THE ARCHITECTURE OF DIATOMIC MOLECULES

PART I: THEORY

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ABSTRACT

Consider a *"real" (i.e. not artificially gedanken)* quantum mechanical clock in the rest frame of reference. This can be a molecular, or an atomic, or a nuclear entity, of "*characteristic mass*" M_0, doing a regular *"clock labour*", in a space of "*size*" $\mathcal{R}_0$, throughout a "*unit period time*" T_0. In our previous work, we established that, in a *"real"* wave-like description, if the *"characteristic mass*" M_0 of the object is multiplied by the arbitrary number γ, then the *size of space* $\mathcal{R}_0$, in which this object is installed, shrinks as much, and the *total energy* E_0 of the object, is increased as much.

This occurrence *(were the object in consideration indeed, "real"),* yields at once the *"quantum mechanical invariance"* of the quantity $E_0M_0\mathcal{R}_0^2$, through either *relativistic* or *non-relativistic* quantum mechanical description, whichever is appropriate for the case in hand; interestingly, the quantity $E_0M_0\mathcal{R}_0^2$ happens to be *Lorentz invariant,* and strapped to h^2. Note that *primarily,* what we do is not a "*dimension analysis*". Anyhow, the invariance of $E_0M_0\mathcal{R}_0^2$ in regards to an *overall mass change,* would not work, if the wave-like object in hand is not "*real*", though of course, there still would be no problem in regards to a *dimension analysis.*

Herein, we consider the cast $E_0M_0\mathcal{R}_0^2 \sim h^2$ we establish, along the Born&Oppenheimer Approximation, applied to the Schrodinger description of a diatomic molecule. This yields a fundamental relationship, i.e. $T_0 \sim (1/h)\sqrt{g\mathcal{M}_0 m_e}\,\mathcal{R}_0^2$, where $\mathcal{M}_0$ is the *reduced mass of the nuclei,* m_e the *mass of the electron,* and g a *dimensionless* and *relativistically invariant* coefficient; we elaborate on the *proportionality constant* in question, to arrive at the somewhat rigorous relationship $T_0 = [4\pi^2/(\sqrt{n_1n_2}\,h)]\sqrt{g\mathcal{M}_0 m_e}\,\mathcal{R}_0^2$, n_1 and n_2 being *principal quantum numbers to be associated with the electrons making up the bond(s) of the diatomic molecule in hand,* though due to *quantum defects,* they are not *integer numbers.*

It appears immediately that g, *purely* related to the *electronic bond structure of the molecule,* should remain practically *constant,* for *chemically alike bonds.* This allows us to draw the *architectural layout of diatomic molecules,* since the above relationship reduces to an even simpler one, i.e. $T_0 \sim \sqrt{\mathcal{M}_0}\,\mathcal{R}_0^2$ for a *family of chemicaly alike molecules,* and to $T_0 \sim \mathcal{R}_0^2$, for *different electronic states of a given molecule;* this latter is an *approximate relationship* known since 1925, but never disclosed so far.

The *setting* of the *proportionality constant,* and paticularly the *quantum numbers* embodied by the above relationships, requires an elaboration; this, on the basis of H_2 molecule, shall constitute the topic of Part II of this work, thus essentially yielding a calibration of the *composite quantum number* n_1n_2, as well as the identification of the seemingly *ambiguous data;* n_1n_2 turns out to be $\mathcal{R}/\mathcal{R}_0$, $\mathcal{R}$ being the *characteristic length at the given excited state,* and $\mathcal{R}_0$ *the characteristic length of the ground state, provided that the two states are configured similarly.* We should further expect this finding to hold for members of a given *chemical family,* where $\mathcal{R}$ becomes say, the *internuclear distance of a heavier member,* and $\mathcal{R}_0$ the *internuclear distance of the lightest member,* given that the heavier member can be considered to be electronically configured just like the corresponding excited state of the lightest member.

Various applications, in excellent agreement with our finding are presented. Our approach can be easily extenden to *polyatomic molecules*.

INTRODUCTION

This work is issued from a totally different perspective than the one considered herein.[1, 2, 3, 4, 5, 6, 7,8] We have to emphasize that without our *original idea,* it would be *practically impossible* that we could discover the *approach* we are going to present herein, and reproduce our results, now based on a *rigorous quantum mechanical derivation.*

Thus, it was the author's original idea that *in order to insure the validity of the theory of relativity in regards to any entity existing in nature, the matter architecture and the internal dynamics this displays, ought to be made in just a given manner.*

In effect a *natural entity,* has got an *internal dynamics,* thus it works as a *clock;* this bears a *clock period,* T_0; the mechanism in question involves a *"characteristic mass"* M_0, which we call the *"clock mass",* and is installed in a *space of size* $\mathcal{R}_0$.[3]

The *"clock mass"* is a concept we would like to introduce, to represent the *"compound mass"* doing the *"clock labour"* of the wave-like object in hand. One may define different *clock masses* for the same object in regards to different motions this displays. The *clock mass* within the frame of the *hydrogen atom's Schrödinger description* is the *reduced mass* of the proton and the electron. The *clock mass* turns out to be the *reduced mass* $\mathcal{M}_0$ of the atoms regarding the *rotational motion of a diatomic molecule.* In this context, the *clock mass* is the mass one comes out with, when he can reduce the Schrödinger description of a many-body wave-like object, to a one-body wave-like object. In the case of the *vibrational motion of a diatomic molecule,* the *clock mass* of the vibrational motion can be formulated as $m_e (\mathcal{M}_0 / m_e)^{1/2}$ (based on the *electron mass* m_e), etc.[3]

Anyway the *clock mass* does not seem to be an *obvious mass,* unless the motion of concern is simple. We shall denote throughout, the *clock mass* by M_0.

Our *key idea* yielding *(through a totally different way, than the one presented herein)* our original results, is as follows.

The *Lorenzt tranformations* on T_0, M_0 and $\mathcal{R}_0$, *were the wave-like object in hand brought to a uniform translational motion,* or similarly, the *transformations that these quantities would undergo, were the object planted into a gravitational field,* can only hold, if the intrinsic relationship *(drawn by quantum mechanics)* between T_0, M_0 and $\mathcal{R}_0$, bears the form [$T_0 \sim M_0\mathcal{R}_0^2$].[1, 2, 3, 4, 5, 6]

We have to emphasize that the *Lorentz invariant cast* $T_0 \sim M_0\mathcal{R}_0^2$, thus happens to be *immediate* requirement of the *constancy of the speed of light in regards to all inertial frames of reference*.

This cast turns out to be $T_0 \sim \sqrt{g\mathcal{M}_0 m_e}\,\mathcal{R}_0^2$ for diatomic molecules, in fact for any molecule, T_0 being the molecule's vibrational period, associated with the bond we would take in consideration, M_0 the nuclei reduced mass, m_e the electron's mass, R_0 the bond length, and g a *dimensionless and relativistically invariant coefficient.*

On the other hand, the *proportionality constant* depicted by $T_0 \sim \sqrt{gM_0 m_e}\,\mathcal{R}_0^2$ is, as we shall disclose, basically made of 1/h. We say *"basically",* because, there is also a "*geometry factor*", as well as "*quantum numbers*" coming into play.

This was our finding, rooted to *the special theory of relativity,* which in fact gave birth to all of the results that we shall rederive in the present work through a straightforward approach, now based on only *quantum mechanics.*

We will limit ourselves first to *atomic,* chiefly *molecular* wave-like bodies. More specifically, we are going to focus *primarily* on *diatomic molecules.*

Thus herein we are going to derive the above relationship between T_0, M_0, and $\mathcal{R}_0$ for a diatomic molecule, based on the Born and Oppenheimer (B&O) approximation. Note that as we shall disclose, the outcome is somewhat *rigorous,* though it is based on the B&O approximation.

In Section 2, we present an *essential relationship* between the *total energy* E_0 of the wave-like object in hand, its *size* of concern and its *clock mass.* We shall call this relationship the *universal matter architecture cast* (UMA). We summarize its derivation in Appendix A. The B&O approximation is summarized, next, in Section 3.

The relationship $T_0 \sim \sqrt{gM_0 m_e}\,\mathcal{R}_0^2$ is thence derived, in Section 4.

In this relationship, it becomes clear that g, is a quantity *purely* related to the *electronic bond structure* of the molecule. We anticipate thus that g, should remain practically *constant* for *chemically alike bonds.* This allows us right away, to draw an *architectural foundation* and a *totally new systematization for diatomic molecules,* since the above relationship reduces to an even simpler one, i.e. $T_0 \sim \sqrt{M_0}\,\mathcal{R}_0^2$, for a family of *chemicaly alike molecules.*

This, were the quantum numbers overlooked, further reduces to $T_0 \sim \mathcal{R}_0^2$, for different *electronic states* of a given molecule; this latter is an *approximate relationship* known since 1925, but never disclosed so far. The proportionality constant in question indeed, embodies essentially *non-trivial quantum numbers.* They are pinned down in Section 5. The subsequent elucidation is undertaken in section 6. A conclusion is presented in Section 7.

This terminates the content of the present Part I.

The disclosure of the *proportionality constant* embodied by the above relationships, requires an elaboration; this, particularly on the basis of H_2 molecule, shall constitute the topic of Part II of this work, thus essentially yielding the calibration of of the *composite quantum number* n_1n_2, as well as the identification of the seemingly ambiguous data .

Various applications, in excellent agreement with our unique approach are presented.

Our work can easily be extended our work to *polyatomic molecules.*

We like to stress that we found practically nothing achieved in the literature, along the line we pursue herein.

2. THE UMA CAST

For a *"real"* atomistic or molecular wave-like object, i.e. a wave-like object existing in nature, we have shown elsewhere the following theorem, *first,* on the basis of the Schrodinger Equation, as complex as this may be, *then* on the basis of the Dirac Equation, whichever may be appropriate, in relation to the frequency of the internal dynamics of the object in hand.[4] A *"real"* atomistic and molecular wave-like object, involves a *potential energy* made of only "*Coulomb Potential energies". *Thence even a relativistic Dirac description embodying potential energies made of potential energies other than Coulomb Potentials energies, may indeed not represent a *"real"* description.

Theorem 1: In a *"real wave-like description" (thus, not embodying artificial potential energies),* composed of I electrons and J nuclei, if the *(identical)* electron masses m_{i0}, i = 1,..., I, and different nuclei masses m_{j0}, j = 1,…, J, belonging to the object, are overall multiplied by the *arbitrary number* γ, then *concurrently, a)* the *total energy* E_0 associated with the given internal motion of the object, is increased as much, *and b)* the *size* R_0 to be associated with this motion contracts as much; in *mathematical words* this is

$$\{ [(m_{i0},\ i = 1,..., I) \rightarrow (\gamma m_{i0},\ i = 1,..., I)],\ [(m_{j0},\ j = 1,…, J) \rightarrow (\gamma m_{j0},\ j = 1,…, J)] \}$$

$$\Rightarrow \{ [E_0 \rightarrow \gamma E_0],\ [\mathsf{R}_0 \rightarrow \frac{R_0}{\gamma}] \} . \qquad (1)$$

A general derivation of this occurrence is presented in Appendix A.

Note that, for every particle of mass m_0 belonging to the wave-like object in hand, the term $h^2\nabla^2/(8\pi^2 m_0)$ takes place, within the frame of the wave-like description of this object. This makes that, as we shall soon undertake from a different angle, *multiplying* all of the masses m_0's of concern by an arbitrary number, is identical to *dividing* h^2 of $[h^2\nabla^2/(8\pi^2 m_0)]$ by this number, and the output Eq.(1) through the latter operation will still hold *(provided that the wave-like object is "real", i.e. embodies just Coulomb potential energy terms).*

Interestingly, *multiplying all of the masses by a given number* and *multiplying* h^2 by *a given number,* within the frame of the wave-like description in consideration, at the first glance, do not really evoke the *same sense.* As we gather, *multiplying all of the masses by a given number (i.e. altering all of the masses by the same amount),* to many of us, seems a *useless artificial operation.* Quite on the contrary, *undertaking a similar operation with* h^2 can be quickly associated with a *quantum jump to an excited state.*

Thus, as trivial as it may be, the *equivalence* of *multiplying* h^2 *by a given number* to *dividing all of the masses by this number*, seems worth to be framed separately.

This constitutes our Theorem 2.

Theorem 2: *Altering* brutally, *as much as this may not make any immediate physical sense,* all of the masses that take place within the frame of a wave-like description by a given amount, is identical to dividing h^2 in this description by the same number, *may this latter operation be in the aim of the formulation of an eigenstate.*

Anyhow, as we shall detail below, *changing* all of the masses that take place within the frame of the wave-like description, may very well not be *meaningless* at all. Anyway, we are going to stand on this theorem, to benefit from the output of Theorem 1, in the case where indeed one aims to formulate an eigenstate via the introduction of quantum numbers, *right next* to h^2, in the wave-like description in consideration.

Regarding Theorem 1 note that, since the *clock mass* M_0 is just a mass, manufactured based on different masses embodied by the object in hand; multiplying these masses by γ, alters M_0 just as much.

Eq.(1) immediately yields the invariance of the quantity $E_0 M_0 \mathsf{R}_0^2$. This is *remarkable,* since this quantity is as well Lorentz invariant *(were the object brought into a uniform translational motion).*

Theorem 2 yields the invariance of the quantity $E_0 (M_0 / h^2) \mathsf{R}_0^2$, were M_0 left unperturbed, and h^2 instead, is multiplied by a *given number.*

The elements composing the quantity $E_0 M_0 \mathsf{R}_0^2$ anyway are all, somewhat *quantized quantities.* Therefore we anticipate that $E_0 M_0 \mathsf{R}_0^2$ ought to be in relation with a *Lorentz invariant, universal constant,* incorporated by the wave-like description in question.

Thus the quantity $E_0 M_0 R_0^2$ should be *"strapped"* to the square of the Planck Constant, h^2 *(being proportional to it, through a rather complex, dimensionless, and relativistically invariant quantity, which is somewhat a characteristic of the bond structure of the wave-like object in hand).* This is further elaborated in Appendix A.

The foregoing findings make the content of our Theorems 3 and 4.

Theorem 3: For any real wave like obect, the product $E_0 (M_0 / h^2) \mathsf{R}_0^2$ remains invariant, were M_0 arbitrarily altered; the same holds when instead, h^2 is multiplied by an arbitray number.

Theorem 4: The quantity $E_0 M_0 \mathsf{R}_0^2$ is *strapped* to h^2.

Thus in short, following the elaboration we preset in Appendix A,

$$E_0 M_0 R_0^2 \sim h^2 \ . \tag{2}$$

We call this occurrence, the UMA (Universal Matter Architecture) Cast.

The *proportionality constant* depicted by Eq.(2) shall be worked out separately.

Note further that *primarily* what we do is not a "*dimension analysis*". In effect, Theorem 3 would not work [i.e. $E_0(M_0/h^2)R_0^2$ would not be invariant in regards to a mass change], if the wave-like object in question is not *"real*", though of course, *dimension-wise* there would still be no problem.

One may question the *meaningfulness* of an *overall mass change,* we considered within the frame of Theorem 1. Indeed, an overall mass change of the entity in hand, at the first glance, seems meaningless.

Yet as seen, it already allowed us to land at Theorems 3 and 4, condensed into Eq.(2). We will see that this latter relationship shall still constitute a *valuable tool* within the frame of the particular case of the *electronic description* of a diatomic molecule *(where the clock mass reduced merely to* m_e*, the electron mass),* yielding a unique systematization of molecular spectroscopic data.

Secondly one should recall that an *overall mass change* is after all, not that meaningless, since it indeed comes into play were the object brought to a *uniform translational motion,* or were it planted into a *gravitational field.* Thence one better urges to examine what happens to its quantum mechanical description, under such circumstances.

Finally we will soon see that Theorem 1, more specifically Theorem 2, is amazingly interesting in determining *quantum numbers* to be associated with excited levels of a wave-like object, as complex as this may be.

3. BORN AND OPPENHEIMER (B&O) APPROXIMATION

The non-relativistic quantum mechanical description of a diatomic molecule can be achieved via the usual Schrödinger Equation, involving the *"two nuclei"* and the surrounding "*electrons":*

$$\begin{aligned}&-\frac{h^2}{8\pi^2}\left(\frac{1}{m_A}\nabla_A^2+\frac{1}{m_B}\nabla_B^2+\frac{1}{m_e}\sum_i\nabla_{ie}^2\right)\psi_{A,B,e}\\&+\left(\sum_{i,i'}\frac{e^2}{r_{ii'}}+\frac{Z_A Z_B e^2}{r_{AB}}-\sum_i\frac{Z_A e^2}{r_{Ai}}-\sum_i\frac{Z_B e^2}{r_{Bi}}\right)\psi_{A,B,e}=E_{A,B,e}\psi_{A,B,e}\end{aligned} \ . \tag{3}$$

Here the *subscripts* "$_A$" and "$_B$" designate the *nuclei,* and "$_e$" designates the *electrons.* We have then the following notation.

m_A : mass of A
m_B : mass of B
Z_A : atomic number of A
Z_B : atomic number of B
m_e : electron's mass
e : electron's charge
r_{Ai} : i^{th} electron's distance to A
r_{Bi} : i^{th} electron's distance to B
$r_{ii'}$: distance between the i^{th} and the i^{th} electron
r_{AB} : distance in between the nuclei
$\psi_{A,B,e}$: eigenfunction associated with the molecule
$E_{A,B,e}$: eigenvalue associated with the molecule

Note that the above description is quite satisfactory, since the *relatively slow motion* of the nuclei can indeed be fairly treated by a *non-relativistic approach.*

Eq.(3), through B&O approximation, is reduced into the *separate descriptions* of the *"nuclear"* and *"electronic"* motions.

We thus come, as usual, to solve separately the two following non-relativistic Schrödinger Equations, written with the familiar notation[9]:

$$\left[-\frac{h^2}{8\pi^2}\left(\frac{1}{m_A}\nabla_A^2+\frac{1}{m_B}\nabla_B^2\right)+\frac{1}{2}k_0\left(r_{AB}-r\right)^2\right]\psi_{A,B}=E_{A,B}\psi_{A,B} \quad , \qquad (4)$$

$$\left(-\frac{h^2}{8\pi^2 m_e}\sum_i \nabla_{ei}^2\psi_e+\sum_{i,i'}\frac{e^2}{r_{ii'}}+\frac{Z_A Z_B e^2}{r_{AB}}-\sum_i\frac{Z_A e^2}{r_{Ai}}-\sum_i\frac{Z_B e^2}{r_{Bi}}\right)\psi_e=E_e\psi_e \quad . \qquad (5)$$

Eq.(4) describes the *nuclei vibrational motion,* about the *internuclear distance* r_{AB} to be input to this equation *(for a given electronic state of the molecule),* whereas Eq.(5) describes the *electronic motion* around the two *"fixed"* nuclei. Thus, one solves Eq.(5), for a given electronic state, in order to determine how the *electronic energy* E_e varies with respect to r_{AB}, and find the internuclear distance r_{AB}, which makes minimum E_e, more precisely $E_e(r_{AB})$; we call $r_{AB\mathit{min}}$ and $E_{e\mathit{min}}$, respectively, the internuclear distance and the eigenvalue in question *(for the given electronic state);* this is then $r_{AB\mathit{min}}$ as r_{AB}, to be input to Eq.(4). Normally $E_{e\mathit{min}}$ is negative; yet below, by $E_{e\mathit{min}}$ we shall mean $|E_{e\mathit{min}}|$.

The *force constant* k_0 to be input to Eq.(4) is given by

$$k_0=\left.\frac{\partial^2 E_e\left(r_{AB}\right)}{\partial r_{AB}^2}\right|_{r_{AB}=r_{AB\min}} \quad . \qquad (6)$$

Knowing k_0 and r_{AB} related to the *ground electronic state of the diatomic molecule* in hand, one can subsequently construct Eq.(4), and solve it, as usual for the *vibrational,* also *rotational* eigenvalues $E_{A,B}$, associated with the *electronic state* of the molecule of concern.

ψ_e is the *electronic motion eigenfunction* associated with the eigenvalue $E_e(r_{AB})$, and $\psi_{A,B}$ is the *nuclei motion eigenfunction* associated with the eigenvalue $E_{A,B}$.

$E_{A,B}$ can be expressed, with the familiar notation, as

$$E_{A,B} = \frac{j(j+1)h^2}{8\pi^2 I_{AB}} + \left(v + \frac{1}{2}\right) h\,\varpi_{A,B};\ j = 0,1,...;\ v = 0,1,...; \qquad (7)$$

here I_{AB} is the *"moment of inertia"* of the nuclei:

$$I_{AB} = M_{AB}\ r_{AB}^2\ , \qquad (8)$$

where M_{AB} is the nuclei reduced mass.

$\varpi_{A,B}$ is the *classical vibrational frequency* of the molecule, the inverse of which, $T_{A,B}$, is the classical vibrational period of the molecule. $T_{A,B}$ is given, as usual, by

$$T_{A,B} = 2\pi\sqrt{\frac{M_{AB}}{k_0}}\ . \qquad (9)$$

Thus, along this definition, $E_{A,B}$ [as expressed by Eq.(7), above], is the solution of Eq.(4), for the *nuclear motion of the molecule.*

4. THE *"VIBRATION PERIOD"*, VERSUS THE *"DIATOMIC MOLECULE CLOCK MASS"* AND THE *"INTERNUCLEAR DISTANCE"*

The B&O approach, together with the UMA Cast, stated above, i.e. Eq.(2), allows us to draw an *elegant relationship* for the *vibrational motion of a diatomic molecule,* in terms of *different masses* taking part in the internal motion of the molecule, and the "*internuclear distance*" coming into play.

Eq.(2) indeed should be valid within the frame of Eq.(5)*, since this latter embodies potential energy terms, each just in the *Coulombian form.* On the other hand m_e *(the electron mass)* is the *only mass,* coming into play in this equation.

Thence Eq.(2), on the basis of Eq.(5), shall be written as

$$E_{e\,min}\, m_e\, r^2_{AB\,min} \sim h^2 \qquad \text{[written out of Eq.(5)]}\ . \qquad (10)$$

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* Eq.(2) holds within the frame of Eq.(3). It must also in *principle* hold within the frame of Eq.(4). But here, the original structure of the Schrödinger Equation had been perturbed by the introduction of the *approximate Morse potential*. So, whether Eq. (2) holds within the frame of Eq.(4) is not trivial. Nevertheless, as it is summarized in Appendix A, Eq.(2) ought to hold for any wave-like object, existing in nature, which we call a *"real wave-like object"*.

The *proportionality constant* to be introduced in this relationship shall soon be worked out.

$E_e(r_{AB})$ can be as usual expressed fairly in terms of the force constant k_0, defined by Eq.(5), as

$$E_e(r_{AB}) = E_{e\mathit{min}} + \frac{1}{2}\ k_0\,(r_{AB} - r_{AB\mathit{min}})^2\ . \tag{11}$$

It should be emphasized that this relationship does not display *characteristics* such as *“anharmonicity”* and *“dissociation”;* but throughout this work we are going to deal with only *the lowest vibrational level of the states* of concern. Thus, even when we deal with an *exited electronic state,* Eq.(11) is quite valid for the *lowest vibrational level* of it.

$E_e(r_{AB})$ vanishes at the abscissa r_{AB}, which we can define with respect to $r_{AB\mathit{min}}$, i.e.

$r_{AB} = p\ r_{AB\mathit{min}}$ [value which makes $E_e(r_{AB})$, vanish] ; (12)

p is an *unknown parameter* at this stage, though it appears to be roughly around 2.

Eqs.(11) and (12), provides us with the possibility of expressing $E_{e\mathit{min}}$, as

$$E_{e\mathit{min}} = \frac{1}{2}\ k_0\,(p-1)^2\ r^2_{AB\mathit{min}}\quad . \tag{13}$$

We plug the RHS of this equation in Eq.(10); next, we use Eq.(9) to eliminate the force constant k_0; thus we arrive at the simple expression for $T_{A,B}$, i.e.

$$T_{A,B} \sim \frac{1}{h}\sqrt{g_k \mathsf{M}_{AB} m_e}\ r^2_{AB}\ , \tag{14}$$

where g_k is defined as

$$g_k = \frac{(p-1)^2}{2}\quad . \tag{15}$$

note that the *subscript* “$_k$” stands for the *force constant* k.

At this stage we can simplify our notation. Thus from now on we shall call $T_{A,B}$, T_0; $\varpi_{A,B}$, ϖ_0; M_{AB}, M_0, and r_{AB}, r_0.

The quantity

$$M_0 = \sqrt{\mathsf{M}_0 m_e}\quad , \tag{16}$$

has the dimension of a *mass;* we call it the *“vibrational clock mass”* to be associated with the *vibrational motion of the diatomic molecule* in hand.

The *proportionality constant* in Eq.(14) shall embody *a geometry factor,* and as we shall figure out, *quantum numbers.* A *geometry factor* of 2π originates from the use of Eq.(10) [where h^2 may be read as $h^2/4\pi^2$, and accordingly, 2π is left after the square rooting, on the way to Eq.(14)]; an other 2π factor originates from the use of Eq.(9); thus altogether, a *geometry factor* of $4\pi^2$ shall be expected to multiply Eq.(14).

The *quantum numbers* to be introduced in Eq.(14) turn out to be more peculiar, and we elabourated on this, below. Nonetheless, one can sense that [h^2] in Eq.(10), should be in fact read as usual, as [n^2 h^2], more precisely as [n_1n_2 h^2], n_1 and n_2 being *principal quantum numbers of electrons making up the bond(s) of the diatomic molecule in hand.* Note yet that, these numbers shall not be *nice integer numbers,* as one may be inclined to expect at a first glance.

Eq.(14), thus becomes

$$T_0 = \frac{4\pi^2}{h\sqrt{n_1 n_2}} \sqrt{gM_0 m_e}\; r_0^2 \,. \qquad (17)$$

where g is an *overall dimensionless quantity;* it is different than g_k, since it also involves a similar quantity, which we call g_{IN}, coming into play within the frame of Eq.(10); note that the *subscript* "$_{IN}$" stands for "invariance", since g_{IN} is associated with the *invariant quantity* $E_0M_0R^2$. A discussion is provided about the *significance* of the dimensionless coefficient g_{IN}, in Appendix A.

Note that the geometric average of n_1n_2 appearing here, is solely due to the *square rooting* of $n_1n_2h^2$, we undertook on the way.

This relationship, though g is not known beforehand, is *rigorous*. In fact, despite the B&O approximation we adopted, also the *approximate Morse potential* we introduced at the level of Eq.(10), g *(to be determined),* ultimately insures the equality of Eq.(17).

More profoundly, Eq.(17) displays a striking feature; it is that, *"space" (size)* and *"time" (period of time)* are *separable* from each other, if *"mass" (clock mass)* were considered the *"size"* and *"period of time"* dependent function. Though we arrived at Eq.(17), through an approximation, henceforth its *cast,* concerning the *separability* in question, still appears to be rigoruos.

One may recall that, such a *separability* does not at all seem obvious. Note that in effect*, "moments"* and *"locations"* are, through the *Lorentz transformations,* interrelated *(and are not independent from each other),* in regards to transformations beween inertial frames of reference. However *(Lorentz transformations of) "differences of instants"* and *"differences of locations",* well happen to be independent from each other. It should be this fact, which makes the setting of *"size"* and *"period of time"* in a wave like object, are *independently* linked to the *"clock mass"* quantity.

It becomes clear that, g is purely related to the *electronic structure* of the molecule's bond. Thus, for *alike bonds*, in a given *chemical family,* we come to expect g, to remain virtually the same.

Indeed note that, already without the use of quantum numbers, the plots of T_0 versus $\sqrt{M_0}r_0^2$, for members of a given chemical family, exhibit nicely increasing, almost faultless, smooth curves. We present *eight examples* in Figures 1 - 7.

We call g, the "*molecular bond looseness factor*", for as one can check, the inverse of it is roughly proportional to the *dissociation energy* of the molecule.

Our approach allows us to draw a *whole new systematization of diatomic molecules,* and more.

The introduction of quantum numbers n_1n_2 though, requires a demonstration. Next, they should be somehow determined. This is what we shall now achieve. (A detailed study shall be undertaken on the basis of H_2 molecule, through Part II of this work.)

5. ELABORATION ON THE QUANTUM NUMBERS

The presence of quantum numbers in Eq.(17), is right awayinduced by the *identification* of the RHS of Eq.(2) as h^2. This equation is further transformed into Eq.(10), written for the mere *electronic description* of the molecule [cf. Eq.(5)].

The *excited electronic eigenstates* of the molecule should anyway involve quantum numbers. [†] The simplicity of Eq.(2) or Eq.(10), as implied by Theorem 4, *clearly* leaves *no other room* to *quantum numbers that shall come into play in these equations,* other than that, *right next* to h^2.

Thus a composite quantum number $\mathcal{N}$ (i.e. *the product of the two principal quantum numbers to be associated with the bond electrons, in the case of a diatomic molecule),* should come to multiply h^2, in Eq.(2) or Eq.(10), regarding an *excited eigenstate,* in just the same way the *square of an integer quantum number* related to an excited state of the *simplest* wave-like objects *(for example, the hydrogen atom),* comes in a similar relationship, to multiply to h^2.

This *piece of information* makes that, were $\mathcal{N}$ somehow known, one can introduce it *right next* to h^2, into the *framework* of the *ground level wave-like description (i.e. the Hamiltonian)* of the entity in hand, and consequently determine the *eigenvalue,* and the *characteristic length* induced by the *resulting formulation.*

Though there is a *peculiarity.*

Eq.(10), in the simplest case of the hydrogen atom, shall *(with the usual notation)* be written as

---

[†] Any excited eigenstate shall obviously involve quantum numbers. But here, we are particularly interested in *electronic excited eigenstates.*

$$8\pi^2 E_n g_{IN} m_e \mathcal{R}_n^2 = n^2 h^2 \quad ; \qquad \text{(10, rewritten)}$$

(for the hydrogen atom, g_{IN} *is unity)*

here E_n is the *total energy* of the n^{th} electronic state, $\mathcal{R}_n$ is the corresponding *characteristic size,* and n the *principal quantum number;* g_{IN} is a coeffcient related to the electronic configuration we visualized *(next to the geometry factor),* at the level of Eq.(10).

In the case of the hydrogen atom, g_{IN} is *unity,* regardless n. Thus, in these case 1) g_{IN} is *unity* at the ground state, *but also* 2) g_{IN} remains the same at all electronic levels.

Neither property holds for systems of higher complexities, though as we show, an equation similar to Eq.(10) can well be written for any diatomic molecule, or further any wave-like entity.

Since g_{IN} [of Eq.(10)], more generally g [of Eq.(17)] appear to be *purely* related to the *electronic structure* of the entity in hand, we expect them to remain the same, for *alike electronic configurations.* This hold within the frame of alike electronic states of a given molecule, as well as within the frame of alike ground states of molecules belonging to a given chemical family.

However, as one jumps from the ground state of a complex system, such as that of a diatomic molecule, to an excited state of this entity, it is not obvious that the electronic configuration shall stay the same; in fact, generally it will not. Take for instance the *hydrogen molecule.* Its excited electronic states a priori, will not bear the same electronic configuration as that of the ground state, unless the two electrons are excited in a complete symmetry. Even then, the *shielding effects* may not be the same.

This is the peculiarity we wanted to clarify.

Thus, as the molecule jumps from its ground state to an excited state, in general, it is not only that, h^2 is multiplied within the framework of the wave-like description, by the appropriate quantum number; but we should further represent the *change* that takes place in the electronic structure. That can be taken care of, by a corresponding change in the coefficient g_{IN} of Eq.(10).

In fact, altering h^2 and altering both h^2, together with g_{IN} so that the ratio h^2/g_{IN} is changed by the same amount, within the frame of Eq.(10), are *mathematicaly equivalent operations,* yet as discussed, *physically* they appear to be quite different.

Thereby we can conceive an *excited electronic state* as achieved in two steps: 1) Switching the ground state electronic configuration into the new configuration by just changing g_{IN}. 2) Jumping from this configuration to the new quantum state.

For electronic state configured like the ground state, we will have to achieve only the second step.

This, yields the content of our Theorem 5.

Theorem 5: Were the atomic or molecular wave-like object in hand, at a given electronic state, characterized by the *composite quantum number* $\mathcal{N}$, then the *eigenvalue* and *characteristic length* associated with this state, become the output of the formulation one obtains by multiplying h^2 with $\mathcal{N}$, in the *framework of the ground state description*, provided that the two states are configured similarly.

So the introduction of appropriate quantum numbers in Eq.(10), next to h^2 *(within the framework of the wave-like description),* in order to take care of the *excited electronic eigenstates* of the molecule as complex as this may be, appears to be as standard as this is, for the simplest atomic object, *provided that the two states are configured similarly.*

We can predict the solution of the *new set* up, through Theorem 1. It can be obtained based on a *reformulation* of this theorem. Thus we establish our Theorem 6 regarding an excited electronic level of the wave-like object in hand.

Theorem 6: In a *"real wave-like ground description"* if, in the aim of expressing an excited eigenstate, h^2 is multiplied by the *composite quantum number* $\mathcal{N}$ *(the inverse of te eigenvalue related to this eigenstate, were the ground state energy normalized to unity),* then *concurrently, a)* the magnitude of the *total ground energy* E_0 associated with the given wave-like object, is decreased much, to become E, the *new eigenvalue, and b)* the corresponding *ground state size* R_0 stretches as much, to become R, the *new size,* provided that the two states are configured similarly; in *mathematical words* this is

$$[h^2 \rightarrow \mathcal{N} h^2] \quad \Rightarrow \{[E_0 \rightarrow E = \frac{E_0}{\mathcal{N}}], [\mathsf{R}_0 \rightarrow \mathsf{R} = \mathcal{N}\mathsf{R}_0]\}. \qquad (18)$$

This draws an additional aspect of the *meaningfulness of multiplying the overall mass* of the wave-like object by a given number, since this turns out to be identical to dividing h^2 of the wave-like description in hand, by the same number, or vice-versa.

Note that Theorem 6 holds for any excited eigenstate *(rotational, vibrational, electronic, or else).*

This theorem, for *excited states* of the molecule, configured like the ground state, yields at once

$$\mathcal{N} = \frac{\mathsf{R}}{\mathsf{R}_0} \quad . \tag{19}$$

(Composite quantum number of the excited eigenstates, were this configured like the ground state)

This interestingly holds no matter how complex the molecule may be.

Accordingly we establish our next theorem.

Theorem 7: The *composite quantum number* to be associated with an excited eigenstate, is the mere ratio of the *size the object displays at this excited state,* to the *size the object displays at the ground state,* provided that the two states are configured similarly.

Theorem 7 can be checked for the electronic states of hydrogen atom. It is surprising that it holds for any object and for any excited eigenstate the object may involve.

What if the *electronic structure* of the excited state is not the same as that of the ground state?

The answer is fortunately not complicated. Since the the coefficient g_{IN} in Eq.(10) comes to multiply the *mass of the electron,* which happens to be the only mass taking place in the description of the electronic motion of the diatomic molecule, *any change* in g_{IN}, evidently can be represented by a *corrresponding hypothetical change in the mass of the electron.*

If further, we are *concomitantly* to consider a *quantum number* $\mathcal{N}$ to be associated with the excited eigenstate in question *(i.e. configured in a different way than the ground state), then* based on Eq.(10), this state can well be described by merely altering h^2/m_e in the framework of the ground state of the molecule by $\mathcal{N}(g_{IN})_{initial}/(g_{IN})_{final}$, where the subscripts "$_{initial}$" and "$_{final}$" refer respectively to the *ground state* and the *excited electronic state* in consideration.

The ultimate output, is at once framed by Theorems 1 and 2.

Theorem 8: The *ratio* of the *size* a diatomic molecule displays at an *excited excited state,* to the *size it displays at the ground state,* is equal to $\mathcal{N}(g_{IN})_{initial}/(g_{IN})_{final}$, i.e. the *composite quantum number* to be associated with the excited state, *times* a coefficient, the inverse of which quantifies how much the overall *ground state electronic configuration* is altered.

In what follows we shall solely focus on excited electronic eigenstates [since we visualize Eq.(17), for just the lowest vibrational state of an electronic eigenstate].

Note that the usage of Eq.(19) along Eq.(17) requires that the coefficient g is not altered as the molecule passes from its ground level to the given excited electronic state, so that we can plot T, the largest vibrational period at the given *excited electronic state*, versus $\mathcal{N}^{-1/2}\mathcal{R}_0^2$, where $\mathcal{R}_0$ is the size of concern, at this eigenstate.

6. THE DISCLOSURE OF THE AGED EMPIRICAL RELATIONSHIP $\varpi_0 r_0^2$ = Constant, AND THE COMPLETE SET OF H_2 ELECTRONIC VIBRATIONAL DATA: A NEW SYSTEMATIZATION OF DIATOMIC MOLECULES

Recall that the following empirical relationship, evoking very much Eq.(17), had been established for a given diatomic molecule, back in 1925, yet not unveiled so far:[10, 11, 12, 13, 14]

$$\varpi\, r^2 = \text{Empirical Constant}\,; \qquad (20)$$

(approximate relationship written in 1925
for the electronic states of a given molecule)

here, ϖ is the *ground vibration frequency,* i.e. the inverse of the *vibrational period* T, *related to a given electronic state of the molecule,* and r the corresponding *internuclear distance.*

The *"Empirical Constant"* is then to be determined separately, for each diatomic molecule.

Eq.(20) bears the same cast as that of Eq.(17) *(as far as the dependency of the vibrational period on the internuclear distance is concerned);* yet it does not include the *quantum numbers.*

Eq.(17), together with Theorem 6, instead suggests that we should look at the relationship

$$T = \frac{4\pi^2}{h\sqrt{\dfrac{r}{r_0}}}\sqrt{g\mathcal{M}_0 m_e}\, r^2 = \frac{4\pi^2}{h}\sqrt{g\mathcal{M}_0 r_0 m_e}\, r^{3/2}\ , \qquad (21)$$

(relationship written for the largest vibrational period
of excited electronic states of a given molecule)

where r_0 is the *internuclear distance* at the *very ground state,* as usual.

r/r_0 taking place in the above relationship, following Theorem 6, is just the *composite quantum number* to be associated with the electronic state taken in consideration.

Eq.(21) makes that based on any molecule, regarding electronic states bearing similar configurations, for which g, the *bond looseness factor,* remains about the same, T^2 versus r^3 should display a *straight line.*

The *approximate empirical constant* of Eq.(20), can now be evaluated from Eq.(21), as

$$\text{Empirical Constant } = \frac{\sqrt{\mathcal{N}}\,h}{4\pi^2\sqrt{g\mathbf{M}_0 m_e}}\ ; \qquad (22)$$

recall that $\mathcal{N}$ is the *composite quantum number*, i.e. r/r_0 (staying indeed roughly the *same,* were r is not far from r_0), making up that the "*constant"* is question is indeed only *approximately,* a constant, supposing anyway that the electronic states in question, are configured similarly, so that g stays practically constant, throughout.

This entirely discloses the mechanism behind the *approximate empirical relationship* [Eq.(22)], established back in 1925.

Thus, Eq.(22) makes that, it is not *really* the quantity ωr^2 which is a *constant* for electronic states of a given molecule, configured similarly, but based on Eq.(19), *more likely* it is the quantity

$$\text{Constant} = \omega r^{3/2}\,. \qquad (23)$$

(written by the author, for similar electronic states of a given molecule)

This *new constant* then is

$$\text{Constant } = \frac{h}{4\pi^2\sqrt{g\mathbf{M}_0 m_e r_0}}\ ; \qquad (24)$$

(written by the author for similar electronic states of a given molecule)

recall that r_0 dominates the *internuclear distance, at the ground state.*

As an example, T^2 versus r^3 for H_2 molecule, is sketched in Figure 8. Thus some 23 states out of 29, for which data is available, are neatly aligned. Herein, we included H_2^+, which too seems to display the same g as that of H_2 ground state; we find $g \approx 0.8$. The remaining 6 electronic excited states of H_2 seem to be configured *differently.* We call these *"ambiguous states"* (the previous 23, being seemingly all configured approximately like the molecule's ground state).

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The study of the electronic vibrational data of H_2 molecule is undertaken in details in Part II.

To analyze the remaining 6 data (out of 29), we note, out of Eq.(14) that, switching *the nuclei reduced mass* M_0 of *alkali molecules or alkali hydrides* into *that of the hydrogen molecule,* should virtually transpose the *corresponding vibrational period,* into the *vibrational period of* H_2 *electronic state of* of the *same electronic character;* recall that switching the *nuclei mass* does not practically affect the *electronic structure* of the molecule, and accordingly we should expect that *amongst* H_2 *electronic states* there are states, configured like *the ground electronic states of alkali molecules and alkali hydrides.*

Therefore we anticipate that the *6 ambiguous electronic states* of H_2 should be configured just like the respective *ground electronic states of alkali molecules and alkali hydrides,* and vice versa.

6. SYSTEMATIZATION OF GROUND STATES OF ALL DIATOMIC MOLECULES

Our approach makes that we can visualize Eq.(21) not only regarding the *electronic states of a given molecule,* but also regarding the *ground states of molecules belonging to a given chemical family,* thus exhibiting *similar electronic configurations,* with virtually the same g.

Let us elaborate on this a little.

Above we have rigorously proven that Eq.(15) holds for any diatomic molecule, i.e.

$$T_0 = \frac{4\pi^2}{h\sqrt{n_1 n_2}} \sqrt{g \mathcal{M}_0 m_e r_0^2} \ , \qquad (15) \ \textit{(rewritten)}$$

$n_1 n_2$ being quantum numbers induced by the Planck Constant [cf. Eq.(10)(rewritten)].

Within the frames of Theorems 6 and 7, regarding the electronic states of a given molecule, we have established that $n_1 n_2$ turns out to be the ratio of the internuclear distance of the molecule at the given excited state, to the internuclear distance of the molecule at the ground state, provided that these states are configured alike.

We have further demonstrated that already the cast $T_0 \sim \sqrt{\mathcal{M}_0} r^2$ holds fairly well regarding diatomic molecules belonging to a given chemical family, thus being configured similarly, so that g stays virtually the same, throughout each one of the Figures 1-7.

Further straightening up of these curves, requires to specify $n_1 n_2$.

At this stage consider Figure 8, where we analyzed H_2 spectroscopic data, and found out that the *ambiguous states* are configured like *alkali hydrides,* and Li_2.

This suggests that, *quantum mechanically* we can well describe, say the ground state of Li_2, on the basis of an *equivalent* H_2 excited state.

Therefore the corresponding quantum numbers $n_1 n_2$, we propose to associate with Li_2 ground state, in comparison with the H_2 ground state, following Eq.(18) and Theorem 7, becomes the mere ratio of the internuclear distance of Li_2 at its ground state, to the internuclear distance of H_2 at its ground state, given that the H_2 and Li_2 bonds, are configured similarly.

Hence, we rewrite Eq.(21) *(not for the excited levels of a given molecule),* but for the *ground states of molecules* belonging to a given chemical family, and accordingly being configured alike:

$$T_{0i} = \frac{4\pi^2}{h\sqrt{\frac{r_{0i}}{r_{00}}}} \sqrt{g\mathcal{M}_{0i}}\, r_{0i}^2 = \frac{4\pi^2}{h} \sqrt{g\mathcal{M}_{0i} r_{00}}\, r_{0i}^{3/2} \; ; \qquad (25)$$

(written by the author for the ground vibrational period of molecules belonging to a given chemical family)

here T_{0i} is the *ground state largest vibrational* period of the ith member of the chemical family in consideration; $\mathcal{M}_{0i}$ is the reduced mass and; r_{0i} is the ground state internuclear distance of this member; r_{00} is *the internuclear distance of the ground state of the family's member,* chosen as the *reference molecule;* more precisely we pick up as the member bearing the lowest vibrational period.

Therefore T_{0i}^2 versus $\mathcal{M}_{0i} r_{0i}^3$ for *chemically alike molecules,* should display a *linear behavior,* the slope of which shall furnish g, to be associated with the chemical family in consideration.

Thus we can now write an equation similar to Eq.(21), in regards to the ground states of molecules belonging to a given chemical family:

$$\text{Constant} = \frac{\omega_{0i}\mathcal{M}_{0i} r_{0i}^2}{\sqrt{n_1 n_2}} = \omega_{0i}\mathcal{M}_{0i} r_{00} r_{0i}^{3/2} \; , \qquad (26)$$

(written by the author, for the ground states of chemically alike molecules)

where ω_{0i} is the inverse of the ground state *vibrational period* of the molecule of concern.

The *constant* in question shall be expressed as

$$\text{Constant} = \frac{h}{4\pi^2\sqrt{g m_e}} \,. \tag{27}$$

Although r_{00} is a constant within a given chemical family, we still included it, in the RHS of Eq.(26), to define our constant to be the same for all chemical families, if g remained the same, thus as suggested by the RHS of Eq.(27).

In Figures 9-15, based on experimental data,[13, 15, 16] we present T_{0i} versus $\sqrt{\mathbf{M}_{0i} r_{0i}^3}$, for *seven chemical families,* for which the coefficient g, stays indeed neatly constant. The constancy of $\omega_{0i}\mathbf{M}_{0i} r_{0i}^{3/2}$ in harmony with Eqs.(26) and (27), is *quantitatively* demonstrated, in *(the fifth column of)* Tables 1-7.

g's are calculated from Eq.(27) for different chemical families, and are presented in Table 8. Note that g's vary between 0.79 and 0.01.

Note that following Eqs. (26) and (27), the *value of constancy* of $\omega_{0i}\mathbf{M}_{0i} r_{0i}^{3/2}$ depends, both on g and r_{00} *(the reference internuclear distance of the family of concern),* which makes that the *"constants"* calculated in *(the fifth columns of)* Tables 1-7, differ.

Note further that, the *standart deviation* on the constants in question, is roughly *ten percent.* There seems to be *two reasons* for this. The *first one* is that chemically alike molecules, on the contrary to our assumption, are not exactly configured similarly, which may make that g is not a constant throughout. *The second one* is that our supposition that the RHS Eq.(18), can be used to replace the the *composite quantum number* $n_1 n_2$ in Eq.(15), even for chemically alike molecules *(where we choose the molecule with the lowest vibrational period, as the reference molecule),* may not be rigorous. Along this line it seems interesting to recall that, when we use the *principal quantum numbers associated with the bond electron*s, *straight,* to compose $n_1 n_2$, instead of using Eq.(18), we come out with the *constancy* of $\omega_{0i}\mathbf{M}_{0i} r_{0i}^2 / \sqrt{n_1 n_2}$, not any worse than that of $\omega_{0i}\mathbf{M}_{0i} r_{0i}^{3/2}$ [cf. Eq.(26)].[7,8]

Since g happens to be roughly, *inversely proportional to the dissociation energy of the molecule,* as one can observe from Table 1, it indeed decreases as the bond becomes stronger. Thus, the smaller g is, the higher is the number of the covalent bonds, making the overall bond of the diatomic molecule, or the higher is the number of free electrons an atom possesses, the looser will be the bond it will make with, say, an halogen, thus the higher will g be, etc. [17]

Table 1 Checking the Validity of Eq.(23), for Alkali Molecules

Molecules	M_0 (amu)	T_0 (cm^{-1} x10^{3}c)	r_0 ($\overset{\circ}{A}$)	$\frac{T_0}{\sqrt{M_0}\, r_0^{3/2}}$	$\lvert \text{Relative Error} \rvert$ as Referred to the Average
H_2	0,50	0,24	0,74	0,53	0,52
Li_2	3,50	2,89	2,67	0,35	0,01
LiNa	5,33	3,89	2,90	0,34	0,03
Na_2	11,50	6,34	3,08	0,35	0,01
NaK	14,48	8,06	3,50	0,32	0,08
K_2	9,49	10,80	3,92	0,45	0,29
KRb	26,83	13,2	4,07	0,31	0,11
Rb_2	42,47	17,3	4,21	0,31	0,12
RbCs	52,04	20	4,42	0,30	0,15
Cs_2	66,47	23,8	4,64	0,29	0,17
Average				0,36	0,15

Table 2 Checking the Validity of Eq.(23), for O_2 - like Molecules

Molecules	M_0 (amu)	T_0 (cm^{-1} x10^{3}c)	r_0 ($\overset{\circ}{A}$)	$\frac{T_0}{\sqrt{M_0}\, r_0^{3/2}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
O_2	8,00	0,64	1,21	0,17	0,21
S_2	15,99	1,39	1,89	0,13	0,07
Se_2	39,97	2,56	2,16	0,13	0,07
Te_2	63,82	4,00	2,59	0,12	0,14
SO	10,67	0,90	1,49	0,15	0,07
Average				0,14	0,11

Table 3 Checking the Validity of Eq.(23), for N_2 - like Molecules

Molecules	M_0 (amu)	T_0 (cm^{-1} x10^{3}c)	r_0 ($\mathring{A}$)	$\frac{T_0}{\sqrt{M_0}\, r_0^{3/2}}$	$\lvert \mathrm{RelativeError} \rvert$ as Referred to the Average
N_2	7,00	0,43	1,09	0,14	0,06
P_2	15,49	1.29	1,89	0,12	0,06
PN	9,65	0,76	1,49	0,13	0,00
Average				0,13	0,04

Table 4 Checking the Validity of Eq.(23), for Halogens

Molecules	M_0 (amu)	T_0 (cm^{-1} x10^{4}c)	r_0 ($\mathring{A}$)	$\frac{T_0}{\sqrt{M_0}\, r_0^{3/2}}$	$\lvert \mathrm{RelativeError} \rvert$ as Referred to the Average
F_2	11,21	9,50	1,44	1,64	0,06
Cl_2	17,96	17,49	1,99	1,47	0,15
Br2	31,15	39,96	2,28	2,08	0,19
I_2	46,87	63,47	2,67	2,13	0,22
BrF	15,04	15,35	1,76	1,69	0,02
ClF	12,93	12,31	1,63	1,64	0,05
ICl	26,23	27,42	2,32	1,51	0,13
Average				1,74	0,12

Table 5 Checking the Validity of Eq.(23), for CsBr - like Molecules

Molecules	M_0 (amu)	T_0 (cm^{-1} x10^{4}c)	r_0 ($\mathring{A}$)	$\frac{T_0}{\sqrt{M_0}\, r_0^{3/2}}$	$\lvert\text{Re lativeError}\rvert$ as Referred to the Average
CsBr	52,63	49,92	3,14	1,24	0,51
CsI	71,63	64,94	3,41	1,22	0,49
NaCl	26,46	13,95	2,51	0,68	0,17
NaBr	31,98	17,86	2,64	0,74	0,09
NaI	35,15	19,45	2,90	0,66	0,19
KF	25,64	12,78	2,55	0,62	0,24
KCl	35,95	18,59	2,79	0,67	0,19
KBr	43,55	26,26	2,94	0,79	0,03
KI	47,48	29,89	3,23	0,75	0,08
RbCl	39,53	25,07	2,89	0,81	0,01
Average				0,82	0,20

Table 6 Checking the Validity of Eq.(23), for BF - like Molecules

Molecules	M_0 (amu)	T_0 (cm^{-1} x10^{4}c)	r_0 ($\mathring{A}$)	$\frac{T_0}{\sqrt{M_0}\, r_0^{3/2}}$	$\lvert\text{Re lativeError}\rvert$ as Referred to the Average
BF	7,26	6,72	1,26	1,76	0,26
BCl	12,06	8,38	1,72	1,07	0,24
BBr	14,77	9,66	1,88	0,98	0,31
AlCl	20,95	15,24	2,13	1,071	0,24
AlBr	26,64	20,11	2,29	1,12	0,20
InCl	31,71	26,82	2,31	1,36	0,03
InI	56,72	60,32	2,86	1,66	0,18
TlCl	35,09	29,87	2,55	1,24	0,12
TlBr	52,27	57,98	2,68	1,83	0,30
TlI	66,67	78,31	2,87	1,97	0,40
Average				1,41	0,23

Table 7 Checking the Validity of Eq.(23), for CO - like Molecules

Molecules	M_0 (amu)	T_0 (cm^{-1} x10^{4}c)	r_0 ($\mathring{A}$)	$\frac{T_0}{\sqrt{M_0} r_0^{3/2}}$	$\lvert \text{Relative Error} \rvert$ as Referred to the Average
CO	4,67	6,86	1,13	2,64	0,47
CS	7,86	8,73	1,53	1,65	0,09
SiO	8,13	10,18	1,51	1,92	0,07
SiS	13,43	14,93	1,93	1,52	0,16
GeO	10,23	13,15	1,65	1,94	0,08
SnO	12,27	14,09	1,84	1,61	0,10
SnS	20,62	25,25	2,06	1,88	0,04
PbO	14,00	14,85	1,92	1,49	0,17
PbS	23,49	27,72	2,39	1,55	0,14
Average				1,80	0,15

Table 8 Bond Looseness Factors of the Chemically Alike Diatomic Molecules

Chemical Family	Bond Looseness Factor (g)
H_2, Li_2, Na_2, K_2	0.79
O_2, S_2, Se_2, Te_2, OS	0.05
N_2, P_2, PN	0.04
F_2, Cl_2, Br_2, I_2, BrF, ClF, ICl	0.04
CsF, CsBr, CsI, NaCl, NaBr, NaI, KF, KCl, KBr, KI, RbCl	0.01
BF, BCl, BBr, AlCl, AlBr, InCl, NBr, InI, TlCl, TlBr, TlI	0.05
CO, CS, SiO, SiS, GeO, SnO, SnS, PbO, PbS	0.13

7. CONCLUSION

Note that Eq.(21) frames the force constant k of the molecule at the excited state of concern, as

$$k = \frac{fe^2}{r^3} \ , \tag{28}$$

along

$$fe^2 = \frac{h^2}{4\pi^2 r g_{IN} m_e} \ ; \tag{29}$$

here, e is the electron charge, and f is a dimensionless constant.

Eq.(28) dimension-wise, is somewhat obvious, if one proposes to relate the force constant to the internuclear distance. This correlation was in effect proposed sometime ago, by Bratoz et al., for alkali hydrides,[18,19] for which f is reported to be 2. Our estimation, based on the data[12] is, on the average, 2.6.

f was subsequently obtained by Salem and Ohwada[20,21] which then, based on *empirical presumptions,* chiefly for molecules containing alkali atoms, leads to

$$f = \frac{1}{2}(N_i + 1)(N_j + 1) \ , \tag{28}$$

where N_i and N_j, are the respective number of electrons residing outside of the complete shells of the atoms making up the diatomic molecule.

Note thence that, under this form f, thus g, indeed stay constant, just the way we had originally conjectured.

Eq.(28) yields 8 for alkali halides, whereas based on the data, and on the average, we come out with 11.1.

Recall nonetheless that in order to obtain our results, we followed a totally different path, than that induced by Eq.(28). Moreover we arrived at our result, primarily regarding the *electronic states of a given molecule.* The literature we reviewed does not coop at all with such an aspect.

Note further that recent trials, on the *"problem of transferable spectroscopic constants",* despite satisfactory results they may furnish, are far from displaying how the *fundamental quantities* of *mass, space* and *time (i.e. clock mass, clock size and period of time of the clock motion),* are structured in interrelation with each other, in the architecture of molecules,[22] in fact just the way Eq.(21) reveals.

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As far as we gather, the *invariance* of $E_0M_0R_0^2$ through, a general quantum mechanical description, based on an *overall mass change,* in relation to a *real wave-like body,* seems to have been *overlooked* for more than half a century *(presumably because no meanigfulness was attributed to such a procedure),* even worse, despite the evidence of *(though approximate) empirical data* (i.e. $\varpi_0 r_0^2$ = Constant), evoking it clearly, and worse of all, despite the fact that, it is well known as a *relativistic invariant.* It is in reality, via this occurrence that quantum mechanics should work as the *internal machinery of special theory of relativity,* were the object in hand brought to a uniform translational motion, or as well, the *internal machinery of the end result of general theory of relativity,* were the object transplanted into a gravitational field.[3,6] We have to recall that within the frame of the special theory of relativity, the *invariance* of $E_0M_0R_0^2$ becomes a straightforward consequence of the *constancy of the speed of light,* in regards to all inertial frames of reference.

But here, not to attract *conservative reactions,* we did not insist on this inspiring idea.

The quantity $E_0M_0R_0^2$ is further *“strapped”* to h^2, so that for any *real wave-like object* the relationship, $E_0M_0R_0^2 \sim h^2$ [Eq.(2)] holds.

We find it exciting to emphasize that, *fundamentally* the spcecial theory of relativity makes it necessary that, already at rest, a wave-like entity ought to be built in just a given way, and this makes that *“space size”*, *“clock mass”* and *“period of time”* as well as *“energy”,* one can associate with the *internal motion* the object displays, must be interrelated in just the way delineated by Eq.(2). We called this occurrence the UMA Cast. A general derivation of this result is presented in Appendix A. Note that, primarily what we did here, is not a “*dimension analysis*”. Anyhow the occurrence we disclose (as shown in Appendix A), would not work if the wave-like object in hand is not *“real*”, though of course, there still would be no problem in regards to a *dimension analysis.*

The UMA Cast, together with the B&O approximation, applied to a diatomic molecule, led us to an *elegant relationship* between the period of oscillation T_0, the *clock mass* M_0, and the *internuclear distance* R_0, to be associated with a diatomic molecule, more specifically, $T_0 = [4\pi^2/(\sqrt{n_1n_2}h)]\sqrt{gM_0m_e}\,R_0^2$ [Eq.(17)], where M_0 is the *nuclei reduced mass,* m_e the *mass of the electron,* n_1 and n_2 *principal quantum numbers* to be associated with the electrons making up the bond(s) of the molecule in hand, and g a coefficient related *solely* to the *bond electronic structure.* The “*clock mass*” M_0, regarding the vibrational motion then becomes $\sqrt{M_0m_e}$ [Eq. (16)].

More profoundly, Eq.(17) displays a striking feature; it is that, *“space” (size)* and *“time” (period of time)* are *separable* from each other, if *“mass” (clock mass)* were considered the *size* and *period of time* dependent function. Though we arrived at Eq.(17), through an approximation, henceforth, its *cast,* concerning the *separability* in question, still appears to be rigoruos.

One may recall that, the *separability* of *“space”* and *“time”* does not at all seem obvious. Recall that in effect, *“moments”* and *“locations”* are, through the *Lorentz transformations,* interrelated *(and are not independent from each other),* in regards to transformations beween inertial frames of reference. However *(Lorentz transformations of) “differences of instants”* and *“differences of locations”,* well happen to be independent from each other. It is indeed this fact, which should be responsible of the setting of *“size”* and *“period of time”,* in a wave-like object, *independently linked* to the *“clock mass”* .

Eq.(19) is especially valid in regards to the excited electronic states of a given diatomic molecule. We figured thus that the *composite quantum number* $n_1 n_2$ turns out to be R/R_0, where R is the internuclear distance of the diatomic molecule of concern, at the given excited electronic state, and R_0 the internuclear distance at the ground electronic state, provided that both states are configured similarly. *(Note that, at the given electronic state, we visualize just the lowest vibrational state.)*

Thus for a given diatomic molecule, we expect T^2 versus R^3, to behave as a straight line passing by the origin, for electronic states bearing alike configuration, thus the same g.

We test our approach successfully on the basis of H_2 molecule, and beyond.

Were R close to R_0, Eq.(17) reduces to $T_0 \sim R_0^2$. This latter relationship was established empirically in 1925. Unfortunately, it was up to our approach, left out totally uninterpreted.

Our finding about the *composite quantum number,* led us to extend our approach to chemically alike diatomic molecules.

Consider for instance the alkali molecules. Then Li_2 can well be considered as built at excited level of H_2 configured like Li_2, the corresponding composite number to be introduced into Eq.(17) then being, R/R_0, where R is the ground internuclear distance of the latter molecule. The same should be valid for Na_2, etc.

Given that H_2, Li_2, Na_2, etc, are all expected to be configured the same at the bond level, they should all bear the same bond looseness factor.

Thus T^2 versus $M_0 R^3$ for molecules belonging to a given family, should behave as a straight line passing from the origin.

*

It is important to note that our relationship $T_0 = [4\pi^2/(\sqrt{n_1 n_2}h)]\sqrt{gM_0 m_e}\,R_0^2$, bears the *form* of the de Broglie relationship (cf Appendix A).

This induces the following interesting facts:

The UMA Cast [Eqs. (2), (14) and (17)], we derived out of the Schrodinger Equation or Dirac Equation,[23,24] constitutes a "*concise integral form*" of the Heisenberg Uncertainty Principle.[25,26]

This eases much the teaching of the *"Uncertainty Principle"* which can be reformulated a follows: Within a real wave-like object, the *clock* period, the clock *mass* and the clock *size*, should be structured in just a given manner, and this to be governed by the Planck Constant).

It is further important to note that, say the familiar expression about the *vibrational period of a diatomic molecule*, i.e. $T_0 = 2\pi\sqrt{M_0 / k_0}$, herein we dealt with, displays no feature at all about the UMA cast, and we would be unable to show that the cast of this period relationship can be reduced to the UMA Cast, without our original idea rooted to the special theory of relativity. This point is elaborated in Appendix A.

Thence, it is not obvious at all that, any *"real*" quantum mechanical object should be structured in accordance with the UMA Cast we disclose.

What we developed over here, can be extended to *triatomic molecules*, and beyond.

We conjecture that, due to the nature of the framework we have drawn, it can be extended as well, to the *nuclear world*, with hopefully no great difficulty. We like to stress that we found nothing achieved in the literature, along the line we pursued herein.

APPENDIX A

INVARIANCE BASED ON MASS VARIATION, MANUFACTURED BY WAVE MECHANICS: THE "UMA CAST"

Consider an *atomistic* or *molecular* wave-like object, *"existing in nature".* Such an object shall embody a Coulomb potential energy, thus involving a *spatial dependency propotional to the inverse of the distance between the interacting electrical charges.* We shall call it a *"real wave-like object",* and the *potential energy* it embodies, a *"real potential energy".* So by *"real",* we mean *"not artificially gedanken".* Note that the results we are going to derive herein, do not *generally* hold if the potential energy considered for a wave-like description, is not a *"real"* one.

In this appendix we deal with the quantum mechanical description of basically *atomistic and molecular real wave-like objects.* Yet, this can be extended to *real nuclear objects* with no great difficulty.

A-1. IN A REAL WAVE-LIKE DESCRIPTION, IF MASS IS INCREASED, THEN SIZE OF THE OBJECT CONTRACTS AS MUCH, AND THE TOTAL ENERGY EXPANDS IN THE SAME AMOUNT

For a *real atomistic* or *molecular* wave-like object, herein we show the *following theorem,* on the basis of the Schrodinger Equation, as complex as this may be. Our approach can be extended to a similar demonstration on the basis of the Dirac Equation as well.[4] However, here we shall omit this latter exercise.

Theorem A-1: In a *"real wave-like description" (thus, not embodying artificial potential energies),* composed of I electrons and J nuclei, if the *(identical)* electron masses m_{i0}, i = 1,..., I, and different nuclei masses m_{j0}, j = 1,…, J, involved by the object, are overall multiplied by the *arbitrary number* γ, then *cocurrently, a)* the *total energy* E_0 associated with the given internal motion of the object, is increased as much, *and b)* the *size* R_0 to be associated with the given motion contracts as much; in mathematical words this is

$$\{ [(m_{i0}, i = 1,..., I) \rightarrow (\gamma\, m_{i0}, i = 1,..., I)],\ [(m_{j0}, j = 1,\ldots, J) \rightarrow (\gamma\, m_{j0}, j = 1,\ldots, J)] \}$$

$$\Rightarrow \{ [E_0 \rightarrow \gamma E_0],\ [\mathsf{R}_0 \rightarrow \frac{\mathsf{R}_0}{\gamma}] \} .$$

Let us accentuate that, if the object is, say an *atom,* then R_0 is *(no matter how we define it, provided that it is compatible with the Planck Constant)* the radius of it; if the object is a diatomic molecule, R_0 is the internuclear distance, etc. R_0, in fact, may be just *any length* one may pick, within the framework of the object in hand, and Theorem A-1, as can be shown, shall still be valid.

We would like to emphasize that the content of Theorem A-1 is well known on the basis of the hydrogen atom. Yes indeed. *(In fact this is not really an overall mass change one considers, regarding the hydrogen atom framework, but the change of the nucleus proton number.)* Anyway, a *general overall mass change* in a given entity was not so far considered, perhaps because *no immediate meaningfulness* is attributed to it; thus the results of such a procedure are not provided in the literature.

However, as we shall see, not only the *exercise* we aim to, leads us to a useful relationship, but also, the object interestingly undergoes an overall *mass transformation* were it brought to a *uniform translational motion* or were it embedded in a *gravitational field,* or in fact just in *any field* it eventually interacts with. Thus it turns out to be quite interesting to examine the results of an overall mass change on the basis of a wave-like entity.

Proof of the First Part of Theorem A-1

For our purpose, we consider the (*time independent*) Schrödinger Equation, i.e. with the familiar notation, written for a *"real"* atomistic or a molecular wave-like object composed of J nuclei, of respective masses m_{j0}, j = 1,…, J, and I electrons *(altogether)*, of *(the same)* mass m_{i0}, i = 1,..., I:

$$\left(-\sum_{j}\frac{h^2}{8\pi^2 m_{j0}}\nabla_j^2-\sum_{i}\frac{h^2}{8\pi^2 m_{i0}}\nabla_i^2-\sum_{i,j}\frac{Z_{j0}e^2}{r_{ij0}}+\sum_{i,i'}\frac{e^2}{r_{ii'0}}+\sum_{j,j'}\frac{Z_{j0}Z_{j'0}e^2}{r_{jj'0}}\right)\psi_0(\underline{r}_0)$$

$$=E_0\psi_0(\underline{r}_0)\,. \qquad \text{(A-1)}$$

E_0 is the eigenvalue and $\psi_0(\underline{r}_0)$ the related eigenfunction; Z_{j0} is the atomic number of the j^{th} nucleus; r_{ij0} is the distance between the i^{th} and the j^{th} particles.

Thus, multiply the masses m_{i0} (i = 1,..., I), and m_{j0} (j = 1,…, J), in Eq.(A-1) by γ; the eigenfunction and the related eigenvalue will accordingly be altered:

$$\left(-\sum_{j}\frac{h^2}{8\pi^2\gamma m_{j0}}\nabla_j^2-\sum_{i}\frac{h^2}{8\pi^2\gamma m_{i0}}\nabla_i^2-\sum_{i,j}\frac{Z_{j0}e^2}{r_{ij0}}+\sum_{i,i'}\frac{e^2}{r_{ii'0}}+\sum_{j,j'}\frac{Z_{j0}Z_{j'0}e^2}{r_{jj'0}}\right)\psi_{new}(\underline{r}_0)$$

$$=E\,\psi_{new}(\underline{r}_0)\,. \qquad \text{(A-2)}$$

This is the same as

$$\left(-\sum_{j}\frac{h^2}{8\pi^2 m_{j0}}\nabla_j^2-\sum_{i}\frac{h^2}{8\pi^2 m_{i0}}\nabla_i^2-\sum_{i,j}\frac{Z_{j0}e^2}{\frac{r_{ij0}}{\gamma}}+\sum_{i,i'}\frac{e^2}{\frac{r_{ii'0}}{\gamma}}+\sum_{j,j'}\frac{Z_{j0}Z_{j'0}e^2}{\frac{r_{jj'0}}{\gamma}}\right)\psi_{new}(\underline{r}_0)$$

$$=\gamma\,E\,\psi_{new}(\underline{r}_0)\,. \qquad \text{(A-3)}$$

Let now

$$\underline{r}_0\rightarrow\underline{r}=\gamma\underline{r}_0\,, \qquad \text{(A-4)}$$

together with

$$\psi(\underline{r})\equiv\psi_{new}(\underline{r}_0)\,. \qquad \text{(A-5)}$$

Since

$$\frac{\partial\psi(r_0)}{\partial u_0}=\frac{\partial\psi(r)}{\partial u}\frac{\partial u}{\partial u_0}\ ;\ u_0=x_0,y_0,z_0;\ u=x,y,z; \qquad \text{(A-6)}$$

we have

$$\frac{\partial\psi(r_0)}{\partial u_0}=\gamma\frac{\partial\psi(r)}{\partial u}\,. \qquad \text{(A-7)}$$

Eq.(A-3) thus becomes

$$\left(-\sum_{j}\frac{h^2}{8\pi^2 m_{j0}}\gamma^2\nabla_j^2-\sum_{i}\frac{h^2}{8\pi^2 m_{i0}}\gamma^2\nabla_i^2-\sum_{i,j}\frac{Z_{j0}e^2}{\frac{r_{ij0}}{\gamma}}+\sum_{i,i'}\frac{e^2}{\frac{r_{ii'0}}{\gamma}}+\sum_{j,j'}\frac{Z_{j0}Z_{j'0}e^2}{\frac{r_{jj'0}}{\gamma}}\right)\psi(\underline{r})$$

$$=\gamma\, E\psi(\underline{r})\,. \tag{A-8}$$

Dividing by γ^2, and using Eq. (A-4), this yields

$$\left(-\sum_{j}\frac{h^2}{8\pi^2 m_{j0}}\nabla_j^2-\sum_{i}\frac{h^2}{8\pi^2 m_{i0}}\nabla_i^2-\sum_{i,j}\frac{Z_{j0}e^2}{r_{ij}}+\sum_{i,i'}\frac{e^2}{r_{ii'}}+\sum_{j,j'}\frac{Z_{j0}Z_{j'0}e^2}{r_{jj'}}\right)\psi(\underline{r})$$

$$=\frac{E}{\gamma}\psi(\underline{r})\,. \tag{A-9}$$

In comparison with Eq. (A-1), we can deduce at once that

$$\frac{E}{\gamma}=E_0\;\Rightarrow E=\gamma E_0\quad \text{(c.q.f.d.)}\,. \tag{A-10}$$

Thus, we achieved partly the demonstration of Theorem A-1.

Proof of the second part of Theorem A-1

Next we focus on a size of interest $\mathcal{R}_0$ *(say the "size of an atom", or the "internuclear distance" in a diatomic molecule of concern),* to be associated with the wave like object in hand. $\mathcal{R}_0$ shall be determined based on the solution of Eq.(A-1). Following the mass perturbation, $\mathcal{R}_0$ becomes $\mathcal{R}_{0new}$, and this latter shall be found, based on the solution of Eq.(A-2). According to Eq.(A-4), $\mathcal{R}_{0new}$ is transformed into $\mathcal{R}$, i.e. $\mathcal{R}=\gamma\mathcal{R}_{0new}$. (Note that according to this equation, any distance, say r_0 we would consider, becoming r_{onew} due to the mass change, is transformed into r, so that $r=\gamma\, r_{onew}$. Thus the derivation presented herein, in fact holds for any distance, thence also for a given specific distance $\mathcal{R}_0$ we would pick up.)

R is to be determined as the solution of Eq.(A-9). But since this equation is identical with Eq.(1) [along Eq.(A-10)], the solution of Eq.(A-9) in regards to $\mathcal{R}$, is the *"original size"* of interest, i.e. $\mathcal{R}_0$.

Hence

$$\gamma \mathsf{R}_{0\mathrm{new}} = \mathsf{R}_0 , \tag{A-11}$$

or the same

$$\mathsf{R}_{0\mathrm{new}} = \frac{\mathsf{R}_0}{\gamma} \quad \text{(c.q.f.d.)} . \tag{A-12}$$

This ends the demonstration of Theorem A-1.

Though this proof is rigorous, we still happened to attract conservative reactions. For this reason, below, we present a cross check of the latter demonstration. To simplify an otherwise heavy notation, for the present purpose, we shall consider just the hydrogen atom's Schrodinger description, thus in spherical symmerty, yet without any loss of generality regarding the validity of our cross check exercise.

Cross Check of the Second Part of Theorem A-1

The size R_0 in question, can be described first, by expressing the wave function in question, $\psi_0(r_0)$, out of the Schrodinger Equation, and then deriving $\psi_0(r_0)$ with respect to r_0, i.e. the polar coordinate. Note that we should in fact look for R_0 which makes $\partial\psi_0^2(r_0)/\partial r_0$ vanish; but [since, ordinarily $\psi_0(r_0) \neq 0$], this is the same as R_0 which makes $\partial\psi_0(r_0)/\partial r_0$ vanish.

Thus with the familiar notation (M_0 being the reduced mass of the proton and the electron):

$$\psi_0(r_0) = -\frac{\nabla^2\psi_0(r_0)}{\dfrac{8\pi^2 M_0}{h^2}\left(E_0 + \dfrac{Z_0 e^2}{r_0}\right)} , \tag{A-13}$$

$$\frac{\partial\psi_0(r_0)}{\partial r_0} = 0 = -\frac{h^2}{8\pi^2 M_0}\,\frac{\left\{\dfrac{\partial}{\partial r_0}\left[\nabla^2\psi_0(r_0)\right]\right\}\left(E_0 + \dfrac{Z_0 e^2}{r_0}\right) + \left[\nabla^2\psi_0(r_0)\right]\left(\dfrac{Z_0 e^2}{r_0^2}\right)}{\left(E_0 + \dfrac{Z_0 e^2}{r_0}\right)^2} ; \tag{A-14}$$

thus

$$\left\{\left[\frac{\partial}{\partial r_0}\left[\nabla^2\psi_0(r_0)\right]\right]\Bigg|_{r_0=\mathsf{R}_0}\right\}\left(E_0 + \frac{Z_0 e^2}{\mathsf{R}_0}\right) + \left\{\left[\nabla^2\psi_0(r_0)\right]\Big|_{r_0=\mathsf{R}_0}\right\}\left(\frac{Z_0 e^2}{\mathsf{R}_0^2}\right) = 0 . \tag{A-15}$$

This is the equation which will yields $\mathcal{R}_0$.

In order to assess how $\mathcal{R}_0$ will be affected when M_0 is multiplied by γ, we can consider Eq.(A-14), where we shall accordingly replace E_0 by γE_0, and $\psi_0(\underline{r}_0)$ by $\psi(\underline{r}_0)$:

$$\left\{\frac{\partial}{\partial r_0}\left[\nabla^2\psi(r_0)\right]\right\}\left(\gamma E_0+\frac{Z_0e^2}{r_0}\right)+\left[\nabla^2\psi(r_0)\right]\left(\frac{Z_0e^2}{r_0^2}\right)=0\,. \tag{A-16}$$

Using Eqs. (A-4), (A-5), (A-6) and (A-7), this can be rearranged to yield

$$0=\frac{\gamma\partial}{\partial r}\left[\frac{\gamma^2\partial^2\psi(r)}{\partial r^2}+\frac{2\gamma}{r}\frac{\gamma\partial\psi(r)}{\partial r}\right]\left(\gamma E_0+\frac{Z_0e^2}{r_0}\right)+\left[\frac{\gamma^2\partial^2\psi(r)}{\partial r^2}+\frac{2\gamma}{r}\frac{\gamma\partial\psi(r)}{\partial r}\right]\left(\frac{Z_0e^2}{r_0^2}\right). \tag{A-17}$$

Let us divide this by γ^4, and use Eq.(A-4) :

$$0=\frac{\partial}{\partial r}\left[\frac{\partial^2\psi(r)}{\partial r^2}+\frac{2}{r}\frac{\partial\psi(r)}{\partial r}\right]\left(E_0+\frac{Z_0e^2}{r}\right)+\left[\frac{\partial^2\psi(r)}{\partial r^2}+\frac{2}{r}\frac{\partial\psi(r)}{\partial r}\right]\left(\frac{Z_0e^2}{r}\right). \tag{A-18}$$

Through a comparison with Eq.(A-13), it becomes clear that the value r, or [according to Eq.(A-4)], γr_0 which satisfies this equation should be the *(previous)* R_0. Let us call R_{0new}, the corresponding new value of r_0. Thus:

$$\gamma\mathcal{R}_{0new}=\mathcal{R}_0 \tag{A-11}$$

or the same

$$\mathcal{R}_{0new}=\frac{\mathcal{R}_0}{\gamma}\quad\text{(c.q.f.d.)}\,. \tag{A-12}$$

This ends the cross check of the demonstration of the second part of Theorem A-1. Note again that for the purpose of this cross check we adopted the simple Schrodinger frame, but just to simplify the rather heavy notation. Otherwise Eq.(A-18) is valid for any *"real"* quantum mechanical frame, as complicasted as this may be, and in fact, that is what we have achieved above, through a rigorous and elegant way to prove the second part of Theorem A-1.

Thus we would like to emphasize that Theorem A-1 holds no matter how complicated the wave-like object is. Thence the *vector*

$[(m_{i0},\ i = 1,...,I),\ (m_{j0},\ j= 1,\ldots,\ J),\ E_0,\ \mathcal{R}_0]$,

composed of the original electron massses m_{i0}, i = 1,...,I, the original nuclei masses (m_{j0}, j= 1,…, J), the original eigenfunction E_0, and the original size R_0, associated with the wave-like object, belongs to the *set of vectors*

$[(\gamma m_{i0},\ i = 1,...,I),\ (\gamma m_{j0},\ j= 1,\ldots,\ J),\ \gamma E_0,\ \mathcal{R}_0/\gamma],\ \forall\gamma$.

Therefore it should be stressed that the *total energy expansion* and the *size compression* occur *conjointly*, regarding the mass tranformation in question.

Note that our derivation holds, if various potential energies to be input in the Schrödinger Equation involve *spatial dependencies propotional to the inverse of the respective distances between the interacting electric charges.* In addition, if any of these potential energies were to bear the form $(z_{j0}z_{j'0})e^2/r^n_{jj'0}$ (in regards to the charges $z_{j0}e$ and $z_{j'0}e$, at a distance $r_{jj'}$ from each other), the derivation we achieved, would not hold, unless n=1. [It is clear that, otherwise, we could not obtain Eq.(A-9), for $(z_{j0}z_{j'0})e^2/r^n_{jj'0}$ in this equation, could not be transformed into $z_{j0}z_{j'0}e^2/r_{jj'}$, through the rearrangement in question.] Note further that the foregoing derivation would not either hold through a (*relativistic*) Dirac description, if this does not involve potential energies in the form $z_{j0}z_{j'0}e^2/r_{jj'0}$, for the atomistic or molecular wave-like object in consideration.

We would like to emphasize that, the condition n=1, is imposed by the *special theory of relativity;* thus a *potential energy* not bearing this form (*whether in a non-relativistic wave-like description, or even in a Dirac relativistic wave-like description*), is a *violation* of the special theory of relativity,[1, 2, 3] such a violation would further deteriorate the results we presented herein.

A-2. THE INVARIANCE OF THE QUANTITY {(TOTAL ENERGY) x (CLOCK MASS) x (SİZE)^2} IN REGARDS TO THE CHANGE IN MASS

We define the *"clock mass",* as a mass to be associated with the *internal dynamics* of the wave-like object in hand. Thus it is the *"clock mass"* which does the *"clock labour"* depicted by the internal dynamics of concern (cf. the text). Below M_0 will represent the clock mass.

Via Theorem A-1, through the transformation $[M_0 \rightarrow \gamma M_0]$, the quantity $E_0 M_0 R_0^2$, becomes $[\gamma E_0][\gamma M_0][R_0^2/\gamma^2]$, hence remains *invariant.*
Therefore, we establish *at once,* our next theorem.

Theorem A-2: In a *real wave-like description,* in regards to the transformation $[M_0 \rightarrow \gamma M_0]$, the product $E_0 M_0 R_0^2$ remains invariant.

Note once again that, this theorem would not hold, if the right potentials were not used in our original description, i.e. Eq.(A-1).

Actually, under the overall mass transformation we have considered *(through a "real" quantum mechanical description),* we have to note that the invariance of (total energy x mass x length^2) holds for any mass m_0, also for any piece of length r_0, the object involves.

Furthermore it is interesting to note that, the *quantum mechanical* invariance of the quantity (total energy x mass x length^2) *(based on an overall mass change, as we conisdered, in the already non-relativistic quantum mechanical description),* further happens to be an invariance, depicted by the *special theory of relativity.*
Fundamentally, it is this latter finding which, constituted the start point of our entire work. Our finding evokes that in order to be compatible with the *"special theory of relativity",* also with the *"general theory of relativity"; "mass", "space" (i.e. size)* and *"time" (i.e. period of time),* or *"energy",* to be associated with the internal dynamics of a given entity, must be structured through just a *"given way of interrelation"* with each other, i.e. the frame displayed by the *invariance* stated in Theorem A-2.

Thus, amongst all the possible $E_0m_0r_0^2$'s we can compose, based on *different masses* m_0 and *different pieces of length* r_0 the object depicts, obviously $E_0M_0R_0^2$ too remains, both *quantum mechanically (regarding the overall mass change we considered),* and *relativistically (regarding a uniform translational motion),* invariant.

This seems to bear a profound meaning, given that $E_0M_0R_0^2$ constitutes a very particular composition.

Indeed, it is true that any quantity (energy x mass x length^2) manufactured out of any *given mass,* any *wall clock* of given *energy,* and any *stick meter* put together, *(when brought to a uniform translational motion) relativistically* remains *invariant,* and this does not of course induce any given interrelation regarding the three totally *independent* quantities in question. It should not however be the same, if these three quantites are somewhat interrelated, to display *quantum mechanically,* the same invariance *(based on an overall mass perturbation);* all the more, $E_0M_0R_0^2$ is nailed to the *universal constant* h^2, for all *simple systems (such as the hydrogen atom, diatomic molecule in rotation, alpha disintegrating nucleus)* we know of.

Henceforth for any wave-like object, we expect the quantity $E_0M_0R_0^2$ (made of the *total energy* of the object, a *particular mass* M_0, i.e. its *clock mass* corresponding to the motion of concern of the wave-like object in hand, and a *pariticular size* R_0, i.e the *characteristic size of space* the motion in question is displayed), to be girdled to h^2.

Below we elaborate on our claim.

Note again that, we did not arrive to this result, through a *dimension analysis;* moreover, let us precise that our conclusion would not hold if the *potential energy* term the wave-like description embodies, were not made of *Coulomb potential energies.*

A-3. DE BROGLIE RELATIONSHIP FOR A COMPLEX SYSTEM AND THE VALUE OF THE INVARIANCE $E_0 M_0 R_0^2$

One way of evaluating the value of $E_0 M_0 R_0^2$, is to determine E_0 out of its *kinetic* and *potential* components, based on an *"appropriate de Broglie relationship"* that we shall introduce, and the Virial Theorem.[27, 28]

De Broglie in 1924, in his doctorate thesis[29], applied his relationship (relating the wave length λ_0 of the particle of concern, to its momentum $m_0 v_0$), i.e.

$$\lambda_0 = \frac{h}{m_0 v_0} , \tag{A-19}$$

to the *stationary electron* revolving around the *proton,* for which then, λ_0 is considerd to be $2\pi r_0$, r_0 being the radius of the orbit. This, beautifully yields the Bohr Postulate[30], stated earlier in 1913, for the hydrogen atom's *ground state:*

$$2\pi r_0 \, m_0 v_0 = h . \tag{A-20}$$

This further, taking the square of both sides and rearrenging the outcome, allows us to calculate the *electron's kinetic energy,* K_0:

$$K_0 = \frac{h^2}{8\pi^2 m_0 r_0^2} . \tag{A-21}$$

On the other hand the *potential energy* U_0, of the electron, achieving its motion in a Coulombian field via the de Broglie relationship [i.e. Eq.(A-19)], can be calculated to be

$$U_0 = -\frac{h^2}{4\pi^2 m_0 r_0^2} . \tag{A-22}$$

Note that one could not obtain this result, if the attraction force between the electron and the proton did not behave as, exactly $1/r_0^2$.

This makes that the *total energy* E_0 of the *hydrogen atom electron,* comes to be

$$E_0 = -\frac{h^2}{8\pi^2 m_0 r_0^2} . \tag{A-23}$$

The above frame, and chiefly Eq.(A-20), constitutes a *unique application* of the de Broglie relationship, beyond its being a *general particle-wave duality* basis regarding a particle exhibiting a *free translational motion*.

Actually, almost after *fifty years* he wrote his thesis, de Broglie in 1973, complained that quantum mechanics did not really grow in conformity with his original ideas, although he does not state how it should have grown.[31]

Nevertheless we believe, there is a bearing in de Broglie worries. That is, the basic philosophy through which de Broglie has applied his relationship to the hydrogen atom [Eq.(A-20)], is almost forgatten.

This latter application however can be followed to land at our original idea, i.e. shortly speaking, *"mass", "space"* and *"time"* or *"energy"* ought to be structured in just a given manner in any atomistic and molecular wave-like object, just in accordance with the cast of Eq.(A-23), particularly owing to the *Coulombian type of interactions* displayed by the electric charges of the object of concern.
Thence, we believe that, if quantum mechanics is *ill grown,* or did not allow any deeper grasp of a huge collection of molecular data *(unveiling practically not much),* this is because, there had been actually *no de Broglie relationship written for a complex object,* undergonig a given motion.

Having given deep thoughts to the subject, henceforth, we conjecture the following de Broglie relationship for the *complex wave-like object* in consideration, of total energy E_0, and *clock mass* M_0, doing a stationary *clock labour* moved with an *average velocity* v_0, in a space of *characteristic size* R_0:

$$R_0 = \frac{h/2\pi}{g_B M_0 v_0} , \qquad \text{(A-24)}$$

where g_B is a *relativistically invariant and dimensionless constant,* usually not far from *unity,* which we propose to work out separately; [2, 32] note particularly that g_B turns to be exactly unity, within the frame of the wave-like description of the hydrogen atom.

Herein we suppose that the object in question undertakes only *one motion,* so that we do not have to deal with a superposition of motions, such as for instance a *"rotation* plus, a *"vibration"*. We will soon elabourate on the case in which one has a superposition of motions.

Thus, Eq.(A-24) allows us to evaluate the *average kinetic energy* K_0 of the wave-like object displaying the internal dynamics of concern, just the way we did above, for the electron of the hydrogen atom:

$$K_0 = \frac{h^2}{8\pi^2 g_B^2 M_0 R_0^2} . \qquad \text{(A-25)}$$

Thus the *average kinetic energy* of the wave-like object in hand, comes to be proportional to $h^2/M_0 R_0^2$.

On the other hand, its *average potential energy (provided that it is made of Coulombian potential energies),* according to Virial Theorem, is the double of its kinetic energy[4,5], i.e.

$$U_0 = -\frac{h^2}{4\pi^2 g_B^2 M_0 R_0^2} ; \qquad \text{(A-26)}$$

thus this too, is proportional to $h^2/M_0\mathbf{R}_0^2$.

Note that here the use of the Virial Theorem does not interfere at all with the *mass transformation* we have considered above.

Both the kinetic energy and the potential energy of the wave-like object in hand, being proportional to $h^2/M_0\mathbf{R}_0^2$, its total energy must also be proportional to $h^2/M_0\mathbf{R}_0^2$; or the same, $E_0M_0\mathbf{R}_0^2$ is proportional to h^2; more specifically, the total energy E_0 becomes

$$E_0 = -\frac{h^2}{8\pi^2 g_B^2 M_0 \mathbf{R}_0^2} \quad . \qquad \text{(A-27)}$$

This draws the following theorem.

Theorem A-3: In a *real atomistic or molecular wave-like description,* the quantity $E_0M_0\mathbf{R}_0^2$ is proportional to h^2.

Henceforth $E_0M_0\mathbf{R}_0^2$ is not only an *invariant* regarding an *overall mass perturbation* within the frame of the quantum mechanical description of a *"real"* object, but is further strapped to h^2; this is deep, since $E_0M_0\mathbf{R}_0^2$ is *relativistically invariant* too. Let us stress that we could not derive Eq.(A-27), if the *potential energy* depicted by the object were not made of *Coulomb Potentials.*

It should still be recalled that Eq.(A-27), thus Theorem A-3, is equivalent to associating *(on the contrary to the general wisdom)* a *simple* de Broglie relationship with the wave-like object in hand *(as complex as this may be).* The fact that we do not know g_B beforehand, may though seem not to advance us much. As we show, this is fortunately not the case.

Indeed g_B appears to be solely dependent on the *electronic configuration* of the object in hand. Thus consider for example the H_2 molecule. We shall thus expect g_B to stay practically the same for the excited electronic levels of H_2 bearing electronic configurations similar to that of the ground state of H_2. We elabourate on this elsewhere. [33]

Nonetheless mathematically speaking, Eq.(A-27) constitutes a definition of g_B. Via the usual weighting and integration of Eq.(A-1) over the appropriate space domain, and the *Virial Theorem,* note further that, we land at an equation which is *formally* equivalent to Eq.(A-27):

$$E_0 = \frac{h^2}{8\pi^2}\int_{\text{space}} \psi_0(\underline{r}_0)\left[\sum_j \frac{\nabla_j^2}{m_{j0}} + \sum_i \frac{\nabla_i^2}{m_{i0}}\right]\psi_0(\underline{r}_0)\,dV = -\frac{h^2}{8\pi^2 g_B^2 M_0 \mathbf{R}_0^2} \ , \qquad \text{(A-27)}$$

.

which yields a *better hint* about g_B.

In the case of the *electronic description of a diatomic molecule,* for instance [cf. Eq.(5) of the text], the expression about g_B^2 reduces to

$$g_B^2 = \frac{1}{\mathcal{R}_0^2 \int_{\text{space}} \psi_e(\underline{r}_0)\left[\sum_i \nabla_i^2\right]\psi_e(\underline{r}_0)\,dV} \;; \qquad \text{(A-28)}$$

here the subscript "$_i$" refers to the i$^{\text{th}}$ electron; recall that $\psi_e(\underline{r}_0)$ is the *wave function* associated with the electronic motion of the molecule in consideration, and $\mathcal{R}_0$ is the *characteristic length,* i.e. the *average internuclear distance* for a diatomic molecule.

A-4. DISCUSSION

Theorem A-1 is well known on the basis of *hydrogen atom. (In fact this is not really an overall mass change one considers, regarding the hydrogen atom framework, but the change of the nucleus proton number.)* Yet presumably, because there was no apparent reason, it was not considered on a *general basis.*

Multiplying *all of the masses,* the object in hand embodies, does not indeed seem to mean much at a *first glance.* However, not only that this *exercise* led us to a *useful relationship (i.e.* $E_0M_0R_0^2 \sim h^2$*),* but also the object, interestingly, undergoes such a *mass transformation* were it brought to a *uniform translational motion,* or were it embedded in a *gravitational field,* or in fact just in *any field* it eventually interacts with.

The relationship we ended up with (Theorem A-3, i.e. the Universal Matter Architecture Cast, shaping, the *"total energy",* the *"size",* and the *"masses"* to be associated with the wave-like object in hand, *in relation with each other,* through h^2), appears to be straightforward on the basis of non-relativistic or even relativistic wave-like descriptions of simple configurations, such as *"electron in the box", "hydrogen atom",* and the *"nucleus"* regarding *"alpha disintegration",* etc. Our approach shows however that the UMA cast ought to hold, for any *"real"* quantum mechanical description *(thus, embodying only Coulomb potential energy terms),* as cumbersome as this may be. We believe the *significance* of this cast, as simple as it may look, has been overlooked, up to our approach.

Our result may still seem somewhat obvious, since one may think he can quickly establish the UMA Cast (Theorem A-3), via a *dimension analysis.* Yet one must keep in mind that *(either through a non-relativistic approach or even through a relativistic approach, it would not matter),* the UMA cast would not occur, if the object considered is not a *"real"* one, though of course, there would still be no problem *dimension-wise.*

Here is a good example which at a first approach shows no feature at all about the UMA Cast: the familiar *expression about the vibrational period of a diatomic molecule,* i.e.

$$T_0 = 2\pi\sqrt{\frac{\mathsf{M}_0}{k_0}}\;, \qquad \text{(A-29)}$$

with T_0 the *inverse of the fundamental vibration frequency* ϖ_0, M_0 the reduced mass of the vibrating molecules, and k_0 the vibration force constant.

Obviously, E_0 and T_0 are related to each other [cf. Eqs.(A-25) and (A-27)]; thus Theorem A-3 should apply for T_0^{-1} replacing E_0, and accordingly h, replacing h^2. After all, Theorem A-3, yields [Eq.17) of the text]

$$T_0 = \frac{4\pi^2}{\sqrt{n_1 n_2}\, h} \sqrt{g M_0 m_e}\, R_0^2 ; \qquad \text{(A-30)}$$

here m_e is the *mass of the electron,* g a *constant* related to the *electronic configuration of the molecule,* thus to g_B [cf. Eq.(A-28)]; n_1 and n_2 are *principal quantum numbers* of electrons making up the bond(s) of the diatomic molecule in hand, and R_0 the ground state *internuclear distance.* We have to keep in mind though due to quantum defects, n_1 and n_2 are not integers. We have in effect figured out that the composite quantum number $n_1 n_2$ is merely R/R_0, for an excited state, where the internnuclear distance, is R., provided that the two states are configured

We would like to note that Eq.(A-30), utimately turns out to be a relationship equivalent to *Bohr's postulate,* i.e. Eq.(A-20) or *more fundamentally,* a relationship equivalent to Eq.(A-19), the *de Broglie relationship,* to be associated with the diatomic molecule of concern, i.e. Eq.(A-24).

It took us, already on the basis of H_2^+ molecule, a whole work to show especially that, Eq.(A-29) can indeed be formulated in harmony with the UMA Cast^2 *(and this, before we could generalize it for the entire body of diatomic molecules).*

Thence, it is not obvious at all that, any *wave-like* object should be structured in accordance with the UMA Cast we disclose.

Note that as seen, the *clock mass* M_0, we referred to, becomes $m_e\sqrt{M_0/m_e}$ for the *vibrational motion of a diatomic molecule.*

Generalization of the UMA Cast for an Object Bearing More than one Motion

Here is *another example* not clearly disclosing the UMA Cast, which will allow us to generalize it for more than one motion the wave-like object may display; this is the expression of the total energy E_0 embodying the vibrational motion together with the rotational motion, displayed by a diatomic molecule, i.e.

$$E_0 = E_{\text{Vibration}} + E_{\text{Rotation}} , \qquad \text{(A-31)}$$

or *(with the definitions given above)*

$$E_0 = (v+\frac{1}{2})h\varpi_0 + J(J+1)\frac{h^2}{8\pi^2\mathsf{M}_0\mathsf{R}_0^2} - \frac{J^2(J+1)^2h^4}{128\pi^6\varpi_0^2(\mathsf{M}_0\mathsf{R}_0^2)^3} \ , \qquad \text{(A-32)}$$

where as usual, v is the *vibrational quantum number,* and J the *rotational quantum* number.[34]

The only term which appears to *match* openly with the UMA Cast, is the second term in the RHS of Eq.(A-32), and this, if we neglect the third one; then indeed

$$E_{\text{Rotation}}\mathsf{M}_0 R_0^2 \cong J(J+1)\frac{h^2}{8\pi^2} \ . \qquad \text{(A-33)}$$

Note however that the first term [in the RHS of Eq.(A-32)], can be rewritten, with the use of Eq.(A-30) as

$$E_{\text{Vibration}}\sqrt{g\mathsf{M}_0 m_e}\,\mathsf{R}_0^2 = (v+\frac{1}{2})\sqrt{n_1n_2}\,\frac{h^2}{4\pi^2} \ . \qquad \text{(A-34)}$$

Thus now this too, agrees well with our Theorem A-3.

Furthermore, we can use Eq.(A-30) once again, to transform the third term of the RHS of Eq.(A-32), i.e.

$$\frac{J^2(J+1)^2h^4}{128\pi^6\varpi_0(\mathsf{M}_0\mathsf{R}_0^2)^3} = \frac{J^2(J+1)^2}{\sqrt{n_1n_2}}\frac{h^2}{32\pi^4\mathsf{M}_0\mathsf{R}_0^2}\frac{gm_e}{\mathsf{M}_0} \ . \qquad \text{(A-35)}$$

With this, we can work out the *rotational energy* [cf. Eq.(A-32)], and check whether it matches with the UMA Cast. It luckily does:

$$E_{\text{Rotation}}\mathsf{M}_0\mathsf{R}_0^2 = J(J+1)\frac{h^2}{8\pi^2} + \frac{J^2(J+1)^2}{\sqrt{n_1n_2}}\frac{h^2}{32\pi^4}\frac{gm_e}{\mathsf{M}_0} \ , \qquad \text{(A-36)}$$

or, indeed

$$E_{\text{Rotation}}\mathsf{M}_0\mathsf{R}_0^2 = J(J+1)\frac{h^2}{8\pi^2}\left[1+\frac{J(J+1)}{\sqrt{n_1n_2}\,4\pi^2}\frac{gm_e}{\mathsf{M}_0}\right] \ . \qquad \text{(A-37)}$$

Therefore this too, comes to approve our Theorem A-3. Note that the second term in the bracket is quite negligible as compared to 1, due to the very small value of the ratio m_e/M_0 *(the electron mass divided by the nuclei reduced mass).*

The above derivation, while disclosing the UMA Cast, further allows us to *immediately* generalize it, in the case where we have a *superposition* of K different *(clock)* motions, each of energy E_{0i}, displayed by the same wave-like clock of *grand total energy,* $E_{0(\text{Grand Total})}$. We call the outcome TheoremA- 4.

Theorem A-4: If $E_{0(\text{Ground Total})}$ is composed of k components, so that

$$E_{0(\text{Grand Total})} = \sum_{k=1}^{K} E_{0k} \quad , \tag{A-38}$$

then each component E_0 can be expressed as

$$E_{0k} = p_k \frac{h^2}{M_{0k} R_{0k}^2} ; \tag{A-39}$$

therefore

$$E_{0(\text{Grand Total})} = \sum_{k=1}^{K} p_k \frac{h^2}{M_{0k} R_{0k}^2} \quad . \tag{A-40}$$

Here M_{0k} is the *clock mass,* R_{0k} the *clock size,* and p_i the appropriate proportionality constant *(including basically a geometry factor and a rather complex quantum number)* to be associated with the kth motion of the wave-like object in hand.

Thus Theorem A-4 in short states that, the previous Theorem A-3 holds separately for each motion, the internal dynamic of the object, may involve.

The Relationship $8\pi^2 g_B^2 m_e r^2 |E| = n_1 n_2 h^2$ holds well Regarding the *Excited Electronic Levels* (E) and the Corresponding *Internuclear Distances* (r) in a Diatomic Molecule, Particularly in H_2 Molecule [35]

The only *basic energy type* we have not specified in this appendix is the *"electronic energy".* Thus we should underline an immediate conclusion of Theorem A-4, in the case of a *diatomic molecule,* particularly, on the basis of the Bohr & Oppenheimer approximation. According to this, *as summarized in the text,* the descriptions regarding the *electronic motion* of the bond on the one hand, and the *nuclei vibrational motion* on the other hand, can be fairly separated from each other.

The resulting Schrödinger equation about the description regarding the *electronic motion* embodies, only the *electron mass;* furthermore the *overall potential energy* input to this equation is made of just *Coulomb potential energy terms,* which makes that this description is a *"real"* one [which is our condition in regards to the validity of Theorem A-3 or Eq.(A-27)].

Thus Eq.(A-27), for the *electronic motion* of the bond in consideration, becomes

$$8\pi^2 g_B^2 m_e r^2 |E| = n_1 n_2 h^2 . \tag{A-41}$$

Here m_e is the *electron mass (here playing the role of the "characteristic mass").* E is the *electronic energy of the molecule in hand, at the given state,* and r the *internuclear distance of the molecule at this state.* n_1 and n_2 *(as explained in the text)* are the *principal quantum numbers* to be associated with the *bond electrons;* more specifically, essentially based on Theorem A-1, $n_1 n_2 = r / r_0$ (cf. Theorem 6 of the text).

Note that g_B^2 of Eq.(A-41), corresponding to what we called g_{IN} at the level of Eq.(10) of the text.

E is negative. But to simplify our notation, below we will call E, *the magnitude of the electronic energy* of concern.

E *(as a positive quantity)* is usually given as

$$E = E_0 - T_e \quad , \tag{A-42}$$

where E_0 is the magnitude of the *ground state electronic energy* of the molecule, and T_e a tabulated quantity.

Eq.(A-42) together with Theorem A-4 becomes

$$T_e = E_0 - \left(\frac{h^2}{8\pi^2 m_e g_B^2} \right) \frac{1}{r r_0} \quad , \tag{A-43}$$

For *electronic states configured like the ground state,* we expect the coefficient g_B to remain practically the same.

Thence the plot of T_e for the states, configured similarly, versus 1/r, should come out as a decreasing *straight line.* The intersection of this with the T_e axis, shall furnish E_0, the *ground state electronic energy,* and the slope in question shall furnish the coefficient g_B.

Note that Eq.(A-43) is valid for any diatomic molecule. We checked its suitability elsewhere, on the basis of H_2, the only molecule providing us with the sufficient amount of data.

Recall further that, Eq.(A-39) can be well written, through a *heuristic approach* based on the *Heisenberg uncertainty principle,* and the *Virial Theorem, yet deveiling not much for the rest.*

Disclosure of the Aged Empirical Relationship, $\varpi R^2 =$ Constant

We would like to recall a *final example* we undertook in the text [cf. Eq.(18)] which, on the contrary to the previous examples, matches in an evident manner with the UMA Cast, but amazingly not notified as such, i.e.

$$\varpi R^2 = \text{Constant}, \tag{A-44}$$

an *approximate empirical relationship* between the *(lowest) vibrational frequency* ϖ and the *internuclear distance* R, established back in 1925, for a given diatomic molecule's electronic states;[8] with indeed no *successful explanation* up to now, the constant is to be determined *(empirically)* for the molecule of interest.

Interestingly enough Eq.(A-44) though, can immediately be deduced from Eq.(A-30) [Eq.(17) of the text]. Thence the *mysterious constant* of 1925, becomes

$$\text{Constant} = \frac{h\sqrt{n_1 n_2}}{4\pi^2 \sqrt{M_0 g m_e}} \quad ; \qquad \text{(A-45)}$$

According to our Theorem A-4, $n_1 n_2$ stays indeed about the same, in regards to the electronic states for which the internuclear distance is not far from R_0 the internuclear distance at the ground state.

Thence through the UMA Cast, we draw *a whole new systematization of diatomic molecules*, and this, in a totally different manner than that we followed in Reference 3.

This should remind us that the UMA Cast, overall, had in effect been no more *visible* than the empirical finding, $\varpi R^2 = \text{Constant}$ is, which again, was left unveiled since 1925. [Note that it turned out to be even harder to identify the RHS of Eq.(A-32) as an UMA Cast.] So, one better not consider it, as trivial as he may think, it now seems.

We should vitally recall that the UMA Cast we disclose is indeed invariant through the occurrences dealt with both the *"special theory of relativity"*, and the *"general theory of relativity"*. That is in fact how *originally* we arrived at it;[1,2,3,4,5] we elaborated on the proposition that, it is this cast that works as the *internal machinery* of the occurrences one observes through the framework of these two fundamental theories, and even more.

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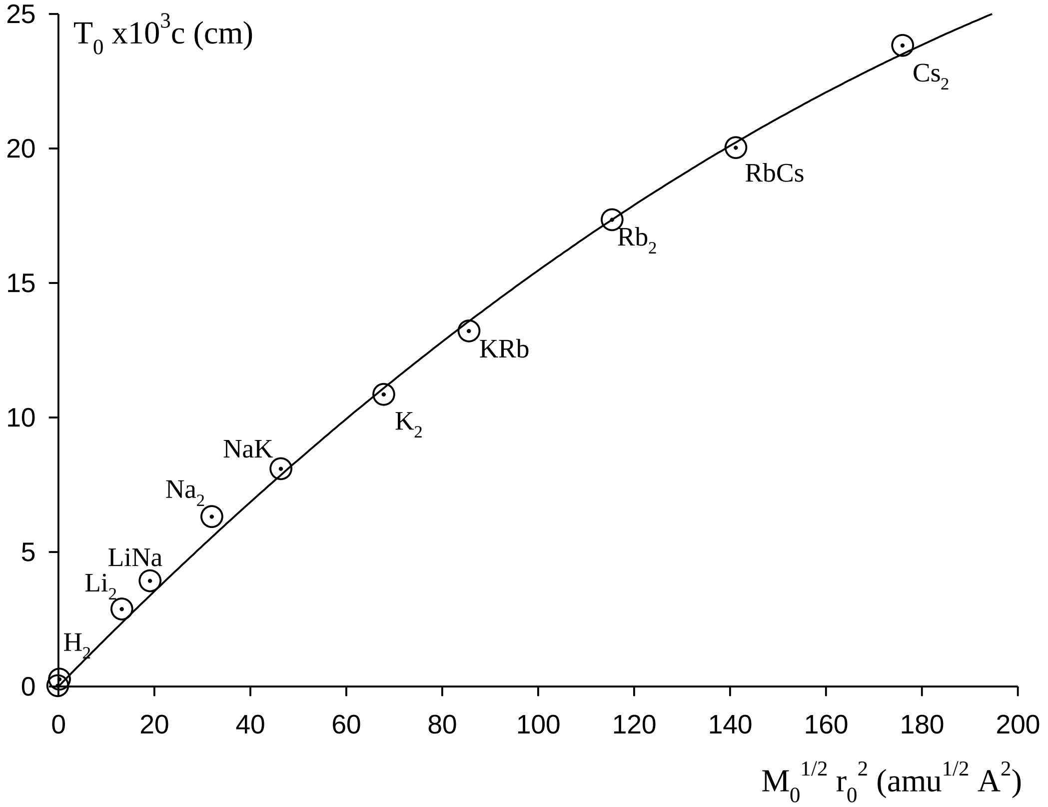

Figure 1 Period of alkali molecules versus $M_0^{1/2} r_0^2$

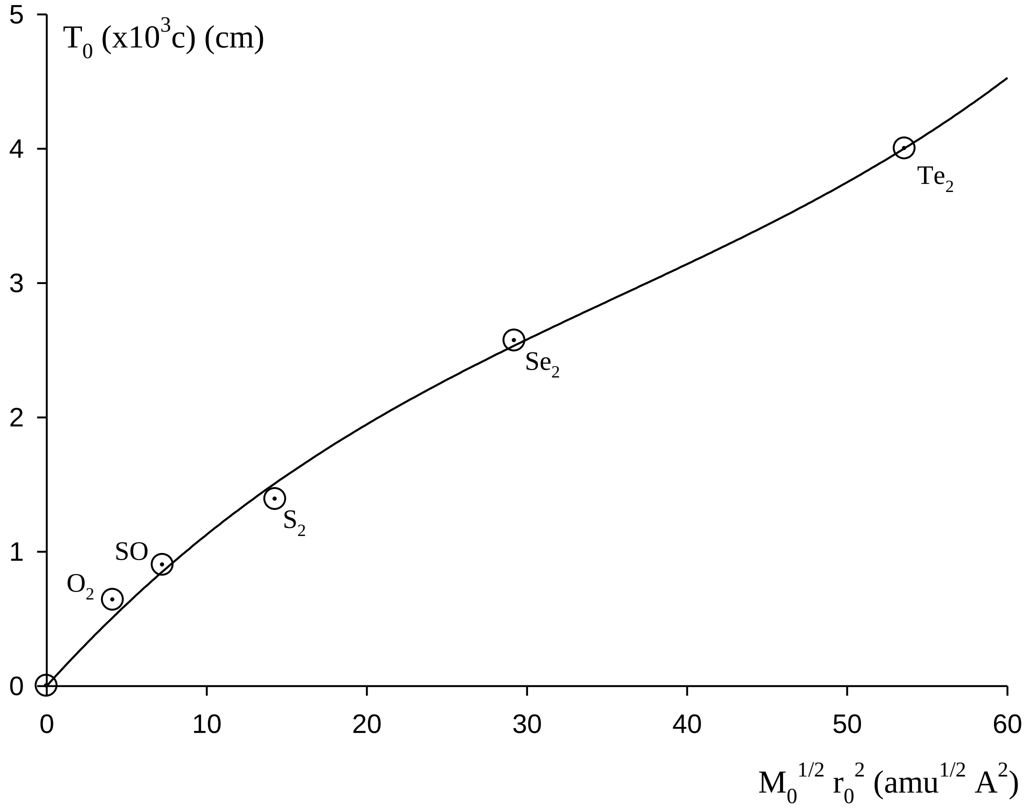

Figure 2 Period of (O_2, S_2, Se_2, Te_2) versus $M_0^{1/2}r_0^{\,2}$

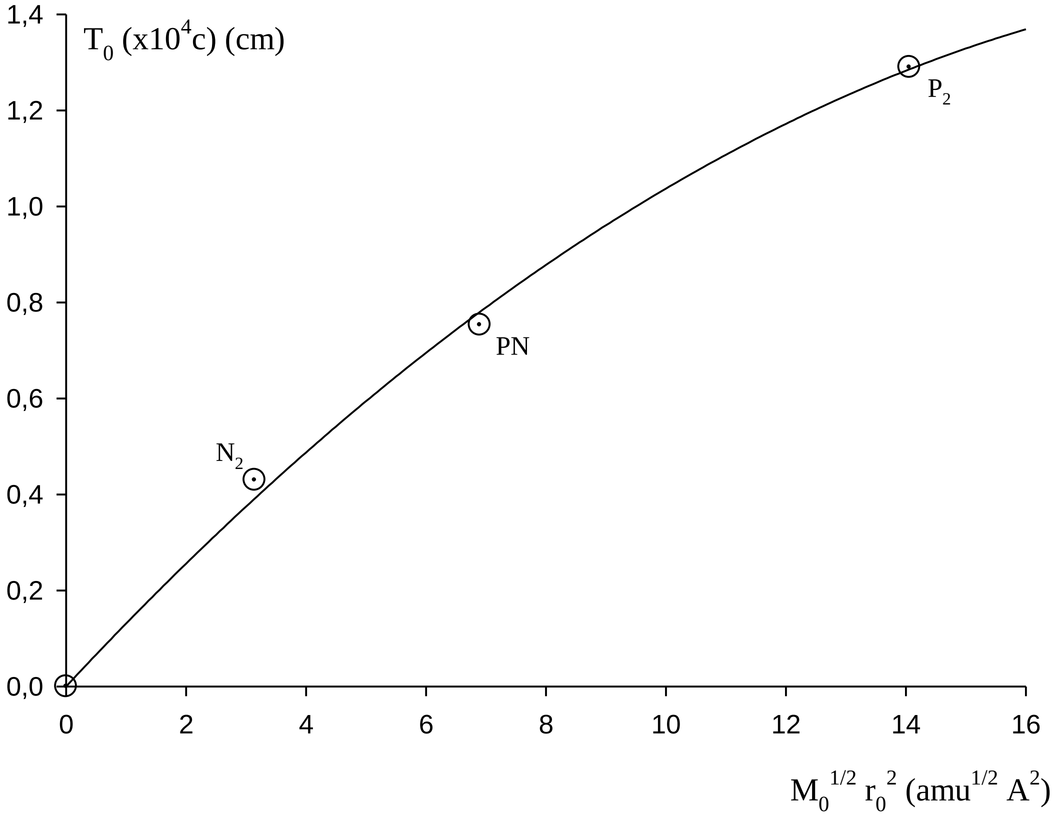

Figure 3 Period of (N_2, PN, P_2) versus $M_0^{1/2}\, r_0^{\ 2}$

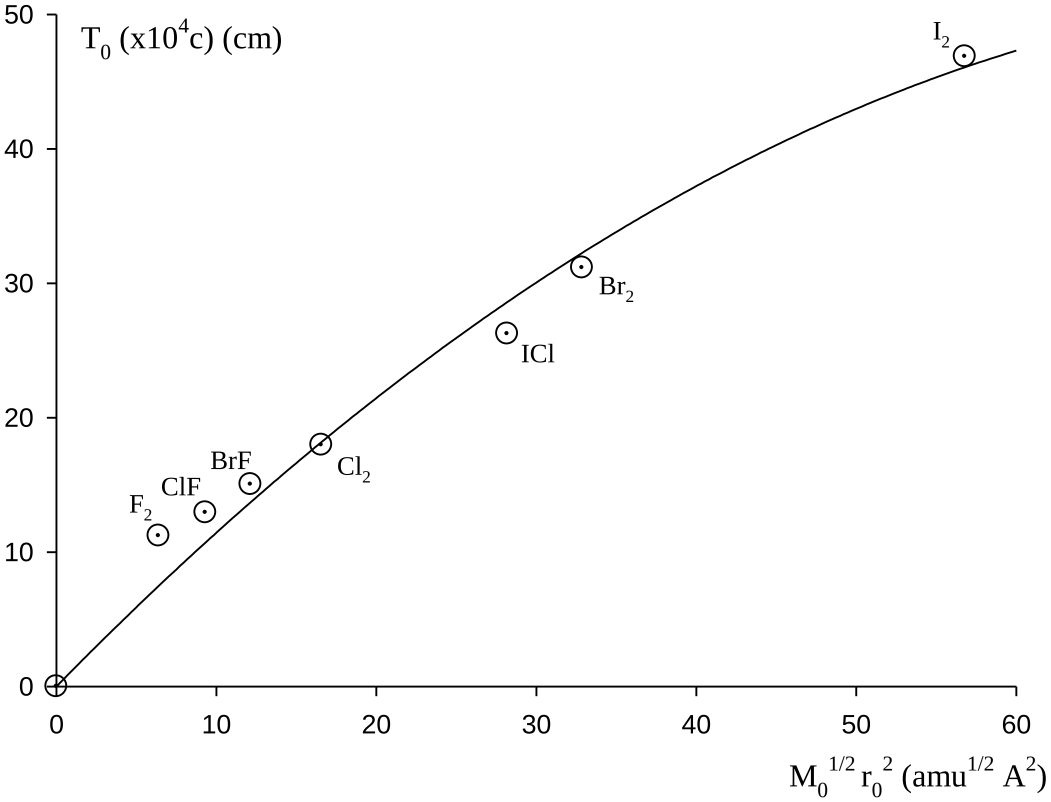

Figure 4 Period of diatomic molecules, made of combinations of halogen atoms, versus $M_0^{1/2} r_0^{\,2}$

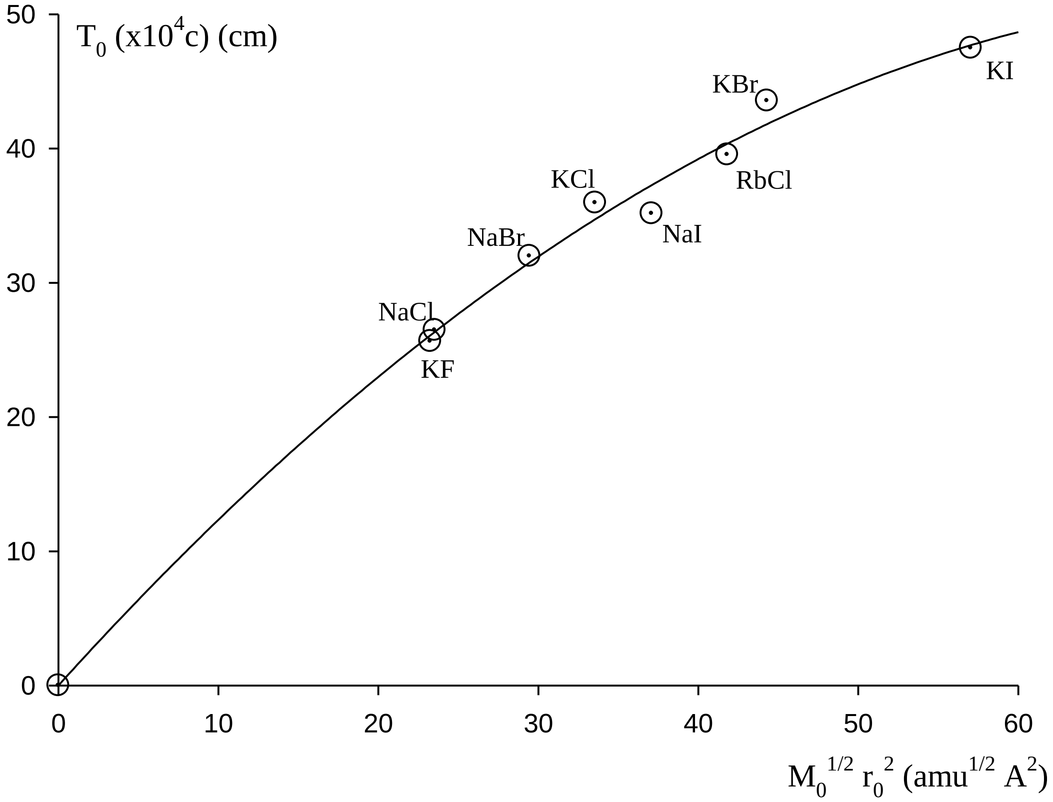

Figure 5 Period of different alkali-halogen molecules versus $M_0^{1/2}$ r_0^2

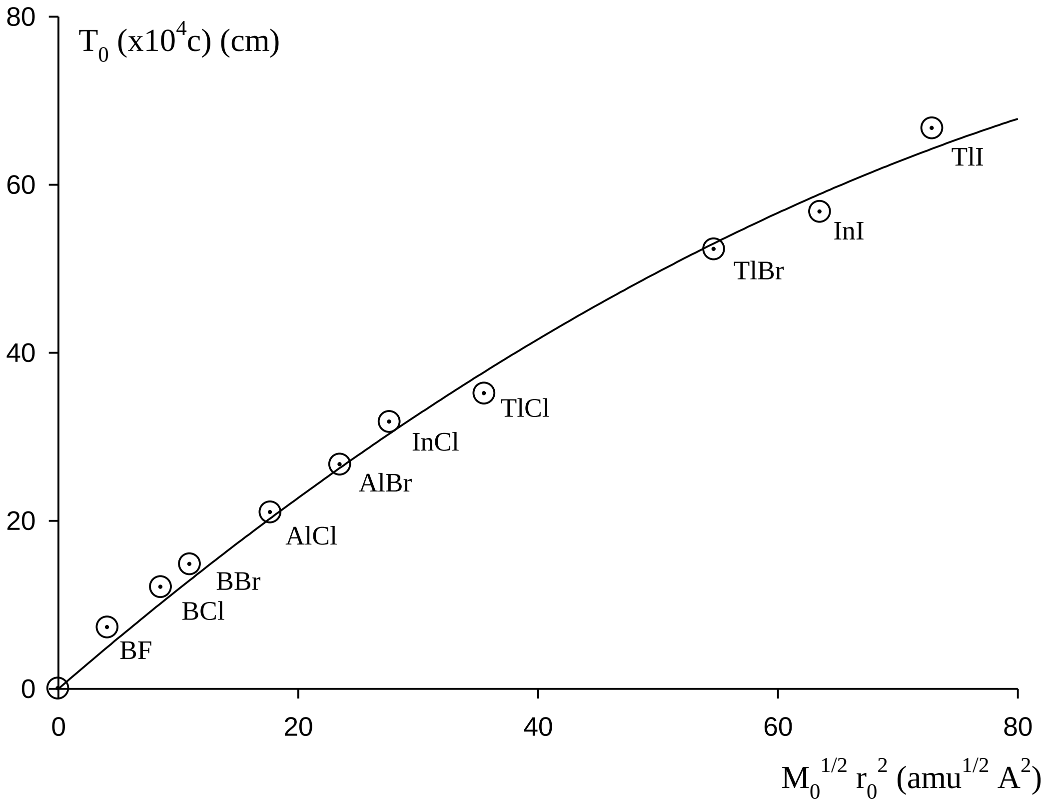

Figure 6 Period of diatomic molecules, made of atoms belonging to respectively the 3th and 7th columns of the periodic table, versus $M_0^{1/2}\ r_0^{\ 2}$

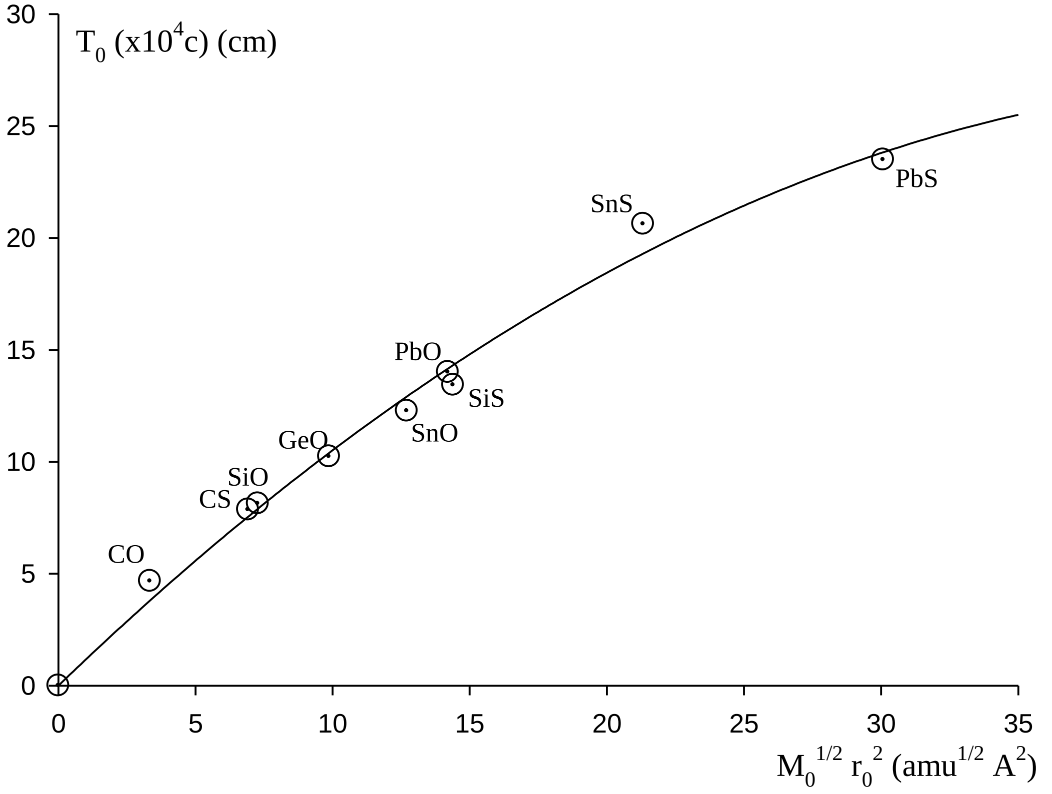

Figure 7 Period of diatomic molecules, made of atoms belonging to respectively the 4th and 6th columns of the periodic table, versus $M_0^{1/2}\, r_0^{\ 2}$

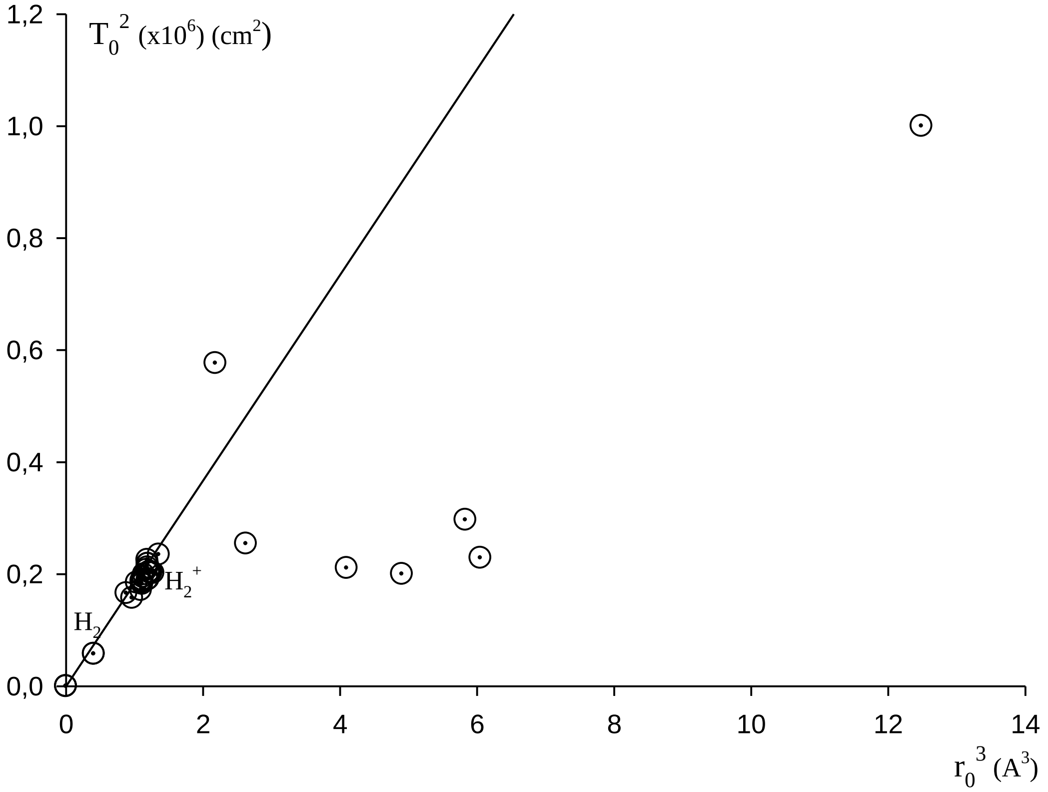

Figure 8 [Vibrational Period]^2 versus [Internuclear Distance]^3 for Different Electronic States of H_2 molecule

(The states corresponding to experimental data *off the straight line* have been identified to be configured like the *ground states* of respectively, alkali hydrides and Li_2)

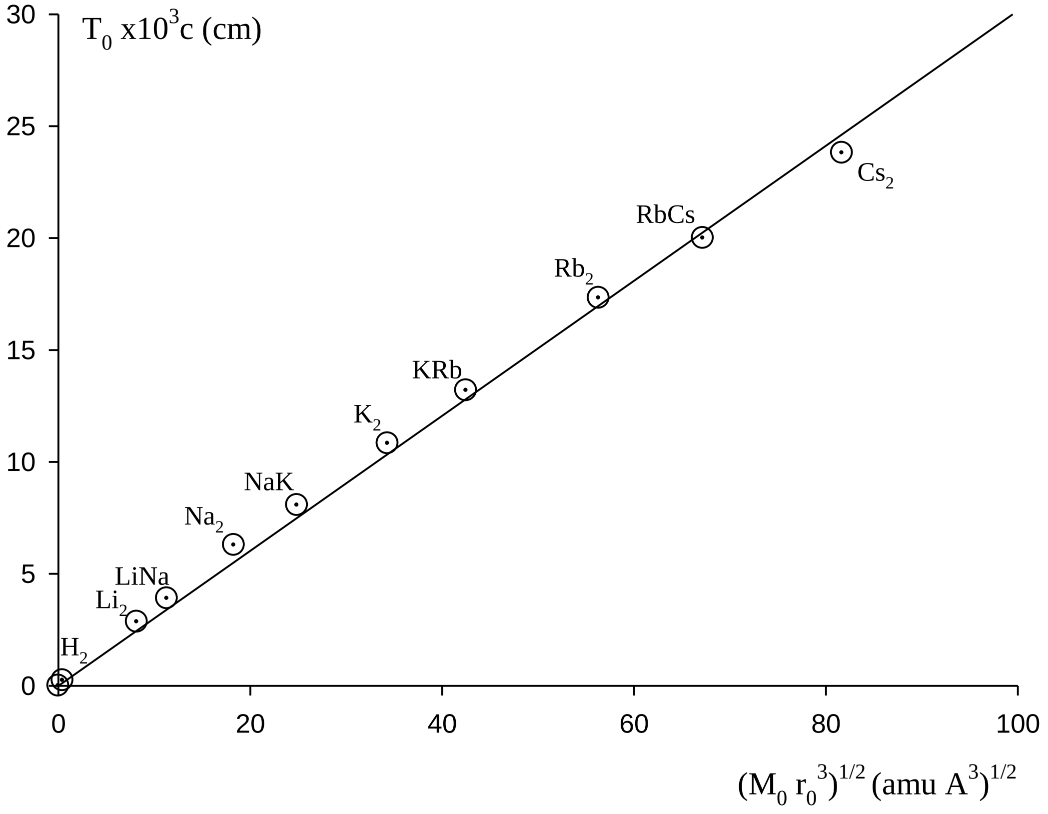

Figure 9 Period of alkali molecules versus $(M_0\ r_0^3)^{1/2}$

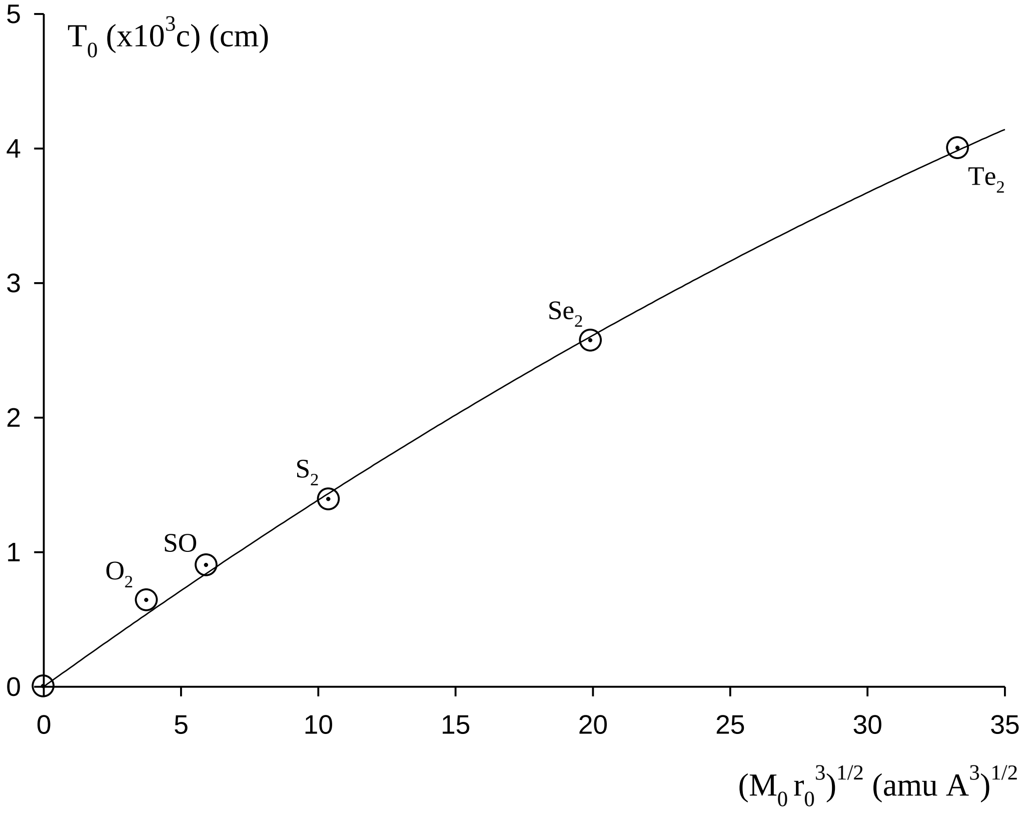

Figure 10 Period of (O_2, S_2, Se_2, Te_2) versus $(M_0 r_0^3)^{1/2}$

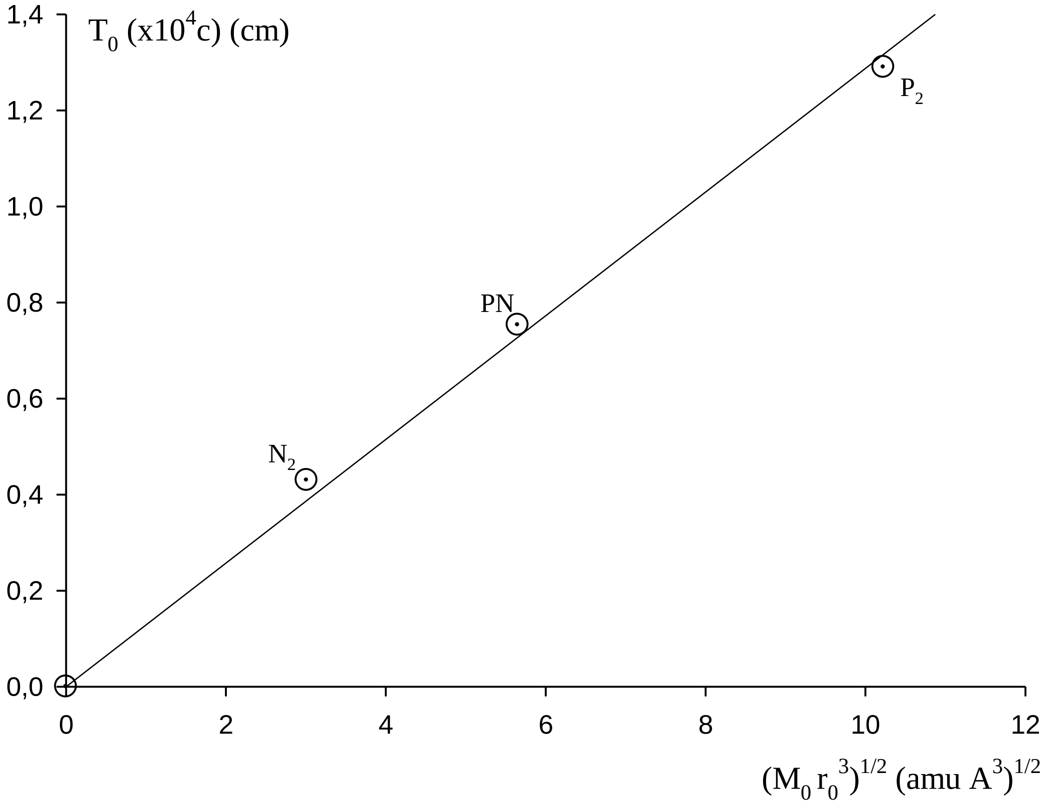

Figure 11 Period of (N_2, PN, P_2) versus $(M_0 r_0^3)^{1/2}$

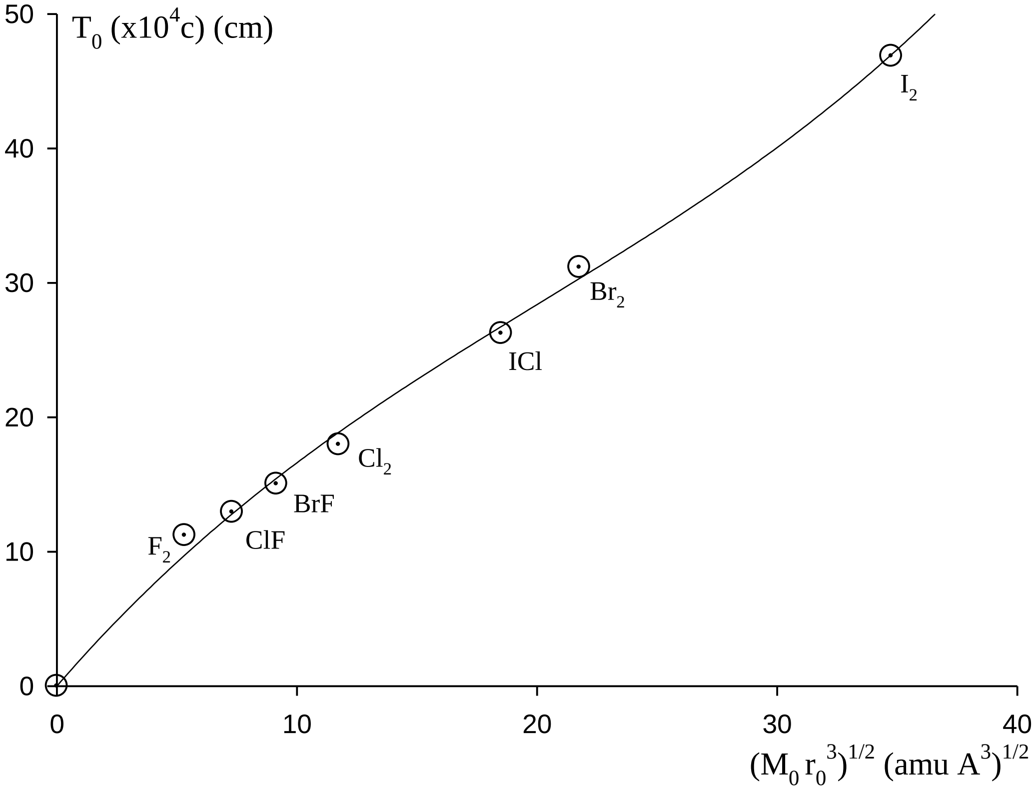

Figure 12 Period of diatomic molecules, made of combinations of halogen atoms, versus $(M_0 r_0^3)^{1/2}$

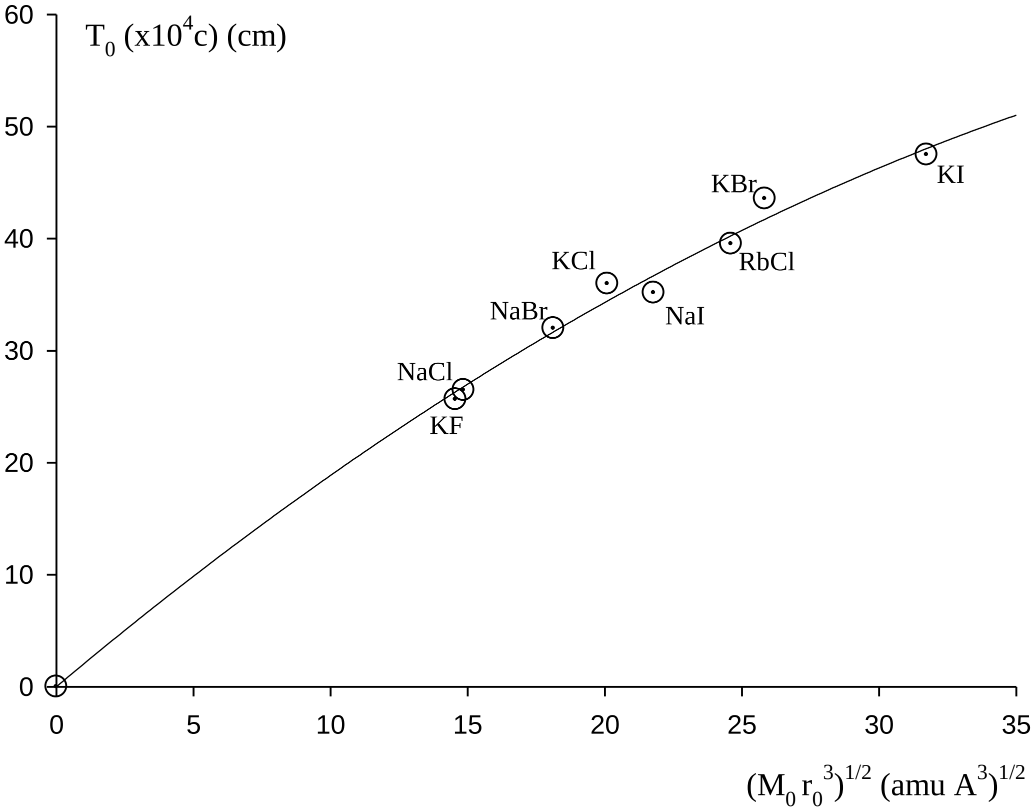

Figure 13 Period of different alkali-halogen molecules versus $(M_0 r_0^3)^{1/2}$

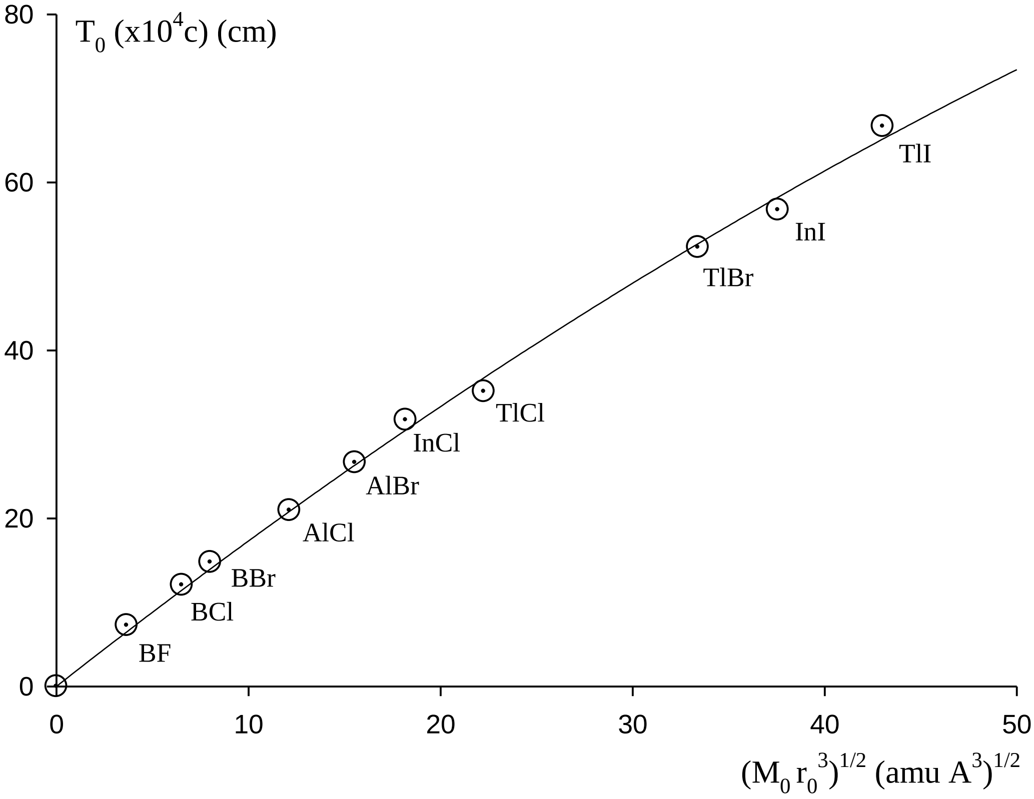

Figure 14 Period of diatomic molecules, made of atoms belonging to respectively the 3th and 7th columns of the periodic table, versus $(M_0 r_0^3)^{1/2}$

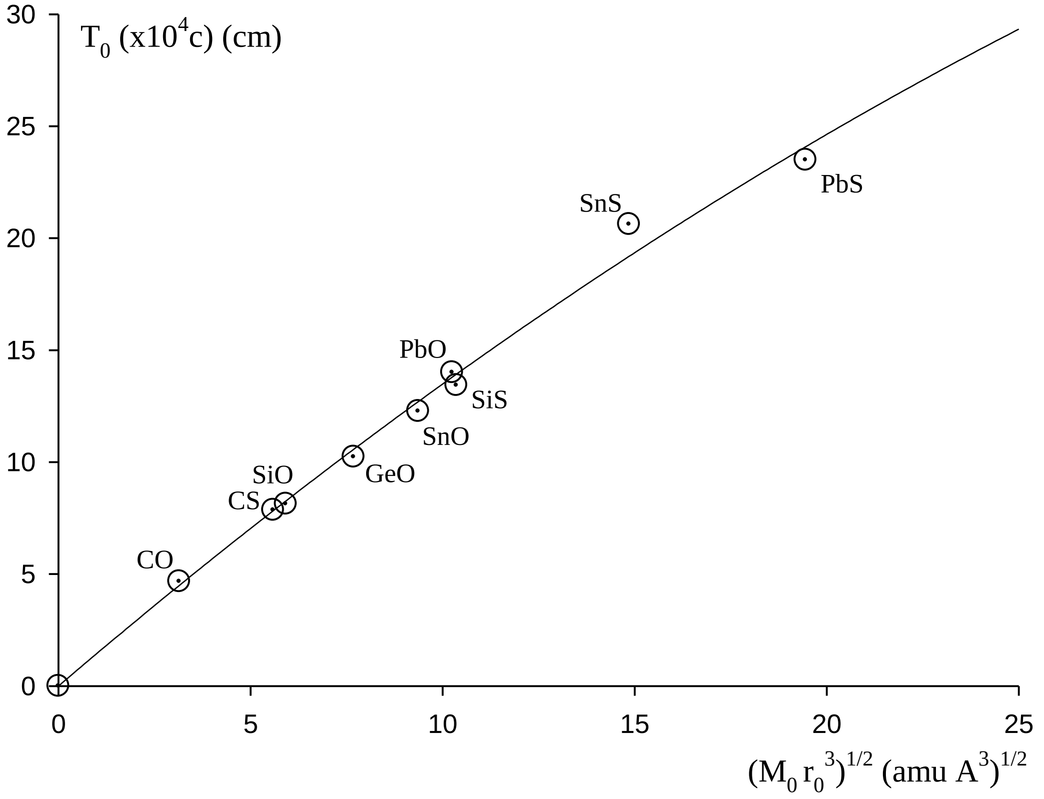

Figure 15 Period of diatomic molecules, made of atoms belonging to respectively the 4th and 6th columns of the periodic table, versus $(M_0 r_0^3)^{1/2}$

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