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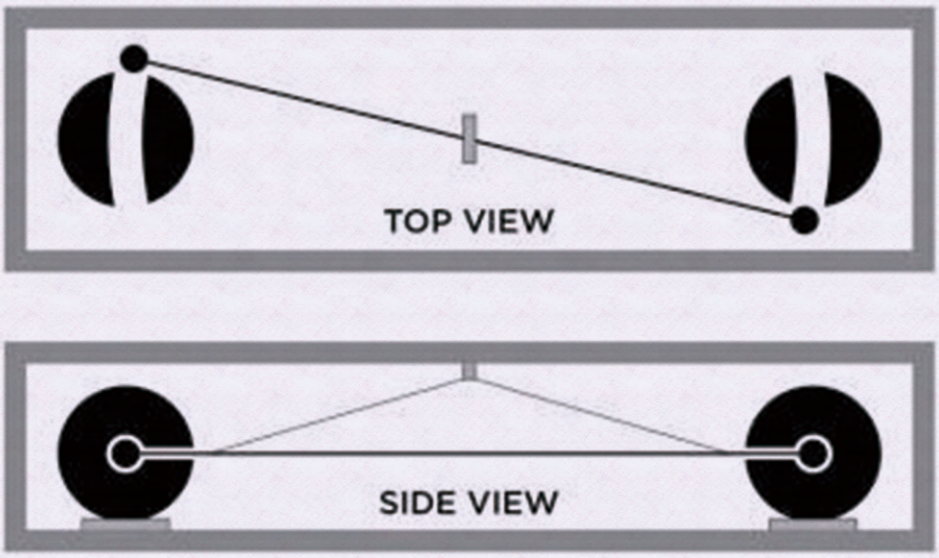


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# An Axion Interpretation of the ANITA Events

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## Abstract

We suggest that the unusual events observed by the ANITA experiment originate from axion particles traversing the Earth. Under the influence of the geomagnetic field, the axion may oscillate into a photon and vice-versa. To amplify the axion transition into photon, we consider that the phenomenon takes place at resonance, where the effective photon mass is equal to the axion mass. This requirement fixes the axion mass at 44 eV. An axion at this mass scale reproduces the cold dark matter scenario. If our interpretation prevails, with the help of axions we can establish an axion tomography of the Earth.

## Keywords

Axion, Axion-Photon Interaction, Earth's Magnetic Field, Cosmology, Dark Matter, Multimessenger Astronomy

## 1. Introduction

The Antarctic Impulsive Transient Antenna (ANITA) experiment has observed two air shower events with energy ~500 PeV emerging from the Earth with exit angles ~30˚ above the horizon [1] [2]. The steep arrival angle implies that the candidate particle propagates a distance inside the Earth of the order of the Earth's radius $R_E$ (6371 km).

One might think the neutrino lies at the origin of the ANITA unusual events. The neutrinos interact with the nucleons through the weak charged current, resulting in absorption, and the weak neutral current, which implies a redistribution of the neutrino energy. For a detailed analysis see [3], where a Mellin transform of the neutrino transport equation provides the shadowing factor of ultra-high high energy neutrinos. The neutrino-nucleon cross-section rises with energy and at energies above a few TeV, the Earth is becoming opaque to neutrinos. The option of a $\tau$ lepton decay, generated from a $\tau$ neutrino, is disfavored also when we take into consideration the SM cross-sections [1]. We are engaged then

to search for a solution next or beyond the Standard Model. In the present work, we examine the prospect that the axion particle might serve this purpose.

## 2. The Axion Proposal

Let us recall that the raison d'être of the axion particle is the strong CP problem. The QCD Lagrangian respects all symmetries (P, C, CP…). At low energies, the non-linear nature of the theory introduces a non-trivial vacuum which violates the CP symmetry. The CP-violating term is parameterized by $\theta$ and experimental bounds indicate that $\theta < 10^{-9}$. This is a very small number, and the smallness of this parameter creates what is known as the strong CP problem. An elegant solution has been offered by Peccei-Quinn [4]. A global $U(1)_{PQ}$ symmetry is introduced, the spontaneous breaking of which provides the cancellation of the $\theta$-term. As a byproduct, we obtain the axion field, the Nambu-Goldstone boson of the broken $U(1)_{PQ}$ symmetry. There are extensive reviews covering the theoretical aspects and the experimental searches for the axion [5] [6] [7].

A general feature of the axion is its two-photon coupling

$$L_{a_{\gamma\gamma}} = -\frac{1}{4} gaF_{\mu\nu}\tilde{F}^{\mu\nu} = ga\vec{E}\cdot\vec{B} \tag{1}$$

where $a$ is the axion field, $F_{\mu\nu}\left(\tilde{F}^{\mu\nu}\right)$ the (dual) electromagnetic field strength tensor and $g$ the photon-axion coupling constant. Accordingly, in the presence of a magnetic field $\vec{B}$, a photon may oscillate into an axion and vice-versa. A prototype experiment in the search for solar axions is the CAST experiment, which set the limit $g < 10^{-10}$ GeV$^{-1}$ [8] [9]. The CAST experiment involves a magnetic field $B = 9$ T and a magnetized region $L = 9.3$ m. Therefore, the relevant scale $(BL)^2$ is $(BL)^2 \approx 7000$ T$^2$m$^2$. Our proposal involves Earth's magnetic field, a magnetic dipole with a mean value $B_0 \approx 3\times10^{-5}$ T on the Earth's surface. The weakness of the geomagnetic field $B$ is compensated by the larger $L$ value, of the order of Earth's radius $R_E$. Therefore, in our case, the scale is $(BL)^2 \approx 36{,}100$ T$^2$m$^2$. This increased value allows a higher accuracy and the exploration of a new range of $g$ and $m_a$ (coupling constant and axion mass respectively) [10] [11].

## 3. Calculation and Results

Consider a travelling photon of energy $E$ and let us define as $z$-axis the direction of photon's propagation. The polarization of the photon $\vec{A}$ lies then at the $x$-$y$ plane. The photon is moving in the presence of the geomagnetic field $\vec{B}$. The component of $\vec{B}$ parallel to the direction of motion does not induce photon-axion mixing. Following Equation (1), the transverse magnetic field $\vec{B}_T$ couples to $A_{\parallel}$, the photon polarization parallel to $\vec{B}_T$ and decouples from $A_{\perp}$, the photon polarization orthogonal to $\vec{B}_T$. The photon-axion mixing is governed by the following equation:

$$\left(E - i\partial_z + \boldsymbol{M}\right)\begin{pmatrix} A_{\parallel} \\ a \end{pmatrix} = 0 \tag{2}$$

The 2-dimensional matrix $\boldsymbol{M}$ is

$$\boldsymbol{M} = \begin{pmatrix} -\frac{m_\gamma^2}{2E} & \frac{gB_\mathrm{T}}{2} \\ \frac{gB_\mathrm{T}}{2} & -\frac{m_a^2}{2E} \end{pmatrix} \tag{3}$$

For a photon, moving in a medium with number density of electrons $N_e$, the effective photon mass $m_\gamma$ is given by

$$m_\gamma^2 = \frac{4\pi\alpha N_e}{m_e} \tag{4}$$

Assuming that Earth's material contains an equal number of protons and neutrons, we obtain the estimate [12] [13]

$$N_e \sim \rho/(2m_N) \tag{5}$$

Therefore

$$m_\gamma^2 = \frac{2\pi\alpha}{m_e m_N}\rho \tag{6}$$

The density of the Earth as a function of the distance is rather well known and very close to the two-density model description, in which the core and the mantle each have a separate and constant energy [14]. We take the core of the Earth to be a sphere whose radius is $R_2$ = 3490 km and whose constant density is 11.0 g/cm$^3$. The mantle, a spherically symmetric shell of constant density 4.4 g/cm$^3$, surrounds the core and extends out to $R_E$ = 6371 km. For a nadir angle ~60˚, our particle crosses the Earth at a distance 5517 km far from the center, traversing a distance of 6371 km within the Earth. Moving entirely within the mantle, $\rho$ = 4.4 g/cm$^3$ and the effective photon mass is $m_\gamma$ ~44 eV.

Matrix $\boldsymbol{M}$ is diagonalized through the angle Θ with

$$\tan 2\Theta = \frac{2gB_\mathrm{T}E}{m_a^2 - m_\gamma^2} \tag{8}$$

Defining

$$D = \frac{1}{2E}\left[\left(m_a^2 - m_\gamma^2\right)^2 + 4g^2B_\mathrm{T}^2E^2\right]^{1/2} \tag{9}$$

$$\sin 2\Theta = \frac{gB_\mathrm{T}}{D} \tag{10}$$

we obtain for the probability that an axion converts into a photon after travelling a distance $s$

$$P(a \to \gamma) = \sin^2 2\Theta \ \sin^2 \frac{Ds}{2} \tag{11}$$

A resonance phenomenon occurs, offering the maximum probability, when

$$m_a = m_\gamma \tag{12}$$

We gather that the most favorable value for the axion mass is $m_a$ ~44 eV. Proceeding along these lines we obtain that at resonance and for values of $Ds \ll 1$

$$P(a \to \gamma) = \frac{1}{4} g^2 B_T^2 s^2 \tag{13}$$

Putting the appropriate numbers ($g = 10^{-10}$ GeV$^{-1}$, $B = 3 \times 10^{-5}$ T, $s = R_E$) we obtain

$$P(\alpha \to \gamma) = 10^{-16}. \tag{14}$$

## 4. Conclusions

Let us summarize our findings. We suggest that highly energetic axions traverse the Earth and they are becoming photons under the influence of the geomagnetic field. These photons create the showers observed by ANITA. The photon polarization is parallel to the geomagnetic field in the Antarctica and therefore we expect a strongly horizontally polarized ($H_{pol}$) signal. Indeed this is observed by the ANITA experiments [1] [2]. The proposed mechanism suggests a mass scale for the axion at 44 eV. The physical properties of the QCD axion are to large extent determined by the scale $f_a$ of the PQ symmetry breaking, similar to how the low energy pion interactions are fixed by the pion decay constant $f_\pi$. Next to QCD interactions, we should include the electroweak interactions and also the gravitational interactions [15]. Thus, the obtained mass scale of 44 eV is not unnatural. A proposed experiment [16] is dedicated to explore axions in a mass range around several eV. What is most interesting is that our axion can solve also the dark matter issue. Cosmological N-body simulations with dark matter indicate that an axion with a mass around a hundred eV will provide power spectra almost indistinguishable from ΛCDM [17] [18]. Thus two problems disappear with a single suggestion.

One might wonder what the origin of these energetic axions is. We can imagine that the inverse phenomenon takes place at gigantic extragalactic scale. VHE photons in the presence of magnetic fields at their source suffer conversion into axions, thus avoiding absorption by $\gamma\gamma$ collisions on the extragalactic background light. Through this mechanism, we obtain a spectrum of "hard" axions [19]. These axions may reach our planet. If our model prevails, then these axions crossing the Earth may be useful in order to establish an axion tomography of the Earth. Notice that a neutrino tomography of the Earth has been already achieved [12] [13] [20]. On the other hand, a fraction of these axions may be converted into photons in the Milky Way. These VHE photons should be of prime interest to the CTA experiment [21]. A multimessenger exploration of space and particle physics is opened.

There are other proposals to address the unusual ANITA events. It has been suggested that an axion pulse is transformed into an electromagnetic pulse in Earth's ionosphere [22]. Subsequently, the down-going radio wave is reflected in the Antarctic ice, giving rise to the peculiar events. In another direction, a supersymmetric interpretation has been advanced to explain the ANITA events [23]. Clearly, we need more data to unravel the underlying mechanism.

**Note Added:** Our work was followed by the findings of the XENON1T expe-

riment (https://arxiv.org/pdf/2006.09721.pdf) reporting an excess of events, attributed most probably to axions.

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## Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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# The Primordial Principle of Self-Interaction

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## Abstract

The Standard Model of Particle Physics treats four fields—the gravitational, electromagnetic, weak and strong fields. These fields are assumed to converge to a single field at the big bang, but the theory has failed to produce this convergence. Our theory proposes *one* primordial field and analyzes the evolution of this field. The key assumption is that *only* the primordial field exists—if any change is to occur, it must be based upon self-interaction, as there is nothing other than the field itself to interact with. This can be formalized as the *Principle of Self-interaction* and the consequences explored. I show that this leads to the linearized Einstein field equations and discuss the key ontological implications of the theory.

## Keywords

Self-Interaction, Principles of Physics, Electromagnetism, Gravitomagnetism, "Weak Field" Approximation, Kasner Metric, Iterated Solutions, Gauge Theory of Gravity, Primordial Principle

## 1. Introduction

Newton, in his analysis of gravity, concluded that it made no sense to imagine a truly empty vacuum with nothing in it; something must be there, to transmit force from one place to another. This "something" is the gravitational field. Later Einstein reached the same conclusion [1]: "*there is no such thing as an empty space, i.e., a space without a field. Spacetime does not claim existence on its own, but only as a structural quality of the field… there exists no space 'empty of field'*". Einstein thus conceived of physical reality as a field.

The concept of field evolved from Faraday to Maxwell to Hertz [2]; then Heaviside [3] extended Newton's gravitation field in analogy with the electromagnetic field. Einstein's nonlinear gravity can be linearized to produce Heaviside's equations and the gravitational waves implied by these equations have been de-

tected [4]. Contributors to quantum field theory assigned a gauge theory to every fundamental particle such that Feynman incorporated gravity as the 31st field [5]. Eventually, Susskind [6] claimed the equivalent of up to 500 fields account for the multiverse.

The current status of gravitational field theory is marked by two questions. The Standard Model poses that electromagnetic, gravitomagnetic, weak and strong fields converge at the big bang, yet this convergence fails without supersymmetry, which has effectively been eliminated at the LHC [7]. This suggests new approaches be explored. The other question, posed by Will and Poisson [8], concerns the "*unreasonable effectiveness*" of the weak field approximation. This paper directly addresses this question.

The plan of this paper is as follows:

**Section 1**, the Introduction, traces the history of fields in physics and discusses the failure of convergence to a primordial field.

**Section 2**, the *Principle of Self-interaction*, introduces the concept of primordial field as the original entity that existed or came into existence "*in the beginning*". As nothing else existed, any physical interaction could only be with the primordial field itself. Based on this formulation of physics, I propose a "change operator", acting on the field and represent the change as the field acting on itself. This yields the *self-interaction equation*. I then solve this equation for a scalar aspect of the field and interpret this scalar as *time*, in which case the solution has a frequency property. I then consider a vector field aspect and formulate a vector equation.

**Section 3** treats "*contact with Newton's equation*" as a means of linking the symbolic formulation of self-interaction to physical reality. We find that Newton's equation of gravity can be derived from the *self-interaction equation*, and compare the primordial self-interaction to the interaction between separate entities.

**Section 4** introduces Hestenes' *Geometric Calculus* as the most appropriate mathematical formalism for physics, based on the fact that every geometric algebra entity has both an algebraic interpretation *and* a geometric interpretation. In addition, Geometric Calculus deals with multi-vectors composed of different types of entities. For example, we found a scalar solution and a vector solution to the self-interaction equation; therefore we combine both solutions into a multi-vector representation. The *geometric product* of two vectors is introduced as the fundamental operation and the *dual* operator, $i$, is also introduced. The self-interaction equation is redefined in the Geometric Calculus formalism.

**Section 5** expands the redefined self-interaction equation in terms of the fundamental constituents introduced in section 4, and then the expansion of the equation is regrouped in terms of "like terms" appearing on each side of the equation. This process yields four equations which are presented in terms of the fundamental constituents.

**Section 6** interprets the four equations, derived in section 5, in terms of the associated physics; the result is a set of equations known as the "weak field equa-

tions" of general relativity.

**Section 7** derives the gravitomagnetic wave equations and discusses the recent detection of gravitomagnetic waves.

**Section 8** discusses *momentum* in the primordial field and describes how terms that would seem to cancel mathematically can exist if separated in space. The addition of these terms completes the linearized field equations first derived by Heaviside and later derived from Einstein's general relativistic nonlinear field equations.

**Section 9** discusses the fact that it has been impossible to successfully apply adjunct linear "Lorenz condition" stipulation to Einstein's "generally covariant" formulation of general relativity. The Geometric Calculus is used to formulate the gravitomagnetic gauge field equations and to derive the Lorenz gauge condition.

**Section 10** presents the key finding of the theory of gravity based on the Principle of Self-interaction: the fact that "field strength" does *not* appear in this theory. That distinguishes our linear gravitomagnetic field equations from the equivalent field equations derived from general relativity. Relativists assume that these equations apply only for "weak" gravitational fields, whereas our theory is "*strength-independent*", and applies for all strengths.

**Section 11** discusses the fact that Einstein's nonlinear field equations can be derived iteratively from the linearized field equations we have derived from our theory of the self-interacting primordial field.

**Section 12** presents conclusions and reiterates the "strength-independent" nature of the self-interaction solution, enabling a physical interpretation of the Kasner metric solution of Einstein's equations. Other applications will be treated in future papers. We summarize by emphasizing that self-interaction theory of gravity presents a novel reinterpretation of gravity that addresses current confusions associated with the success of the post-Newtonian approach to relativity.

## 2. The Principle of Self-Interaction

Perhaps the simplest assumption upon which to base a universe is that the universe either existed, or came into existence, as a primordial entity. That is, "*in the beginning*" this primordial entity, and *nothing else*, existed. If nothing else existed, there was nothing to interact with the primordial entity except itself. To be specific we call this entity a physical field.

Our physics tools are generally designed to relate changes in one physical entity to another entity. For example the basic equation

$$\nabla f = s \tag{1}$$

relates change (represented by operator $\nabla$, undefined) in a field (represented by $f$, undefined) to a source $s$. If our primordial field is represented by $f$, and change is represented by mathematical operator $\nabla$, then $s$ does not exist apart from $f$. And change must have occurred if the primordial field evolved to the current state of our universe. Today, changes occur when things "*interact with each other*", but, if *nothing else existed* to interact with the primordial field, any

interaction could only be the field interacting with itself, and we denote this by *ff*. So change based on self-interaction is described by the equation

$$\nabla f = ff \tag{2}$$

This fundamental *Principle of Self-interaction* describes changes in the primordial field *f* as it interacts with itself.

In the following, we assume minimal knowledge of physics, while at the same time we assume knowledge of logic and mathematics, as necessary. As we cannot model the universe based only on two symbols $\nabla$ and *f*, we assume some *aspect* or property *p* of the field and ask how the field changes with respect to this aspect. In other words $\nabla = \partial/\partial p$ where $f = f(p)$. The self-interaction equation becomes:

$$\frac{\partial}{\partial p} f(p) = f(p) f(p). \tag{3}$$

This fundamental equation has solution, $f = -p^{-1}$.

$$\frac{\partial}{\partial p}\left(-p^{-1}\right) = \left(-p^{-1}\right)\left(-p^{-1}\right) \Rightarrow -\left(-p^{-2}\right) = +p^{-2} \tag{4}$$

This implies a scalar property or aspect of the primordial universe. The most fundamental scalar in physics is almost certainly time *t*, therefore we initially identify $p = t$ and $f(t) = -1/t$. The field appears to have a frequency aspect and we postpone interpretation of the $-$ sign. Parameter *t* is cosmological time, the same time everywhere in the universe. It represents a distance (duration in time) from a beginning to the present state. To find a 3-space vector solution to $\nabla f = ff$ we promote $\nabla$ and *f* to $\vec{\nabla}$ and $\vec{f}$ for parameter $\vec{r} = \{x, y, z\}$. The self-interaction equation becomes

$$\vec{\nabla}\vec{f} = \vec{f}\vec{f}. \tag{5}$$

This combination is not well defined in vector calculus, so we expand the meaning of the change operation to project change onto the field, and use the inner product or dot product to represent self-interaction:

$$\vec{\nabla} \cdot \vec{f} = \vec{f} \cdot \vec{f}. \tag{6}$$

Physical fields have energy density proportional to the square of the fields; $\rho_E = \vec{f} \cdot \vec{f} = f^2$. For unity speed of light ($c = 1$) we have mass equivalent density $\rho_m = \rho_E$ and we find $\vec{\nabla} \cdot \vec{f} = \rho_E$.

## 3. Contact with Newton's Gravity

Einstein's general relativity field equations are unphysical differential geometry equations unless, and until, they make contact with Newton's equation; we apply the same criterion to the primordial field equation. Specifically, we write

$$\vec{\nabla} \cdot \vec{G} = \vec{G} \cdot \vec{G}. \tag{7}$$

If we assume that $\vec{f}$ is gravitational field $\vec{G}$, we recall that, unlike the electromagnetic field, the gravitational field energy is negative, as it is necessary to

add energy to free a body captured in a gravity well. Thus energy density $\rho_E$ is negative and (for $c=1$) $\rho_m = \rho_E$ and *the self-interaction equation* becomes

$$\vec{\nabla}\cdot\vec{G} = -\rho_m . \tag{8}$$

If Newton's gravitational constant $g=1$, this is seen to be Newton's equation of the gravitational field. Therefore our primordial field is tentatively identified as the gravitational field. Although it may be assumed that gravity is sourced by mass, Calabi [9] asked: "*Could there be gravity in our universe even if space is vacuum totally devoid of matter*?" His answer, that curvature makes gravity without matter possible, establishes a feasible identification of the primordial field. Let us return to the self-interaction Equation (7). Danforth first showed, [10] circa 2007, that this equation has solution

$$\vec{G}(\vec{r}) = \frac{1}{\vec{r}} \equiv \frac{\vec{r}}{r^2} \quad \text{such that} \quad \vec{G}\cdot\vec{G} = \frac{1}{r^2} = \rho_E \tag{9}$$

We compare this with Newton's force law

$$\vec{F} = -\frac{gmm'}{r^2} = -gmm'\frac{\vec{r}}{r^3} \equiv m'\vec{G}_N \tag{10}$$

describing the force of gravity on test mass $m'$ a distance $r$ from the source of the field, $m$. Let us use unit test mass $m'=1$ and keep $g=1$ and set $\vec{G}_N = \vec{F}/m' = \left(m/r^3\right)\vec{r} = \rho_m\vec{r}$. Although we have suppressed the display of $m'$ and $g$, these constants enter into any dimensional check, so that if Newton's gravitational constant has units $|g| = l^3/mt^2$ we find $\left|\vec{G}_N\right| = |g\rho r| = \left|\frac{l^3}{mt^2}\frac{m}{l^3}\frac{l}{1}\right| = \frac{l}{t^2}$, which correctly has dimensions of acceleration.

In the following, we set Newton's gravitational constant $g=1$. This scalar dimensional constant is always present and has dimensions $|g| = l^3/mt^2$ whether we display it or suppress its display. Similarly, we let test mass $m'=1$ retaining the result shown in Equation (10): $\vec{F} = m'\vec{G}_N$. Thus:

$$\text{Newtonian:} \quad \vec{G}_N = \frac{gm\vec{r}}{r^3} \tag{11}$$

$$\text{Primordial:} \quad \vec{G} = \frac{g\vec{r}}{r^2} \tag{12}$$

If the forces are identical these two equations imply $m=r$. We choose the origin of the gravitational system $(0,0,0)$ to be the center-of-mass and consider the test mass $m'$ to be located at $\vec{r} = (x,y,z) \equiv (r,\theta,\phi)$. In Newtonian problems, the mass $m$ is located at the origin and $m'$ at $\vec{r}$.

We see that the gravitational field derived from Newton's force law has dependence $\vec{G}_N \sim \vec{r}/r^3$ while the solution of the primordial field self-interaction Equation (9) has dependence $\vec{G} \sim \vec{r}/r^2$. How can we explain this difference?

The difference between the gravitational acceleration due to fixed mass $m$, distance $r$ from the test mass $m'$, and a primordial field $\vec{G}$ tested at the same point (see **Figure 1**) is as follows: for mass $m$ all of the mass contributes to the

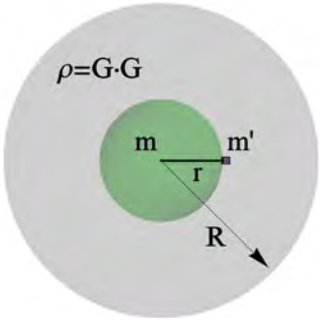


**Figure 1.** Mass $m$ at $\vec{r}$.

field $\vec{G}$ at $\vec{r}$. For the primordial field, assumed spherically symmetric, Birkhoff's *Shell theorem* [11] implies that only the mass density *inside* the sphere of radius $r$ (centered on the origin at the "center of mass") contributes to the field at the test point. Mass $m$ inside the sphere is (modulo $4\pi/3$)

$$m = r^3(\rho) = r^3\left(\vec{G}\cdot\vec{G}\right) = r^3\left(\frac{1}{r^2}\right) = r. \tag{13}$$

This is the result implied by Equations (11) and (12). Thus the Newtonian force on the test mass at $\vec{r}$, due to mass *m inside the sphere*, is

$$\vec{G}_N = \frac{\vec{F}}{m'} = \frac{gm\vec{r}}{r^3} \Rightarrow \frac{gr\vec{r}}{r^3} = \frac{g\vec{r}}{r^2} = G(r), \tag{14}$$

and self-interaction of primordial field at $\vec{r}$ is correctly given by the *self-interaction equation*. In order to derive this result, we modified equation $\vec{\nabla}\vec{f} = \vec{f}\vec{f}$ by specializing in the inner product represented by "$\cdot$". We next generalize our tool-set to solve the unmodified equation.

## 4. Geometric Calculus

Our goal is to create a physical model, or a physical theory of reality, based on minimal knowledge of physics at the time of creation and on the most effective mathematics. As our world has both logical relationships and shapes, the only mathematical field in which every mathematical term has both an algebraic *and* a geometric interpretation is Hestenes' geometric calculus [12], with its fundamental theorem on a smooth $m$-dimensional manifold $M$ with boundary $\partial M$:

$$\int_M \mathrm{d}^m x\,\partial F = \oint_{\partial m} \mathrm{d}^{m-1} x\,F \tag{15}$$

This theorem is compatible with and contains Gauss's theorem, Stokes theorem, Green's theorem, and the Cauchy integral formula, in coordinate-free formalism [13]. The type of geometric algebra entities in a (3 + 1)D universe are *scalar*, *vector*, *bivector*, and *trivector* or *pseudo-scalar*. The fundamental geometric algebra operation, the *geometric product* of two vectors $\vec{u}$ and $\vec{v}$, is:

$$\vec{u}\vec{v} = \vec{u}\cdot\vec{v} + \vec{u}\wedge\vec{v}. \tag{16}$$

The geometric product of two vectors yields a multi-vector consisting of inner product $\vec{u}\cdot\vec{v}$, which is a scalar projecting one vector into the other, and outer

product $\vec{u}\wedge\vec{v}$, which is a bivector, a directed area representing the rotation of $\vec{u}$ into $\vec{v}$. The scalar product is identical to the vector dot product. The bivector can be related to the vector cross product as seen in Figure 2.

$$\vec{u}\wedge\vec{v} = i\vec{u}\times\vec{v} \tag{17}$$

Bivector $\vec{u}\wedge\vec{v}$ is a directed area with no defined shape, while $\vec{u}\times\vec{v}$ is an axial vector, which is *not* included as a vector in vector analysis, but which is required to represent magnetic fields. The term $i$ is the dual operator that transforms cross-product into wedge, as shown, or vice versa: $\vec{u}\times\vec{v} = -i\vec{u}\wedge\vec{v}$. An axial vector can be envisioned as a vector cross product, but its rotational aspect can be represented as a bivector. The negative sign associated with $-t^{-1}$ is interpreted to mean *left-handed* circulation of the local field with rotational frequency $\sim t^{-1}$.

In geometric calculus, as in vector calculus, the derivative operator $\vec{\nabla}$ is viewed as a vector. Therefore the geometric product of $\vec{\nabla}$ with field $\vec{f}$ is as follows

$$\vec{\nabla}\vec{f} = \vec{\nabla}\cdot\vec{f} + \vec{\nabla}\wedge\vec{f}\,. \qquad gradient = divergence + curl \tag{18}$$

This relation *gradient = divergence + curl* is not true in any other mathematical formalism.

Scalar derivative $\partial_t$ operating on scalar function $f(t)$ yields $f(t) = -t^{-1}$ for self-interaction equation $\partial_t f(t) = f(t)f(t)$, while a primordial field with aspects of distance in time and space leads to a directional field $\vec{f}$. If these aspects are separable with respect to time and space, we resolve our field into two primary *subfields*, $\vec{G}(r)$ and $\vec{C}(t)$ and express the primordial field

$$\overline{f} = \vec{G} + i\vec{C} \tag{19}$$

where $\vec{G}(r)$ is a vector and $\vec{\bar{C}}(t)$ is a bivector formed by the dual operator $i$ operating on the $\vec{C}(t)$ field vector. The nature of $\vec{G}\sim\vec{r}^{-1}$ and the nature of $\vec{C}\sim -t^{-1}$, where the ~ symbol implies proportionality; scalar constants may be required to match experimental measurement of $\vec{G}(r)$ and $\vec{\bar{C}}(t)$. The overbar denotes a multivector. If $\vec{\nabla}$ is the vector derivative with respect to space, and $\partial_t$ is the scalar derivative with respect to time, then for changes in space and time, we generalize change operator $\overline{\nabla}$ to include both derivatives, and field $\overline{f}$ to include both subfields:

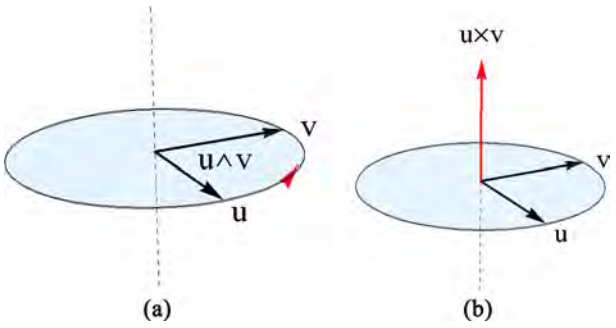


Figure 2. (a) Wedge product; (b) Cross product.

$$\overline{\nabla f} = \overline{ff} \quad \Rightarrow \quad \left(\vec{\nabla} + \partial_t\right)\left(\vec{G} + i\vec{C}\right) = \left(\vec{G} + i\vec{C}\right)\left(\vec{G} + i\vec{C}\right). \tag{20}$$

## 5. Expansion of Primordial Field Equation

$$\left(\vec{\nabla} + \partial_t\right)\left(\vec{G} + i\vec{C}\right) = \left(\vec{G} + i\vec{C}\right)\left(\vec{G} + i\vec{C}\right) \tag{21a}$$

First we multiply out all terms, noting that the dual operator *i* commutes with all vectors.

$$\vec{\nabla}\vec{G} + \partial_t\vec{G} + i\vec{\nabla}\vec{C} + i\partial_t\vec{C} = \vec{G}\vec{G} + i\vec{G}\vec{C} + i\vec{C}\vec{G} - \vec{C}\vec{C} \tag{21b}$$

Next we expand the geometric products on both sides and then group like terms.

$$\begin{aligned} &\vec{\nabla}\cdot\vec{G} + i\vec{\nabla}\times\vec{G} + \partial_t\vec{G} + i\vec{\nabla}\cdot\vec{C} - \vec{\nabla}\times\vec{C} + i\partial_t\vec{C} \\ &= \vec{G}\cdot\vec{G} + i\vec{G}\times\vec{G} + i\vec{G}\cdot\vec{C} - \vec{G}\times\vec{C} + i\vec{C}\cdot\vec{G} - \vec{C}\times\vec{G} - \vec{C}\cdot\vec{C} - i\vec{C}\times\vec{C} \end{aligned} \tag{21c}$$

Observing that a curl of a vector with itself is identically zero we delete terms $\vec{G}\times\vec{G}$ and $\vec{C}\times\vec{C}$. We also note that $\vec{G}\times\vec{C} + \vec{C}\times\vec{G} = 0$. The remaining terms should be grouped by like terms.

$$\vec{\nabla}\cdot\vec{G} + i\vec{\nabla}\times\vec{G} + \partial_t\vec{G} + i\vec{\nabla}\cdot\vec{C} - \vec{\nabla}\times\vec{C} + i\partial_t\vec{C} = \vec{G}\cdot\vec{G} + i\vec{G}\cdot\vec{C} + i\vec{C}\cdot\vec{G} - \vec{C}\cdot\vec{C} \tag{21d}$$

First we group scalars; next scalars multiplied by the dual operator, then vector terms and finally vectors multiplied by *i*. This expansion of the self-interaction equation yields four equations:

$$\vec{\nabla}\cdot\vec{G} = \vec{G}\cdot\vec{G} - \vec{C}\cdot\vec{C} \tag{22a}$$

$$i\vec{\nabla}\cdot\vec{C} = i2\vec{G}\cdot\vec{C} \tag{22b}$$

$$\partial_t\vec{G} - \vec{\nabla}\times\vec{C} = 0 \tag{22c}$$

$$i\vec{\nabla}\times\vec{G} + i\partial_t\vec{C} = 0 \tag{22d}$$

These equations derive from the self-interaction of the primordial field according to our *Self-interaction Principle*, based on the simplest assumptions. They are quite explicit, yet to proceed further we need to make use of what more we know of physical reality. For example, we know that physical fields are *real* and *have energy*. Ohanian and Ruffini state: [14] "*The gravitational field may be regarded as the material medium sought by Newton*; *the field is material because it possesses an energy density*." For example, energy-momentum density of the electromagnetic fields $\vec{E}$ and $\vec{B}$ are given by $E^2 + B^2 + \vec{E}\times\vec{B}$. Therefore we assume that $\vec{G}\cdot\vec{G}$ and $\vec{C}\cdot\vec{C}$ represent energy density, and $\vec{G}\times\vec{C}$ represents momentum density. We know that energy has mass equivalence such that energy density $\rho_E = \rho_m c^2$; if $c = 1$ then $\rho_E = \rho_m$. Additionally, we know that Einstein's general relativity field equations are simply differential geometry until they make contact with real physics in the form of Newton's equation. Therefore we conclude that we too must again make contact with Newton's equation.

## 6. Interpretation of Primordial Field Equation

When we apply our knowledge to the first scalar Equation (22a), we interpret

$\vec{G}$ as the gravitational field and $\vec{G}\cdot\vec{G}$ as the *self-energy density* of the gravitational field. Ignoring the complication of $\vec{C}\cdot\vec{C}$ we have $\vec{\nabla}\cdot\vec{G}=\rho$. Calling on additional information, we know that gravitational energy is *negative* since we must apply *positive* energy to a body captured in a gravitational field in order for it to escape the field, hence the mass density $\rho\sim-\vec{G}\cdot\vec{G}$ and we obtain:

$$\vec{\nabla}\cdot\vec{G}=-\rho \quad \textit{Newton's gravitational equation} \tag{23a}$$

This implies that $\vec{C}\cdot\vec{C}$ has positive energy so that equivalent mass density $-\vec{C}\cdot\vec{C}$ in Equation (22a) contributes correctly to Newton's equation. It has recently been shown that rotational energy in molecules is equivalent to mass [15], therefore the circulational energy of the C-field yields the appropriate sign. In other words, we have derived Newton's equation of the gravitational field from our *Principle of Self-interaction* as required.

Our next interpretation also relies on analogy with the electromagnetic field, where $\vec{E}\cdot\vec{B}=0$, since the fields are orthogonal to each other. Obviously, our C-field is the *gravitomagnetic* field, sometimes called cogravitation [16]. Existence of this field was positively established circa 2011 by the *Gravity Probe B* experiment [17]. If we assume that $\vec{G}\cdot\vec{C}=0$ then Equation (22b) becomes

$$\vec{\nabla}\cdot\vec{C}=0. \tag{23b}$$

Again analogous to $\vec{\nabla}\cdot\vec{B}=0$, this implies that no gravitomagnetic "pole" exists and also that the gravitomagnetic field can be derived from a gauge equation $\vec{C}=\vec{\nabla}\times\vec{A}$ since $\vec{\nabla}\cdot\vec{\nabla}\times\vec{A}\equiv 0$.

We obtained terms $-\vec{C}\times\vec{G}$ and $-\vec{G}\times\vec{C}$. When we add these and note that $\vec{G}\times\vec{C}=-\vec{C}\times\vec{G}$ we initially assume that these terms cancel. We will revisit these terms later. Until then we have:

$$\vec{\nabla}\times\vec{C}=\partial_t\vec{G} \tag{23c}$$

By now it's obvious from the electromagnetic analogy that the last equation is

$$\vec{\nabla}\times\vec{G}=-\partial_t\vec{C} \tag{23d}$$

Grouping these for convenience we obtain:

$$\begin{aligned}&\vec{\nabla}\cdot\vec{G}=-\rho, \qquad &&\vec{\nabla}\times\vec{G}=-\partial_t\vec{C}\\ &\vec{\nabla}\cdot\vec{C}=0, \qquad &&\vec{\nabla}\times\vec{C}=+\partial_t\vec{G}\end{aligned} \tag{24}$$

These equations, derived from the *Self-interaction Principle*, were derived by Oliver Heaviside in 1893, and later from Einstein's relativistic field equations, as the "*weak field equations*".

## 7. Gravitational Wave Equations

The Maxwell-like field equations invite the following procedure, based on the vector identity:

$$\vec{\nabla}\times\left(\vec{\nabla}\times\vec{V}\right)=\vec{\nabla}\left(\vec{\nabla}\cdot\vec{V}\right)-\nabla^2\vec{V}, \tag{25}$$

where the last term can be written $-\vec{\nabla}\cdot\left(\vec{\nabla}\vec{V}\right)$. The first term on the right va-

nishes at all times for $\vec{V}=\vec{C}$ since $\vec{\nabla}\cdot\vec{C}\equiv 0$. For no mass density $\rho=0$, and for minimal field density $\rho\approx 0$, we have $\vec{\nabla}\cdot\vec{G}\approx 0$, leaving the relation $\vec{\nabla}\times\left(\vec{\nabla}\times\vec{V}\right)=-\nabla^2\vec{V}$. Substitute first $\vec{G}$ and then $\vec{C}$ into this identity.

$$\vec{\nabla}\times\left(\vec{\nabla}\times\vec{G}\right)=-\nabla^2\vec{G}\Rightarrow\vec{\nabla}\times\left(-\frac{\partial\vec{C}}{\partial t}\right)=-\frac{\partial}{\partial t}\left(\vec{\nabla}\times\vec{C}\right)\Rightarrow-\frac{\partial^2\vec{G}}{\partial t^2} \tag{26a}$$

$$\vec{\nabla}\times\left(\vec{\nabla}\times\vec{C}\right)=-\nabla^2\vec{C}\Rightarrow\vec{\nabla}\times\left(+\frac{\partial\vec{G}}{\partial t}\right)=+\frac{\partial}{\partial t}\left(\vec{\nabla}\times\vec{G}\right)\Rightarrow-\frac{\partial^2\vec{C}}{\partial t^2} \tag{26b}$$

Summarizing, we have obtained the wave equations

$$-\nabla^2\vec{G}+\frac{\partial^2\vec{G}}{\partial t^2}=0\quad\text{and}\quad-\nabla^2\vec{C}+\frac{\partial^2\vec{C}}{\partial t^2}=0 \tag{27}$$

Dimensional analysis indicates that a velocity-squared term is needed, so we assume $v=1$ and include the symbolic speed in the equation.

$$-\nabla^2\vec{G}+\frac{1}{v^2}\frac{\partial^2\vec{G}}{\partial t^2}=0,\quad-\nabla^2\vec{C}+\frac{1}{v^2}\frac{\partial^2\vec{C}}{\partial t^2}=0 \tag{28}$$

The 2017 [18] detection of inspiralling neutron stars established that the speed of light in an absolute frame, defined by the Cosmic Microwave Background, is the same as the speed of propagation of gravity through the same frame which is pervaded by gravity. Will [19] analyzes the connection between gravity and speed of light by correlating electromagnetic parameters $\mu,\varepsilon$ with Newton's gravitational constant $g$ in terms of $TH\varepsilon\mu$ formalism of Lightman and Lee. We have:

$$c=\frac{1}{\sqrt{\varepsilon_0\mu_0}}\Rightarrow\left[\varepsilon(g)\mu(g)\right]^{-1/2}=\left[\left(\frac{-1}{4\pi g}\right)_{\varepsilon}\left(\frac{-4\pi g}{c^2}\right)_{\mu}\right]^{-1/2}=\left(c^{-2}\right)^{-1/2}=c \tag{29}$$

Since it is now known that velocity $v$ in Equations (28) is equal to the speed of light we observe that the *Principle of Self-interaction* predicts gravitational waves.

## 8. Momentum in the Primordial Field

We now revisit the two terms appearing in the expansion of the *Self-interaction Equation* (21c) which we deleted based on $\vec{G}\times\vec{C}+\vec{C}\times\vec{G}=0$. We did so due to antisymmetry $\vec{G}\times\vec{C}=-\vec{C}\times\vec{G}$. However since $\vec{E}\times\vec{B}$ is the momentum energy density of the electromagnetic field; we interpret $-\vec{C}\times\vec{G}$ as the momentum energy density of the gravitomagnetic field. The energy density has equivalent mass density, and momentum density implies that energy is moving with velocity $\vec{v}$. Hence we rewrite $-\vec{C}\times\vec{G}$ as $-\rho\vec{v}$ and obtain the complete set of Heaviside equations:

$$\begin{aligned}&\vec{\nabla}\cdot\vec{G}=-\rho, &&\vec{\nabla}\times\vec{G}=-\partial_t\vec{C}\\&\vec{\nabla}\cdot\vec{C}=0, &&\vec{\nabla}\times\vec{C}=-\rho\vec{v}+\partial_t\vec{G}\end{aligned} \tag{30}$$

This requires some physical explanation. First, we note that $\vec{G}\times\vec{C}$ cancels $\vec{C}\times\vec{G}$ if they are the same vectors. Based on the significance of the gravitational

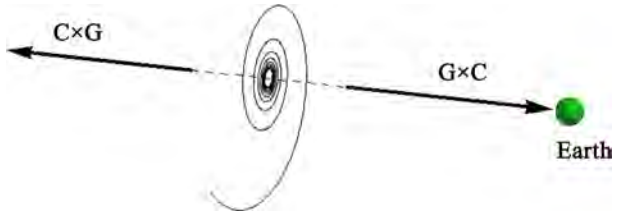


Figure 3. Inspiraling stars.

waves detected from in-spiraling neutron stars, we re-examine this interpretation. Obviously, observed from Earth, the momentum expressed by $\vec{G}\times\vec{C}$ is $\vec{G}(\vec{r})\times\vec{C}(t)$ as symbolized in Figure 3.

But imagine that the earth is positioned at the *far* side of the inspiraling stars. In this case, the momentum vector observed would be $\vec{G}(-\vec{r})\times\vec{C}(t)$ and would have the opposite apparent circulation, changing the sign of the momentum term. The position of Earth is arbitrary, and physics tells us that the inspiraling stars produced gravitational radiation in *both* directions, so we conclude that, instead of canceling, both momentum terms exist, and that is why we include the $\rho\vec{v}$ term in Equation (30). Finally, we generalized from the velocity $v=c$ of the gravitational radiation to encompass subluminal momentum density with $v<c$. Physical reasoning causes us to restore the terms that we originally canceled for mathematical reasons.

## 9. Gauge Field Equations

We anticipate problems with energy-momentum tensors in general relativity; unambiguous gauge fields simply cannot be defined, therefore we will reformulate our field Equation (21) by defining $\rho=\vec{G}\cdot\vec{G}-\vec{C}\cdot\vec{C}$ and $\vec{p}=\rho\vec{v}\sim\vec{G}\times\vec{C}$ where mass density current $\vec{p}$ (momentum density) is the analog of the electromagnetic charge density current $\vec{j}$. The source multivector becomes $\overline{p}=\rho+\vec{p}\equiv\rho(1+\vec{v})$ and the reformulated multivector field equation becomes:

$$\left(\vec{\nabla}+\partial_t\right)\overline{f}=\overline{p}\,. \tag{31}$$

As we have seen, this structure supports the wave operator:

$$\partial_\mu\partial^\mu=\left(\nabla^2-\partial_t^2\right). \tag{32}$$

The following, modeled after Arthur [20] is motivated by Kauffmann's [21] statement that:

> "There is no way to successfully apply adjunct linear "Lorenz condition" stipulation to the Einstein equation when it is presented in the customary "generally covariant" form:
>
> $$G_{\mu\nu}=-\left(8\pi g/c^2\right)T_{\mu\nu}\,. \tag{33}$$

Let us multiply Equation (31) by operator $\left(\vec{\nabla}-\partial_t\right)$ to obtain the sourceless wave equation on the left-hand side and the term $\left(\vec{\nabla}-\partial_t\right)(\rho+\vec{p})$ on the right,

and recall that the scalar and vector potentials of electromagnetism give rise to scalar wave equations with $\rho$ and $\vec{j}$ as multivector source $\overline{j} = \rho + \vec{j}$. Arthur suggests that we find a single wave equation relating the four momentum $\overline{A}$ to $\overline{j}$. Our analogy replaces current density $\vec{j}$ by momentum density $\vec{p}$ to obtain

$$\left(\nabla^2 - \partial_t^2\right)\overline{A} = \overline{p} \tag{34}$$

which, using Equation (31), we rewrite as

$$\left(\vec{\nabla} + \partial_t\right)\left(\vec{\nabla} - \partial_t\right)\overline{A} = \left(\vec{\nabla} + \partial_t\right)\overline{f} \tag{35}$$

This allows us to factor $\left(\vec{\nabla} + \partial_t\right)$ from each side to obtain

$$\overline{f} = \left(\vec{\nabla} - \partial_t\right)\overline{A} + \overline{f}' \tag{36}$$

where $\overline{f}'$ is any solution of the homogeneous (source free) Equation (28); $\left(\vec{\nabla} + \partial_t\right)\overline{f}' = 0$. For simplicity, we choose $\overline{f}' = 0$, and recall that $\left(\nabla^2 - \partial_t^2\right)$ is a scalar. Therefore, if we multiply $\overline{A}$ by a scalar in Equation (34), we see that, since the multivector $\overline{p}$ is a scalar plus a vector, and $\overline{A}$ must have the same form as $\overline{p}$, we must write a multivector

$$\overline{A} = -\phi + \vec{A} \tag{37}$$

which is analogous to the electromagnetic gauge field four-vector. Next expand Equation (36):

$$\overline{f} = \left(\vec{\nabla} - \partial_t\right)\overline{A} = \left(\vec{\nabla} - \partial_t\right)\left(-\phi + \vec{A}\right) \tag{38}$$

$$\vec{G} + i\vec{C} = -\vec{\nabla}\phi + \vec{\nabla}\cdot\vec{A} + \vec{\nabla}\wedge\vec{A} + \partial_t\phi - \partial_t\vec{A}$$

As always, each type of term must satisfy the equation separately; so, matching scalar, vector, and bivector terms, we obtain the following equations:

$$\begin{aligned} 0 &= \partial_t\phi + \vec{\nabla}\cdot\vec{A} \\ \vec{G} &= -\vec{\nabla}\phi - \partial_t\vec{A} \\ i\vec{C} &= \vec{\nabla}\wedge\vec{A} \Leftrightarrow \vec{C} = \vec{\nabla}\times\vec{A} \end{aligned} \tag{39}$$

Since the field $\overline{f}$ has no scalar terms, we set the scalar terms to zero. From Newton's theory, we have $\phi \sim m/r$, thus the gravitational field agrees with Newton plus a gauge term. The last Equation (39c) follows from (23b) $\vec{\nabla}\cdot\vec{C} = 0$. A dimensional analysis performed almost anywhere along the way will suggest that the gauge field $\vec{A}$ has dimensions of velocity $\vec{A} \sim \vec{v}$. In analogy with electromagnetic theory, the product of charge $q$ with gauge field $\vec{A}$ yields electromagnetic momentum $\vec{p}_q = q\vec{A}$, therefore our analogous product of mass with gauge field yields gravitomagnetic gauge field momentum $\vec{p}_m = m\vec{A} \equiv m\vec{v}$. Since this is the momentum in gravitomagnetism, we assume our assignment $\vec{A} \Rightarrow \vec{v}$ is correct. We check this by examining term $-\partial_t\vec{A}$ in Equation (39), where we find that the term represents an acceleration $\partial_t\vec{v}$ that is dimensionally compatible with gravitational acceleration $\vec{G}$.

Finally, scalar Equation (39a) is dimensionally correct, since $\vec{\nabla}\cdot\vec{A} \sim \frac{\partial}{\partial x}\frac{\partial x}{\partial t} \sim \frac{\partial}{\partial t}$. But most significantly, this equation, in electromagnetic field theory is the *Lorenz condition*, and thus we consider this the gravitomagnetic Lorenz condition that is missing in general relativity. Great effort has been expended in relativity to establish an adjunct stipulation of the Lorenz condition $\partial_\mu A^\mu = 0$. Kauffmann substitutes this into the "poster child" of gauge imposition in electromagnetic theory, $\partial_\mu \partial^\mu A^\nu - \partial^\nu \partial_\mu A^\mu = j^\nu$, and simplifies the relation to

$$\partial_\mu \partial^\mu A^\nu = j^\nu . \tag{40}$$

This "stipulation" is equivalent to Equation (34), suggesting that our approach has been correct. In summary, the much desired gravitomagnetic *Lorenz gauge condition* that is still missing from general relativity is obtained rather directly from the *Principle of Self-interaction*.

## 10. Consequences of the Self-Interaction Principle

The key factor concerning our derivation of the Heaviside-Einstein equations (30) is the fact that "field strength" never enters the equation. Our description of the field as "primordial" implies field strengths associated with the big bang, in strong contrast to the century old perception of *weak field approximation*. The *Self-Interaction Principle* replaces the "weak field approximation" with the "all-field equations"—the equations hold for *all* finite strengths of the gravitational field. That is the key lesson to be learned from this theory.

Will observes that "*most of our understanding of gravitational radiation has come from approximations to Einstein's equations*." And Padmanabhan analyzes a Lagrangian for the two body problem in the post-Newtonian approximation and finds that the perihelion precession per orbit "*miraculously matches with the corresponding expression for a test body in the Schwarzschild metric. No simple reason for this conclusion is known and it is an issue worth thinking about*".

The self-interaction theory contradicts this prevailing view by applying to *any* gravitational field, regardless of strength. It addresses Will's statement that "*we have no good understanding of why this approximation to general relativity should be so effective*." Will reviews binary pulsars and inspiralling compact binaries, including black holes, and the surprising *fact that the approximate calculations agree with those of numerical relativity for very strong fields*. He notes no obvious reason to expect weak field equations to work for inspiralling black holes, but they do.

The *Self-Interaction Principle* provides the reason. It is "strength-independent"; it never makes assumptions about "weak field" approximation.

## 11. The Equivalence of Linear and Nonlinear Formulation of Gravitation

The *mass-energy density* approach of field theory is equivalent to Einstein's me-

tric-based theory of *curved space-time*. Although Einstein's metric-based general relativity is by far the most familiar theory of gravity, a number of approaches have formulated gravity as a gauge theory. In 1954, Gupta constructed a theory in which the "source" couples to the massless spin-2 field $h_{\mu\nu}$ as the energy-momentum tensor, *including the energy momentum of the* $h_{\mu\nu}$ *field itself.* The coupling induces a cubic term in the Lagrangian, resulting in a corresponding cubic term ${}^{3}T^{\mu\nu}$ in the energy momentum tensor, which is then included in the source [22]. This in turn generates a quartic term ${}^{4}T^{\mu\nu}$, and so on. This considers the stress-energy carried by the linearized gravitational field, $h_{\mu\nu}$ and *iteratively corrects* for it and then corrects the corrections. This alternate way to derive general relativity has been developed and explored by Gupta (1954), Kraichnan (1955), Thirring (1961), Feynman (1963) Weinberg (1965) and Deser (1970).

The most significant aspect of the gauge approach is that, per Feynman [23]: "*this iterative procedure generates an infinite series that can be summed to yield the full nonlinear Einstein equation*." Similarly, Misner, Thorne and Wheeler [24]: "*Just as one can 'descend' from general relativity to linearized theory by linearizing about flat space time so can one 'bootstrap' one's way back up from linearized theory to general relativity*…". The two formalisms are equivalent.

Although linear equations are transformable into non-linear via iterative analysis, the nonlinear equations did not just "snap into being". As Padmanabhan noted, it is necessary to know *beforehand* that the final field equations have to match with those in Einstein's theory, in order to introduce the extra assumptions to obtain it, but these extra assumptions are essentially equivalent to the result we're attempting to derive! So Einstein's equations did not just fall out of an analysis of gravity; or even *the Equivalence Principle*; many issues still have yet to be resolved. One simply cannot obtain an expression for the energy-momentum tensor for the spin-2 field that is unique and gauge invariant; instead one can obtain a large class of non-unique theories. This has resulted in numerous "Einstein-like" theories, a number of which are finally being eliminated by the real gravitational wave data that is increasingly being detected.

Ohanian and Ruffini observe that "*almost all of the result that had been the subject of experimental investigation can be described by the linear approximation … the deflection of light, the time delay of light, gravitational time dilation, gravitational lensing, and gravitational radiation emerge from the linear approximation*." Recently Will [25] derived a new contribution to Mercury's perihelion advance, based in part on interaction between Mercury's motion and the gravitomagnetic field of moving planets; a contribution 100 times larger than the second-post-Newtonian contribution.

Poisson and Will [26] begin their development of post-Newtonian theory by postulating a form of the metric and ask "*which guiding principle can be invoked to justify the choices made…? The answer is simply that no such principle exists…*" The central theme of their book is "*the physics of weak gravitational*

*fields*." A reason for this approach is that "*no exact solution to Einstein's equation has ever been found that describes a simple double-star system and orbital motion*." Thus the focus on *weak field approximation* is utilitarian of necessity, as they conclude that "*Almost no physically useful exact solutions of the theory* (*of general relativity*) *are known*." Yet "*we have no good understanding of why this approximation to general relativity should be so effective*," since "*neutron stars…have very strong internal gravity*".

In contrast, the *Self-Interaction Principle* makes no field strength assumption, other than the implicit assumption that the strength of the field at the big bang is included in the theory.

## 12. Conclusions

Despite equivalence of the linear formalism to Einstein's nonlinear form, the "weak field approximation" terminology has misled physicists to believe that *real* gravitation is described by space-time curvature corresponding to the nonlinear formalism, although Feynman, Padmanabhan, Weinberg, and others insist that curved spacetime is *not* a necessary conception of gravity.

Familiarity with the Schwarzschild and Kerr metrics convince many that the "proper" theory of gravity is general relativity. Nevertheless, these metric solutions are static; they represent a geometric solution that does not evolve over time, given a fixed mass, *M*. For a *dynamic space-time*, an exact metric solution to Einstein's field equations has existed for over 90 years, yet its interpretation has been "obscure and questionable". This Kasner metric has recently been interpreted [27] in terms of self-interaction equations, and a meaningful physical theory derived.

We have worked from the assumption that our universe evolved from a single primordial field. The corresponding *Principle of Self-interaction* produces the known gravitomagnetic field equations; however, in contrast with the "weak field approximation" assumption, a self-interacting field *remains* self-interacting—it does *not* become *non*-self-interacting due simply to a physicist's deleting nonlinear terms for ease of solution. Therefore the most significant aspect of the derivation of the gravitational field equations from the self-interaction principle is that there is absolutely no mention of field strength. Derivation from the *Principle of Self-interaction* instead yields *all-strength-field-equations* of the gravitational field.

The space-time curvature aspect of gravity is based on an approximate equivalence principle that holds only at a mathematical point. On the other hand, there is another assumed equivalence that some find remarkable; Ohanian and Ruffini state:

> "That the exact nonlinear equations are implied by the linear equations… is a remarkable feature of Einstein's theory."

We restate this as follows:

That Einstein's exact nonlinear equations are implied by our linear equations… is a remarkable feature of the Principle of Self-interaction.

This offers a new ontological understanding of physical reality.

## Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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# Brownian Motion in an External Field Revisited

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## Abstract

In many interesting physical examples, the partition function is divergent, as first pointed out in 1924 by Fermi (for the hydrogen-atom case). Thus, the usual toolbox of statistical mechanics becomes unavailable, notwithstanding the well-known fact that the pertinent system may appear to be in a thermal steady state. We tackle and overcome these difficulties hereby appeal to firmly established but not too well-known mathematical recipes and obtain finite values for a typical divergent partition function, that of a Brownian particle in an external field. This allows not only for calculating thermodynamic observables of interest, but for also instantiating other kinds of statistical mechanics' novelties.

## Keywords

Divergent Partition Functions, Statistical Mechanics, Fisher Information

## 1. Introduction

In many interesting physical examples, the partition function is divergent [1] [2] [3] [4]. Thus, the usual toolbox of statistical mechanics becomes unavailable, notwithstanding the well-known fact that the pertinent system may appear to be in a thermal steady state (see, for instance [5] [6] [7] [8] [9]) and references therein]. Our goal here is to deal with a specific divergent partition function, and obtain a finite value for it. This permits to compute new observables of interest and also to develop some hopefully new statistical mechanics' insights.

## 2. The Central Issue

### 2.1. Partition Function

We will consider here the partition function for Brownian motion in an external

field, given by [4]

$$\mathcal{Z} = \int_{-\infty}^{\infty} \mathrm{e}^{\frac{\beta U_0}{1+x^2}} \mathrm{d}x, \tag{2.1}$$

with $\beta = 1/(k_B T)$ and $k_B$ = Boltzmann's constant. Change now variables to $y = 1 + x^2$. Taking advantage now of well-known features of Schwartz' theory of distributions [10], we can recast the integral that defines $\mathcal{Z}$ in the fashion

$$\mathcal{Z} = \int_1^{\infty} (y-1)^{-\frac{1}{2}} \mathrm{e}^{\frac{\beta U_0}{y}} \mathrm{d}y \equiv \lim_{\nu \to 1} \int_1^{\infty} y^{\nu-1} (y-1)^{-\frac{1}{2}} \mathrm{e}^{\frac{\beta U_0}{y}} \mathrm{d}y, \tag{2.2}$$

and remember that the limit of an integral equals the integral of the limit. We consult then the Table of Ref. [11] and find that our current integral is a special case of the more general one

$$W = \int_u^{\infty} x^{\nu-1} (x-u)^{\mu-1} \mathrm{e}^{\frac{\beta}{x}} \mathrm{d}x = B(1-\mu-\nu, \mu) u^{\mu+\nu-1} \phi\left(1-\mu-\nu; 1-\nu, \frac{\beta}{u}\right). \tag{2.3}$$

Here $B$ is the well-known beta function and $\phi$ the confluent hypergeometric function, that reads, appealing to the Gamma function $\Gamma$,

$$B = \Gamma(1-\mu-\nu)\Gamma(\mu)/\Gamma(1-\nu). \tag{2.4}$$

Comparing integrals, we see at this stage that the right hand side of (2.2) will coincide with $W$ in (2.3) by setting

$$\mu = 1/2; \ \nu = 1; \ u = 1, \tag{2.5}$$

so that these special values are to be inserted in

$$W = \Gamma(1-\mu-\nu)\left[\Gamma(\mu)/\Gamma(1-\nu)\right] u^{\mu+\nu-1} \phi\left(1-\mu-\nu; 1-\nu, \frac{\beta}{u}\right). \tag{2.6}$$

Note also that

$$\Gamma(1/2) = \sqrt{\pi}; \ \Gamma(-1/2) = -2\sqrt{\pi}. \tag{2.7}$$

We have a $\Gamma(0)$ in a denominator now. This induces us to appeal once again to [11] to employ the useful relation

$$\lim_{\gamma \to 0} \phi(\alpha; \gamma; s) = z\alpha\phi(\alpha+1; 2; z), \tag{2.8}$$

so that we can finally arrive at the result

$$\mathcal{Z} = \pi\beta U_0 \phi\left(\frac{1}{2}; 2; \beta U_0\right), \tag{2.9}$$

our desired finite form. We see that we arrive at $\mathcal{Z}$ via a straightforward path. The essential step here is that of consulting an appropriate table of integrals and performing adequate manipulations. Note that at very low temperatures quantum effects raise their head and our treatment becomes invalid. Below it will be shown that one also encounters problems or exceedingly high temperatures. We have found a finite partition function for our Brownian problem and proceed to calculate with it, below, important quantifiers of statistical mechanics.

### 2.2. Units for Our Graphs

We find it convenient to plot our thermal quantities versus $y = k_B T / U_0$ in the range $0 \le y \le 1$. Given the smallness of $k_B$, this encompasses an immense $T$-range, since $k_B$ is of the order of $10^{-23}$ in its appropriate units. In particular, we plot the logarithm of the partition function in **Figure 1**. We appreciate the fact that it converges to a definite value as $T$ grows.

## 3. Other Thermal Quantities

### 3.1. Mean Energy

One has

$$\langle \mathcal{U} \rangle = -\frac{\partial \ln \mathcal{Z}}{\partial \beta}, \tag{3.1}$$

so that

$$\langle \mathcal{U} \rangle = -\frac{1}{\mathcal{Z}}\left[\pi U_0 \phi\left(\frac{1}{2};2;\beta U_0\right) + \frac{\pi \beta U_0^2}{4}\phi\left(\frac{3}{2};3;\beta U_0\right)\right]. \tag{3.2}$$

Note that at very low temperatures quantum effects raise their head and our classical treatment becomes invalid.

### 3.2. Entropy $\mathcal{S}$

We have

$$S = \frac{\partial\left(k_B T \ln Z\right)}{\partial T}, \tag{3.3}$$

so that

$$\mathcal{S} = \ln\left[\pi \beta U_0 \phi\left(\frac{1}{2};2;\beta U_0\right)\right] - \frac{\beta}{\mathcal{Z}}\left[\pi U_0 \phi\left(\frac{1}{2};2;\beta U_0\right) + \frac{\pi \beta U_0^2}{4}\phi\left(\frac{3}{2};3;\beta U_0\right)\right], \tag{3.4}$$

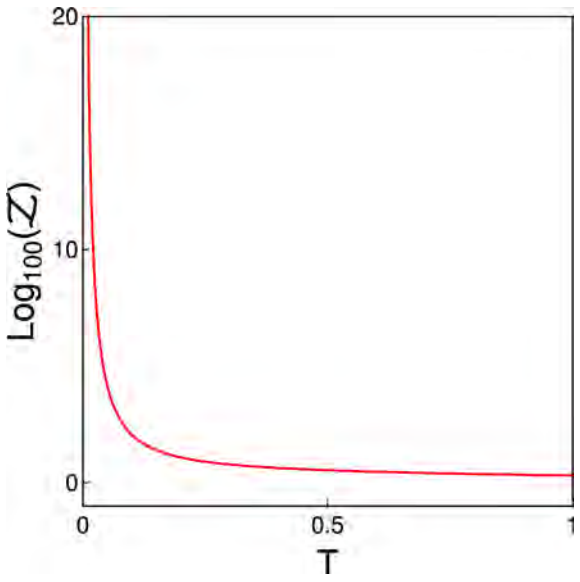


**Figure 1.** Logarithm of the partition function in appropriate units (see text).

that is plotted in Figure 2. Note that at very low temperatures, quantum effects raise their head and our treatment becomes invalid. This is evident whenever $S$ becomes negative at low $T$. A new effect is observed at very large $T$. Whenever $T \geq 10^{22}$, the treatment becomes invalid as well. Such high-$T$ outcome is typical of classical self-gravitating systems [12] [13] [14].

### 3.3. Specific Heat $\mathcal{C}$

One defines it as

$$\mathcal{C} = -\frac{\beta}{T}\frac{\partial \langle \mathcal{U} \rangle}{\partial \beta}, \tag{3.5}$$

so that

$$\begin{aligned}\mathcal{C} = &-\frac{1}{Z^2}\left[\pi U_0 \phi\left(\frac{1}{2};2;\beta U_0\right)+\frac{\pi\beta U_0^2}{4}\phi\left(\frac{3}{2};3;\beta U_0\right)\right]\\ &\times\left[\frac{\pi\beta U_0}{T}\phi\left(\frac{1}{2};2;\beta U_0\right)+\frac{\pi\beta^2 U_0^2}{4T}\phi\left(\frac{3}{2};3;\beta U_0\right)\right]\\ &+\frac{1}{\mathcal{Z}}\left[\frac{\pi\beta U_0^2}{2T}\phi\left(\frac{3}{2};3;\beta U_0\right)+\frac{\pi\beta^2 U_0^3}{8T}\phi\left(\frac{5}{2};4;\beta U_0\right)\right],\end{aligned} \tag{3.6}$$

depicted in Figure 3. Note that at very low temperatures, quantum effects raise their head and our treatment becomes invalid. Thus, the third thermodynamics' law is violated here. Interestingly enough there is a Schottky anomaly. This is an effect typical of solid-state physics: the specific heat at low temperature exhibits a peak. When $T$ is high, the specific heat decreases. A new effect is observed at very large $T$. The specific heat becomes negative. Such outcome is typical of classical self-gravitating systems [12] [13] [15].

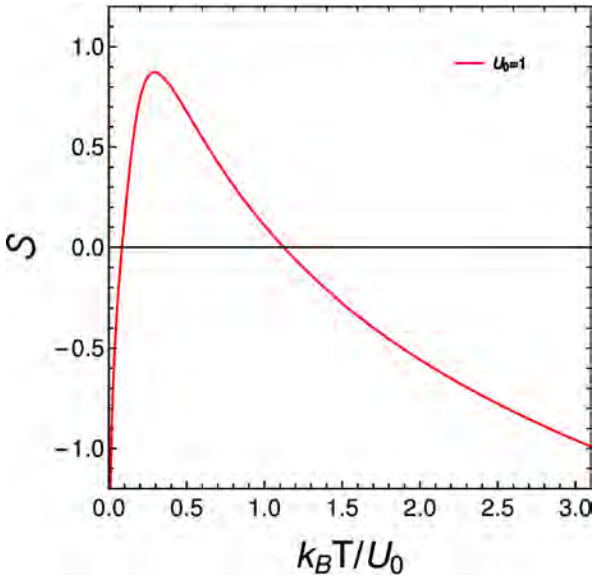


Figure 2. Entropy in appropriate units. Negative values at low $T$ reflect on quantum effects that need to be considered. Those at high $T \geq 10^{22}$ are discussed in the text.

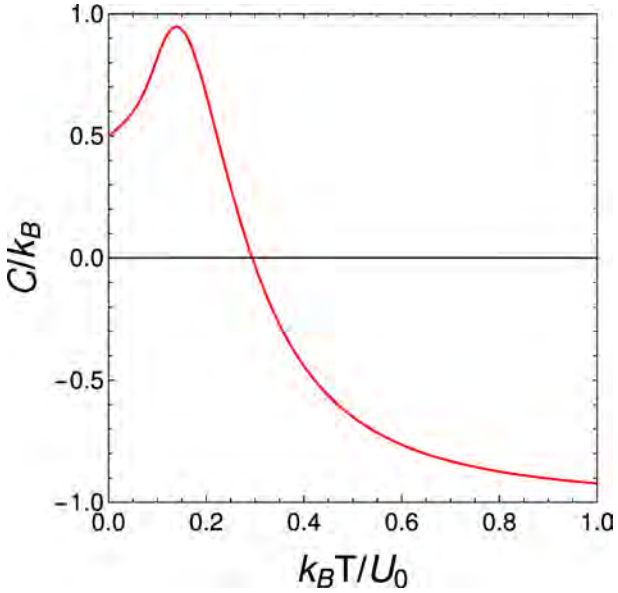


**Figure 3.** Specific heat in appropriate units. The third thermodynamics' law is violated here because our treatment is classical. A Schottky effect is clearly visible (see text).

## 4. Moment Generating Functions

We pass to the moment generating function for our extant probability distribution function (PDF) $f(x)$ [consult (2.1)]

$$f(x)=\frac{e^{\frac{\beta U_0}{1+x^2}}}{\mathcal{Z}}, \tag{4.1}$$

where $\mathcal{Z}$ is given by (2.1). In the naive traditional treatment, these moments diverge. The mean value for $x^{2n+1}$, $(n=1,2,3,\cdots)$ vanishes by parity. That of $x^{2n}$ becomes

$$\left\langle x^{2n}\right\rangle=\frac{1}{\mathcal{Z}}\int_{-\infty}^{\infty}x^{2n}e^{\frac{\beta U_0}{1+x^2}}dx. \tag{4.2}$$

Appeal again to the variables change $y=1+x^2$ and face

$$\left\langle x^{2n}\right\rangle=\frac{1}{\mathcal{Z}}\int_{1}^{\infty}(y-1)^{n-\frac{1}{2}}e^{\frac{\beta U_0}{y}}dy, \tag{4.3}$$

so that, proceeding in a fashion similar to that above we find

$$\left\langle x^{2n}\right\rangle=\frac{\beta U_0}{\mathcal{Z}}\Gamma\left(-n+\frac{1}{2}\right)\Gamma\left(n+\frac{1}{2}\right)\phi\left(\frac{1}{2}-n;2;\beta U_0\right), \tag{4.4}$$

Thus, we get for the moment generating function $\mathcal{M}_1(t)$

$$\mathcal{M}_1(t)=\frac{\beta U_0}{\mathcal{Z}}\sum_{n=0}^{\infty}\frac{t^{2n}}{(2n)!}\Gamma\left(\frac{1}{2}-n\right)\Gamma\left(\frac{1}{2}+n\right)\phi\left(\frac{1}{2}-n;2;\beta U_0\right). \tag{4.5}$$

As particular cases, we obtain the values

$$\left\langle x^{2}\right\rangle=-\frac{\pi\beta U_0}{\mathcal{Z}}\phi\left(-\frac{1}{2};2;\beta U_0\right), \tag{4.6}$$

and

$$\left\langle x^4 \right\rangle = \frac{\pi\beta U_0}{\mathcal{Z}}\phi\left(-\frac{3}{2};2;\beta U_0\right). \tag{4.7}$$

The first one is plotted in **Figure 4**. We encounter again here the high temperature effect already reported in [2] [12] [13] (and references therein) and in precedent graphs: a high temperature upper bound, beyond which our treatment becomes invalid. Such bound manifests itself in making negative these types of expectation values at temperatures of the order of $10^{22}$ Kelvin. For reference, 100 seconds after the Big Bang it is estimated that the temperature is of a billion K-degrees, and 0.0001 seconds after the Big Bang it is of about $T = 10^{13}$ K [16].

## 5. Fisher Information Measure (FIM)

Given a continuous probability distribution function (PDF) $f(x)$ with $x \in \Delta \subset \mathbb{R}$ and $\int_\Delta f(x)\mathrm{d}x = 1$, its associated *Shannon Entropy* $\mathcal{S}$ is, as we saw above,

$$\mathcal{S}(f) = -\int_\Delta f \ln(f)\mathrm{d}x \tag{5.1}$$

a quantifier of global nature that it is not very sensitive to strong changes in the distribution that may take place in a small-sized region. This is not the case for *Fisher's Information Measure* (FIM) $\mathcal{F}$ [17] [18], which constitutes a quantifier of the gradient content of $f(x)$, being accordingly quite sensitive even to small localized perturbations. One writes

$$F(f) = \int_\Delta \frac{1}{f(x)}\left[\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right]^2 \mathrm{d}x = 4\int_\Delta \left[\frac{\mathrm{d}\psi(x)}{\mathrm{d}x}\right]^2 \tag{5.2}$$

FIM can be interpreted in variegated fashions. 1) As a quantifier of the ability

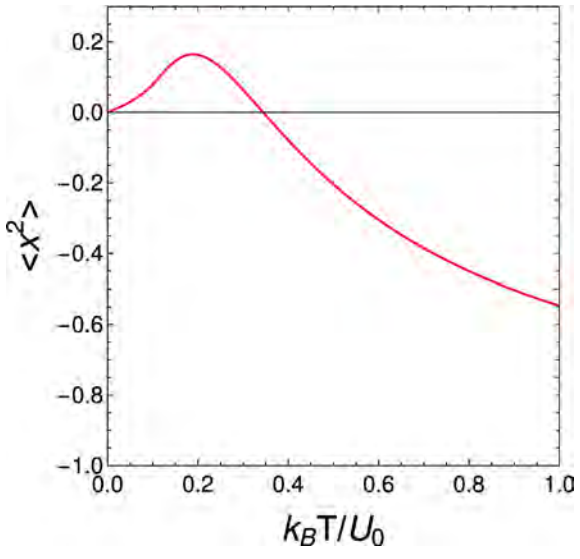


**Figure 4.** $\left\langle x^2 \right\rangle$ values in appropriate units (see text). The unphysical negative values emerge at temperatures higher than $10^{22}$ Kelvin.

to estimate a parameter. 2) As the amount of information that can be extracted from a set of measurements. 3) A quantifier of the state of disorder of a system or phenomenon [18], and finally, at more recent times 4) As a strict measure of order [19] [20] [21]. In the above definition of FIM the division by $f(x)$ is not desirable if $f(x)\to 0$ at certain $x$-values. We bypass this issue by working with a real probability amplitudes $f(x)=\psi^2(x)$ [17] [18], which is a simpler form (no divisors), while showing that $\mathcal{F}$ simply measures the gradient content of $\psi(x)$. The gradient operator significantly influences the contribution of minute local $f$-changes in FIM's values. Thus, this quantifier is called a local measure [18].

For the $f$ of (3.5) one has

$$\mathcal{F}(f)=\frac{2}{\mathcal{Z}}\int_0^\infty \mathrm{e}^{\frac{\beta U_0}{1+x^2}}\left[\frac{\mathrm{d}\mathrm{e}^{\frac{\beta U_0}{1+x^2}}}{\mathrm{d}x}\right]^2\mathrm{d}x, \tag{5.3}$$

or

$$\mathcal{F}(f)=\frac{8\beta^2U_0^2}{\mathcal{Z}}\int_0^\infty \frac{x^2}{\left(1+x^2\right)^2}\mathrm{e}^{\frac{\beta U_0}{1+x^2}}\mathrm{d}x. \tag{5.4}$$

Changing variables in the fashion $y=1+x^2$ we get

$$\mathcal{F}(f)=\frac{4\beta^2U_0^2}{\mathcal{Z}}\int_1^\infty y^{-2}(y-1)^{\frac{1}{2}}\mathrm{e}^{\frac{\beta U_0}{y}}\mathrm{d}y, \tag{5.5}$$

that after evaluation yields for the Fisher information measure the value

$$\mathcal{F}(f)=2\beta U_0, \tag{5.6}$$

clearly a very large positive number, given the smallness of the Boltzmann constant entering the denominator. Let us look for the Cramer-Rao (CR) product $\left[\mathcal{F}(f)\left\langle x^2\right\rangle_f\right]$, that is always $\geq 1$ [18]. The CR relation has been linked to the Heisenberg uncertainty relation (HUR) for the $D$-dimensional quantum central problem [22]. Still further, Frieden has shown that all UHRs can be derived from the CR relation [18].

We need a value for $\left\langle x^2\right\rangle$, that we take from (4.4). The Cramer-Rao product $\left\langle x^2\right\rangle\mathcal{F}$ is then

$$\mathcal{F}(f)\left\langle x^2\right\rangle=-\frac{2\pi\beta^2U_0^2}{\mathcal{Z}}\phi\left(-\frac{1}{2};2;\beta U_0\right). \tag{5.7}$$

The CR product is plotted in **Figure 5**. We see that it is indeed $\geq 1$ till we reach a very high temperature, of the order of $10^{22}$ Kelvin, at which our probability distribution no longer makes sense. We have already encountered above this effect, in connection with $\left\langle x^2\right\rangle$-graph, the entropy, and the specific heat.

## 6. Conclusions

In deceptively simple fashion, we have regularized the partition function for Brownian functions moving in an external potential, thus solving a very old

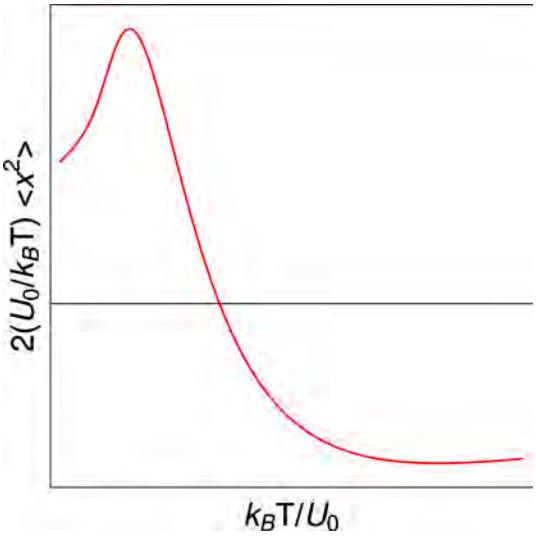


**Figure 5.** The product of $\langle x^2 \rangle$ times Fisher's information measure (Cramer-Rao) (in appropriate units). The well-known associated bound is seen to be violated for temperatures higher than $10^{22}$ Kelvin (see text).

problem. Some other special cases were already treated by the present authors. One is that of the $Z$-expression in the case of Newton's gravity [12], where the divergences are of a different nature from the ones here discussed. A second case is that of Fermi's problem, cited in the Introduction [23]. Our treatment displays two noticeable features.

- Being of a classical nature, it fails at very low temperatures, where quantum effects become predominant.
- At extremely high temperatures, of the order of $10^{22}$ Kelvin, we face a $T$-upper bound. This fact has already been reported, in another context, by Refs. [12] [13]. Our partition function is saying to us that the system can not exist at such high temperatures.

Summing up: We were here tackling partition function' divergences, a physically-motivated mathematical problem, that we indeed solved. As for applications, the most we can say at this stage is that we have at our disposal a new canonical probability distribution. Can one use the concomitant partition function $Z$ in a concrete problem? To answer this question, more research is needed. We guess that with this $Z$ some density distribution might be constructed that could describe a quasi-stationary solution in some suitable scenario.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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# A Simple Model for the Calculation of Diffusion Coefficient in a Periodic Potential

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## Abstract

Motivated by developing a simple model to calculate the diffusion coefficient in moderate friction region, a simplified model is proposed to deal with the diffusion of Brownian particles in a periodic potential. Where the internal noise is a Gaussian white noise, and the basic cell of the periodic potential is composed of a parabolic potential linked with a harmonic potential. When the particles cross the joint point of the potential, a time coarse-graining scheme is used to obtain a simple analytical expression of the probability distribution. The particles drift and diffuse from the first barrier to the second barrier, the passing probability over the second barrier corresponding to the escape rate becomes decrease serves as the long-jump probability. The theoretical result is confirmed by numerical simulation results. The approach can be extended to color noise case.

## Keywords

Diffusion Coefficient, Periodic Potential, Brownian Motion

## 1. Introduction

The diffusion of Brownian particles in a spatially periodic potential is a topic of great interest in many scientific areas of physics, chemistry, and biology [1] [2] [3]. Much effort has been devoted to the study of Brownian motion in periodic potentials. The diffusion coefficient has been investigated through numerical, simulation, and analytic approaches.

The matrix-continued-fraction method was employed to investigate the Brownian motion in one and two-dimensional periodic potentials. The diffusion coefficient was obtained through numerical calculation of the dynamic structure factor [4] [5] [6] [7]. Some characteristics of the diffusion coefficient were found, such as the resonant diffusion in one-dimensional periodic potential due to the

interplay between two oscillatory motions [4], the anomalous dependence of the diffusion coefficient on the friction $D \propto \gamma^{-\sigma}$ with $\sigma < 1$ in a coupled two-dimensional potential [5]. It is found that the coupling between two degrees of freedom always reduces the multiple-jump probability and then lowers the diffusion coefficient [6]. The diffusion-path approximation and quasi-2D approximation were examined by numerical results [7]. The former strongly overestimates the diffusion coefficient at large couplings, and the latter always gives rather good results.

Many diffusion features of Brownian particles in a periodic potential have been revealed by numerical simulations. For nonseparable and anisotropic potentials, molecular dynamics simulation found that the diffusion coefficient presents different dependence on friction in low friction regime as compared with separable potentials, which is directly related to the occurrence of long jumps [8]. For two-dimensional periodic or random potentials, superdiffusion, large-step diffusion, normal diffusion, and subdiffusion were observed through Langevin simulations [9]. These rich varieties of behaviors emerge naturally from an ordinary Langevin equation for a system described by ordinary canonical Maxwell-Boltzmann statistics, without injecting special assumptions such as Levy flights or special memory effects into models of surface diffusion. The Langevin simulation results show that the diffusion coefficient behaves as $D \propto \gamma^{-\sigma}$ with $0 < \sigma < 1/3$ in a two-dimensional periodic potential due to the coupling between the x and y degrees of freedom [10].

Some analytical approaches have been developed to study the diffusion of Brownian particles in a periodic potential. By expanding the distribution function into suitable eigenfunctions, a general method was given in Ref. [11] to calculate the distribution and correlation function of the diffusive motion of particles in a one-dimensional periodic potential. The one-dimensional diffusion in potentials which have a finite number of jumps in their value and in their derivative was investigated. The jump conditions of the eigenfunctions of the corresponding Fokker-Planck-operator were derived and applied to a periodic potential [12]. The modified PGH theory [13] is applied to the motion of a particle moving on a periodic potential influenced by friction and Gaussian thermal noise [14], a uniform expression for the diffusion coefficient valid for any friction value was derived, and the finite barrier corrections were also taken into account. A semiclassical theory for the diffusion of a particle moving on a periodic potential was presented in Ref. [15]. The analytical expressions for the diffusion coefficient and and hopping length distribution are valid for memory friction and any value of friction. Two kinds of approximate schemes, the quasi-2D approximation and the effective potential approach were employed to calculate the two-dimensional diffusion rate constant of a particle driven by a white or colored noise [16]. The theoretical result is qualitatively in agreement with the numerical result. Kramers theory was used to derive simple expressions for the hopping distribution in multidimensional activated surface diffusion

[17]. The derived expressions are valid on condition that the average energy loss of the particle as it goes from one barrier to the next is of the order of $k_BT$ or more.

Although some analytical methods have been developed, simple and exact method is still deserve explored. Combine the physical picture of diffusion and the random walk model, a model to calculate the diffusion coefficient in the turnover region of damping is proposed in the present work. The proposed method provides a simple and exact approach to calculate the diffusion coefficient. Based on this approach, the diffusion of Brownian particles in the usual cosine periodic potential can be deal with by resort to the perturbation theory. The theoretical results for the applied periodic potential are confirmed by Langevin simulation results.

## 2. A Simplified Model for Calculation of Diffusion Coefficient

We consider a Brownian particle moving in a periodic potential with a basic cell composed of a parabolic potential barrier linked smoothly with a harmonic potential well, which is subjected to a Gaussian white noise. The equation of motion of the particle reads

$$\dot{x} = v, \quad \dot{v} = -\gamma v - \frac{1}{m}\frac{\partial V}{\partial x} + \frac{1}{m}\xi(t), \tag{1}$$

where $m$ is the mass of the Brownian particle, $\gamma$ is the damping coefficient, and $V(x)$ is the periodic potential, its basic cell is given by

$$V(x) = \begin{cases} V_b - \frac{1}{2}m\omega_b^2 x^2, & \text{region I;} \\ \frac{1}{2}m\omega_0^2 (x-2)^2, & \text{region II;} \\ V_b - \frac{1}{2}m\omega_b^2 (x-4)^2, & \text{region III.} \end{cases} \tag{2}$$

The three parts in a basic cell of the piecewise potential are connected smoothly at $x = x_{c1}, x_{c2}$ (**Figure 1**), $V_b$ is the height of the potential barrier, $x_{c1} = 1$, $x_{c2} = 3$, $V_b = 1$, $\omega_0 = 1$, $\omega_b = 1$, and $m = 1$ are taken in the present work. Such a potential can serve as a zero-order approximation of a cosine periodic potential. The Gaussian white noise obeys the fluctuation-dissipation theorem: $\langle \xi(t)\xi(t') \rangle = 2m\gamma k_B T \delta(t-t')$, $k_B$ is the Boltzmann constant and $T$ the temperature.

The probability density function in every potential barrier or potential well can be obtained exactly. However, the exact form of probability density after several step jumps is a high dimension integration due to the particle passes through the joint points with stochastic times. The problem is in essence a complex nonlinear one. To simplify the calculation, we construct a time coarse-grain model: the particle passes the joint point $x_{c1}$ with mean passage time of the corresponding potential barrier region. The initial velocity of the particle starting diffusion from the barrier top is set to the average velocity calculated by the Kramers for-

mula. We label the first potential barrier, the first potential well, and the second potential barrier as region I, II, and III, respectively, as shown in Figure 1. The transition probability density and probability density in the region I for an initial $\delta$ distribution of the probability density reads [18]

$$W_1(x,v,t;x_0,v_0,0)=N_1\exp\left[-\alpha_1x^2-\beta_1v^2-\gamma_1xv\right], \tag{3}$$

where

$$\alpha_1=1/2\sigma_{11}^{-1}(t),\beta_1=1/2\sigma_{22}^{-1}(t),\gamma_1=\sigma_{12}^{-1}(t),N_1=\frac{1}{2\pi}\left[4\alpha_1\beta_1-\gamma_1^2\right]^{1/2}. \tag{4}$$

The expressions of the second order moments $\sigma_{ij}$ can be found in Ref. [18]. The equivalent probability density of the particle at $x_{c1}$ is obtained by concentrating all probabilities the particle appearing in region I with $x>0$ on this point at the mean first passage time $t_1$ according to the coarse-grain approximation, that is

$$W_{01}(x,v,t_1)=N_{20}\exp\left[-b_1(v-\overline{v}_1)^2\right]\delta(x-x_{c1}), \tag{5}$$

with $b_1=\beta_1,\overline{v}_1=-\gamma_1x_{c1}/(2\beta_1)$, and $N_{20}=1/2\sqrt{\beta_1/\pi}$. The mean first passage time $t_1$ is given by

$$\begin{aligned}t_1&=\int_0^\infty \mathrm{d}t\int_0^1\mathrm{d}x\int_\infty \mathrm{d}vW_1(x,v,t;x_0,v_0,0)\\&=\int_0^\infty \mathrm{d}t\frac{N_1\pi}{\sqrt{4\alpha_1\beta_1-\gamma_1^2}}\mathrm{erf}\left(\sqrt{\alpha_1-\frac{\gamma_1^2}{4\beta_1}}x_{c1}\right)\end{aligned} \tag{6}$$

The total probability for the particle appearing in region I for $x>0$ has been normalized as 1. The transition probability density [18] in region II is given by

$$\begin{aligned}&P_2(x,v,t;x_{c1},v_1,t_1)\\&=N_2\exp\left(-\alpha_2(x-\overline{x}_2')^2-\beta_2(v-\overline{v}_2')^2-\gamma_2(x-\overline{x}_2')(v-\overline{v}_2')\right).\end{aligned} \tag{7}$$

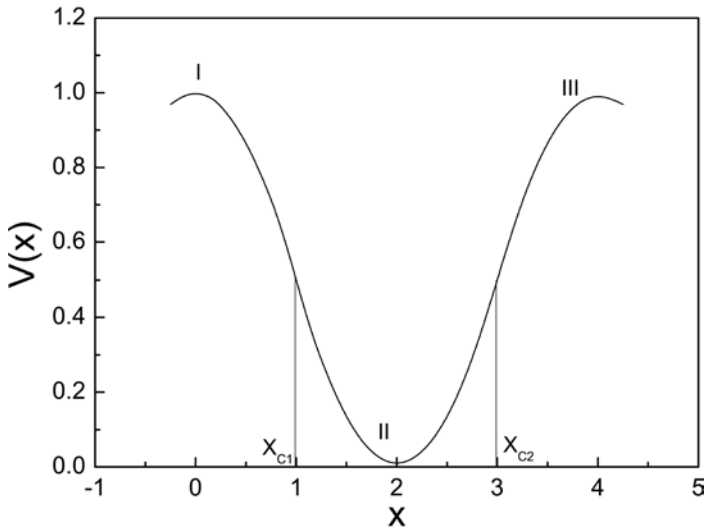


Figure 1. The potential profile. $x_{c1},x_{c2},\cdots$ are the joint points of parabolic barriers and harmonic potential wells.

where

$$\begin{aligned}&\bar{x}_2' = G_{11}x_{c1} + G_{12}v_1, \bar{v}_2' = G_{21}x_{c1} + G_{22}v_1,\\&\alpha_2 = 1/2\,\sigma_{11}^{-1}(t), \beta_2 = 1/2\,\sigma_{22}^{-1}(t), \gamma_2 = \sigma_{12}^{-1}(t),\\&N_2 = \frac{1}{2\pi}\left[4\alpha_2\beta_2 - \gamma_2^2\right]^{1/2},\end{aligned} \tag{8}$$

all of these quantities are defined in region II. The probability density in region II is then obtained

$$\begin{aligned}&W_2(x,v,t) = \int_{-\infty}^{\infty} \mathrm{d}v_1 \int_{-\infty}^{\infty} \mathrm{d}x_1 W_{01}(x_1,v_1,t_1) P(x,v,t;x_1,v_1,t_1)\\&= N_0 N_2 \sqrt{\frac{\pi}{D_2}} \exp\left(-a_2(x-\bar{x}_2)^2 - b_2(v-\bar{v}_2)^2 - c_2(x-\bar{x}_2)(v-\bar{v}_2)\right),\end{aligned} \tag{9}$$

where

$$\begin{aligned}&\bar{x}_2 = G_{11}\bar{x}_1 + G_{12}\bar{v}_1, \bar{v}_2 = G_{21}\bar{x}_1 + G_{22}\bar{v}_1,\\&D_2 = b_1 + \alpha_2 G_{12}^2 + \beta_2 G_{22}^2 + \gamma_2 G_{12} G_{22},\\&a_2 = \frac{4b_1\alpha_2 + \left(4\alpha_2\beta_2 - \gamma_2^2\right)G_{22}^2(t_2-t_1)}{4D_2},\\&b_2 = \frac{4b_1\beta_2 + \left(4\alpha_2\beta_2 - \gamma_2^2\right)G_{12}^2(t_2-t_1)}{4D_2},\\&c_2 = \frac{4b_1\gamma_2 - 2\left(4\alpha_2\beta_2 - \gamma_2^2\right)G_{12}(t_2-t_1)G_{22}(t_2-t_1)}{4D_2}.\end{aligned} \tag{10}$$

The transition probability density in region III is given by

$$\begin{aligned}&P_3(x,v,t;x_{c2},v_2,t_2)\\&= N_3 \exp\left(-\alpha_3(x-\bar{x}_3')^2 - \beta_3(v-\bar{v}_3')^2 - \gamma_3(x-\bar{x}_3')(v-\bar{v}_3')\right).\end{aligned} \tag{11}$$

Where

$$\begin{aligned}&\bar{x}_3' = G_{11}x_{c2} + G_{12}v_2, \bar{v}_3' = G_{21}x_{c2} + G_{22}v_2,\\&\alpha_2 = 1/2\,\sigma_{11}^{-1}(t), \beta_2 = 1/2\,\sigma_{22}^{-1}(t), \gamma_2 = \sigma_{12}^{-1}(t),\\&N_2 = 1\Big/\left(2\pi\sqrt{\det(\sigma)}\right),\end{aligned} \tag{12}$$

All these quantities are defined in region III. The probability density in region III is expressed as

$$W_3(x,v,t) = \int_{t_1}^{t} \mathrm{d}t_2 \int_{-\infty}^{\infty} \mathrm{d}v_2 v_2 W_2(x_{c2},v_2,t_2) P_3(x,v,t;x_{c2},v_2,t_2). \tag{13}$$

The escape probability at time $t$ crossing over the second barrier top is

$$P_e(t) = \int_0^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}v W_3(x,v,t), \tag{14}$$

Performing the Gaussian integrations over $x$ and $v$, the escape probability can be expressed as

$$\begin{aligned}P_e(t) = &\int_{t_1}^{t} \mathrm{d}t_2 \int_{-\infty}^{\infty} \mathrm{d}v_2 v_2 \frac{1}{2}\sqrt{\frac{\pi}{D_2}} N_0 N_2 \mathrm{erfc}\left[-\sqrt{\alpha_3 - \frac{\gamma_3^2}{4\beta_3}}\bar{x}_3'\right]\\&\times \exp\left[-a_2(x_{c2}-\bar{x}_2)^2 - b_2(v_2-\bar{v}_2)^2 - c_2(x_{c2}-\bar{x}_2)(v-\bar{v}_2)\right].\end{aligned} \tag{15}$$

In random walk model, the diffusion coefficient is expressed as [19] [20]

$$D = k\left\langle l^2 \right\rangle = k\sum_n (nd)^2 P_n, \tag{16}$$

where $d$ is the spatial periodic of the potential, $P_n$ is the probability of n-step jumps, and $k$ is the Kramers rate calculated by the Kramers formula in spatial diffusion regime, which is still valid for damping out of spatial diffusion regime due to the parabolic potential barrier. When the center of the probability packet moves toward to the second barrier, the passing probability over the barrier top increases rapidly at almost a constant rate $k_e = \frac{\mathrm{d}P_e}{\mathrm{d}t}$, as shown by the numerical results. When the center of the probability packet moves back to the potential well, the passing probability over the second potential barrier only increases due to diffusion and then becomes slow. We take the critical probability $P_c$ that the increase of $P_e(t)$ as a function of time from rapid to slow as the long jump probability (more than one step). Thereafter the process in the first basic cell is repeated periodically, which is a part of our simplified model. The probabilities for n-step jumps is then given by

$$P_n = P_c^{n-1}(1-P_c)(n=1,2,\cdots) \tag{17}$$

such a geometric progression jump probability distribution is a good approximation for several step jumps, as shown by simulation results (see Fig. 6 of Ref. [8]).

## 3. Comparison with Langevin Simulation Results

To check the accuracy of the diffusion coefficient obtained by the simplified model,

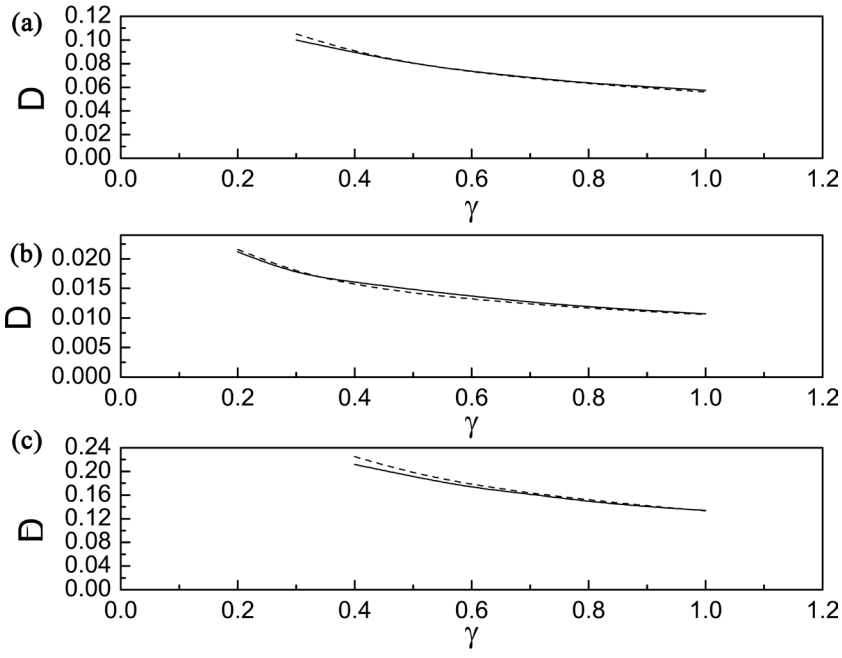


**Figure 2.** The diffusion coefficient as a function of damping. Where the potential barrier height $V_b = 1$, the spatial periodic $d = 4$. (a) for $T = 0.2$, (b) for $T = 0.3$, and (c) for $T = 0.4$.

we simulate the Langevin Equations (1) by second order Runge-Kutta algorithm. The number of test particles and the time step are taken as $N = 3\times10^5$ and $\Delta t = 2\times10^{-3}$, respectively. As shown in **Figure 2**, the theoretical results match the simulation results well in moderate friction region. Such a region is common in surface diffusion problem. The maximal error for applied parameters is less than 6% until lower reduced potential barrier height $V_b/k_BT = 2.5$. The moderate friction region is called the turnover region in escape theory, which is not covered by the original Kramers escape theory. The calculation of escape rate (a factor of diffusion coefficient, see Eq. (16)) and diffusion coefficient in this region is lack of a simple method.

## 4. Conclusion

A simple model is proposed to calculate the diffusion coefficient for Brownian particles moving in a periodic potential. The basic cell of the periodic potential is composed of a parabolic potential barrier linked with a harmonic potential well smoothly, which can serve as a zero-order approximation of a cosine periodic potential. Further theoretical results for the common cosine periodic potential can be obtained by perturbation theory. The theoretical result for the applied potential is confirmed by the simulation result in moderate friction region, which is an often encountered region in surface diffusion problem. The proposed approach can be generalized conveniently to color noise case.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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# Lemaître Transformations of the Interior Schwarzschild Metric

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## Abstract

A Lemaître transformation is set up for the free fall in the interior of a stellar object using the frame of the interior Schwarzschild solution. The metric is calculated in comoving coordinates and field strengths are derived for this metric.

## Keywords

Interior Schwarzschild Metric, Lemaître Transformations, Freely Falling Systems

## 1. Introduction

In this short note, we supplement investigations of an earlier paper [1] on free fall inside a non-rotating stellar object, which is described by the interior Schwarzschild solution. In the above mentioned paper, we had set up a Lorentz transformation that describes the physics of an observer who is moving in free fall through a tube bored through the center of the star. We assign a matrix to this Lorentz transformation that describes a coordinate transformation with which the metric of the interior Schwarzschild solution can be brought into a form that corresponds to Lemaître's relation for free fall in the exterior Schwarzschild field.

We also discuss the form parameter of the metrics in Schwarzschild static coordinates and Lemaître coordinates, and derive the field quantities from tetrads corresponding to the metric in Lemaître form.

## 2. Free Fall Inside a Star

We started with the metric of the Schwarzschild interior solution

$$\mathrm{d}s^2 = \frac{1}{1-\frac{r^2}{\mathcal{R}^2}}\mathrm{d}r^2 + r^2\mathrm{d}\vartheta^2 + r^2\sin^2\vartheta\mathrm{d}\varphi^2 - \frac{1}{4}\left[3\cos\eta_g - \cos\eta\right]^2\mathrm{d}t^2 \qquad (2.1)$$

in the form given by Flamm [2]. The lapse function of the metric is

$$a_T = \frac{1}{2}\left[3\cos\eta_g - \cos\eta\right]. \tag{2.2}$$

Here, $r$ is the radial coordinate, $\eta$ is the polar angle of a cap of a sphere with radius $\Re$, representing geometrically the interior Schwarzschild solution. $\eta_g$ is the polar angle at the boundary surface separating the interior solution from the exterior solution.

From

$$v_T^2 + a_T^2 = 1 \tag{2.3}$$

we deduced the velocity of free fall

$$v_T = -\sqrt{1 - \frac{1}{4}\left(3\cos\eta_g - \cos\eta\right)^2} \tag{2.4}$$

and with $\alpha_T = a_T^{-1}$ the assigned Lorentz factor

$$\alpha_T = \frac{2}{3\cos\eta_g - \cos\eta}. \tag{2.5}$$

Finally, we obtain the Lorentz transformation

$$L^{1}_{1'} = \alpha_T, \quad L^{1}_{4'} = -i\alpha_T v_T, \quad L^{4}_{1'} = i\alpha_T v_T, \quad L^{4}_{4'} = \alpha_T \tag{2.6}$$

operating in the [1,4]-slice of the model. We use the original Minkowski notation with

$$x^4 = i(c)t.$$

At the boundary one has $\eta = \eta_g$ and thus

$$v_T^g = -\sin\eta_g, \quad \alpha_T^g = \frac{1}{\cos\eta_g} = \frac{1}{\sqrt{1 - v_T^{g\,2}}}.$$

The cap of the sphere provides the relations

$$r = \Re\sin\eta, \quad \cos\eta = \sqrt{1 - \frac{r^2}{\Re^2}}. \tag{2.7}$$

From Flamm's paper [2] we read $\rho = 2\Re$, where

$$\rho = \sqrt{\frac{2r^3}{M}}, \quad \Re = r\sqrt{\frac{r}{2M}}$$

is the curvature radius of the Schwarzschild parabola and the radius of a cap of a sphere. Thus, we have $\sin\eta = \sqrt{2M/r}$. Finally, we obtain at the boundary

$$v_T^g = -\sqrt{\frac{2M}{r_g}}, \quad \alpha_T^g = \frac{1}{\sqrt{1 - \frac{2M}{r_g}}}$$

the values for an observer freely falling in the exterior field having reached the boundary.

Thus, using for the velocity the expression

$$v_T(r) = -\sqrt{1-\frac{1}{4}\left(3\sqrt{1-\frac{2M}{r_g}} - \sqrt{1-\frac{2Mr^2}{r_g^3}}\right)^2} \tag{2.8}$$

we are prepared for a drawing. We note that at the center of the star $(r=0)$ the velocity of the freely falling observer would reach the velocity of light for $r_g^{\min} = 2.25M$ . We call this the *inner horizon* of the Schwarzschild model. This is the minimal extension of a star of mass $M$ in geometrical units. We extended the problem for an object freely falling from an arbitrary position outside of the star [3] [4]. This is depicted in **Figure 1**.

The surface of the stellar object is indicated by the dashed lines. One can recognize the smooth transition of the velocities from the exterior region to the interior region. The pressure of the star would be infinitely high at the inner horizon $r_{\min} = 2.25M$ . Hence, it is evident that one has to accept that $r_g > r_{\min}$ . Since $r_{\min} > 2M$ a formation of a black hole is not possible with the frame of the complete Schwarzschild model. In [5] we have shown that a collapsing star can reach the inner horizon only asymptotically, *i.e.*, after an infinitely long time.

## 3. The Lemaître Transformation

The fact that the free fall velocity of an object in the exterior field can be easily prolongated into the interior raises the question whether a coordinate transformation changes the interior metric into a form which has the structure of the exterior Lemaître metric can be found. Since the problem can be reduced to the [1,4]-slice of the model, it is sufficient to read from the interior metric (2.1) the bein-vectors

$$\overset{1}{e}_1 = \alpha_I = \frac{1}{\sqrt{1-\frac{r^2}{\Re^2}}} = \frac{1}{\cos\eta}, \quad \overset{4}{e}_4 = a_T, \quad \overset{1}{e}^1 = a_I = \sqrt{1-\frac{r^2}{\Re^2}} = \cos\eta, \quad \overset{4}{e}^4 = \alpha_T . \tag{3.1}$$

With the Lorentz transformation (2.6), we are able to transform the beine into the freely falling system with $\overset{m'}{e}_i = L_m^{m'}\overset{m}{e}_i$, still using the static coordinate system

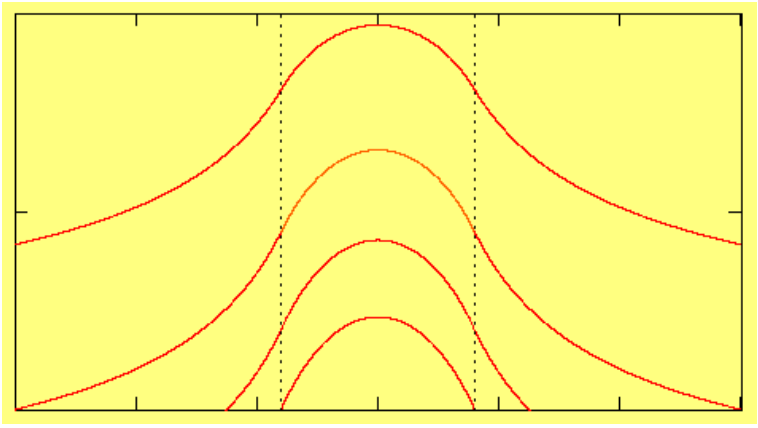

**Figure 1.** Free fall through the interior of a stellar object.

(*i*). We try to diagonalize the bein system with an additional coordinate transformation:

$$\overset{m'}{e}_{i'} = L^{m'}_{m}\,\overset{m}{e}_{i}\,\Lambda^{i}_{i'}, \tag{3.2}$$

$$\begin{aligned} &\Lambda^{1}_{1'} = -\alpha_T v_T a_I, \quad \Lambda^{1}_{4'} = -i\alpha_T v_T a_I, \quad \Lambda^{4}_{1'} = -i\alpha_T^2 v_T^2, \quad \Lambda^{4}_{1'} = \alpha_T^2 \\ &\Lambda^{1'}_{1} = -\frac{\alpha_T \alpha_I}{v_T}, \quad \Lambda^{1'}_{4} = -i, \qquad \Lambda^{4'}_{1} = -i\alpha_T v_T a_I, \quad \Lambda^{4'}_{1} = 1 \end{aligned}. \tag{3.3}$$

Indeed, we obtain

$$\overset{1'}{e}_{1'} = -v_T, \quad \overset{4'}{e}_{4'} = 1, \quad \overset{1'}{e}_{1'} = -\frac{1}{v_T}, \quad \overset{4'}{e}_{4'} = 1, \tag{3.4}$$

recalling that $v_T$ is pointing inwards and thus is a negative quantity.

It is easy to show that

$$\Lambda^{j'}_{[i|k]} = 0, \quad \Lambda^{j}_{[i'|k']} = 0 \quad \Rightarrow \Lambda^{j'}_{i} = x^{j'}{}_{|i}, \quad \Lambda^{j}_{i'} = x^{j}{}_{|i'}, \tag{3.5}$$

proving that the new Lemaître coordinates are holonomic. Restricting ourselves to the [1,4]-slice of the model, we obtain for the line element

$$\mathrm{d}s^2 = v_T^2 \mathrm{d}r'^2 - \mathrm{d}t'^2, \tag{3.6}$$

using comoving coordinates $\{r', t'\}$. Evidently, taking $v_T$ at the boundary the line element (3.6) coincides with the well-known Lemaître line element of the exterior solution. Comparing it with the line element in the non-comoving coordinates in the canonical form given by (2.1), we recognize that the *form parameter* is $k = 1$ for the static line element and $k = 0$ for the freely falling coordinate system. We recall that *k* is misleadingly called *curvature parameter* by cosmologists and $k = 0$ is believed to describe a *globally flat* geometry. Once more, we convince ourselves that $k = 0$ indicates a *locally flat* system, *i.e.*, a system being in free fall. More on this topic one could be found in our papers [6] [7].

In addition, we read from (3.6) that the time $t'$ is the same for all observers at any point during the free fall. The coordinate time coincides with the proper time and is the universal time for all freely falling observers.

Since the lapse function is $g_{4'4'} = 1$, one cannot draw gravitational forces from the metric of the freely falling system. This is just what we expect from Einstein's elevator principle [6]. We calculate the Ricci-rotation coefficients from the comoving bein system (3.4). At first we obtain

$${}'U_{4'} = A_{1'4'}{}^{1'} = -\overset{1'}{e}_{1'}\overset{1'}{e}_{1'|4'} = \frac{1}{v_T} v_{T|4'} = \frac{1}{v_T}\left(-i\alpha_T v_T\right) v_{T|1} = -i\alpha_T v_{T|1}.$$

For further processing one derives from Equation (2.7) the relations $\mathrm{d}r = \Re\cos\eta\,\mathrm{d}\eta$, $\mathrm{d}x^1 = \left(1/\cos\eta\right)\mathrm{d}r = \Re\mathrm{d}\eta$ and finally

$$\eta_{|1} = \frac{1}{\Re}.$$

Differentiating (2.4) one arrives at

$$v_{T|1} = -\frac{1}{2}\frac{a_T}{v_T}\frac{1}{\Re}\sin\eta$$

and lastly we get with $\alpha_T = 1/a_T$ the tidal force

$$'U_{m'} = \left\{0,0,0,i\frac{\sin\eta}{v_T}\frac{1}{2\Re}\right\}. \tag{3.7}$$

Once again using (2.4) one obtains with $v_T^g = -\sin\eta_g$ and $\rho_g = 2\Re$

$$'U_{m'}^g = \left\{0,0,0,-\frac{i}{\rho_g}\right\}, \tag{3.8}$$

the corresponding expression for the free fall in the exterior field at the boundary. We note that we could also apply the inhomogeneous transformation law of the Ricci-rotation coefficients to transform the force of gravity [1] into (3.7). For $\eta = 0$, *i.e.*, at the center of the star one has $'U_{m'} = 0$.

This investigation is not merely an academic exercise. Benish [8] has treated the question whether the theoretically discussed process of free fall in the interior could be supported by an experiment. He proposed a torsion balance, similar to the one used in the Cavendish experiment. Two massive spheres can move through greater spheres on approximately radial orbits and thus could perform an oscillatory motion. The velocity of this motion could be detected on the axis of the suspension by optical devices. The design proposed by Benish is shown in Figure 2.

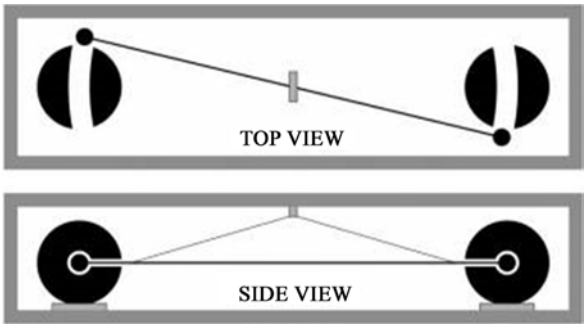


Figure 2. Experiment proposed by Benish.

## 4. Conclusion

We investigated the free fall through a non-rotating stellar object. We found that the velocity of free fall in the exterior Schwarzschild field is smoothly prolongated into the interior. According to Einstein's elevator principle no gravitational forces can be detected by a freely falling observer, but tidal forces act on him. We found a transformation from non-comoving coordinates to comoving coordinates and a metric in Lemaître form. The form parameters of the metrics change from $k = 1$ to $k = 0$ by this transformation, demonstrating that $k = 0$ is an indicator for free fall.

## Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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# Variational Calculation of the Doubly-Excited States Nsnp of He-Like Ions via the Modified Atomic Orbitals Theory

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## Abstract

In this paper, we have declined the formalism of the method of the Modified Atomic Orbital Theory (MAOT) applied to the calculations of energies of doubly excited states 2*snp*, 3*snp*, and 4*snp* Helium-like systems. Then we also applied the variational procedure of the Modified Atomic Orbital Theory to the computations of total energies, excitation energies of doubly-excited states 2*snp*, 3*snp*, 4*snp* types of Helium-like systems. The results obtained in this work are in good agreement with the experimental and theoretical values available.

## Keywords

Modified Atomic Orbital Theory, Doubly Excited States, Excitation Energy, Helium-Like Systems

## 1. Introduction

Much theoretical research has revealed that the helium atom exhibits a strong electron-electron correlation. Since the early experiment by Madden and Codling [1], Madden and Ederer [2], and theoretical explanation by Cooper *et al.* [3], doubly-excited states of helium-like atoms have been the target of a number of theoretical approaches. The increasing interest of physicists in these studies over the years is connected with the understanding of collisional and radiational processes which take place in hot astrophysical and laboratory plasma [4]. The greatest attention has been concentrated on the study of doubly-excited states [5]. Some of these doubly-excited states in two-electron systems have been iden-

tified in the solar flare [6] and in the solar corona [7] and revealed experimentally by the studies of double Rydberg resonances in negative ions of rare gases [8] [9]. The investigations of the intrashell S states of two-electron systems are advanced and due to the group theoretical method [10] [11] which allowed intrashell states to be approximately classified and some of these properties were studied [12] [13].

So, most atomic spectra can be treated in term of singly excitation of singly or mixed configurations [14] [15]. After Herrick and Sinanoglu [11], higher-energy Rydberg envelopes contain doubly-excited states which are generally labelled in the usual spectroscopic notation $\left(Nl,nl'\right)^{2S+1}L^{\pi}$ with $n=N,N+1,\cdots$. In these notations, $N$ and $n$ denote respectively the principal quantum numbers of the inner and the outer electron, $l$ and $l'$ are respectively orbital quantum numbers, $S$ the total spin, $L$ the total angular momentum and $\pi$ the parity of the system.

Various methods have been performed to understand electron-electron correlation effects in doubly $\left(Nl,nl'\right)^{2S+1}L^{\pi}$ excited states of He-like systems. Although many accurate data have been tabulated for these doubly excited states, the methods used require in general, complexity in the Variationnal procedure along with the use of computational codes.

Many theoretical studies have been done on doubly-excited states $\left(Nl,nl'\right)^{2S+1}L^{\pi}$. Among these methods, we have the theoretical and experimental methods [16]-[23]. The variational method of time-independent perturbation from Ray and Mukherjee was applied for the calculation of the total energies of the $2s^2$, $2p^2$ and $3d^2$ states of He, $Li^+$, $Be^{2+}$, and $B^{3+}$ [24]. Sakho used the semi-empirical procedure of the Screening Constant by Unit Nuclear Chargemethod (SCUNC) to calculate the energies of doubly excited states $(Nsnp)\ {}^1P_o$ helium-like systems [25].

In all these ab initio methods, energies of $\left(Nl,nl'\right)^{2S+1}L^{\pi}$ doubly-excited states of *He* isoelectronic sequence can't be expressed in an analytical formula. In addition, most of these preceding methods require large basis-set calculations involving a fair amount of mathematics complexity.

The Modified Atomic Orbital Theory is a purely theoretical method initiated by Sakho [26]. This theory stems from Slater's orbital theory [27]. This theory (MAOT) has been known for its simplicity, as it is a very suitable calculation method that has yielded enormous results from simple semi-empirical formulas without resorting to a computer program in solving resonant photoionization problems. It was subsequently that Sakho [25] studied the resonance energies of the $2s^22p^4\ ({}^1D_2)\ ns$, $nd$, $2s^22p^4\ ({}^1S_0)\ ns$, $nd$, and $2s^22p^5\ ({}^3P_2)$ states from of the metastable $2s^22p^5\ ({}^2P_{1/2})$ state and the ground $2s^22p^5\ ({}^2P_{3/2})$ state of the $Ne^+$ ion. Thus the variational principle, which is a purely theoretical method, takes advantage of the principle of variation. This variational method is a computational technique to provide approximate solutions to solving the Schrödinger equation. In the following, after a brief review of Slater's orbital theory, we apply for the first time the variational procedure of the Modified

Atomic Orbitals Theory to the calculations of total energies, excitation energies of doubly excited 2s$n$p, 3s$n$p, 4s$n$p states of types helium-like systems. This procedure consists of determining the variational parameter $\alpha$ and the screening constant $\sigma$, from the construction of a correlated wave function.

## 2. Theory

### 2.1. Brief Description of the Modified Atomic Orbitals Theory

In the context of the Modified Atomic Orbitals Theory (MAOT), the total energy of a $(n\ell)$—given orbital is expressed as Rydberg units [28].

$$E(n\ell) = -\frac{\left[Z-\sigma(\ell)\right]^2}{n^2}. \tag{1}$$

For the $(Nl, nl')^{2S+1}L^{\pi}$ doubly excited states, the total energy of an atomic system of many M electrons is expressed as follows

$$E = -\sum_{i=1}^{M}\frac{\left[Z-\sigma_i\left(^{2S+1}L^{\pi}\right)\right]^2}{n_i^2}. \tag{2}$$

### 2.2. Construction of the Wave Function

In the construction of the correlated wave function, a product of hydrogen-type wave functions is performed in which variational parameters are introduced. Thus, in the case of atomic systems, these criteria are generally determined by the screen effects exerted by the electrons on each other by the spin-orbit interaction, etc.

The hydrogen wave functions for $|n,l,m_l\rangle$ states are radial and have the same shape. They are non-normed and it's obtained from the radial coordinates ($r$) and an exponential factor.

So for different states, we get:

For 4s ($l = 0$):

$$R_{4,0}(r) = \frac{24}{96}\times\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\times\left(1-\frac{3\times Z}{4\times a_0}\times r+\frac{Z^2}{8\times a_0^2}\times r^2-\frac{Z^3}{192\times a_0^3}\times r^3\right)\times \mathrm{e}^{-\frac{Z\times r}{4\times a_0}} \tag{3}$$

For 4p ($l = 1$):

$$R_{4,1}(r) = \frac{5}{16\sqrt{2}}\times\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\times\left(\frac{Z}{a_0}\times r-\frac{1}{4}\times\frac{Z^2}{a_0^2}\times r^2+\frac{1}{80}\times\frac{Z^3}{a_0^3}\times r^3\right)\times \mathrm{e}^{-\frac{Z\times r}{4\times a_0}} \tag{4}$$

For 3s ($l = 0$):

$$R_{3,0}(r) = \frac{1}{3\sqrt{3\pi}}\times\left(\frac{z}{a_0}\right)^{\frac{3}{2}}\times\left(1-\frac{2}{3}\times\frac{Z}{a_0}\times r+\frac{2}{27}\times\frac{Z^2}{a_0^2}\times r^2\right)\times \mathrm{e}^{-\left(\frac{Z\times r}{3\times a_0}\right)} \tag{5}$$

For 3p ($l = 1$):

$$R_{3,1}(r) = \frac{2\times\sqrt{2}}{27\times\sqrt{\pi}}\times\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\times\left(\frac{Z}{a_0}\times r-\frac{Z^2}{6\times a_0^2}\times r^2\right)\times \mathrm{e}^{-\left(\frac{Z\times r}{3\times a_0}\right)} \tag{6}$$

For 2s ($l = 0$):

$$R_{2,0}(r) = \frac{2}{4\times\sqrt{2\pi}}\times\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\times\left(1-\frac{Z}{2\times a_0}\times r\right)\times \mathrm{e}^{-\left(\frac{Z\times r}{2\times a_0}\right)} \tag{7}$$

For 2p ($l = 1$):

$$R_{2,1}(r) = \frac{1}{4\times\sqrt{2\pi}}\times\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\times\left(\frac{Z}{a_0}\times r\right)\times \mathrm{e}^{-\left(\frac{Z\times r}{2\times a_0}\right)} \tag{8}$$

To build the wave functions of $(Nl, nl')^{2S+1}L^{\pi}$ type, the product of the radial portions $R_{n,l}(r)$ is produced while considering the electrons (1) and (2) heliumoid systems, whose radial coordinates are respectively $r_1$ and $r_2$. As part of the independent particle model where electronic correlation phenomena are neglected, (Coulombian repulsion, spin-orbit interaction, etc.), the product of the functions is given as follows:

For the function 2s2p:

$$2\mathrm{s} = \left(1-\frac{Z}{2\times a_0}\times r_1\right)\times \mathrm{e}^{-\left(\frac{Z\times r_1}{2\times a_0}\right)} \quad \text{and} \quad 2\mathrm{p} = \left(\frac{Z}{a_0}\times r_2\right)\times \mathrm{e}^{-\left(\frac{Z\times r_2}{2\times a_0}\right)}$$

$$\Psi(2\mathrm{s}2\mathrm{p}) = \left[\left(1-\frac{Z}{2\times a_0}\times r_1\right)\times\left(\frac{Z}{a_0}\times r_2\right)\right]\times \mathrm{e}^{-\frac{Z}{2\times a_0}\times r_1}\times \mathrm{e}^{-\frac{Z}{2\times a_0}\times r_2} \tag{9}$$

For the function 3s3p:

$$3\mathrm{s} = \left(1-\frac{2\times Z}{3\times a_0}\times r_1+\frac{2\times Z^2}{27\times a_0^2}r_1^2\right)\times \mathrm{e}^{-\left(\frac{Z}{3\times a_0}\times r_1\right)} \quad \text{and}$$

$$3\mathrm{p} = \left(\frac{Z}{a_0}\times r_2-\frac{Z^2}{6\times a_0^2}\times r_2^2\right)\times \mathrm{e}^{-\left(\frac{Z}{3\times a_0}\times r_2\right)}$$

$$\Psi(3\mathrm{s}3\mathrm{p}) = \left(\left(1-\frac{2\times Z}{3\times a_0}\times r_1+\frac{2\times Z^2}{27\times a_0^2}r_1^2\right)\times\left(\frac{Z}{a_0}\times r_2-\frac{Z^2}{6\times a_0^2}\times r_2^2\right)\right) \times \mathrm{e}^{-\left(\frac{Z}{3\times a_0}\times r_1\right)}\times \mathrm{e}^{-\left(\frac{Z}{3\times a_0}\times r_2\right)} \tag{10}$$

For the function 4s4p:

$$4\mathrm{s} = \left(1-\frac{3\times Z}{4\times a_0}\times r+\frac{Z^2}{8\times a_0^2}\times r^2-\frac{Z^3}{192\times a_0^3}\times r^3\right)\times \mathrm{e}^{-\left(\frac{Z\times r_1}{4\times a_0}\right)}$$

$$4\mathrm{p} = \left(\frac{Z}{a_0}\times r-\frac{1}{4}\times\frac{Z^2}{a_0^2}\times r^2+\frac{1}{80}\times\frac{Z^3}{a_0^3}\times r^3\right)\times \mathrm{e}^{-\left(\frac{Z\times r_2}{4\times a_0}\right)}$$

$$\Psi(4\mathrm{s}4\mathrm{p}) = \left(\left(1-\frac{3\times Z}{4\times a_0}\times r_1+\frac{Z^2}{8\times a_0^2}\times r_1^2-\frac{Z^3}{192\times a_0^3}\times r_1^3\right) \times\left(\frac{Z}{a_0}\times r_2-\frac{1}{4}\times\frac{Z^2}{a_0^2}\times r_2^2+\frac{1}{80}\times\frac{Z^3}{a_0^3}\times r_2^3\right)\right)\times \mathrm{e}^{-\left(\frac{Z\times r_1}{4\times a_0}\right)}\times \mathrm{e}^{-\left(\frac{Z\times r_2}{4\times a_0}\right)} \tag{11}$$

Taking into account the phenomena of electron-electron correlation effects occurring in *He*-like systems, the nuclear charge of the exponential factor is substituted in favor of the effective charge $Z^*$, and in atomic unit, the Bohr radius $a_0 = 1$.

So these functions become:

For the wave function 2s*n*p:

$$\Psi(2\text{snp}) = \left(\left(1 - \frac{Z}{2\times a_0}\times r_1\right)\times\left(\frac{Z}{a_0}\times r_2\right)\right)\times \mathrm{e}^{-\frac{Z^*}{n}(r_1+r_2)} \tag{12}$$

For the wave function 3s*n*p:

$$\Psi(3\text{snp}) = \left(\left(1 - \frac{2\times Z}{3\times a_0}\times r_1 + \frac{2\times Z^2}{27\times a_o^2} r_1^2\right)\times\left(\frac{Z}{a_0}\times r_2 - \frac{Z^2}{6\times a_0^2}\times r_2^2\right)\right)\times \mathrm{e}^{-\frac{Z^*}{n}(r_1+r_2)} \tag{13}$$

For the wave function 4s*n*p:

$$\begin{aligned}\Psi(4\text{snp}) = &\left(\left(1 - \frac{3\times Z}{4\times a_0}\times r_1 + \frac{Z^2}{8\times a_0^2}\times r_1^2 - \frac{Z^3}{192\times a_0^3}\times r_1^3\right)\right.\\ &\left.\times\left(\frac{Z}{a_0}\times r_2 - \frac{1}{4}\times\frac{Z^2}{a_0^2}\times r_2^2 + \frac{1}{80}\times\frac{Z^3}{a_0^3}\times r_2^3\right)\right)\times \mathrm{e}^{-\frac{Z^*}{n}(r_1+r_2)}\end{aligned} \tag{14}$$

where the effective charge number $Z^*$ is given by:

$$Z^* = Z\left(1 - \frac{\sigma(Nl, nl')}{Z}\right) \tag{15}$$

With $\sigma(Nl, nl')$ the screen constant relating to these states.

## 2.3. Determining the Screen Constant

To determine the screen constant, we start from the relation:

$$E(\alpha) = \langle H\rangle(\alpha) = \frac{\langle\Psi(\alpha)|H|\Psi(\alpha)\rangle}{\langle\Psi(\alpha)|\Psi(\alpha)\rangle} \tag{16}$$

And Hamiltonian of the helium isoelectronic series in given by (in atomic units):

$$H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \tag{17}$$

The average value of this expression (17), while using the closure relation reflecting the fact that the $|r_1, r_2\rangle$ kets are continuous bases in the state space of the two electrons:

$$\iint \mathrm{d}r_1^3\mathrm{d}r_2^3\,|r_1, r_2\rangle\langle r_1, r_2| = \mathbb{1} \tag{18}$$

From this relation we can from (21):

$$\begin{aligned}&E(\alpha)\iint \mathrm{d}^3r_1\mathrm{d}^3r_2\,\langle\Psi(\alpha)||r_1, r_2\rangle\times\langle r_1, r_2||\Psi(\alpha)\rangle\\ &= \iint \mathrm{d}^3r_1\mathrm{d}^3r_2\,\langle\Psi(\alpha)||r_1, r_2\rangle\hat{H}\langle r_1, r_2||\Psi(\alpha)\rangle\end{aligned} \tag{19}$$

The development of (19) gives:

$$\begin{aligned} &E(\alpha)\iint \mathrm{d}^3r_1\mathrm{d}^3r_2\Psi(r_1,r_2,\alpha)\times\Psi^*(r_1,r_2,\alpha) \\ &=\iint \mathrm{d}^3r_1\mathrm{d}^3r_2\Psi(r_1,r_2,\alpha)\hat{H}\Psi^*(r_1,r_2,\alpha) \end{aligned} \tag{20}$$

The normalization constant denoted $N$ is given by:

$$NE(\alpha)=\iint \mathrm{d}^3r_1\mathrm{d}^3r_2\Psi(r_1,r_2,\alpha)\hat{H}\Psi^*(r_1,r_2,\alpha) \tag{21}$$

And from this relation (24), we obtain:

$$N=\iint \mathrm{d}^3r_1\mathrm{d}^3r_2\left|(r_1,r_2,\alpha)\right|^2 \tag{22}$$

To facilitate the development of these expressions, we made a change of variable of some parameters of the Equation (20). It was later that we posed in elliptical coordinates:

$$s=(r_1+r_2);t=(r_1-r_2);u=r_{12} \tag{23}$$

And the element of elementary volume gives:

$$\mathrm{d}\tau=\mathrm{d}r_1^3\mathrm{d}r_2^3=2\pi^2\left(s^2-t^2\right)u\mathrm{d}s\mathrm{d}t\mathrm{d}u \tag{24}$$

Applying these changes of variables in Equation (23) the preceding expression of the normalization constant denoted $N$ is in elliptic coordinate:

$$\begin{aligned} NE(\alpha)=\int_0^\infty \mathrm{d}s\int_0^s \mathrm{d}u\int_0^u \mathrm{d}t\Bigg\{&u\left(s^2-t^2\right)\times\left[\left(\frac{\partial\Psi}{\partial s}\right)^2+\left(\frac{\partial\Psi}{\partial t}\right)^2+\left(\frac{\partial\Psi}{\partial u}\right)^2\right]+2\left(\frac{\partial\Psi}{\partial u}\right) \\ &\times\left[s\left(u^2-t^2\right)\frac{\partial\Psi}{\partial s}+t\left(s^2-u^2\right)\frac{\partial\Psi}{\partial t}\right]-\Psi^2\left[4Zsu-s^2+t^2\right]\Bigg\} \end{aligned} \tag{25}$$

Since we did not take into account the Coulomb repulsion, so: $\frac{\partial\Psi}{\partial u}=0$.

The normalization constant becomes:

$$NE(\alpha)=\int_0^\infty \mathrm{d}s\int_0^s \mathrm{d}u\int_0^u \mathrm{d}t\left\{u\left(s^2-t^2\right)\times\left[\left(\frac{\partial\Psi}{\partial s}\right)^2+\left(\frac{\partial\Psi}{\partial t}\right)^2\right]-\Psi^2\left[4Zsu-s^2+t^2\right]\right\} \tag{26}$$

To determine the values of the screen constant $\sigma$ and the variational parameter $\alpha$, we start from this equation, which is the sum of three integral data as follows:

$$NE(\alpha)=E_1(\alpha)+E_2(\alpha)+E_3(\alpha) \tag{27}$$

The development of this expression (27) makes it possible to obtain the value of $\sigma$ and $\alpha$ by the formula:

$$\frac{\mathrm{d}E(\alpha_i)}{\mathrm{d}\alpha_i}=0 \tag{28}$$

The expressions corresponding to $E_1(\alpha)$, $E_2(\alpha)$, and $E_3(\alpha)$, are:

$$E_1(\alpha)=\int_0^\infty \mathrm{d}s\int_0^s \mathrm{d}u\int_0^u \mathrm{d}t\,u\left(s^2-t^2\right)\times\left(\frac{\partial\Psi}{\partial s}\right)^2 \tag{29}$$

$$E_2(\alpha)=\int_0^{\infty}\mathrm{d}s\int_0^{s}\mathrm{d}u\int_0^{u}\mathrm{d}t\,u\left(s^2-t^2\right)\times\left(\frac{\partial\Psi}{\partial t}\right)^2 \tag{30}$$

$$E_3(\alpha)=-\int_0^{\infty}\mathrm{d}s\int_0^{s}\mathrm{d}u\int_0^{u}\mathrm{d}t\left[4Zsu-s^2+t^2\right]\Psi^2 \tag{31}$$

The normalization constant is as follows:

$$N=\int_0^{\infty}\mathrm{d}s\int_0^{s}\mathrm{d}u\int_0^{u}\mathrm{d}t\,u\left(s^2-t^2\right)\times\Psi^2 \tag{32}$$

With these changes of variables, the correlated wave functions of the states 2s*n*p, 3s*n*p, and 4s*n*p become:

$$\Psi(2\mathrm{s}2\mathrm{p})=-\frac{1}{8}\times\left((s-t)\times(s\times z+t\times z-4)\right)\times\mathrm{e}^{-\alpha s} \tag{33}$$

$$\begin{aligned}\Psi(3\mathrm{s}3\mathrm{p})=\frac{1}{1296}\times\Big[&z\times(s-t)\times(s\times z-t\times z-12)\times\left(s^2\times z^2+2\times s\times t\times z^2\right.\\&\left.-18\times s\times z+t^2\times z^2-18\times t\times z+54\right)\Big]\times\mathrm{e}^{-\alpha s}\end{aligned} \tag{34}$$

$$\begin{aligned}\Psi(4\mathrm{s}4\mathrm{p})=-\frac{1}{983040}\times\Big(&z\times(s-t)\times\left(s^2\times z^2-2\times s\times t\times z^2-40\times s\times z\right.\\&+t^2\times z^2+40\times t\times z+320\Big)\times\left(s^3\times z^3+3\times s^2\times t\times z^3-48\times s^2\times z^2\right.\\&+3\times s\times t^2\times z^3-96\times s\times t\times z^2+576\times s\times z+t^3\times z^3\\&\left.-48\times t^2\times z^2+576\times t\times z-1536\right)\Big)\times\mathrm{e}^{-\alpha s}\end{aligned} \tag{35}$$

## 3. Results and Discussions

In this part, the procedure consists of determining the final expressions of energies, the value of the variational parameter $\alpha$, and the screen constant $\sigma$. Since the calculations used are very complex, and require a lot of changes of variables, with matrices to be manipulated, we have found it necessary to make a first call to a computer program with the software matlab. In this program, we first defined the parameter *s*, *t*, *u*, *a*, and *z* of Equation (23), the expression of the derivative as a function of each parameter, and the square of its derivatives. In a second step, the expressions of ($E_1$, $E_2$, $E_3$ and $N$) of the Equations (29)-(32), as well as their factorials were defined and detailed expression by expression. Then, to simplify some parameters, a matrix calculation was carried out in this program, and relations between these matrices were made to obtain a simple expression of the Equation (27) in order to apply the formula of the Equation (28) to have the approximate values of the screen constant $\sigma$ and the variational parameter $\alpha$.

### 3.1. Expression of the Total Energies

In the case of the variational calculation of the Modified Atomic Orbital theory (MAOT, the expression of the total energy of the doubly-excited states (*N*s*n*p) of an orbital is given by the formula (in Rydberg):

$$E(Nsnp) = -\left(\frac{(Z-\sigma(ns))^2}{N^2}\right) - \left(\frac{(Z-\sigma(np))^2}{n^2}\right) \tag{36}$$

With $N \neq n$ and $\sigma(ns) = \sigma(np)$.

In some cases, a corrective factor may be added to this expression to obtain results that are closer to those found in the literature consulted.

Thus the expressions of the states 2s*n*p, 3s*n*p, and 4s*n*p are detailed as follows:

- For the state 2s*n*p:

$$E(2s2p) = -\left(\frac{(Z-\sigma(ns))^2}{N^2}\right) - \left(\frac{(Z-\sigma(np))^2}{n^2}\right) \tag{37}$$

With $\sigma(ns) = \sigma(np)$ and $N = n$.

- For the state 3s*n*p:

$$E(3s3p) = -\left(\frac{(Z-\sigma(ns))^2}{N^2}\right) - \left(\frac{(Z-\sigma(np))^2}{n^2}\right) \tag{38}$$

With $\sigma(ns) = \sigma(np)$ et $N = n$.

- For the state 4s*n*p:

$$E(4s4p) = -\left(\frac{(Z-\sigma(ns))^2}{N^2}\right) - \left(\frac{(Z-\sigma(np))^2}{n^2}\right) \tag{39}$$

With $\sigma(ns) = \sigma(np)$ and $N = n$.

### 3.2. Expression of the Variational Parameter $\alpha$

The determination of the variational parameter $\alpha$ comes from the expression (28) with:

$$E(\alpha_i) = \sum_{i=1}^{3}\left(\frac{E_i}{N}\right) \tag{40}$$

Thus the calculation program is presented in the **Appendix**, and the variational parameter $\alpha$ of the states 2s2p, 3s3p and 4s4p is given as follows:

$$\alpha = \frac{n+l+l'}{n} Z\left(1-\frac{\sigma(Nl,nl')}{Z}\right) \tag{41}$$

For the state 2s2p:

$$\alpha_2(2s2p) \approx \frac{3}{2} Z\left(1-\frac{1}{2}\times\frac{1}{Z}\right) \tag{42}$$

With $\sigma(2s2p) = 0.5$.

For the state 3s3p:

$$\alpha_3(3s3p) \approx \frac{4}{3} Z\left(1-\frac{3}{12}\times\frac{1}{Z}\right) \tag{43}$$

With $\sigma(3s3p) = 0.25$.

For the state 4s4p:

$$\alpha_4(4s4p) \approx \frac{5}{4}Z\left(1-\frac{3}{7}\times\frac{1}{Z}\right) \tag{44}$$

With $\sigma(4s4p) = 0.428$.

### 3.3. Results and Discussion

In this work, the results obtained are compared with those found in the theoretical and experimental literature. We have calculated the total energies of the states (3s*n*p $^1$P$^o$), (2s*n*p $^1$P$^o$), (4s*n*p $^1$P$^o$) as well as the excitation energies of the states (3s*n*p $^1$P$^o$), (2s*n*p $^1$P$^o$), (4s*n*p $^1$P$^o$). For the states (3snp $^1$P$^o$) the total energies are given in Rydberg and in eV, shown in Table 1 (1 eV = 13.605698 Ryd) shown in Table 2. For the (2s*n*p $^1$P$^o$), (4s*n*p $^1$P$^o$) states, their results are given in eV and represented in Table 3 and Table 4 respectively. Equations (37), (38), (39) have been used for the calculation of its total states energies (3s*n*p $^1$P$^o$), (2s*n*p $^1$P$^o$), (4s*n*p $^1$P$^o$) respectively. About excitations energies, we have taken the energies of the ground state given by Frankowski and Pekeris [29]. These energies are given in ua (1 ua = 2 Rydberg) their values are given as follows: He (−2.90372), $Li^+$ (−7.27991), $Be^{2+}$ (−13.65556), $Be^{3+}$ (−22.03097).

In Tables 1-4, we used the variational computation of the modified atomic orbitals theory (MAOT) of the energies doubly-excited states (3snp $^1$P$^o$), (2snp $^1$P$^o$), (4snp $^1$P$^o$). We compared the results obtained with theoretical results for all of these states, and experimental results existing only for the (3s3p $^1$P$^o$), (2s2p $^1$P$^o$), helium (He) states of Kossmann *et al.* [17], (2s2p $^1$P$^o$), lithium ($Li^+$) from Diehl *et al.* [19], and (4s4p $^1$P$^o$) from Woodru *et al.* [30]. The theoretical results to which we have compared our results are those of Sakho *et al.* [25], Ivanov and Safronova [15], Drake and Dalgarno [22], Ho [18], Biaye *et al.* [21], Bachau

**Table 1.** The total energies of the doubly excited states of (*N*s*n*p) $^1$P$^o$ helium-like systems (*Z* = 2 to 10) in Rydberg (1 Ryd = 13.60569 eV).

| States | | Z | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 3s3p $^1$P$^o$ | −E$^p$ | 0.68056 | 1.68056 | 3.12500 | 5.01389 | 7.34722 | 10.12500 | 13.34722 | 17.01389 | 21.12500 |
| | −E$^s$ | 0.66054 | 1.64784 | 3.07958 | 4.95577 | 7.27640 | 10.04147 | 13.25099 | 16.90496 | 21.00337 |
| | −E$^a$ | 0.67140 | 1.659 40 | 3.09000 | 4.96600 | 7.28600 | 10.04800 | 13.25600 | 16.91000 | 21.00000 |
| | −E$^b$ | 0.66268 | 1.67395 | 3.15417 | 5.10468 | 7.52607 | 10.41871 | 13.78253 | 17.61787 | 21.92494 |
| 3s4p $^1$P$^o$ | −E$^p$ | 0.53168 | 1.31293 | 2.44141 | 3.91710 | 5.74002 | 7.91016 | 10.42752 | 13.29210 | 16.50391 |
| | −E$^s$ | 0.53206 | 1.31269 | 2.44053 | 3.91561 | 5.73790 | 7.90742 | 10.42415 | 13.28811 | 16.49930 |
| | −E$^a$ | 0.54240 | 1.31960 | 2.44400 | 3.91400 | 5.73000 | 7.89600 | 10.40800 | 13.26600 | 16.47200 |
| 3s5p $^1$P$^o$ | −E$^p$ | 0.46278 | 1.14278 | 2.12500 | 3.40944 | 4.99611 | 6.88500 | 9.07611 | 11.56944 | 14.36500 |
| | −E$^s$ | 0.47259 | 1.15756 | 2.14475 | 3.43416 | 5.02579 | 6.91965 | 9.11573 | 11.61403 | 14.41455 |

P: Present results obtained from Equation (38); s: (Sakho *et al.*, 2010) [26], a: (Bachau *et al.*, 1991) [20]; b: (Biaye *et al.*, 2005) [21].

**Table 2.** The total energies of the doubly excited states of ($N$s$n$p) $^1$P$^o$ types of helium-like systems ($Z$ = 2 to 10). Results given in eV (1 Ryd = 13.60569 eV).

| States | | $Z$ | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 3s3p $^1$P$^o$ | $-E^p$ | 9.26 | 22.87 | 42.52 | 68.22 | 99.96 | 137.76 | 181.60 | 231.49 | 287.42 |
| | $-E^s$ | 9.10 | 22.47 | 41.88 | 67.34 | 98.85 | 136.40 | 180.01 | 229.66 | 285.35 |
| | $-E^h$ | 8.28 | 21.14 | 40.05 | 65.01 | 96.01 | 133.06 | 176.16 | 225.30 | 280.49 |
| | $-E^k$ | 9.10 | 22.33 | 42.04 | 67.52 | 99.03 | | | | |
| | $-E^l$ | 9.11 | 22.54 | 42.00 | 67.51 | | | | | |
| | $-E^i$ | 9.10 | | | | | | | | |
| 3s4p $^1$P$^o$ | $-E^p$ | 7.23 | 17.86 | 33.22 | 53.29 | 78.10 | 107.62 | 141.87 | 180.85 | 224.55 |
| | $-E^s$ | 7.66 | 18.42 | 33.90 | 54.10 | 79.03 | 108.68 | 143.06 | 182.16 | 225.98 |
| 3s5p $^1$P$^o$ | $-E^p$ | 6.30 | 15.55 | 28.91 | 46.39 | 67.98 | 93.68 | 123.49 | 157.41 | 195.45 |
| | $-E^s$ | 7.02 | 16.58 | 30.25 | 48.03 | 69.93 | 95.94 | 126.05 | 160.05 | 198.63 |

P: Present results obtained from Equation (38); s: (Sakho *et al.*, 2008) [25]; h: (Ivanov and Safronova, 1993) [16]; i: experimental results (Kossmann *et al.*, 1988) [17]; k: (Wagué, 1987) [31]; l: (Lipsky *et al.*, 1977) [32].

**Table 3.** The total energies of the doubly excited states of ($N$s$n$p) $^1$P$^o$ types of helium-like systems ($Z$ = 2 to 10). Results given in eV (1 Ryd = 13.60569 eV).

| States | | $Z$ | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 2s2p $^1$P$^o$ | $-E^p$ | 17.96 | 46.88 | 89.39 | 145.52 | 215.25 | 298.58 | 395.52 | 506.07 | 630.22 |
| | $-E^s$ | 18.88 | 47.76 | 90.24 | 146.34 | 216.03 | 299.33 | 396.24 | 506.76 | 630.88 |
| | $E^a$ | 18.86 | 47.82 | 90.33 | 146.40 | 216.07 | 299.32 | 396.18 | 506.64 | 630.70 |
| | $-E^h$ | 19.42 | 48.23 | 90.63 | 146.66 | 216.28 | 299.51 | 396.34 | 506.78 | 630.84 |
| | $-E^j$ | 18.87 | 47.84 | 90.34 | 146.42 | 216.09 | 299.34 | 396.20 | 506.20 | 630.84 |
| | $-E^{f,i}$ | 18.88$^i$ | 47.78$f$ | | | | | | | |
| 2s3p $^1$P$^o$ | $-E^p$ | 15.05 | 37.16 | 69.09 | 110.85 | 162.44 | 223.86 | 295.10 | 376.16 | 467.06 |
| | $-E^s$ | 15.95 | 38.23 | 70.34 | 112.28 | 164.04 | 225.63 | 297.05 | 378.29 | 469.36 |
| | $-E^h$ | 15.95 | 37.99 | 69.86 | 111.55 | 163.07 | 224.41 | 295.59 | 376.58 | 467.41 |

P: Present results obtained from Equation (37); s: (Sakho *et al.*, 2008) [25]; a: (Ho, 1980) [18]; h: (Ivanov and Safronova, 1993) [16]; i: experimental results (Kossmann *et al.*, 1988) [17]; f: Experimental data, (Diehl *et al.*, 1999) [19]; j: (Drake and Dalgarno, 1971) [22].

*et al.* [20], Sakho *et al.* [26], Wagué [31], Lipsky *et al.* [32].

Thus in **Table 1**, **Table 2**, containing the states (3snp $^1$P$^o$), we have calculated the total energies of doubly-excited states types (3s$n$p $^1$P$^o$) ranging from ($Z$ = 2 to 10) using Equation (38).

The results found are in perfect agreement with those found in the theoretical and experimental literature consulted and quoted above. For the (3s3p $^1$P$^o$) helium (He) states, we compared our results with those obtained experimentally by

Kossman *et al.* [17], and the results obtained are in perfect agreement.

In Table 3 and Table 4, containing the states (2snp $^1P^o$), and (4s4p $^1P^o$), we used the Equations ((37), (39)) respectively. Then we added to each of these equations a corrective factor to obtain results equivalent to those found in the theoretical and experimental. In Table 3, states (2snp $^1P^o$), we calculated the total energies of doubly excited states of helium-like systems ($Z$ = 2 to 10). Our results found are in good agreement with the theoretical results [16] [22] [25] and experimental [17] [19].

In Table 4, states (4s4p $^1P^o$), we also calculated the total energies of doubly-excited states of helium-like systems ($Z$ = 2 to 10). The results found are in

Table 4. The total energies of the doubly excited states of ($N$s$n$p) $^1P^o$ types of helium-like systems ($Z$ = 2 to 10). Results given in eV (1 Ryd = 13.60569 eV).

| State | | Z | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 4s4p $^1P^o$ | $-E^p$ | 5.24 | 12.91 | 23.98 | 38.46 | 56.33 | 77.61 | 102.29 | 130.37 | 161.85 |
| | $-E^s$ | 5.35 | 13.03 | 24.10 | 38.58 | 56.46 | 77.75 | 102.43 | 132.03 | 162.00 |
| | $E^\alpha$ | 5.29 | 12.95 | 24.01 | 38.46 | 56.31 | 77.56 | 102.43 | 130.27 | 161.72 |
| | $-E^m$ | 5.35 | | | | | | | | |

P: Present results obtained from Equation (39); m: Experimental data, Woodruff and Samson (1982) [30].

Table 5. Excitation energies of the doubly excited states of ($N$s$n$p) $^1P^o$ types of helium-like systems ($Z$ = 2 to 5). Results given in eV (1 Ryd = 13.60569 eV; 1 ua = 2 Rydberg).

| States | | $Z$ | | | |
|---|---|---|---|---|---|
| | | 2 | 3 | 4 | 5 |
| 2s2p $^1P^o$ | $E^p$ | 61.05 | 151.22 | 282.19 | 453.98 |
| | $E^s$ | 60.13 | 150.34 | 281.35 | 453.15 |
| | $E^j$ | 60.13 | | | |
| | $E^{f,i}$ | $60.13^i$ | $150.31^f$ | | |
| 2s3p $^1P^o$ | $E^p$ | 63.97 | 160.94 | 302.50 | 488.64 |
| | $E^s$ | 63.06 | 159.87 | 301.25 | 487.21 |
| 3s3p $^1P^o$ | $E^p$ | 69.75 | 175.23 | 329.07 | 531.28 |
| | $E^s$ | 69.91 | 175.63 | 330.54 | 532.15 |
| | $E^i$ | 69.91 | | | |
| 3s4p $^1P^o$ | $E^p$ | 71.78 | 180.23 | 338.37 | 546.20 |
| | $E^s$ | 71.35 | 179.68 | 337.69 | 545.39 |
| 3s5p $^1P^o$ | $E^p$ | 72.72 | 182.55 | 342.67 | 553.11 |
| | $E^s$ | 71.99 | 181.52 | 341.34 | 551.46 |
| 4s4p $^1P^o$ | $E^p$ | 73.78 | 185.19 | 347.60 | 561.04 |
| | $E^s$ | 73.66 | 185.07 | 347.49 | 560.91 |
| | $E^m$ | 73.66 | | | |

perfect agreement with those found in the literature consulted.

In Table 5, we presented the excitation energies of the doubly-excited states of ($Nsnp$ $^1P^o$) ($N$, $n \leq 5$) types of helium and its assimilated ions. They are calculated from the energies of the ground state given by Frankowski and Pekeris [29]. The results found in this table are in perfect agreement with the results found by the other authors.

## 4. Conclusion

In a global way, we applied the variational procedure of the modified atomic orbitals theory for the computation of total energies and excitation senergies doubly-excited states of the atomic system with several electrons. In order to achieve our results, we used a matlab program for the first time to reduce the complexity of the calculations. This program allowed us to determine the approximate expressions of the variational parameter, and of the screen constant.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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# Appendix

## Appendix A: Calculation Procedure for the Determination of the Radial Wave Function

The procedure for determining the radial wave function is given as follows:

$$R_{n,l}(r)=\left\{\left(\frac{2Z}{na_0}\right)^3\frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}\right\}^{1/2}\mathrm{e}^{-\frac{zr}{na_0}}\left(\frac{2Zr}{na_0}\right)^l L_{n+l}^{2l+1}\left(\frac{2Zr}{na_0}\right) \tag{A1}$$

The associated Laguerre polynomials are linked to the Laguerre polynomials $L_{n+l}(r)$ by the Rodrigue formula:

$$L_n^k(r)=(-1)\frac{\mathrm{d}^k}{\mathrm{d}r^k}L_n(r) \tag{A2}$$

$$L_n(r)=\mathrm{e}^r\frac{\mathrm{d}^n}{\mathrm{d}r^n}\left(r^n\mathrm{e}^{-r}\right) \tag{A3}$$

For different values of $n$ and $l$, the Laguerre polynomials are mutually orthogonal, which then determines the orthogonality of the radial wave functions.

Let's give the example of the 4s wave function:

For the state 4s we have: $n=4$, $l=0$

$$L_{n+l}^{2l+1}\left(\frac{2Zr}{na_o}\right)=L_4^1\left(\frac{2Zr}{na_o}\right)\Rightarrow\frac{\mathrm{d}}{\mathrm{d}r}\left(L_4(r)\right)\left(\frac{2Zr}{na_o}\right) \tag{A4}$$

And;

$$L_4=\mathrm{e}^r\frac{\mathrm{d}^4}{\mathrm{d}r^4}\left(r^n\mathrm{e}^{-r}\right) \tag{A5}$$

By developing this expression, we get:

$$L_4(r)=\mathrm{e}^r\frac{\mathrm{d}^3}{\mathrm{d}r^3}\left(4r^3\mathrm{e}^{-r}-r^4\mathrm{e}^{-r}\right)=\mathrm{e}^r\frac{\mathrm{d}^2}{\mathrm{d}r^2}\left(12r^2\mathrm{e}^{-r}-4r^3\mathrm{e}^{-r}-4r^3\mathrm{e}^{-r}+r^4\mathrm{e}^{-r}\right)$$

$$\begin{aligned}L_4(r)=\mathrm{e}^r\frac{\mathrm{d}}{\mathrm{d}r}\big(&24r\mathrm{e}^{-r}-12r^2\mathrm{e}^{-r}-12r^2\mathrm{e}^{-r}+4r^3\mathrm{e}^{-r}\\&-12r^2\mathrm{e}^{-r}+4r^3\mathrm{e}^{-r}+4r^3\mathrm{e}^{-r}-r^4\mathrm{e}^{-r}\big)\end{aligned}$$

$$\begin{aligned}L_4(r)=\mathrm{e}^r\big(&24\mathrm{e}^{-r}-24r\mathrm{e}^{-r}-24r\mathrm{e}^{-r}+12r^2\mathrm{e}^{-r}-24r\mathrm{e}^{-r}+12r^2\mathrm{e}^{-r}\\&+12r^2\mathrm{e}^{-r}-4r^3\mathrm{e}^{-r}-24r\mathrm{e}^{-r}+12r^2\mathrm{e}^{-r}+12r^2\mathrm{e}^{-r}-4r^3\mathrm{e}^{-r}\\&+12r^2\mathrm{e}^{-r}-4r^3\mathrm{e}^{-r}-4r^3\mathrm{e}^{-r}+r^4\mathrm{e}^{-r}\big)\end{aligned}$$

$$L_4(r)=\left(24-96r+72r^2-16r^3+r^4\right) \tag{A6}$$

Then he comes:

$$L_4^1=\frac{\mathrm{d}}{\mathrm{d}r}L_4(r)=4\left(-24+36\times r-12\times r^2+r^3\right) \tag{A7}$$

Which give,

$$L_{n+l}^{2l+1}\left(\frac{2Z\times r}{na_0}\right)=L_4^1\left(\frac{2Z\times r}{na_0}\right)$$
$$=(-4)\times\left(-24\times\left(\frac{2Z}{4a_0}\right)^0+36\times r\left(\frac{2Z}{4a_0}\right)^1-12\times r^2\left(\frac{2Z}{4a_0}\right)^2+r^3\left(\frac{2Z}{4a_0}\right)^3\right) \quad \text{(A8)}$$

So the determination of the first part of the expression (A1)

$$\left\{\left(\frac{2Z}{na_0}\right)^3\times\frac{(n-l-1)!}{2n\times\left[(n+1)!\right]^3}\right\}^{\frac{1}{2}}$$

For $n=4$ and $l=0$, we have:

$$\left\{\left(\frac{2Z}{na_0}\right)^3\frac{(n-l-1)!}{2n\times\left((n+l)!\right)^3}\right\}^{\frac{1}{2}}=\left\{\left(\frac{Z}{2\times a_0}\right)^3\times\left(\frac{6}{8\times 24^3}\right)\right\}^{\frac{1}{2}}$$
$$=\left\{\left(\frac{Z}{2\times a_0}\right)^3\times\left(\frac{3}{4\times 24^3}\right)^{\frac{1}{2}}\right\}=\left\{\left(\frac{Z}{2\times a_0}\right)^{\frac{3}{2}}\left(\frac{1}{96\times\sqrt{2}}\right)\right\}=\left\{\frac{1}{4\times 96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right\} \quad \text{(A9)}$$

$$\left\{\left(\frac{2Z}{na_0}\right)^3\frac{(n-l-1)!}{2n\times\left((n+l)!\right)^3}\right\}^{\frac{1}{2}}=\left\{\frac{1}{4\times 96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right\} \quad \text{(A10)}$$

Thus, starting from (A8) and (A10);

$$\left\{\frac{1}{4\times 96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right\}\times(-4)\times\left(-24+\frac{18\times Zr}{a_0}-\frac{3\times Z^2r^2}{a_0^2}+\frac{Z^3r^3}{8a_0^3}\right)$$
$$=\left[\frac{1}{96}\left(24-\frac{18Z}{a_0}r+\frac{32Z^2}{a_0^2}r^2-\frac{Z^3}{8a_0^3}r^3\right)\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right] \quad \text{(A11)}$$

Simplifying by 24 we finally obtain the expression of the radial wave function 4s as follows:

$$R_{4,0}=\frac{24}{96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(1-\frac{3Z}{4a_0}r+\frac{Z^2}{8a_0^2}r^2-\frac{Z^3}{192a_0^3}r^3\right)\mathrm{e}^{-\frac{Z\times r}{4a_0}} \quad \text{(A12)}$$

By analogy the wave function 4p is given as follows:

$$R_{4,1}=\frac{5}{16\sqrt{2}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(\frac{Z}{a_0}r-\frac{1}{4}\frac{Z^2}{a_0^2}r^2+\frac{1}{80}\frac{Z^3}{a_0^3}r^3\right)\mathrm{e}^{-\frac{Z\times r}{4a_0}} \quad \text{(A13)}$$

## Appendix B: Principle of Determining the Screen Constant

To determine the screen constant, we start from the relation:

$$E(\alpha)=\langle H\rangle(\alpha)=\frac{\langle\Psi(\alpha)|H|\Psi(\alpha)\rangle}{\langle\Psi(\alpha)|\Psi(\alpha)\rangle} \quad \text{(B1)}$$

And the Hamiltonian H (in atomic unit) is:

$$H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{z}{r_1} - \frac{z}{r_2} + \frac{1}{r_{12}} \tag{B2}$$

The average value of this expression (B2), while using the closure relation reflecting the fact that the $|r_1, r_2\rangle$ kets are continuous bases in the state space of the two electrons:

$$\iint \mathrm{d}r_1^3 \mathrm{d}r_2^3 \left|r_1, r_2\right\rangle\left\langle r_1, r_2\right| = \mathbb{1} \tag{B3}$$

From this relation we can from (B3):

$$\begin{aligned} &E(\alpha)\iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \left\langle \Psi(\alpha)\middle| r_1, r_2\right\rangle \times \left\langle r_1, r_2 \middle| \Psi(\alpha)\right\rangle \\ &= \iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \left\langle \Psi(\alpha)\middle| r_1, r_2\right\rangle \hat{H} \left\langle r_1, r_2 \middle| \Psi(\alpha)\right\rangle \end{aligned} \tag{B4}$$

The development of (B4) gives:

$$\begin{aligned} &E(\alpha)\iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \Psi(r_1, r_2, \alpha) \times \Psi^*(r_1, r_2, \alpha) \\ &= \iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \Psi(r_1, r_2, \alpha) \hat{H} \Psi^*(r_1, r_2, \alpha) \end{aligned} \tag{B5}$$

The normalization constant denoted $N$ is given by:

$$NE(\alpha) = \iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \Psi(r_1, r_2, \alpha) \hat{H} \Psi^*(r_1, r_2, \alpha) \tag{B6}$$

And from this relation (B6), we obtain:

$$N = \iint \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \left|(r_1, r_2, \alpha)\right|^2 \tag{B7}$$

To facilitate the development of these expressions, we made a change of variable of some parameters of the Equation (B5). It was later that we posed in elliptical coordinates:

$$s = (r_1 + r_2); t = (r_1 - r_2); u = r_{12} \tag{B8}$$

And the element of elementary volume gives:

We know that, $\mathrm{d}\tau = \mathrm{d}r_1^3 \mathrm{d}r_2^3$

$$\mathrm{d}\tau = \mathrm{d}r_1^3 \mathrm{d}r_2^3 = 2\pi^2 \left(s^2 - t^2\right) u \mathrm{d}s \mathrm{d}t \mathrm{d}u \tag{B9}$$

Applying these changes of variables in Equation (B7) the preceding expression of the normalization constant denoted N is in elliptic coordinate:

$$\begin{aligned} NE(\alpha) = \int_0^\infty \mathrm{d}s \int_0^s \mathrm{d}u \int_0^u \mathrm{d}t \Bigg\{ & u\left(s^2 - t^2\right) \times \left[\left(\frac{\partial \Psi}{\partial s}\right)^2 + \left(\frac{\partial \Psi}{\partial t}\right)^2 + \left(\frac{\partial \Psi}{\partial u}\right)^2\right] + 2\left(\frac{\partial \Psi}{\partial u}\right) \\ & \times \left[s\left(s^2 - t^2\right)\frac{\partial \Psi}{\partial s} + t\left(s^2 - u^2\right)\frac{\partial \Psi}{\partial t}\right] - \Psi^2\left[4Zsu - s^2 + t^2\right]\Bigg\} \end{aligned} \tag{B10}$$

Since we did not take into account the Coulomb repulsion, so: $\frac{\partial \Psi}{\partial u} = 0$

The normalization constant becomes:

$$NE(\alpha) = \int_0^\infty \mathrm{d}s \int_0^s \mathrm{d}u \int_0^u \mathrm{d}t \left\{ u\left(s^2 - t^2\right) \times \left[\left(\frac{\partial \Psi}{\partial s}\right)^2 + \left(\frac{\partial \Psi}{\partial t}\right)^2\right] - \Psi^2\left[4Zsu - s^2 + t^2\right]\right\} \tag{B11}$$

To determine the values of the screen constant $\sigma$ and the variational parameter $\alpha$, we start from this equation, which is the sum of three integral data as follows:

$$NE(\alpha) = E_1(\alpha) + E_2(\alpha) + E_3(\alpha) \tag{B12}$$

The development of this expression (B12) makes it possible to obtain the value of $\sigma$ and $\alpha$ by the formula:

$$\frac{\mathrm{d}E(\alpha_i)}{\mathrm{d}\alpha_i} = 0 \tag{B13}$$

The expressions corresponding to $E_1(\alpha)$, $E_2(\alpha)$, and $E_3(\alpha)$, are:

$$E_1(\alpha) = \int_0^{\infty} \mathrm{d}s \int_0^{s} \mathrm{d}u \int_0^{u} \mathrm{d}t\, u\left(s^2 - t^2\right) \times \left(\frac{\partial \Psi}{\partial s}\right)^2 \tag{B14}$$

$$E_2(\alpha) = \int_0^{\infty} \mathrm{d}s \int_0^{s} \mathrm{d}u \int_0^{u} \mathrm{d}t\, u\left(s^2 - t^2\right) \times \left(\frac{\partial \Psi}{\partial t}\right)^2 \tag{B15}$$

$$E_3(\alpha) = -\int_0^{\infty} \mathrm{d}s \int_0^{s} \mathrm{d}u \int_0^{u} \mathrm{d}t \left[4Zsu - s^2 + t^2\right] \Psi^2 \tag{B16}$$

The normalization constant is as follows:

$$N = \int_0^{\infty} \mathrm{d}s \int_0^{s} \mathrm{d}u \int_0^{u} \mathrm{d}t\, u\left(s^2 - t^2\right) \times \Psi^2 \tag{B17}$$

With these changes of variables, we obtain the equations presented above in section (2.3): Equation (33; 34; 35).


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