

$$\xi_i = \frac{\sum_{k=1}^{j} m_k x_k}{\sum_{k=1}^{j} m_k} - x_{j+1} \tag{145}$$

---

[10]Infrared spectroscopy.

[11]Nuclear magnetic resonance spectroscopy of atomic nuclei having non null spin like ^{1}H or ^{13}C.

may be the most consistent approach to write the Laplacian operator with relative coordinates, because they satisfy [22, pp 221-224]

$$\sum_{k=1}^{N} \frac{1}{m_k} \frac{\partial^2 \psi}{\partial x_k^2} = \frac{1}{M} \frac{\partial^2 \psi}{\partial \xi_N^2} + \sum_{j=1}^{N-1} \frac{1}{\mu_j} \frac{\partial^2 \psi}{\partial \xi_j^2} \tag{146}$$

where

$$\frac{1}{\mu_j} = \frac{1}{M_j} + \frac{1}{m_{j+1}} \,, \qquad M_j = \sum_{k=1}^{j} m_k \,. \tag{147}$$

However, they do not satisfy the principle of symmetry between relative coordinates x_{ij}. Therefore, a general and symmetric expression of the Laplacian and Hamiltonian operators expressed with relative coordinates was still needed. In this way, let us remind the following theorem.

Theorem 6 (Internal Laplacian theorem [21, p 79]). *The Laplacian Δ of three particles located at the points A, B and C on a line with weights a, b and c satisfies the identity*

$$\Delta = \frac{1}{a} \frac{\partial^2}{\partial A^2} + \frac{1}{b} \frac{\partial^2}{\partial B^2} + \frac{1}{c} \frac{\partial^2}{\partial C^2} = \frac{1}{m} \frac{\partial^2}{\partial G^2} + \frac{a+b}{a\,b} \frac{\partial^2}{\partial D^2} + \frac{b+c}{b\,c} \frac{\partial^2}{\partial E^2}$$
$$+ \frac{a+c}{a\,c} \frac{\partial^2}{\partial F^2} - \frac{2}{a} \frac{\partial^2}{\partial D \partial F} - \frac{2}{b} \frac{\partial^2}{\partial D \partial E} - \frac{2}{c} \frac{\partial^2}{\partial E \partial F} \tag{148}$$

where $D = B - A$, $E = C - B$ and $F = A - C$ are the relative coordinates, $m = a + b + c \neq 0$ and $G = (a\,A + b\,B + c\,C)/m$ is the centre of mass.

Proof: By applying the properties of the partial derivatives. For more detailed steps see [21, p 255]. ∎

Corollary 7. *The internal Laplacian Δ_{int} (without the centre-of-mass coordinate) of three particles in the three-dimensional Euclidean space is*

$$\Delta_{\text{int}} = \frac{a+b}{a\,b} \nabla_{\mathbf{D}}^2 + \frac{b+c}{b\,c} \nabla_{\mathbf{E}}^2 + \frac{a+c}{a\,c} \nabla_{\mathbf{F}}^2$$
$$- \frac{2}{a} \nabla_{\mathbf{D}} \cdot \nabla_{\mathbf{F}} - \frac{2}{b} \nabla_{\mathbf{D}} \cdot \nabla_{\mathbf{E}} - \frac{2}{c} \nabla_{\mathbf{E}} \cdot \nabla_{\mathbf{F}} \tag{149}$$

where $\mathbf{D}$, $\mathbf{E}$ and $\mathbf{F}$ are their relative vectors, and $\nabla_{\mathbf{D}}$ is the gradient operator in the direction of $\mathbf{D}$

$$\nabla_{\mathbf{D}} = \mathbf{e_1} \frac{\partial}{\partial x_{\mathbf{D}}} + \mathbf{e_2} \frac{\partial}{\partial y_{\mathbf{D}}} + \mathbf{e_3} \frac{\partial}{\partial z_{\mathbf{D}}}. \tag{150}$$

Proof: By addition of the three equations (148) obtained for each Cartesian coordinate.   ∎

Recently, Turbiner *et al* deduced the 3-D internal Laplacian for the special case of three equal masses [59, eq 10].

In quantum mechanics, the kinetic energy operator $\hat{T}$ of a system of three particles is proportional to the weighted three-dimensional Laplacian [44, p 85]

$$\hat{T} = -\frac{\hbar^2}{2} \left(\frac{1}{a} \nabla_{\mathbf{A}}^2 + \frac{1}{b} \nabla_{\mathbf{B}}^2 + \frac{1}{c} \nabla_{\mathbf{C}}^2 \right). \tag{151}$$

On the other hand, the first term on the rhs of (148) accounts for the kinetic energy of the centre of mass. In three dimensions, this becomes

$$\hat{T}_{\mathrm{MC}} = -\frac{\hbar^2}{2m} \nabla_{\mathbf{G}}^2 \tag{152}$$

and it is excluded when calculating the internal energy levels of molecules because the total wavefunction is the internal wavefunction times the translational wavefunction, and the total energy is equal to the internal energy plus the translational energy[12]. Therefore, the operator of the internal kinetic energy is proportional to the internal Laplacian (149)

$$\hat{T}_{\mathrm{int}} = -\frac{\hbar^2}{2} \Delta_{\mathrm{int}}. \tag{153}$$

6.1. Energy Levels of the Linear Vibrations of CO_2

The first time we applied the Laplacian (149) was in order to calculate the vibrational levels of carbon dioxide. The CO_2 molecule is linear and has a central carbon atom bonded to two adjacent oxygen atoms at the same mean distances. Since the relative coordinates D, E and F are linearly dependent, we can choose without loss of generality a wavefunction $\psi(D, F)$ only dependent on the relative coordinates D (from one oxygen atom to the carbon) and F (from the carbon atom to the other oxygen). In this case, the unidimensional internal Laplacian is

$$\Delta_{\mathrm{int}}\psi(D, F) = \frac{1}{\mu_{ab}} \frac{\partial^2 \psi}{\partial D^2} + \frac{1}{\mu_{bc}} \frac{\partial^2 \psi}{\partial F^2} - \frac{2}{b} \frac{\partial^2 \psi}{\partial D \partial F}. \tag{154}$$

There are several stable isotopes of carbon (^{12}C, ^{13}C) and oxygen (^{16}O, ^{17}O, ^{18}O), and the most frequent molecule (98.4 %) is ^{12}C^{16}O$_2$, whose vibrational levels

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[12]The translational energy and wavefunction are obtained from the well-solved Schrödinger equation for a free particle in a potential box.

were computed. The relative isotopic masses of ^{12}C and ^{16}O are respectively 12 (by definition) and 15.9949. By introducing the coordinates $x_1 = D - D_{eq}$ and $x_2 = F - F_{eq}$, where D_{eq} and F_{eq} are the oriented distances at the minimum of the vibrational potential energy, and approximating the C=O bond vibration by the harmonic oscillator, which is a well-known and solved quantum system, the Schrödinger equation for the CO_2 linear vibrations then becomes

$$-\frac{\hbar^2}{2}\left(\frac{1}{\mu_{CO}}\frac{\partial^2\psi}{\partial x_1^2} + \frac{1}{\mu_{CO}}\frac{\partial^2\psi}{\partial x_2^2} - \frac{2}{m_C}\frac{\partial^2\psi}{\partial x_1 \partial x_2}\right) + \frac{k_{CO}(x_1^2 + x_2^2)}{2}\psi = E\psi \quad (155)$$

where x_1 and x_2 are the increases in the lengths of both CO bonds with respect to the equilibrium length, k_{CO} is the force constant (in the harmonic oscillator approximation) of each CO bond, $\mu_{CO} = m_C\, m_O/(m_C + m_O)$ is the reduced mass of the carbon and oxygen atoms, and E is the energy of the linear vibrations. This equation can be written as

$$\frac{\partial^2\psi}{\partial x_1^2} + \frac{\partial^2\psi}{\partial x_2^2} - \frac{2\mu_{CO}}{m_C}\frac{\partial^2\psi}{\partial x_1 \partial x_2} - \frac{\mu_{CO}k_{CO}\left(x_1^2 + x_2^2\right)}{\hbar^2}\psi = -\frac{2E\mu_{CO}}{\hbar^2}\psi \cdot \quad (156)$$

The Schrödinger equation in the harmonic oscillator approximation of a single bond is

$$\frac{d^2\psi}{dx^2} - \frac{\mu_{CO}k_{CO}\, x^2}{\hbar^2}\psi = -\frac{2E\mu_{CO}}{\hbar^2}\psi \cdot \quad (157)$$

By introducing the vibrational frequency of the bond $\nu_{CO} = \frac{1}{2\pi}\sqrt{\frac{k_{CO}}{\mu_{CO}}}$ we have

$$\frac{d^2\psi}{dx^2} - \frac{4\pi^2\mu_{CO}^2\nu_{CO}^2 x^2}{\hbar^2}\psi = -\frac{2E\mu_{CO}}{\hbar^2}\psi \cdot \quad (158)$$

In order to compute the energy levels of the linear vibrations of (156), a basis of 64 functions obtained from the multiplication of pairs of 8 eigenstates of each CO bond satisfying (158) was used. The computation itself splits into two separate computations, one for even states and the other for odd states. The wavefunctions of the even states are linear combinations of products of harmonic oscillator eigenstates of both bonds whose quantum number addition is even (for instance 2+0, 1+1, 0+2, 3+1, ...), and for the odd states the addition of quantum numbers is odd (0+1, 1+0, 3+0, 2+1, ...). Both sets of wavefunctions do not mathematically interact between them and each computation is carried out separately for even and odd states. The results of these computations for ^{12}C^{16}O$_2$ are included in Table 1.

The symmetric and antisymmetric vibrational states are indicated as usual with g and u respectively (from the German words *gerade* and *ungerade*). The total wavefunction remains invariant under the exchange of both ^{16}O nuclei because

Table 1. Energy levels of linear vibrations of $^{12}C^{16}O_2$ and infrared transitions from the ground state computed from (156) by means of the approximation of harmonic oscillator potential energy for each CO bond, which is supposed to have a frequency of $\bar{\nu}_{CO} = 1794$ cm^{-1}. e and o respectively indicate even and odd states, and g and u indicate respectively symmetric and antisymmetric states under the exchange of both oxygen nuclei. Experimental data [51, 61] recorded at 296K.

Level	Energy	Transition frequency from 0^e to higher levels			
	Calculated	Calculated		Experimental	Intensity [51, 61]
	$h\nu_{CO}$	$h\nu_{CO}$	cm^{-1}	cm^{-1}	10^{-22}cm^{-1}/molec·cm^{-2}
0^e	0.954110^g	–			
0°	1.608763^g	0.654653	1174.4	1063.8 [51]	9.75
1°	2.207676^u	1.253546	2248.9	2283.5 [1, 51]	9602
1^e	2.263418^g	1.309308	2348.9	2349.1 [1, 61]	955900
2^e	$2.862330^{g,u}$	1.908220	3423.3	3612.8 [1, 61]	10400
2°	2.918076^g	1.963966	3523.4	3714.8 [1, 61]	15800
3^e	3.461243^g	2.507133	4497.8	4853.6 [51, 61]	77.8
3°	3.516985^u	2.562875	4597.8	4977.8 [51, 61]	352
4^e	3.572743^g	2.618633	4697.8	5099.7 [51, 61]	109

they are bosons with spin 0. Since the product of the rotational and vibrational wavefunctions[13] must be symmetric, the g vibrational states will only exist for symmetric rotational wavefunctions, which have even values of J (the rotational quantum number), while the u states will only exist for odd values of J. On the other hand, according to Boltzmann's distribution law, the most populated energy level at room temperature is the ground state with a factor $\exp(\Delta E_{1\leftarrow 0}/k_B T)$ with respect to the first excited state[14]. Therefore, the absorption bands in the IR (infrared) spectrum are the transitions from the ground state. IR absorption and emission bands are composed by many single rotational-vibrational transitions caused by the thermal population of several rotational levels at room temperature.

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[13]The electronic wavefunction of all the molecules in the ground state is always symmetric.

[14]The parameter $\bar{\nu}_{CO} = 1794$ cm^{-1} allows us to calculate the relative population of vibrational levels at room temperature (298.15K) $N(0^o)/N(0^e) = 3.44 \cdot 10^{-3}$ and $N(1^e)/N(0^e) = 1.18 \cdot 10^{-5}$.

The centres of these IR bands are the pure vibrational frequencies [15] considered in Table 1.

The electric dipole moment of the CO_2 molecule is null, but it has an electric quadrupole moment Q that is a symmetric function of second degree of the relative coordinates. Therefore, the main IR transitions will be from 0^e to other even and symmetric states because $\langle e|Q|o \rangle = 0$ and $\langle g|Q|u \rangle = 0$. Other transitions forbidden by the selection rule of the electric quadrupole moment can take place by other ways with lower intensities. The fundamental IR absorption band of CO_2 is observed at 2349 cm^{-1} overlapping a minor band at 2308 cm^{-1} up to the point that they are usually considered a unique band. They can only be resolved in high resolution spectra. A pair of two minor bands are observed at 3613 and 3715 cm^{-1} [1]. If we assign 2349 cm^{-1} to the $1^e \leftarrow 0^e$ transition, we obtain ν_{CO}=1794 cm^{-1} as a parameter. This value is similar to the observed vibration frequencies of the C=O bond in organic molecules going from 1630 to 1850 cm^{-1} [7, p 487]. Then, our computations predict that the transitions $2^e \leftarrow 0^e$ and $2^o \leftarrow 0^e$ should have frequencies of 3423 cm^{-1} and 3523.4 cm^{-1}, while the experimental bands lie at 3612.8 cm^{-1} and 3714.8 cm^{-1}. The frequency difference between both bands of 100.1 cm^{-1} (calculated) and 102 cm^{-1} (experimental) are very similar. The calculated frequencies of the transitions $3^e \leftarrow 0^e$, $3^o \leftarrow 0^e$ and $4^e \leftarrow 0^e$ are about 380 cm^{-1} lower than the experimental ones. The theoretical separation between them is 100 cm^{-1} while the experimental one is about 120 cm^{-1}. All these are good qualitative and semi-quantitative predictions with systematic deviations that can easily be explained by anharmonicity[16]. The CO_2 laser emits at 961.34 cm^{-1} (main band) and 1064.12 cm^{-1} (secondary band) [62, p 24], which correspond to the transition $0^e \leftarrow 0^o$. The spontaneous emission is forbidden by the selection rule of the electric quadrupole moment, which facilitates the inversion of population and accumulation of excited molecules in the 0° state.

Another strong IR band is observed at 667 cm^{-1}, which corresponds to the bending of the CO_2 molecule and is not considered in our computations. It can be treated as a pure harmonic oscillator. An intense transition in the Raman spectrum at 1333 cm^{-1}, not visible in the IR spectrum and usually attributed to the symmetric stretching of CO_2, has been misunderstood since this transition does not appear

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[15]Energy E (in J), frequency ν (in Hz) and wave number $\overline{\nu}$ (in m^{-1}) are proportional quantities according to $E = h\nu = hc\overline{\nu}$ where h and c are respectively Planck's constant and the speed of light. It is customary to measure IR transitions in cm^{-1} so that Table 1 includes their wave numbers. However, in order to make it easy for non-acquainted readers to understand the text, we are calling wave numbers *frequencies*.

[16]The potential curve does not exactly fit a quadratic function and the Morse potential [14, p 135], which is not symmetric with respect to the minimum, is usually applied to calculate the vibrational energy levels of diatomic molecules [24, p 106].
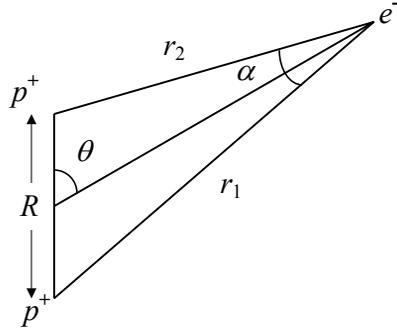
Figure 7. Sketch of the hydrogen molecule-ion H_2^+. p^+ indicate the hydrogen nuclei, which are usually protons, and e^- indicates the surrounding electron.

in our computations of the energy levels of linear vibrations. In fact, it is easy to see that it simply corresponds to the transition $2 \leftarrow 0$ of bending, because $667 \times 2 = 1334$. The method of analysis using the normal modes of vibration leads to uncertainties in the assignment of the IR and Raman bands for molecules with as few atoms as CO_2 [29, p 53], and it should be reviewed under the scope of the *ab initio* calculation of the vibrational energy levels and wavefunctions by means of the internal Hamiltonian here outlined. On the other hand, if one omits the mixed partial derivative in the Hamiltonian (155), the Schrödinger equation reduces to two independent harmonic oscillators without mathematical interaction. In other words, it is then impossible to obtain the full structure of the vibrational energy levels of the molecule. It could explain why scholars resorted to the classic treatment of normal modes of vibration [24, p 135] [34, p 217] [50, p 281], which led them to wrong conclusions like in the case of CO_2.

6.2. Electronic Energy of the Hydrogen Molecule-Ion

The internal Laplacian (149) of the hydrogen molecule-ion H_2^+ is

$$\Delta_{\text{int}} = \frac{1}{\mu_e}\nabla_1^2 + \frac{1}{\mu_e}\nabla_2^2 + \frac{2}{m_p}\nabla_R^2 + \frac{2}{m_p}\nabla_1\cdot\nabla_R + \frac{2}{m_e}\nabla_1\cdot\nabla_2 - \frac{2}{m_p}\nabla_2\cdot\nabla_R \quad (159)$$

where, if $\mathbf{X_i}$ indicate the vectors going from each nuclei to the electron, then $r_1 = \|\mathbf{X_1}\|$, $r_2 = \|\mathbf{X_2}\|$, and $R = \|\mathbf{X_1} - \mathbf{X_2}\|$ as displayed by Fig. 7. The reduced mass of the electron is $\mu_e = m_p m_e/(m_p + m_e)$. Since $m_p \gg m_e$ and then

$\mu_e \cong m_e$, we can take the approximation

$$\Delta_{\text{int}} \cong \frac{1}{m_e}\nabla_1^2 + \frac{1}{m_e}\nabla_2^2 + \frac{2}{m_e}\nabla_1 \cdot \nabla_2 \,. \tag{160}$$

Hence, the Hamiltonian for computing the electronic energy is

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{\hbar^2}{m_e}\nabla_1 \cdot \nabla_2 - \frac{e^2}{4\pi\varepsilon_0 r_1} - \frac{e^2}{4\pi\varepsilon_0 r_2} + \frac{e^2}{4\pi\varepsilon_0 R} \tag{161}$$

where e is the elementary charge, and ε_0 is the vacuum permittivity. In atomic units, that is, by taking $m_e = 1$, $\hbar = 1$, $e = 1$ and $4\pi\varepsilon_0 = 1$, which implies that lengths are measured in Bohr radii ($a_0 = 5.291 \cdot 10^{-11}$ m) and energy in Hartrees (1Ha $= 27.2114$ eV), the Hamiltonian is rewritten as

$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \nabla_1 \cdot \nabla_2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{R} \cdot \tag{162}$$

According to the Born-Oppenheimer approximation, nuclei move very slowly in comparison with electrons, so that R only enters this equation as a parameter of the electronic energy. We will now consider a wavefunction ψ for the ground state of H_2^+ having rotational symmetry around the axis $p - p$, which corresponds to a σ bond and does not therefore depend on the azimuthal angle ϕ. When ψ is given as a function of the spherical coordinates, $\psi(r_1, r_2)$ is enough and no additional dependence on θ_1 or θ_2 is required because it would be redundant. The Schrödinger equation then becomes

$$\begin{aligned}
\hat{H}\psi = &-\frac{1}{2}\left(\frac{\partial^2\psi}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial\psi}{\partial r_1}\right) - \frac{1}{2}\left(\frac{\partial^2\psi}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial\psi}{\partial r_2}\right) \\
&-\frac{r_1^2 + r_2^2 - R^2}{2r_1r_2}\frac{\partial^2\psi}{\partial r_1\partial r_2} + \left(-\frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{R}\right)\psi = E\psi
\end{aligned} \tag{163}$$

where

$$\frac{r_1^2 + r_2^2 - R^2}{2r_1r_2} = \cos\alpha \tag{164}$$

according to the law of cosines, since α is the angle between the vectors $\mathbf{X_1}$ and $\mathbf{X_2}$ (see Fig. 7). It is easy to check that this Hamiltonian is the same as the Hamiltonian of one electron expressed in cylindrical coordinates (without dependence on the azimuthal coordinate ϕ) with the $p - p$ axis taken as the z-axis. In the same way, if we introduce the elliptic coordinates[17] $\xi = (r_1 + r_2)/R$ and $\eta = (r_1 - r_2)/R$,

---

[17]The elliptic coordinates ξ and η together with the azimuthal angle ϕ that accounts for the rotation of the elliptic coordinate system around the z-axis are called *prolate spheroidal coordinates* [56, 58].

the Hamiltonian (163) becomes

$$\hat{H} = \frac{1}{R} - \frac{2}{R^2(\xi^2 - \eta^2)} \left(\frac{\partial}{\partial \xi} \left[(\xi^2 - 1) \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[(1 - \eta^2) \frac{\partial}{\partial \eta} \right] + 2R\xi \right) \quad (165)$$

which is coincident with that of Pauling and Wilson [44, p 333] but omitting the explicit dependence on the azimuthal angle ϕ as explained above. The Schrödinger equation is separable in this case, a fact that was used by Burrau [8] to solve exactly the Schrödinger equation for the electronic energy of the hydrogen molecule-ion (see also [12]). However, the Hamiltonian given in (163) is better adapted to the coordinate dependence of the electrostatic potential energy and can provide easier calculations. Before evaluating the energy from $\langle \psi | \hat{H} | \psi \rangle$, we must calculate $\mathrm{d}V$. From the Pythagorean theorem (Fig. 7) we have

$$\begin{aligned} r_1^2 &= r^2 \sin^2 \theta + \left(r \cos \theta + \frac{R}{2} \right)^2 = r^2 + Rr \cos \theta + \frac{R^2}{4} \\ r_2^2 &= r^2 \sin^2 \theta + \left(r \cos \theta - \frac{R}{2} \right)^2 = r^2 - Rr \cos \theta + \frac{R^2}{4}. \end{aligned} \quad (166)$$

The differentiation of the above equation yields

$$\begin{aligned} r_1 \mathrm{d}r_1 &= r\mathrm{d}r + \frac{R}{2} \cos \theta \mathrm{d}r - \frac{R}{2} r \sin \theta \mathrm{d}\theta \\ r_2 \mathrm{d}r_2 &= r\mathrm{d}r - \frac{R}{2} \cos \theta \mathrm{d}r + \frac{R}{2} r \sin \theta \mathrm{d}\theta \end{aligned} \quad (167)$$

whence

$$r_1 r_2 \mathrm{d}r_1 \wedge \mathrm{d}r_2 = Rr^2 \sin \theta \mathrm{d}r \wedge \mathrm{d}\theta = \frac{R}{2\pi} \mathrm{d}V \quad (168)$$

because the differential of the volume element in the spherical coordinates is $\mathrm{d}V = 2\pi r^2 \sin \theta \mathrm{d}r \wedge \mathrm{d}\theta$ (after integration of $\mathrm{d}\phi$ from 0 to 2π). Then, the volume element is

$$\mathrm{d}V = \frac{2\pi}{R} r_1 r_2 \mathrm{d}r_1 \wedge \mathrm{d}r_2. \quad (169)$$

In order to carry out integration, we must take into account that r_1 and r_2, although being independent variables, cannot have any values. Look at Fig. 7 and notice that R, r_1 and r_2 are sides of a triangle that satisfy the triangular inequalities

$$R + r_1 \geq r_2 , \qquad R + r_2 \geq r_1 , \qquad r_1 + r_2 \geq R \quad (170)$$

whose intersection is the semi-infinite stripe shown in Fig. 8, which is the region of integration. We introduce the elliptic coordinates $u = r_1 + r_2$, $v = r_2 - r_1$, which are more adapted to its boundaries, to have

$$r_1 = \frac{u - v}{2} , \qquad\qquad r_2 = \frac{u + v}{2} \quad (171)$$
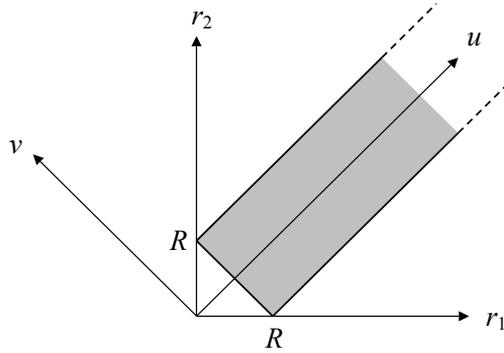
Figure 8. The allowed values of r_1 and r_2 for H_2^+ are the points included inside the semi-infinite stripe.

$$\mathrm{d}r_1 \wedge \mathrm{d}r_2 = \frac{1}{2}\mathrm{d}u \wedge \mathrm{d}v \;, \qquad\qquad \mathrm{d}V = \frac{\pi}{4R}(u^2 - v^2)\mathrm{d}u \wedge \mathrm{d}v \;. \qquad (172)$$

6.2.1. LCAO Computations

The LCAO (Linear Combination of Atomic Orbitals) wavefunction was early applied to H_2^+ [17]. The bonding wavefunction of the ground state is an addition of a variational modification of the $1s$ states of each hydrogen atom [14, p. 233]

$$\psi = N(\mathrm{e}^{-ar_1} + \mathrm{e}^{-ar_2}) \qquad (173)$$

where a is a variational parameter. In order to calculate the normalization constant N, one computes

$$
\begin{aligned}
1 = \langle \psi | \psi \rangle &= N^2 \int_V (\mathrm{e}^{-2ar_1} + \mathrm{e}^{-2ar_2} + 2\mathrm{e}^{-a(r_1+r_2)})\mathrm{d}V \\
&= \frac{N^2\pi}{2R} \int_R^{+\infty} \int_{-R}^{R} \mathrm{e}^{-au}(\cosh av + 1)(u^2 - v^2)\mathrm{d}u \wedge \mathrm{d}v \qquad (174) \\
&= \frac{2\pi N^2}{a^3}\left(1 + \mathrm{e}^{-aR}\left(\frac{a^2R^2}{3} + aR + 1\right)\right)
\end{aligned}
$$

according to Appendix 2, whence

$$N^2 = \frac{a^3}{2\pi\left(1 + \mathrm{e}^{-aR}\left(\frac{a^2R^2}{3} + aR + 1\right)\right)}. \qquad (175)$$

If one applies the Schrödinger equation (163) to this wavefunction taking into account that

$$\frac{\partial^2 \psi}{\partial r_1 \partial r_2} = 0 \qquad (176)$$

one obtains

$$\hat{H}\psi = N\left[\left(\frac{1}{R} - \frac{a^2}{2} - \frac{1}{r_1} - \frac{1}{r_2}\right)\left(e^{-ar_1} + e^{-ar_2}\right) + a\left(\frac{e^{-ar_1}}{r_1} + \frac{e^{-ar_2}}{r_2}\right)\right]. \quad (177)$$

The fact that the mixed partial derivative of the LCAO wavefunction is null is not a minor detail. Likely, it explains the success this kind of wavefunctions have had in quantum chemistry. Wrong Hamiltonians of most atoms and molecules omit mixed partial derivatives, but if $(\nabla_i \cdot \nabla_j)\psi = 0$, they can then provide right results. From (177), we have

$$\langle\psi|\hat{H}|\psi\rangle = \frac{1}{R} - \frac{a^2}{2} - N^2\int_V \frac{r_1 + r_2}{r_1 r_2}\left(e^{-2ar_1} + e^{-2ar_2} + 2e^{-ar_1 - ar_2}\right)\mathrm{d}V$$

$$+ N^2 a\int_V \frac{(r_2 e^{-ar_1} + r_1 e^{-ar_2})(e^{-ar_1} + e^{-ar_2})}{r_1 r_2}\mathrm{d}V$$

$$= \frac{1}{R} - \frac{a^2}{2} + \frac{N^2 a\pi}{R}\int_R^{+\infty}\int_{-R}^{R} e^{-au}(u\cosh av + v\sinh av)\mathrm{d}u \wedge \mathrm{d}v \quad (178)$$

$$+ \frac{N^2(a-2)\pi}{R}\int_R^{+\infty} u e^{-au}\mathrm{d}u\int_{-R}^{R}\mathrm{d}v - \frac{2N^2\pi}{R}\int_R^{+\infty} u e^{-au}\mathrm{d}u\int_{-R}^{R}\cosh av\,\mathrm{d}v$$

$$= \frac{1}{R} - \frac{a^2}{2} + \frac{2\pi N^2 e^{-aR}}{a^2}\left[ae^{aR} + (aR+1)\left(a - 2 - \frac{2\sinh aR}{aR}\right)\right]$$

after integration. By introducing the normalization constant, one finds that the energy of the ground state of the hydrogen molecule-ion is [33, p. 365]

$$\langle\psi|\hat{H}|\psi\rangle = \frac{1}{R} - \frac{a^2}{2} + \frac{a\left[ae^{aR} + (aR+1)\left(a - 2 - \frac{2\sinh aR}{aR}\right)\right]}{e^{aR} + \frac{a^2 R^2}{3} + aR + 1}. \qquad (179)$$

The minimum energy $E = -0.58650649$ Ha occurs at $a = 1.238$ and $R_m = 2.003\,a_0 = 1.0598 \cdot 10^{-10}$ m, which means a bonding energy of -0.08650649 Ha$= -2.354$ eV since the energy of the hydrogen atom is approximately -0.5 Ha. The experimental values are $1.06 \cdot 10^{-10}$ m and -2.6507101 eV. With the help of equation (179), we computed the electronic energy for several values of R close to R_m. In each case, we took the value of the variational parameter a yielding the minimum energy. The progressive change of the variational parameter with R reflects how the cloud of electronic charge self-adapts to the change of the

internuclear distance. Results are shown in Table 2. The dependence of E (in Ha) on R (in a_0, Bohr radii) fits the quadratic function

$$E \cong 0.046787\ R^2 - 0.187578\ R - 0.398498 \qquad (180)$$

which implies a force constant $k = 0.093574$ Ha/$a_0^2 = 145.685$ N/m. The reduced mass of both protons is $\mu = m_p/2 = 8.36311 \cdot 10^{-28}$ kg. The relation between the force constant and the frequency of the harmonic oscillator is

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \qquad (181)$$

which finally gives a vibrational frequency of the H-H bond of $6.6427 \cdot 10^{13}$ Hz = 2215.77 cm^{-1} to be compared with the experimental value of 2255.5 cm^{-1} [42].

6.2.2. Variational Computations

Firstly, we tested the wavefunction $\psi = N\mathrm{e}^{-\frac{a(r_1+r_2)}{2}}$ where a is the variational parameter. The electronic energy E_e that follows from the Schrödinger equation (163) is

$$E_e = \langle\psi|\hat{H}|\psi\rangle = \frac{1}{R} + \frac{(3a^2 - 12a)(aR+1)}{2(a^2R^2 + 3aR + 3)} \ . \qquad (182)$$

The minimum energy $E = -0.58136837$ Ha occurs at $a = 1.364$ and $R = 1.8472\ a_0 = 0.977 \cdot 10^{-10}$ m, which yields a minimum of the bonding energy of -0.08136837 Ha$= -2.2141$ eV. Notice that, at the axial points between both nuclei, $r_1 + r_2 = R$ and ψ is then constant, which is hardly realistic. Therefore, we improved it by including the profile of a catenary between both nuclei

$$\psi = N\mathrm{e}^{-\frac{a(r_1+r_2)}{2}}\cosh\frac{b(r_2-r_1)}{2} = N\mathrm{e}^{-\frac{au}{2}}\cosh\frac{bv}{2} \ . \qquad (183)$$

Now, ψ is no longer constant on the axis between both H atoms. A wavefunction equivalent to (183) was already outlined in 1929 [23], but nowadays we can access computer tools that were not available at that time. Application of the Schrödinger equation (163) to (183) yields

$$\begin{aligned}
\hat{H}\psi &= \left[\frac{1}{R} - \frac{a^2+b^2}{4} + \left(\frac{a}{2}-1\right)\left(\frac{1}{r_1}+\frac{1}{r_2}\right) + \frac{b^2-a^2}{4}\cdot\right. \\
&\left. \frac{r_1^2 + r_2^2 - R^2}{2r_1r_2}\right]\psi + \frac{b}{2}\left(\frac{1}{r_1}-\frac{1}{r_2}\right)N\mathrm{e}^{-\frac{a(r_1+r_2)}{2}}\sinh\frac{b(r_2-r_1)}{2}\cdot
\end{aligned} \qquad (184)$$

Let us calculate the following integral

$$
\begin{aligned}
1 = \int_V \psi^2 \mathrm{d}V &= \frac{\pi N^2}{8R} \int_R^{+\infty} \int_{-R}^R \mathrm{e}^{-au}(1 + \cosh bv)(u^2 - v^2)\mathrm{d}u \wedge \mathrm{d}v \\
&= \frac{\pi N^2 \mathrm{e}^{-aR}}{6a^3b^3R} \Big[a^2b^3R^3 + 3ab^3R^2 + 3b^3R \\
&\quad + 3(ab^2R - a^2 + b^2)\sinh bR + 3a^2bR\cosh bR \Big]
\end{aligned}
\tag{185}
$$

whence the normalization constant is

$$
N^2 = \frac{6a^3b^3Re^{aR}}{\pi L}
\tag{186}
$$

with L given by

$$
\begin{aligned}
L = {}& a^2b^3R^3 + 3ab^3R^2 + 3b^3R + 3(ab^2R - a^2 + b^2)\sinh bR \\
& + 3a^2bR\cosh bR \ .
\end{aligned}
\tag{187}
$$

With the help of Appendix 2, we calculate the other integrals

$$
\begin{aligned}
\int_V \frac{r_1 + r_2}{r_1 r_2}\psi^2 \mathrm{d}V &= \frac{\pi N^2}{2R}\int_R^{+\infty} u\,\mathrm{e}^{-au}\mathrm{d}u \int_{-R}^R (1 + \cosh bv)\mathrm{d}v \\
&= \frac{6ab^2(aR + 1)(bR + \sinh bR)}{L}
\end{aligned}
\tag{188}
$$

$$
\begin{aligned}
\int_V \frac{r_1^2 + r_2^2 - R^2}{2r_1 r_2}\psi^2 \mathrm{d}V &= \frac{\pi N^2}{8R}\int_R^{+\infty}\int_{-R}^R \mathrm{e}^{-au}(u^2 + v^2 - 2R^2) \\
&\quad \times (1 + \cosh bv)\mathrm{d}u \wedge \mathrm{d}v = \frac{1}{L}\Big[-a^2b^3R^3 + 3ab^3R^2 + 3b^3R \\
&\quad + 3(ab^2R + a^2 + b^2)\sinh bR - 3a^2bR\cosh bR \Big]
\end{aligned}
\tag{189}
$$

$$
\begin{aligned}
N^2 \int_V &\frac{r_2 - r_1}{r_1 r_2}\mathrm{e}^{-a(r_1+r_2)}\sinh\frac{b(r_2 - r_1)}{2}\cosh\frac{b(r_2 - r_1)}{2}\mathrm{d}V \\
&= \frac{\pi N^2}{2R}\int_R^{+\infty}\mathrm{e}^{-au}\mathrm{d}u \int_{-R}^R v\sinh bv\,\mathrm{d}v = \frac{6a^2b(bR\cosh bR - \sinh bR)}{L}
\end{aligned}
\tag{190}
$$

whence the electronic energy $E_e = \langle \psi | \hat{H} | \psi \rangle$ follows

$$
\begin{aligned}
E_e = {}& \frac{1}{R} - \frac{a^2 + b^2}{4} + \left(\frac{a}{2} - 1\right)\frac{6ab^2(aR + 1)(bR + \sinh bR)}{L} \\
& + \frac{b^2 - a^2}{4L}\Big[-a^2b^3R^3 + 3ab^3R^2 + 3b^3R \\
& + 3(ab^2R + a^2 + b^2)\sinh bR - 3a^2bR\cosh bR \Big] \\
& + \frac{3a^2b^2}{L}(bR\cosh bR - \sinh bR) \ .
\end{aligned}
\tag{191}
$$

The minimum energy -0.6024431 Ha occurs at $a = 1.3544$, $b = 0.9191$ and $R = 1.9977\, a_0 = 1.0571 \cdot 10^{-10}$ m, yielding a minimum of the bonding energy of -0.1024431 Ha $= -2.7876$ eV. In comparison, Scott et al. [56] obtained a minimum electronic energy of $-0.6026\,3461\,9106\,5398$ Ha and $R = 1.997\,1933\,1996\,9992\, a_0$ by solving the Schrödinger equation in prolate spheroidal coordinates. For several values of the internuclear distance R, we have calculated the values of a and b that minimize the energy (Table 2). The values of the electronic energy E_e for these values of R are plotted in Fig. 9 and fit the quadratic function

$$E_e \cong 0.0506293 R^2 - 0.2024291 R - 0.4001012 \qquad (192)$$

Table 2. Electronic energy E_e of the ground state of H_2^+ as a function of R (the internuclear H-H distance) calculated by means of the equations (179) (LCAO) and (191) (biparametric variational). The values of the variational parameters that minimize the energy for each value of R are indicated together with the minimum energy.

R	a	LCAO E	a	b	Biparametric variational E
(a_0)		(Ha)			(Ha)
1.94	1.225	-0.5863073	1.3647	0.9224	-0.6022616
1.95	1.227	-0.5863671	1.3629	0.9221	-0.6023199
1.96	1.229	-0.5864153	1.3611	0.9210	-0.6023666
1.97	1.231	-0.5864530	1.3593	0.9206	-0.6024019
1.98	1.233	-0.5864805	1.3575	0.9201	-0.6024262
1.99	1.235	-0.5864981	1.3558	0.9197	-0.6024398
2.00	1.237	-0.5865059	1.3540	0.9188	-0.6024428
2.01	1.239	-0.5865044	1.3523	0.9182	-0.6024357
2.02	1.241	-0.5864936	1.3505	0.9181	-0.6024185
2.03	1.243	-0.5864738	1.3488	0.9177	-0.6023916
2.04	1.245	-0.5864453	1.3471	0.9172	-0.6023553
2.05	1.247	-0.5864084	1.3454	0.9162	-0.6023097
2.06	1.249	-0.5863631	1.3437	0.9159	-0.6022551
2.07	1.250	-0.5863098	1.3420	0.9153	-0.6021916

which implies a force constant of 0.1012586 Ha/$a_0^2 = 157.649$ N/m. For the H-H system, the reduced mass is respectively a half of the proton mass, i.e.,
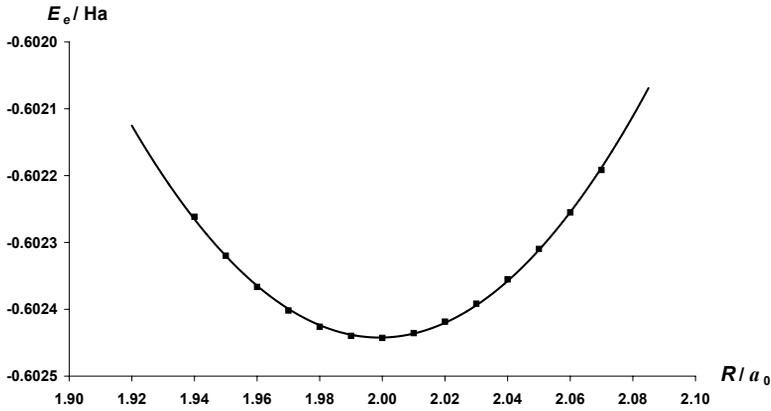
Figure 9. Electronic energy (in Ha) as function of the internuclear distance (in Bohr radii) calculated by means of (191) for the wavefunction (183). The squares are calculated data from Table 2 and the continuous line is the fitting quadratic function (192).

$\mu_{\text{HH}} = m_p/2 = 8.363108 \cdot 10^{-28}$ kg. By means of (181), we obtain a frequency $\nu_{\text{HH}} = 6.9100564 \cdot 10^{13}$ Hz $= 2304.947$ cm^{-1}. For the H-D system, the reduced mass is $\mu_{\text{HD}} = m_p m_d/(m_p + m_d) = 1.114896629 \cdot 10^{-27}$ kg, which yields a frequency $\nu_{\text{HD}} = 5.9847796 \cdot 10^{13}$ Hz $= 1996.308$ cm^{-1}. The experimental values are 2255.5 cm^{-1} [42] and 1914.7 cm^{-1} (centre of the roto-vibrational band, [9]). The vibrational energy of the ground vibrational state is then given by $E_{vib} = h\nu/2$ because protons are not at rest in this state but they also have kinetic energy[18], which added to the electronic energy yields the total energy [11]. The calculated vibrational energies are $5.251055 \cdot 10^{-3}$ Ha for H_2^+ and $4.547923 \cdot 10^{-3}$ Ha for HD^+, which added to the electronic energy yield a total energy of the lowest roto-vibrational level of -0.5971920 and -0.5978952 Ha respectively. As a comparison, the electronic energies obtained from a variation method by Moss [39] were $-0.597\,139\,063\,1234$ and $-0.597\,897\,968\,6450$ Ha respectively, without including the zero-point vibrational energy. The energy necessary for the dissociation of these ions into a hydrogen atom and a proton or deuteron is obtained through

$$E_d = -E_e - 0.5 - E_{vib} \qquad \text{(in Ha)} \qquad (193)$$

---

[18]Therefore, the experimental internuclear distance of $1.06 \cdot 10^{-10}$ m is only a mean value with a strong oscillation.

because the electronic energy of a hydrogen atom is -0.5 Ha under the approximation $\mu_e \cong m_e$. The total molecular energy includes electronic energy, vibrational energy and rotational energy, which is not considered here. In the dissociation, all the energies contribute to the balance of energy, but we consider the molecule at the lowest rotational state with $E_{\mathrm{rot}} = 0$. In this way, our prediction for the H_2^+ is $E_d = 0.602443054 - 0.5 - 5.251055 \cdot 10^{-3} = 0.0971920$ Ha$= 2.644729$ eV. Recently, Liu $et\ al$ [36] have determined that the ionization and dissociation energies of the hydrogen molecule are $E_i(H_2) = 124417.49113(37)$ cm^{-1} and $E_d(H_2) = 36118.06962(37)$ cm^{-1}. They are related to the dissociation energy of the H_2^+ by

$$E_d(H_2^+) = E_d(H_2) + 0.499733567 - E_i(H_2) \qquad \text{(in Ha).} \qquad (194)$$

Because the experimental ionization potential of the H atom is 13.598443 eV$=$ 0.499733567 Ha [53, p 10-208], this differs somewhat from 0.5 Ha owing to the reduced mass of the electron. Therefore, the experimental value of $E_d(H_2^+)$ is 2.6507101 eV. The calculated value only differs by 0.2% from the experimental one. Notice that the well of the electronic energy would yield -2.7876 eV as the bonding energy of H_2^+, lower than the experimental value (-2.6507101 eV) so that at this level of precision the vibrational energy must be taken into account in order to avoid contradiction with the variational theorem, which states that the variational energy is always higher than or equal to its true (experimental) value. Can these results be improved? The answer is yes by considering the full Laplacian (159) instead of its approximation (160), that is, by taking into consideration the correction for the reduced mass of the electron. Moreover, the Born-Oppenheimer approximation is no longer valid in (159) because of the terms $\nabla_1 \cdot \nabla_R$ and $\nabla_2 \cdot \nabla_R$. According to that approximation, the Hamiltonian is the addition of the vibrational and electronic Hamiltonians, and the wavefunction becomes a product of the vibrational and electronic wavefunctions. Then, the energy of the ground state without rotation is the addition of the electronic and vibrational energies, as done above. However, the mixed terms break this simplification. The consequent exact treatment remains to be developed in the future.

6.3. Electronic Energy of the Ground State of Two-Electron Atomic Systems

The two electron atomic systems like He, Li$^+$ and so on are formed by one nucleus and two electrons. Therefore, the internal Laplacian (149) can also be applied to calculate their electronic energy levels. If we take $\mathbf{A} = \mathbf{X}(e_1)$, $\mathbf{B} = \mathbf{X}(n)$ and $\mathbf{C} = \mathbf{X}(e_2)$ then $\mathbf{D} = \mathbf{B} - \mathbf{A} = \mathbf{X}(n) - \mathbf{X}(e_1)$, $\mathbf{E} = \mathbf{C} - \mathbf{B} = \mathbf{X}(e_2) - \mathbf{X}(n)$ and $\mathbf{F} = \mathbf{A} - \mathbf{C} = \mathbf{X}(e_1) - \mathbf{X}(e_2)$. Since one usually denotes $\mathbf{X_1} = \mathbf{X}(e_1) -$
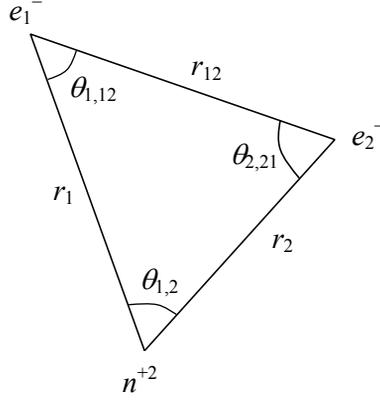
Figure 10.   Sketch of the helium atom with two electrons (e^-) moving around the helium nucleus (n^{+2}).

$\mathbf{X}(n)$, $\mathbf{X_2} = \mathbf{X}(e_2) - \mathbf{X}(n)$ and $\mathbf{X_{12}} = \mathbf{X}(e_2) - \mathbf{X}(e_1)$ (see Fig. 10), it follows that $\mathbf{D} = -\mathbf{X_1}$, $\mathbf{E} = \mathbf{X_2}$ and $\mathbf{F} = -\mathbf{X_{12}}$, whence the internal Laplacian (149) for these systems is

$$\Delta_{\text{int}} = \frac{1}{\mu_e}\nabla_1^2 + \frac{1}{\mu_e}\nabla_2^2 + \frac{2}{m_e}\nabla_{12}^2 - \frac{2}{m_e}\nabla_1\cdot\nabla_{12} + \frac{2}{m_n}\nabla_1\cdot\nabla_2 + \frac{2}{m_e}\nabla_2\cdot\nabla_{12} \quad (195)$$

where $\mu_e = m_e\, m_n/(m_e + m_n)$ is the reduced mass of the electron, very close to its actual mass m_e. Since $m_n \gg m_e$, a very good approximation to this Laplacian is

$$\Delta_{\text{int}} \cong \frac{1}{m_e}\nabla_1^2 + \frac{1}{m_e}\nabla_2^2 + \frac{2}{m_e}\nabla_{12}^2 - \frac{2}{m_e}\nabla_1\cdot\nabla_{12} + \frac{2}{m_e}\nabla_2\cdot\nabla_{12} \,. \quad (196)$$

At the beginning of quantum mechanics, Hylleraas was the first to calculate the energy of the ground state of the helium atom [26, 28]. If the Laplacian (196) is compared with Hylleraas' Hamiltonian for the helium atom (equation 13 of [26], equation 12 of [28]) one sees that Hylleraas omitted the last three terms. For the ground state of helium, the product of two $1s$ functions without angular variables was proposed by Hylleraas (equation 13b of [28]). By introducing the dependence on the interelectronic distance r_{12} in order to take into account the electron correlation, the wavefunction becomes

$$\psi = 1s(r_1)1s(r_2)f(r_{12}) \,. \quad (197)$$

In this case, the Schrödinger equation in spherical coordinates reduces to

$$
\begin{aligned}
\hat{H}\psi = \Big(& -\frac{1}{2}\frac{\partial^2}{\partial r_1^2} - \frac{1}{r_1}\frac{\partial}{\partial r_1} - \frac{1}{2}\frac{\partial^2}{\partial r_2^2} - \frac{1}{r_2}\frac{\partial}{\partial r_2} - \frac{\partial^2}{\partial r_{12}^2} - \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} \\
& - \cos\theta_{1,12}\frac{\partial^2}{\partial r_1\partial r_{12}} - \cos\theta_{2,21}\frac{\partial^2}{\partial r_2\partial r_{12}} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \Big)\psi = E\psi
\end{aligned}
\tag{198}
$$

where $r = \|\mathbf{X}\|$. This equation is given in atomic units, which were explained above for H_2^+. Let us apply (198) to the wavefunction (197) by taking $f(r_{12}) = \exp(r_{12}/2)$

$$
\psi = N\exp(-Zr_1)\exp(-Zr_2)\exp\left(\frac{r_{12}}{2}\right)
\tag{199}
$$

where N is the normalization constant. Since each factor is an eigenfunction of the corresponding pair of terms in the Hamiltonian (from the first to the sixth), one must only evaluate the integral

$$
\begin{aligned}
I(Z) &= -\int_\Omega \psi\left(\cos\theta_{1,12}\frac{\partial^2\psi}{\partial r_1\partial r_{12}} + \cos\theta_{2,21}\frac{\partial^2\psi}{\partial r_2\partial r_{12}}\right)d\Omega \\
&= \frac{Z}{2}\int_\Omega (\cos\theta_{1,12} + \cos\theta_{2,21})\psi^2 d\Omega \ .
\end{aligned}
\tag{200}
$$

This integral has been calculated analytically for $Z = 2$

$$
I(2) = \frac{\displaystyle\int_\Omega (\cos\theta_{1,12} + \cos\theta_{2,21})e^{-4r_1-4r_2+r_{12}}d\Omega}{\displaystyle\int_\Omega e^{-4r_1-4r_2+r_{12}}d\Omega} = \frac{152}{109} \ .
\tag{201}
$$

Then, the electronic energy of the helium atom ($Z = 2$) is

$$
E = -2^2 - \frac{1}{4} + \frac{152}{109} \approx -2.85550\,\text{Ha}
\tag{202}
$$

which is $-77.702\,\text{eV}$, close to the experimental value of $-79.005\,\text{eV}$ obtained from the addition of the first and second ionization potentials of the helium atom [53, p 10-208]. In order to improve this result, we changed ψ for the variational wavefunction $\psi = N\exp\frac{-ar_1-ar_2+br_{12}}{2}$. The application of the Schrödinger equation (198) to this function yields

$$
\begin{aligned}
\hat{H}\psi = \Big[& -\frac{a^2+b^2}{4} + \left(\frac{a}{2} - Z\right)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1-b}{r_{12}} \\
& + \frac{ab}{4}\left(\cos\theta_{1,12} + \cos\theta_{2,21}\right)\Big]N\exp\frac{-ar_1-ar_2+br_{12}}{2} .
\end{aligned}
\tag{203}
$$

Then

$$
E = \langle \psi | \hat{H} | \psi \rangle = -\frac{a^2 + b^2}{4} + N^2 \int_{\Omega} \left[\left(\frac{a}{2} - Z \right) \left(\frac{1}{r_1} + \frac{1}{r_2} \right) \right.
$$
$$
\left. + \frac{1-b}{r_{12}} + \frac{ab}{4} \left(\cos \theta_{1,12} + \cos \theta_{2,21} \right) \right] e^{-ar_1 - ar_2 + br_{12}} d\Omega .
$$
(204)

The normalization constant is obtained from

$$
1 = \langle \psi | \psi \rangle = N^2 \int_{\Omega} e^{-ar_1 - ar_2 + br_{12}} d\Omega .
$$
(205)

We introduce the variables $u = r_1 + r_2$ and $v = r_2 - r_1$. The boundaries of integration are conditioned by the inequalities $|r_1 - r_2| \leq r_{12} \leq r_1 + r_2$, which are equivalent to $-r_{12} \leq v \leq r_{12}$ and $r_{12} \leq u$. After the introduction of the volume element (230) (see Appendix 3), integration is carried out in the following way

$$
\langle \psi | \psi \rangle = N^2 \pi^2 \int_0^{+\infty} e^{-au} du \int_0^u e^{br_{12}} dr_{12} \int_{-r_{12}}^{r_{12}} (u^2 - v^2) dv
$$
(206)
$$
= \frac{4N^2 \pi^2}{b^5} \left(\frac{4}{a} - \frac{2b^2}{a^3} + \frac{8b^4}{(a-b)^5} - \frac{2b^3}{(a-b)^4} - \frac{2b^2}{(a-b)^3} + \frac{4b}{(a-b)^2} - \frac{4}{a-b} \right) .
$$

In the same way, the following results are found

$$
\int_{\Omega} \left(\frac{1}{r_1} + \frac{1}{r_2} \right) e^{-au + br_{12}} d\Omega = \frac{16\pi^2}{b^3} \left(\frac{3b^2}{(a-b)^4} - \frac{2b}{(a-b)^3} \right.
$$
$$
\left. + \frac{1}{(a-b)^2} - \frac{1}{a^2} \right)
$$
(207)

$$
\int_{\Omega} \frac{e^{-au + br_{12}}}{r_{12}} d\Omega = \frac{4\pi^2}{b^4} \left(\frac{2b^3}{(a-b)^4} - \frac{b}{(a-b)^2} + \frac{1}{a-b} + \frac{b^2}{a^3} - \frac{1}{a} \right)
$$
(208)

$$
\int_{\Omega} (\cos \theta_{1,12} + \cos \theta_{2,21}) e^{-au + br_{12}} d\Omega = 2 \int_{\Omega} \frac{u(r_{12}^2 - v^2) e^{-au + br_{12}}}{(u^2 - v^2) r_{12}} d\Omega
$$
(209)
$$
= \frac{16\pi^2}{b^4} \left(\frac{4b^3}{(a-b)^5} - \frac{3b^2}{(a-b)^4} + \frac{2b}{(a-b)^3} - \frac{1}{(a-b)^2} + \frac{1}{a^2} \right) .
$$

The lowest energy obtained from the variational computation is -2.889618 Ha for $a = 3.716$ and $b = 0.509$, that is, -78.63 eV. However, if one applies the old wrong version of the Hamiltonian

$$
\hat{H}_w = -\frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{r_1} \frac{\partial}{\partial r_1} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} - \frac{1}{r_2} \frac{\partial}{\partial r_2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}
$$
(210)

to the same wavefunction, one obtains

$$E_w = \langle \psi | \hat{H}_w | \psi \rangle = -\frac{a^2}{4} + \left(\frac{a}{2} - Z \right) \langle \psi | \frac{1}{r_1} + \frac{1}{r_2} | \psi \rangle + \langle \psi | \frac{1}{r_{12}} | \psi \rangle \cdot \quad (211)$$

For $Z = 2$ (helium atom), the minimum energy is $E_w = -3.225560$ Ha for the parameters $a = 4.85$ and $b = 0.7$, that is, -87.77 eV, not satisfying the variational theorem because it is lower than the experimental value of -79.005 eV.

These results clearly show the exactness of the three-body Hamiltonian (196) and the necessity of their mixed terms, because their omission leads to wrong values of the energy. By introducing the dependence of ψ on r_{12} through the angular variables into the Laplacian of two electrons, Hylleraas guessed [27, eq 5] the right Schrödinger equation for the ground state of helium, whence Pluvinage [46] extracted in 1950 the right Hamiltonian (equation 3 of [52]) identical to our equation (198) after writing $\cos \theta_i$ as a function of r_1, r_2 and r_{12} by means of the cosine theorem.

In Hylleraas's review of the two-electron atomic problem [28] of 1964, the terms containing ∇_{12}^2, $\nabla_1 \cdot \nabla_{12}$ and $\nabla_2 \cdot \nabla_{12}$ in (196) are still missing in his Hamiltonian. Although he had guessed the right expression as function of r_1, r_2 and r_{12} [28, equation 45b], he was not aware that it is only valid for s states having spherical symmetry, such as the ground state of helium, but not for other states having angular dependence, such as p or d, to which (196) must be applied. With Hylleraas' Hamiltonian, further authors obtained good results [45, 55, 60] for the ground state of helium. Notwithstanding this, the lack of consciousness contributed to spread wrong Hamiltonians. This error was continued over time by most authors, such as Pauling (equation 23-32 of [44, p 162]), Dawydow [13, p 306] and Levine (equation 9.49 of [33]), and propagated to students for many years. In recent handbooks, such as [2, p 221], [14, p 179], [35, p 255], [37, p 166] and [54, p 590], the wrong Hamiltonian for the helium atom is still present. The first time we have seen a right Hamiltonian for multielectron atoms including mixed terms is in Ruiz's paper [52]. Thanks to it, she could make very good computations of the electronic energy of the ground state of the boron atom with 0.5% of error. However, this raises the question about how scholars of quantum mechanics could compute results very close to the experimental values by means of wrong Hamiltonians. In 1958, Peckeris [45] wrote "Pending a derivation of the exact solution, the practice has been to follow the classical method of Hylleraas [26] ... leading to", and he then gave the right Schrödinger equation (198).

In Table 3, the energies calculated for two-electron atomic systems from the variational treatment of (204) are compared with the experimental ones obtained by adding the two last ionization potentials of each atom. They show good enough

Table 3. Electronic energy E of two-electron atomic systems calculated by means of (204). The values of the variational parameters a and b that minimize the energy together with its minimum value are indicated. Experimental energies are obtained by adding the last two ionization potentials given in [53, p 10-208].

| | Z | a | b | Variational treatment | | Experimental |
				E (Ha)	E (eV)	E (eV)
He	2	3.716	0.509	-2.889618	-78.6305	-79.005147
Li$^+$	3	5.720	0.528	-7.266819	-197.7402	-198.09429
Be^{+2}	4	7.722	0.537	-13.642909	-371.2424	-371.61526
B^{+3}	5	9.723	0.543	-22.018560	-599.1555	-599.60101
C^{+4}	6	11.724	0.547	-32.393992	-881.4854	-882.08034

agreement. The parameter a approaches $2Z$ while b approaches 0.5, the values corresponding to the eigenfunctions of the Hamiltonian (198) without the terms containing $\cos\theta_{1,12}$ and $\cos\theta_{2,21}$. On the other hand, the energies calculated from the wrong Hamiltonian (210) never satisfy the variational theorem (they lie below the experimental values) and are therefore not listed in this table.

7. Conclusions

The transformation of a quadratic form of the absolute coordinates of three particles into a quadratic form of their centre-of-mass and relative coordinates has applications to the colour space, classical dynamics and quantum mechanics. In the colour space a new set of chromatic coordinates I, J, K are defined as the difference of pairs of the RGB coordinates, which is a fast arithmetic operation with low charge of work for a computer CPU. Luma Y together with two of them form a new system of colour coordinates YJK whose metric gives different weights to the three fundamental colours according to the different sensitivities with which the human eye perceives them. This metric permits defining the norm of a colour, which is identified with its grey level, and the distance between two colours. In Newtonian mechanics, the transformation from the absolute to the relative and centre-of-mass velocities provides a Lagrangian that facilitates obtaining analytic solutions to the dynamics of the three-body problem. The linear dependence of

the relative coordinates is introduced as a holonomic constraint by means of a Lagrange multiplier into the Lagrange equations of motion, which are solved for the system Sun-Earth-Moon. In the first-order approximation, the orbit and the variations of the orbital parameters of the Moon are well described by means of simple periodic functions yielding a treatment that supersedes former complex and non-intuitive theories of Moon's motion. Calculations show very good agreement with observations and fully explain the main problem of the lunar theory. In order to find the Hamiltonian of a quantum system composed by three particles, the transformation of the absolute coordinates into the centre-of-mass and relative coordinates is introduced into their weighted Laplacian. In this way, the internal kinetic energy operator and the Hamiltonian of three particles are obtained and applied to the calculation of the vibrational energy levels of CO_2. Results are consistent with experimental data, but they differ from the analysis based on the method of normal modes of vibration, which seems to have contradictions. The internal Hamiltonian has also been applied to variational computations of the electronic energy of the ground state of the hydrogen molecule-ion, the helium atom and some two-electron atomic systems, and their results agree well with experimental values. On the other hand, wrong Hamiltonians omitting partial derivatives with respect to interelectronic distances yield electronic energies below the experimental values in contradiction with the variational theorem, which states that variational energies are always higher than or equal to the true energy. The introduction of these missing terms into the Hamiltonians will provide faster and better computations yielding a significant economic saving, because nowadays the main part of CPU computation time in college servers is spent on quantum mechanics calculations. This article deals only with the three-body problem owing to lack of space. The more general transformation from the absolute to the relative and centre-of-mass coordinates of N particles was already given in [21, pp 248 and 256] and its applications will be the subject of a future paper.

8. Appendices

Appendix 1. The Forced Oscillator

The general problem to be solved is the differential equation of the forced oscillator under periodic perturbations. It can be described by the differential equation

$$\frac{\mathrm{d}^2 f(t)}{\mathrm{d}t^2} + \omega_0^2 f(t) = c + \sum_{i=0}^{n} (a_i \cos \omega_i t + b_i \sin \omega_i t) , \qquad \omega_i > 0 \qquad (212)$$

where all the ω_i are distinct frequencies, i.e., $\omega_i \neq \omega_j$ for $i \neq j$, and $a_i, b_i, c \in \mathbb{R}$. After applying Laplace transforms to this differential equation one finds

$$s^2 F(s) - s f(0) - f'(0) + \omega_0^2 F(s) = \frac{c}{s} + \sum_{i=0}^{n} \frac{a_i s + b_i \omega_i}{s^2 + \omega_i^2} \qquad (213)$$

where $F(s) = \int_0^\infty e^{-st} f(t) dt$ is the Laplace transform of $f(t)$. By isolating $F(s)$ we obtain

$$
\begin{aligned}
F(s) =& \frac{s f(0) + f'(0)}{s^2 + \omega_0^2} + \frac{c}{s(s^2 + \omega_0^2)} + \frac{1}{s^2 + \omega_0^2} \sum_{i=0}^{n} \frac{a_i s + b_i \omega_i}{s^2 + \omega_i^2} \\
=& \frac{s f(0) + f'(0)}{s^2 + \omega_0^2} + \frac{c}{\omega_0^2 s} - \frac{c s}{\omega_0^2 (s^2 + \omega_0^2)} + \frac{a_0 s + b_0 \omega_0}{(s^2 + \omega_0^2)^2} \\
& + \sum_{i=1}^{n} \left(\frac{1}{s^2 + \omega_0^2} - \frac{1}{s^2 + \omega_i^2} \right) \frac{a_i s + b_i \omega_i}{\omega_i^2 - \omega_0^2}
\end{aligned}
\qquad (214)
$$

after resolving it into simple fractions. The inverse Laplace transform is

$$
\begin{aligned}
f(t) =& \frac{c}{\omega_0^2} + \left(f(0) + \sum_{i=1}^{n} \frac{a_i}{\omega_i^2 - \omega_0^2} + \frac{c}{\omega_0^2} \right) \cos \omega_0 t \\
& + \left(\frac{f'(0)}{\omega_0} + \frac{b_0}{2\omega_0^2} + \sum_{i=1}^{n} \frac{b_i}{\omega_i^2 - \omega_0^2} \right) \sin \omega_0 t \\
& + t \frac{a_0 \sin \omega_0 t - b_0 \cos \omega_0 t}{2\omega_0} + \sum_{i=1}^{n} \left(\frac{a_i \cos \omega_i t}{\omega_0^2 - \omega_i^2} + \frac{b_i \sin \omega_i t}{\omega_0^2 - \omega_i^2} \right)
\end{aligned}
\qquad (215)
$$

which can be written in a more simplified way as

$$
\begin{aligned}
f(t) =& \frac{c}{\omega_0^2} + A \cos \omega_0 t + B \sin \omega_0 t + t \frac{a_0 \sin \omega_0 t - b_0 \cos \omega_0 t}{2\omega_0} \\
& + \sum_{i=1}^{n} \left(\frac{a_i}{\omega_0^2 - \omega_i^2} \cos \omega_i t + \frac{b_i}{\omega_0^2 - \omega_i^2} \sin \omega_i t \right) .
\end{aligned}
\qquad (216)
$$

This treatment can also be applied to any periodic perturbation $g(t)$ with period $T \neq 2\pi/\omega_0$

$$\frac{d^2 f(t)}{dt^2} + \omega_0^2 f(t) = g(t) \qquad (217)$$

by resolving $g(t)$ into Fourier series

$$g(t) = c + \sum_{i=1}^{\infty}(a_i \cos \omega_i t + b_i \sin \omega_i t) \,, \qquad \omega_i = \frac{2i\pi}{T} \cdot \tag{218}$$

Then, the solution to the differential equation (217) is

$$f(t) = \frac{c}{\omega_0^2} + f(0) \cos \omega_0 t + f'(0) \sin \omega_0 t$$
$$+ \sum_{i=1}^{\infty}\left(\frac{a_i}{\omega_0^2 - \omega_i^2}\cos \omega_i t + \frac{b_i}{\omega_0^2 - \omega_i^2}\sin \omega_i t\right) \tag{219}$$

which is a convergent series because it behaves like the sum of the inverse of the squares of the natural numbers.

Appendix 2. Some Definite Integrals

Here, we calculate some definite integrals that are useful for quantum calculations of the system H_2^+

$$\int_R^{+\infty} e^{-au}u^2 du \int_{-R}^R dv = \frac{2e^{-aR}}{a^3}(a^2 R^3 + 2aR^2 + 2R)$$
$$\int_R^{+\infty} e^{-au}du \int_{-R}^R v^2 dv = \frac{2e^{-aR}}{3a}R^3 \tag{220}$$

whence

$$\int_R^{+\infty}\int_{-R}^R e^{-au}(u^2 - v^2)du \wedge dv = \frac{4e^{-aR}}{3a^3}(a^2 R^3 + 3aR^2 + 3R)$$
$$\int_R^{+\infty}\int_{-R}^R e^{-au}(u^2 + v^2)du \wedge dv = \frac{4e^{-aR}}{3a^3}(2a^2 R^3 + 3aR^2 + 3R) \,. \tag{221}$$

We also calculate

$$\int_R^{+\infty} e^{-au}u^2 du \int_{-R}^R \cosh bv \, dv = \frac{2e^{-aR}}{a^3 b}(a^2 R^2 + 2aR + 2)\sinh bR$$
$$\int_R^{+\infty} e^{-au}du \int_{-R}^R v^2 \cosh bv \, dv = \frac{2e^{-aR}}{ab^3}[(b^2 R^2 + 2)\sinh bR - 2bR \cosh bR] \tag{222}$$

whence

$$\int_{R}^{+\infty}\int_{-R}^{R} e^{-au}(u^2 - v^2)\cosh bv\; \mathrm{d}u \wedge \mathrm{d}v$$
$$= \frac{4e^{-aR}}{a^3 b^3}[(ab^2 R - a^2 + b^2)\sinh bR + a^2 bR\cosh bR] \tag{223}$$

$$\int_{R}^{+\infty}\int_{-R}^{R} e^{-au}(u^2 + v^2)\cosh bv\; \mathrm{d}u \wedge \mathrm{d}v$$
$$= \frac{4e^{-aR}}{a^3 b^3}[(a^2 b^2 R^2 + ab^2 R + a^2 + b^2)\sinh bR - a^2 bR\cosh bR] \;. \tag{224}$$

Appendix 3. The Internal Hypervolume Element of the Helium Atom

In order to calculate the internal hypervolume element of the helium atom or any other two-electron atomic system, we can arbitrarily fix the vector $\mathbf{X_1}$ in the z-axis, and then take spherical coordinates for $\mathbf{X_2}$. For fixed values of r_1 and r_2, ψ only depends on r_{12}, that is, on $\theta_{1,2}$ so that we can integrate the ϕ coordinate

$$\mathrm{d}V_2 = 2\pi r_2^2 \sin\theta_{1,2}\mathrm{d}r_2 \wedge \mathrm{d}\theta_{1,2}\;. \tag{225}$$

Finally, we integrate the 4π steradians of $\mathbf{X_1}$

$$\mathrm{d}\Omega = \mathrm{d}V_1 \wedge \mathrm{d}V_2 = 8\pi^2 r_1^2 r_2^2 \sin\theta_{1,2}\mathrm{d}r_1 \wedge \mathrm{d}r_2 \wedge \mathrm{d}\theta_{1,2}\;. \tag{226}$$

Now, let us change the variable $\theta_{1,2}$ for r_{12}. From the cosine theorem we have

$$r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_{1,2} \tag{227}$$

which, by differentiation and exterior product, results in

$$r_{12}\mathrm{d}r_1 \wedge \mathrm{d}r_2 \wedge \mathrm{d}r_{12} = r_1 r_2 \sin\theta_{1,2}\mathrm{d}r_1 \wedge \mathrm{d}r_2 \wedge \mathrm{d}\theta_{1,2} \tag{228}$$

whence

$$\mathrm{d}\Omega = 8\pi^2 r_1 r_2 r_{12}\mathrm{d}r_1 \wedge \mathrm{d}r_2 \wedge \mathrm{d}r_{12}\;. \tag{229}$$

By introducing the change of variables $u = r_1 + r_2$ and $v = r_2 - r_1$ we arrive at the hypervolume element

$$\mathrm{d}\Omega = \pi^2 (u^2 - v^2) r_{12}\mathrm{d}u \wedge \mathrm{d}v \wedge \mathrm{d}r_{12} \tag{230}$$

that was already used by Hylleraas[19] [28].

---

[19]Hylleraas' hypervolume element only differs from (230) in a constant factor that plays no role because it is simplified in the quotient $\langle\psi|\hat{H}|\psi\rangle/\langle\psi|\psi\rangle$.

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