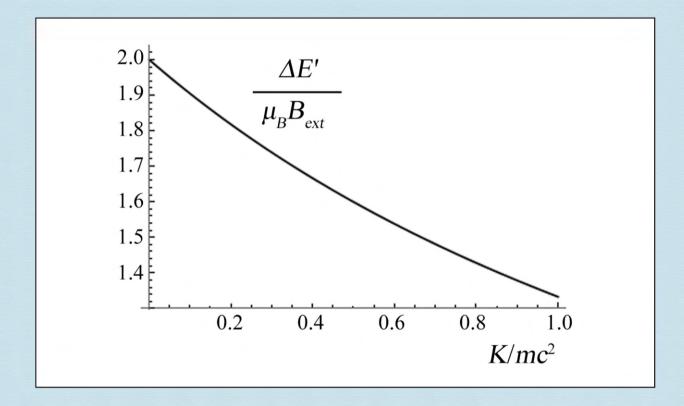


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Quantum Violation of Bell's Inequality: A Misunderstanding Based on a Mathematical Error of Neglect

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Abstract

This paper intends to show how the fabled violation of Bell's inequality by the probabilistic specifications of quantum mechanics derives from a mathematical error, an error of neglect. I have no objection to the probabilities specified by quantum theory, nor to the inequality itself as characterized in the formulation of Clauser, Horne, Shimony, and Holt. Designed to assess consequences of Einstein's principle of local realism, the inequality pertains to a linear combination of four polarization products on the same pair of photons arising in a gedankenexperiment. My assessment displays that in this context, the summands of the relevant CHSH quantity $s(\lambda)$ inhere four symmetric functional relations which have long been neglected in analytic considerations. Its expectation $E[s(\lambda)]$ is not the sum of four "marginal" expectations from a joint distribution, as quantum theory explicitly avoids such a specification. Rather, I show that $E[s(\lambda)]$ has four distinct representations as the sum of three expectations of polarization products plus the expectation of a fourth which is restricted to equal a function value determined by the other three. Analysis using Bruno de Finetti's fundamental theorem of prevision (FTP) yields only a bound for E(s) within (1.1213,2], surely not

 $2\sqrt{2}$ at all as is commonly understood. I exhibit slices of the 4-dimensional polytope of joint P_{++} probabilities actually motivated by quantum theory at the four stipulated angle settings, as it passes through 3-dimensional space. Bell's inequality is satisfied everywhere within the convex hull of extreme distributions cohering with quantum theoretic specifications, even while in keeping with local realism. Aspect's proposed "estimation" of E(s) near to

 $2\sqrt{2}$ is based on polarization products from different photon pairs that do not have embedded within them the functional relations inhering in the rele-

vant gedankenexperiment. When one actively embeds the restrictions into Aspect's estimation procedure, it yields an estimate of 1.7667, although this is not and cannot be definitive. While my analysis supports the subjectivist construction of probability as clarifying issues relevant to the interpretation of quantum theory, the error resolved herein is purely mathematical. It pertains to the reconsideration of Bell violation irrespective of one's attitude toward the meaning of probability.

Keywords

Bell Inequality Defiance, CHSH Formulation, Fundamental Theorem of Probability, Probability Bounds, 4-Dimensional Cuts

1. Introduction

As brash as this may sound, claims that probabilistic specifications of quantum mechanics are inconsistent with local realism and defy Bell's inequality are just plain wrong. This may be difficult to accept, depending on how wedded one is to the outlook that gives rise to defiance of the inequality as it is widely understood. In the eyes of the professional physics community, the matter is now closed. The eminent journal Nature [1] flamboyantly announced the "Death by experiment for local realism" as an introduction to its publication of ambitious experimental results achieved at the Technical University of Delft. These were proclaimed to have closed simultaneously all seven loopholes that had been suggested as possible explanations for the purported violations of the inequality. My claim is that the touted violation of the inequality derives from a mathematical mistake, an error of neglect. Moreover, consequences of the error run through both the analytical development of the defiance structure and the statistical assessment of relevant matters. Its recognition relies only on a basic understanding of functions of many variables and on standard features of applied linear algebra. This presentation is prepared so to be read not only by physicists but by any sophisticated reader who has followed this issue at least at the level of popular description of scientific activity and who is not put off by equations per se.

The defiance of Bell's inequality is one of the seminal results underlying the understanding of quantum theory as it has developed over the past half century. More than seven thousand references to pertinent discussion can be found on Google Scholar, and I do not intend to review the corpus. Most physicists regard the inequality as a condition on freely determined expectation values and their estimates from physical experiments, calculated according to the QM formalism. I consider this viewpoint to be mistaken, for reasons I shall detail herein. However, while surely in a minority camp of objectors, my analysis can be situated within a literature of creditable researchers whose perspective I share. The recent review article of Kupczynski [2] surveys and references more than eighty technical publications in this vein, both longstanding and recent, notably recognized contributions of Fine [3], Hess [4], Hess and Philipp [5], Khrennikov [6], and Kupczynski herself. The review provides many more references from these and other researchers. Of course many of these have been contested, particularly in the perspective of Mermin [7]. Nonetheless, I believe the assessment of the situation that I provide is truly novel, and augments the reservations that have been proposed within the dissenting camp.

It is clear in his own writings that John Bell himself was puzzled by the implications of his inequality [8] [9] [10]. He suspected that something was wrong with the understanding that when coupled with local realism the probabilities of quantum mechanics seem to defy its structure, and he expressed undying confidence that this error would be discovered in due time. I am proposing that I have found the error he sought. I accept all probabilistic assertions supported by quantum theory, and I shall exhibit their implied satisfaction of the inequality bounds which they are widely supposed to defy.

I do not contest the experimental results of the Delft group, nor any of the related experimentation which has followed from the pathbreaking initial work of Alain Aspect and his group [11] [12]. I do contest the inferences they are purported to support. In this note I will first review the derivation of the inequality in the context to which it applies, featuring its relation to Einstein's principle of local realism. The review will focus on the CHSH form of the inequality to which Aspect's optical experimentation is considered to be relevant. Identifying the neglected functional relations that are involved in a thought experiment on a single pair of photons, I will show that claims to quantum defiance of the inequality are mistaken, and show how to derive the actual implications of quantum theory for the probabilities under consideration. Further will be shown why Aspect's computations (and all subsequent extensions) proposed to exhibit empirical confirmation of the inequality defiance are ill considered, and how they ought to be adjusted. This demonstration relies on the computational mechanics of Bruno de Finetti's fundamental theorem of probability. The results are displayed both algebraically and geometrically.

2. The Physical Setup of Four Experiments Providing Context for Bell's Inequality in CHSH Form: A 16-D Problem

We shall review the setup of an optical variant of Bell's experiment, designed by Alain Aspect in the 1980's to take advantage of a formulation of the problem proposed by Clauser, Horne, Shimony, and Holt [13]. The original discussions of the inequality violation were couched in terms of observations of spins of paired electrons. Although specific algebraic details differ for the two types of experimental situation, the conclusions reached would be identical.

An experiment is conducted on a pair of photons traveling in opposite directions along an axis, z, from a common source. As seen in **Figure 1**, the direction one of the photons travels toward detector A on the left is directly opposite to the direction its paired photon travels toward detector B on the right: $\mathbf{z}_A = -\mathbf{z}_B$. At the end of their respective journeys, each of the paired photons engages polarizing material that either allows it to pass through or to be deflected.

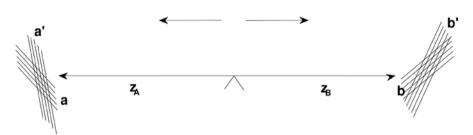


Figure 1. Polarizing material is aligned at the detection stations of *A* and *B*, each with two possible choices of direction in the (x, y) dimension perpendicular to the **z** direction of the incoming photon: direction **a** or **a'** at station *A*, and **b** or **b'** at station *B*.

The detection of a photon that passes through the polarizer is designated by denoting the numerical value of A = +1, while the detection of a photon as blocked is designated by the value of A = -1. The polarizer addressed by photon A is oriented in a variable direction \mathbf{a}^* in the (x, y) plane perpendicular to \mathbf{z}_A . It can be set in either of two specific directions designated as \mathbf{a} and \mathbf{a}' in the experimental setups we shall consider. Similarly, the direction of the polarizer met by the photon at station B can be set at either \mathbf{b} or \mathbf{b}' in its (x, y) plane. Depending on the specific pair of polarization directions $\mathbf{a}^*, \mathbf{b}^*$ chosen for any particular experiment, we shall observe the paired values of either $(A(\mathbf{a}), B(\mathbf{b}))$, or $(A(\mathbf{a}), B(\mathbf{b}'))$, or $(A(\mathbf{a}'), B(\mathbf{b}))$, or $(A(\mathbf{a}'), B(\mathbf{b}'))$. Since the observations of the A and the B photon detections can each equal either +1 or -1 whatever the angle pairing might be, the chosen observation pair $(A(\mathbf{a}^*), B(\mathbf{b}^*))$ will equal one of the four possibilities (+, +), (+, -), (-, +), or (-, -), where the needless numeric values of 1 are suppressed in each designated pairing.

Experimental choices of the two polarizing directions yield a specific *relative* angle between them at stations A and B in any given experiment. Using Aspect's notation that parentheses around a pair of directions denotes the relative angle between them, the experimental detection angle settings $(\mathbf{a}^*, \mathbf{z}_A)$ and $(\mathbf{b}^*, \mathbf{z}_B)$ imply the *relative* angle between polarizers at stations A and B in the (x, y) dimension as $(\mathbf{a}^*, \mathbf{b}^*)$. Bell's inequality is relevant to this context in which the two photon polarization directions can be paired at any one of four distinct relative angles, denoted by the parenthetic pairs (\mathbf{a}, \mathbf{b}) , (\mathbf{a}, \mathbf{b}) , or $(\mathbf{a}', \mathbf{b}')$.

In order to view the relative angles we are talking about, mentally we would need to swing the (x, y) plane around by 180° as it is viewed by the photon directed to station *A*, and superimpose it on the (x, y) plane as it is viewed by the photon directed to station *B*. In this manner we can understand the size and meaning of the relative angles *between* the various values of polarization orientations \mathbf{a}^* and \mathbf{b}^* as seen here in Figure 2, which follows.

The theory of quantum mechanics motivates specification of probabilities for the four observable outcome possibilities of the polarization experiment as depending on the *relative angle* $(\mathbf{a}^*, \mathbf{b}^*)$ between the direction vectors of the

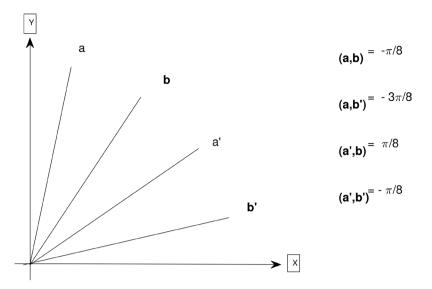


Figure 2. Directional vectors of the polarization angle settings at the observation stations *A* and *B*, viewed in a common axis orientation. The specific relative angle size settings displayed are the extreme violation values, a feature to be discussed.

polarizers at stations *A* and *B*. For any such relative angle pairing, the probabilities specified by quantum theory for the four possible experimental observations $\{++, +-, -+, --\}$ are

$$P\Big[\Big(A\big(\mathbf{a}^*\big) = +1\Big)\Big(B\big(\mathbf{b}^*\big) = +1\Big)\Big]$$

= $P\Big[\Big(A\big(\mathbf{a}^*\big) = -1\Big)\Big(B\big(\mathbf{b}^*\big) = -1\Big)\Big] = \frac{1}{2}\cos^2\big(\mathbf{a}^*, \mathbf{b}^*\big),$
$$P\Big[\Big(A\big(\mathbf{a}^*\big) = +1\Big)\Big(B\big(\mathbf{b}^*\big) = -1\Big)\Big]$$

= $\Big[\Big(A\big(\mathbf{a}^*\big) = -1\Big)\Big(B\big(\mathbf{b}^*\big) = +1\Big)\Big] = \frac{1}{2}\sin^2\big(\mathbf{a}^*, \mathbf{b}^*\big).$ (1)

For efficiency in what follows, we shall denote the four probabilities appearing in Equations (1) by P_{++}, P_{--}, P_{+-} , and P_{-+} when the pertinent angle setting is evident.

These four probabilities surely sum to equal 1, because the sum of $\cos^2 + \sin^2$ of any angle equals 1. A few properties of the joint probability mass function (pmf) they compose should be noticed. Firstly, the four probabilities can be specified by the value of any one of them. The equations (1) stipulate that no matter what the relative angle $(\mathbf{a}^*, \mathbf{b}^*)$ may be, the values of $P_{++} = P_{--}$, and

 $P_{-+} = P_{+-}$. Since the four probabilities do sum to 1 then, the specification of P_{++} as the value p, for example, implies that the pmf vector $[P_{++}, P_{--}, P_{+-}, P_{-+}]$ would be [p, p, (1-2p)/2, (1-2p)/2]. Another implication of this feature is that the probabilities for the paired detection outcomes depend only on the *product* of the two measurements. For both outcomes ++ and -- yield a product of +1 and both outcomes +- and -+ yield a product of -1. Thus, the QM-motivated distribution for the experimental value of the polarization *product* $A(\mathbf{a}^*)B(\mathbf{b}^*)$ is specified by $P[A(\mathbf{a}^*)B(\mathbf{b}^*) = +1] = \cos^2(\mathbf{a}^*, \mathbf{b}^*)$ and

 $P\left[A\left(\mathbf{a}^{*}\right)B\left(\mathbf{b}^{*}\right)=-1\right]=\sin^{2}\left(\mathbf{a}^{*},\mathbf{b}^{*}\right).$

As will be important to recognize in what follows, the expected value (first moment) of this distribution for the detection product is

$$E\left[A(\mathbf{a}^{*})B(\mathbf{b}^{*})\right] = (+1)\cos^{2}(\mathbf{a}^{*},\mathbf{b}^{*}) + (-1)\sin^{2}(\mathbf{a}^{*},\mathbf{b}^{*})$$
$$= \cos^{2}(\mathbf{a}^{*},\mathbf{b}^{*}) - \sin^{2}(\mathbf{a}^{*},\mathbf{b}^{*}) = \cos^{2}(\mathbf{a}^{*},\mathbf{b}^{*})$$
(2)

according to standard double angle formulas. It is worthwhile reminding right here that "the expected value of a probability distribution" is the "first moment" of the distribution. Geometrically, it is the point of balance of the probability mass function weights when they are positioned in space at the places where the possible observations to which they pertain might occur. It is a property of a probability distribution for the outcome of a specific single observable variable. A final peculiarity of Equation (2) to be useful far down the road in this explication is that the expectation value $E\left[A(\mathbf{a}^*)B(\mathbf{b}^*)\right]$ can also be represented as

$$E\left[A\left(\mathbf{a}^{*}\right)B\left(\mathbf{b}^{*}\right)\right] = 2\cos^{2}\left(\mathbf{a}^{*},\mathbf{b}^{*}\right)-1 = 4P_{++}\left(\mathbf{a}^{*},\mathbf{b}^{*}\right)-1.$$
(3)

For the value of $\sin^2(\mathbf{a}^*, \mathbf{b}^*)$ appearing in the final line of Equation (2) can also be written as $1 - \cos^2(\mathbf{a}^*, \mathbf{b}^*)$. Enough of this for now.

Secondly, again no matter what the relative angle $(\mathbf{a}^*, \mathbf{b}^*)$ may be, the marginal probability that the detection observation of the photon equals +1 at either observation station is equal to 1/2. For the standard margining equation for the result of a paired experiment yields

$$P\left[\left(A\left(\mathbf{a}^{*}\right) = +1\right)\right]$$

= $P\left[\left(A\left(\mathbf{a}^{*}\right) = +1\right)\left(B\left(\mathbf{b}^{*}\right) = +1\right)\right] + P\left[\left(A\left(\mathbf{a}^{*}\right) = +1\right)\left(B\left(\mathbf{b}^{*}\right) = -1\right)\right]$ (4)
= $\frac{1}{2}\cos^{2}\left(\mathbf{a}^{*}, \mathbf{b}^{*}\right) + \frac{1}{2}\sin^{2}\left(\mathbf{a}^{*}, \mathbf{b}^{*}\right) = 1/2$

This result codifies a touted feature of physical processes at quantum scales of magnitude, that the photon behaviours of particle pairs are understood to be *entangled*. Since the probability for the joint photon behaviour

 $P\Big[\Big(A(\mathbf{a}^*)=+1\Big)\Big(B(\mathbf{b}^*)=+1\Big)\Big]$ does not factor into the product of their marginal probabilities $P\Big[\Big(A(\mathbf{a}^*)=+1\Big)\Big]$ and $P\Big[\Big(B(\mathbf{b}^*)=+1\Big)\Big]$, the conditional distribution for either one of these events depends on the context of the conditioning behaviour:

$$P\left[\left(A\left(\mathbf{a}^{*}\right)=+1\right)|\left(B\left(\mathbf{b}^{*}\right)=+1\right)\right]=\cos^{2}\left(\mathbf{a}^{*},\mathbf{b}^{*}\right)\neq P\left[\left(A\left(\mathbf{a}^{*}\right)=+1\right)\right]=1/2, \quad (5)$$

and $P\left[\left(A\left(\mathbf{a}^*\right) = +1\right) | \left(B\left(\mathbf{b}^*\right) = -1\right)\right] = \sin^2\left(\mathbf{a}^*, \mathbf{b}^*\right)$, which is different still.

We have concluded what we need to say at the moment about the prescriptions of quantum theory relevant to quantum polarization behaviour of a single pair of prepared photons. Before proceeding to the specification of Bell's inequality, we need to address three issues: what quantum theory professes *not* to say on account of the uncertainty principle, the relevance of the principle of local realism, and a proposal regarding supplementary variables that may impinge on the experimental results.

3. The Uncertainty Principle: What Quantum Theory Disavows

The problem of quantum physics relevant to Bell's inequality concerns the consideration of what might happen in imagined designs of physical situations that are impossible to instantiate. In our developments to this point, we have identified a physical experiment on a pair of photons, polarizing them at one of four exclusive possible relative angle pairings, (\mathbf{a}, \mathbf{b}) , $(\mathbf{a}', \mathbf{b})$, and $(\mathbf{a}', \mathbf{b}')$. We could perform this polarization experiment on a specific pair of photons at any one of these angle pairings. Moreover, we could perform the experiment at all four angle settings if we generated different pairs of photons to engage each of them. However, we cannot perform all four experiments simultaneously on the same pair of photons. The theory of quantum mechanics recognizes this fact explicitly, avowing the uncertainty principle which abnegates all claims regarding the outcome of an experiment that cannot possibly be observed. Not only would any such claim necessarily evade empirical corroboration, but the theoretical algebraic mechanism that is used to identify the quantum probabilities for the results of the polarization experiment embeds this impossibility into its protocol which we shall not detail here. In a word, two measurements of a physical system are recognised to be jointly observable only if the product of the matrix operators that characterise them commutes. Each possible polarization observation pair at a relative angle $(\mathbf{a}^*, \mathbf{b}^*)$ is characterised by its own matrix operator H. Since we have four possible experimental designs under consideration, codified by the paired angle settings (\mathbf{a}, \mathbf{b}) , $(\mathbf{a}, \mathbf{b}')$, $(\mathbf{a}', \mathbf{b})$, and $(\mathbf{a}', \mathbf{b}')$, there are four distinct matrix operators, denoted by $H_{(a,b)}$, $H_{(a,b')}$, $H_{(a',b)}$, and $H_{(a',b')}$, which codify our experimental measurement possibilities. It is a simple matter to determine algebraically that no two of these proposed matrices commute.

All this is to say that the technical manipulations of mathematical quantum theory instantiate formally just what we knew to begin with... that we cannot simultaneously perform the measurement observation of the polarization products at *both* angle settings (\mathbf{a}, \mathbf{b}) and $(\mathbf{a}, \mathbf{b}')$ on the *same pair of photons*, not to speak of $(\mathbf{a}', \mathbf{b})$ and $(\mathbf{a}', \mathbf{b}')$ as well. Although quantum theoretical intrigue allows us to assert probabilities such as $P[(A(\mathbf{a}), B(\mathbf{b})) = (+1, -1)]$ or whatever, it abstains from any prognostication of the form

 $P[(A(\mathbf{a}), B(\mathbf{b})) = (+1, -1) \text{ and } (A(\mathbf{a}), B(\mathbf{b}')) = (+1, +1)]$. This would be a probability assertion regarding simultaneous outcomes of a jointly unobservable pair of events.

Well, who would want to? We shall now find out. Although impossible to perform, we are surely permitted to think about what might happen if we could perform such simultaneous experiments. Enter the realm of a gedankenexperiment. A feature that will be found crucial to the touted violation of Bell's inequality is that it pertains to experimental results supposedly conducted with a single photon pair at all four angle settings. This is very clear in the memorial article of Aspect [14] and many assessments of the inequality that properly recognize this. An example would be the article of Adenier [15]. Many discussants do not. How did such a context for the experiment arise? When the probabilistic pronouncements of quantum theory were formalized, Einstein among others was puzzled by the fact that the conditional probability for the outcome of the experiment at station A depends on both the angle at which the experiment is conducted at station B and on the outcome of that experiment. This matter is codified by the conditional probabilities we have seen in Equations (5). This entanglement of seemingly unrelated physical processes was deemed by Einstein to be a matter of "spooky action at a distance". Along with Podolsky and Rosen [16] he proposed a solution to this enigma, positing that there must be some other factors relevant to what might be happening at the polarizer stations A and B which would account for photon detections that are found to arise. As yet unspecified in the theory, he considered such factors to identify unknown values of "supplementary variables". It was proposed that the probabilities inherent in the results of quantum theory must be representations of scientific uncertainty about the action of these other variables on the two photons at their respective stations. This was their proposed way of accounting for the spooky action at a distance: the "state" of a photon in a polarization experiment, along with the condition of its attendant supplementary variables, involves its disposition to respond to the experiment at any and every one of its relative angle settings.

However, there is one aspect of the matter upon which Einstein wanted to insist: this was termed "the principle of local realism". Although it is central to matters under consideration in this problem, the applicable formulation of this principle, its meaning, and its relevance to the CHSH formulation of Bell's inequality (which we are soon to address) have been matters of contention. In unembellished form, the locality principle merely asserts that physical mechanics engaging at some particular location are not influenced by physical conditions arising in another unconnected locale far removed in space. What this would mean precisely for a gedanken scenario such as we will be considering is a matter of published discussion, notably among Mermin [17], Hess and Philipp [18], and Mermin [19], though many more have been involved. The discussion concerns whether the principle of locality alone is sufficient to establish a factorization that is involved in the CHSH form of Bell's inequality, and how the principle might need to be extended.

Whatever the precise form of its motivation relative to locality, the defiance of Bell's inequality derives from a specific and precise mathematical condition that we will recognize in its development. Fair enough, quantum theory does stipulate the probability for photon behaviour at station *A* with its polarizer direction

a as depending on whether the polarizer direction at *B* is set at **b** or **b'** and on what happens there. However, in any specific instance of the paired experiments conducted at a relative polarization angle (\mathbf{a}, \mathbf{b}) , if the measurement observation at *A* happened to equal $A(\mathbf{a}, \mathbf{b}) = +1$, say, then in this instance the measurement at *A* would have to be the same in any simultaneous gedankenobservation, no matter whether the direction setting at station *B* were **b** or **b'**. That is to say, if the polarization observation $A(\mathbf{a}) = +1$ in a particular experiment on a pair of photons measure in the paired angle design (\mathbf{a}, \mathbf{b}) , then the value of $A(\mathbf{a})$ would also have to equal +1 in a companion experiment on the same pair of photons if the polarization directions were set in the angle pairing $(\mathbf{a}, \mathbf{b}')$. The physical processes occurring at station *A* in any experimental run, uncertain though they may well be, are unrelated to those occurring far away at *B*.

Actually, our mathematical exposition of the probabilistic specifications of quantum theory has already deferred to such an understanding. We have been denoting the photon detection value at station A merely by $A(\mathbf{a})$ rather than denoting it by $A(\mathbf{a}, \mathbf{b})$, even before we have now introduced consideration of this principle of local realism. In the context of locality, the importance of such simplification of the notation was stressed explicitly by Aspect [14]. In fact we had no need to denote the paired direction at B in our notation for $A(\mathbf{a})$ earlier, because we can only do the experiment on a specific photon at one specific possibility pair determining the angle pairing $(\mathbf{a}^*, \mathbf{b}^*)$. So we have merely denoted the observed results as $A(\mathbf{a})$ and $B(\mathbf{b})$, or as $A(\mathbf{a})$ and $B(\mathbf{b}')$. Nonetheless, the QM probabilities of Equation (1) stipulated that each of the paired results of the experiments does depend jointly on the *relative* angle between the two polarization directions.

Despite this notational deference, we should now recognize and expressly declare that this principle of local realism is based upon a claim that lies outside the bounds of matters addressed by the theory of quantum physics. For, as we have noted, it is impossible to make a measurement of both the photon detection product $A(\mathbf{a})B(\mathbf{b})$ and the product $A(\mathbf{a})B(\mathbf{b}')$ on the same pair of photons. So quantum theory explicitly disavows addressing this matter directly, though it is surely a matter of relevance to the interpretation of quantum theoretic prescriptions.

We are ready to conclude this Section by proposing an experimental measurement that lies at the heart of Bell's inequality. We are not yet ready to assess it, nor to explain its relevance to the principle of local realism, but we shall merely air it now for viewing. Peculiar, it is considered to be the result of a gedankenexperiment.

Consider a pair of photons to be ejected toward stations A and B at which the pair of polarizers can be directed in any of the four relative angles we have described. According to the detection of whether the photons pass through the polarizers or are deflected by them, Bell's inequality pertains to an experimental

quantity defined by the equation

$$s \equiv A(\mathbf{a})B(\mathbf{b}) - A(\mathbf{a})B(\mathbf{b}') + A(\mathbf{a}')B(\mathbf{b}) + A(\mathbf{a}')B(\mathbf{b}')$$
(6)

Mathematically, we would refer to this quantity s as a linear combination of four polarization detection products. Any one of the four terms that determine the value of s could be observed in an experiment on a pair of prepared photons. Before we explain why this quantity is of interest, we should recognize right here only that we *can* observe the value of this quantity s if we are to conduct four component experiments on four distinct pairs of photons, each ejected toward stations A and B with the polarizers directed at a different relative angle pairing. However, we *cannot* observe the value of s if it were meant to pertain to all four experiments being conducted simultaneously on the same pair of photons. It just cannot be done, and quantum theory is very explicit about having nothing directly to say about its value. If we are to consider the value of s in such an experimental design, it could only be as the result of a "thought experiment". Enough said for now.

Why would we even be interested by such a "gedankenexperiment" as its perpetrators called it, and what does the supposition of "hidden variables" have to do with the matter?

5. Einstein's Proposal of Hidden Variables Relevant to the Matter

The famous paper [16] which addressed these matters presented ideas that had been brewing for many years [20]. It is now widely known merely as the EPR proposal. The ideas were opposed to those of others who were proclaiming that the experimental and theoretical discoveries of QM support the view that at its fundamental level of particulate matter, the behaviour of Nature is random, and that quantum theory had identified its probabilistic structure. Convinced that "he (the old one) is not playing dice with the universe", EPR proposed that the formulation of quantum theory is incomplete, and quantum probabilities represent our uncertainty about the influence of unspecified supplementary variables. The article stimulated a fury of healthy discussion and argument that I shall not summarize here. Well documented both in the professional journals of physics and in literature of popular science, the discussion has featured considerations of the collapse of a quantum system when subject to observation that disturbs it, the non-locality of quantum processes, and esoteric formulations of the "many worlds" view of quantum theory. What matters for my presentation here is that Einstein's views were widely relegated as a quirky peculiar sideline, and the recognition of randomness as a fundamental feature of quantum activity came to the forefront of theoretical physics.

Enter John Bell. Interested in a reconsideration of Einstein's view, he began his research with an idea to re-establish its validity as a contending interpretation of what we know. However, he was surprised to find this programme at an impasse when he discovered that if the principle of local realism is valid then the probabilistic specifications of quantum theory which we have described above seem to defy a simple requirement of mathematical probabilities. In the context of a hidden variables interpretation of the matter, this seemed to require that the principle of local realism must be rejected. Reported in a pair of articles [8] [9], these results too stimulated a continuation of the flurry which has lasted through the 2015 publication in *Nature* of their apparently definitive substantiation by the research at the Delft University of Technology.

The specification of Bell's inequality can take many forms. The context in which it is addressed in the remainder of my exposition here was presented in an article by Clauser, Horne, Shimony, and Holt [13], commonly referred to as the CHSH formulation. This was the form that attracted still another principal investigator in this story, Alain Aspect. A young experimentalist, he wondered how could such a monumental result of quantum physics pertain only to a thought experiment, devoid of actual physical experimental confirmation. He thought to have devised an experimental method that could confirm or deny the defiance of Bell's inequality. My assessment of his empirical work follows directly from his clear and thoughtful explanation of the situation [14] reported to a conference organized to memorialize Bell's work. My notation is largely the same as Aspect's. I adjust only the notation for expectation of a random variable to the standard form of E(X), replacing his notation of $\langle X \rangle$ which has become standard in mathematical physics in the context of bra-ket notation which I avoid. Here is how it works.

5.1. Explicit Construction of *s* with Hidden Variables

Hidden variables theory proposes that the quantity *s* which we have introduced in Equation (6) should be considered to derive from a physical function of unobserved and unknown hidden variables, whose values might be codified by the vector λ , viz.,

$$s(\lambda) = A(\lambda, \mathbf{a})B(\lambda, \mathbf{b}) - A(\lambda, \mathbf{a})B(\lambda, \mathbf{b}') + A(\lambda, \mathbf{a}')B(\lambda, \mathbf{b}) + A(\lambda, \mathbf{a}')B(\lambda, \mathbf{b}'),$$
(7)

for $\lambda \in \Lambda$. The variable designated by λ here could be a vector of any number of components identifying unknown features of the experimental setup that are relevant to the outcome of the experiment in any specific instantiation. The set designated by Λ is meant to represent the space of possible values of these hidden variables. The status of these variables in the context of any particular experiment is supposed only to depend on the state of the photon pair and its surrounds, independent of the angle setting $(\mathbf{a}^*, \mathbf{b}^*)$ at which the polarizers are directed. According to the deterministic outlook underlying physical theory relying on hidden variables, if we could only know the values of these unspecified variables at the time of any experimental run and have a complete theoretical understanding of their relevance to the polarization behaviour of the photon pair, then we would know what would be the values of the polarization incidence detection of the photon pair at any one or all of the possible angle settings.

Now the personalist subjective theory of probability (apparently subscribed to by Einstein, and surely by Bruno de Finetti and by me) specifies that any individual's uncertain knowledge of the values of observable but unknown quantities could be representable by a probability density over its space of possibilities. Aspect denotes such a density in this situation by $\rho(\lambda)$. For any proponent of quantum probabilities it might well be presumed to be "rotationally invariant" over the full 360° of angles at which the photon may be fluttering toward the polarizer. That is to say, the probabilities for the possible values of the supplementary variables do not depend on the angular direction in (x, y) dimensions of the photons along **z** axes heading toward stations *A* and *B*, rather only on the size of the angle.

Since we avowedly have no idea of what these hidden variables might be, much less what their numerical values may be relevant to any specific experimental run, we can only ponder the "expected value" of $s(\lambda)$ with respect to the distribution specified by $\rho(\lambda)$. The feature of rotational invariance implies that this expectation is the same no matter what be the rotational angle at which the photons flutter relative to their (x, y) plane detections. Let's write this expectation down:

$$E[s(\lambda)] = E[A(\lambda, \mathbf{a})B(\lambda, \mathbf{b})] - E[A(\lambda, \mathbf{a})B(\lambda, \mathbf{b}')] + E[A(\lambda, \mathbf{a}')B(\lambda, \mathbf{b})] + E[A(\lambda, \mathbf{a}')B(\lambda, \mathbf{b}')],$$
(8)

where expectation is assessed with respect to the density $\rho(\lambda)$, yielding then more simply

$$E[s] = E[A(\mathbf{a})B(\mathbf{b})] - E[A(\mathbf{a})B(\mathbf{b}')] + E[A(\mathbf{a}')B(\mathbf{b})] + E[A(\mathbf{a}')B(\mathbf{b}')]$$

as an expectation relative to the random polarization products at these various angles. Equation (8) follows directly from Equation (7) because a rule of probability says that the expectation of any linear combination of random quantities equals the same linear combination of their expectations. Fortunately, we have already reported in Equation (5) that the probabilities of quantum theory identify the expected value of any polarization product at the variable relative polarization angle $(\mathbf{a}^*, \mathbf{b}^*)$ as $E[A(\mathbf{a}^*)B(\mathbf{b}^*)] = \cos 2(\mathbf{a}^*, \mathbf{b}^*)$. So we are ready to proceed.

5.2. Finally, Bell's Inequality

We have now arrived at a place we can state precisely what Bell's inequality says. There is just a little more specificity to detail before we soon will have it. However, I should alert you that there is a little tic in the understanding of Equation (8) to which we shall return after we learn how the inequality is currently understood to be defied by quantum theory. But on the face of it, the validity of Equation (8) is plain as day.

Now re-examining Equation (7), it is apparent that it can be factored into a simplified form:

$$s(\lambda) = A(\lambda, \mathbf{a})B(\lambda, \mathbf{b}) - A(\lambda, \mathbf{a})B(\lambda, \mathbf{b}') + A(\lambda, \mathbf{a}')B(\lambda, \mathbf{b}'), \quad \text{for } \lambda \in \Lambda,$$

$$= A(\lambda, \mathbf{a})[B(\lambda, \mathbf{b}) - B(\lambda, \mathbf{b}')] + A(\lambda, \mathbf{a}')[B(\lambda, \mathbf{b}) + B(\lambda, \mathbf{b}')], \text{ and alternatively}$$

$$= B(\lambda, \mathbf{b})[A(\lambda, \mathbf{a}) + A(\lambda, \mathbf{a}')] - B(\lambda, \mathbf{b}')[A(\lambda, \mathbf{a}) - A(\lambda, \mathbf{a}')]. \quad (9)$$

It is important to notice that once again, in performing this simple factorization of the components $A(\lambda, \mathbf{a})$ and $A(\lambda, \mathbf{a}')$ in this second line, we have implicitly presumed the principle of local realism (and perhaps even more according to the interpretations considered in the discussions among Mermin, Hess, Philipp and others to which we have alluded). For when we consider the first two summands of the first line, $A(\lambda, \mathbf{a})B(\lambda, \mathbf{b})$, and $A(\lambda, \mathbf{a})B(\lambda, \mathbf{b}')$, we should notice that the value of $A(\lambda, \mathbf{a})$ in that first term is evaluated in an experiment at which the paired polarization angle is (\mathbf{a}, \mathbf{b}) , whereas in the second term from which it is factored it is evaluated in an experiment at the relative polarization angle $(\mathbf{a}, \mathbf{b}')$. It is the principle of local realism or its extension, extraneous to any claims of quantum theory, that provides the observed value of $A(\lambda, \mathbf{a})$ must be identical in these two conditions which are impossible to instantiate together. It is only under the condition of this assertion that we would be able to factor this term out of the two expressions. The same goes for the factorization of $A(\lambda, \mathbf{a}')$. This is not a source of any worry. I am merely mentioning this so that we are all aware of what is going on. The same feature of supposition is pertinent to the alternative factorization of the terms $B(\lambda, \mathbf{b})$ and $B(\lambda, \mathbf{b}')$ in the third line from the terms of the first line.

Having arrived at this factorization, it will now take just a little thought to recognize that if the value of the quantity *s* is supposed to be determined from a thought experiment on a single pair of photons, then the numerical value of *s* can equal only either +2 or -2. Of course, if we were to calculate the value of *s* from performing four component experiments with *four different pairs* of photons (something we can actually do), then the four component product values might each then equal either -1 or +1, so the value of *s* might equal any of $\{-4, -2, 0, +2, +4\}$. However, in such a case the factorization we performed in Equation (9) would not be permitted. For each of the observed detection products appearing in the first line would pertain to a different pair of photons whose multiplicands would be free to equal either +1 or -1 as prescribed by experiment. The same possibilities would be accessible if the principle of local realism were not valid. However, if the value of *s* were to be calculated from the results of a thought experiment on the same pair of photons, then its possibilities would be limited according to local realism (and perhaps its extension) merely to

 $\{-2,+2\}$. Here is how to recognize this.

Suppose the values of $B(\lambda, \mathbf{b})$ and $B(\lambda, \mathbf{b}')$ were both observed to equal +1. Then the first term in the factored form of the second line must equal $A(\lambda, \mathbf{a})[B(\lambda, \mathbf{b}) - B(\lambda, \mathbf{b}')] = 0$; and furthermore, the second term in the factored representation would then be $A(\lambda, \mathbf{a}')[B(\lambda, \mathbf{b}) + B(\lambda, \mathbf{b}')]$. The factor

 $A(\lambda, \mathbf{a}')$ equaling either +1 or -1 would then be multiplied by the factor $[B(\lambda, \mathbf{b}) + B(\lambda, \mathbf{b}')]$ which would equal the number +2. Thus, the value of *s* could equal only either -2 or +2. Alternatively, suppose that the values of $B(\lambda, \mathbf{b})$ and $B(\lambda, \mathbf{b}')$ are both observed to equal -1. Then by a similar argument the value of the first factored expression would again equal 0 and the second expression would equal either -1 or +1 multiplied now by -2. Again the computed result of the value of *s* could equal only -2 or +2. I leave it to the reader to confirm the same result for the possible values of *s* if the values of $B(\lambda, \mathbf{b})$ and $B(\lambda, \mathbf{b}')$ were observed to equal either -1 and +1 respectively, or +1 and -1 respectively.

The conclusion is indisputable. If the principle of local realism holds, then the value of *s* that would be instantiated as a result of a thought experiment on the same pair of photons in all four polarization angle settings can equal only -2 or +2. Thus, the expected value E(s) deriving from *any* coherent probability distribution over the four values of the component paired polarization experiments would have to be a number between -2 and +2. Stated algebraically and simply, without all the provisos explaining its content, Bell's inequality is the requirement that $-2 \le E(s) \le +2$.

Well, what do the probabilities of quantum theory imply for the value of E(s)? The answer universally presumed to be correct by proponents of the Bell violation is that when the design of the four experiments on a single pair of photons is constructed at a particular array of angle settings that we shall soon identify, then $E(s) = 2\sqrt{2} = 2.8284$ to four decimal places, a number that exceeds +2. (I shall present the details in the next paragraph.) Moreover, the experimental results of Aspect, as well as the more sophisticated experimentation of succeeding decades, is understood to corroborate this result to many decimal places. I will soon explain how this result is derived as well. However, I will insist on also showing you that not only is this theoretical derivation wrong, but that the calculations used to corroborate this result from experimental evidence are misdirected. Nonetheless, there is nothing at all wrong with the experimental results, which are what they are.

5.3. The Mistaken Violation of Bell's Inequality

It turns out that Bell's inequality is *not* deemed to be defied at *every* four-plex of possible experimental angle settings that we have characterised generically as (\mathbf{a}, \mathbf{b}) , $(\mathbf{a}', \mathbf{b})$, or $(\mathbf{a}', \mathbf{b}')$. At some paired directional settings of the polarizers it seems not to be defied at all. Among other pairings at which it seems to be defied, it is apparently defied more strongly at some pairings than at others. Aspect had thought that if we were to find experimental evidence of the defiance, we should try to find it at the angle pairings for which the theoretical defiance is the most extreme. It is a matter of simple calculus of extreme values to discover that the most extreme violation of the equality should occur at the angle settings $(\mathbf{a}, \mathbf{b}) = -\pi/8$, $(\mathbf{a}', \mathbf{b}) = -\pi/8$, $(\mathbf{a}', \mathbf{b}) = \pi/8$, or $(\mathbf{a}', \mathbf{b}') = -\pi/8$.

(The angle measurements are expressed here in terms of their polar representations. In terms of degrees, the angle $-\pi/8 = -22.5^{\circ}$, while $-3\pi/8 = -67.5^{\circ}$, and $+\pi/8 = +22.5^{\circ}$.) You may wish to examine our **Figure 2** and notice that the angles between the various polarization directions we depicted there correspond to these relative angles. For the record, doubling these angles yields the values of $\pm \pi/4 = \pm 45^{\circ}$ and $-3\pi/4 = -135^{\circ}$ in these instances. And why does that matter?...

Recall Equation (8) and the ensuing sentences. Evaluating E(s) according to this equation at the four angle settings just mentioned requires evaluating the summand component expectations. Each of them in the form $E[A(\mathbf{a}^*)B(\mathbf{b}^*)] = \cos 2(\mathbf{a}^*, \mathbf{b}^*)$, these would then be

$$E[A(\lambda, \mathbf{a})B(\lambda, \mathbf{b})] = \cos 2(\mathbf{a}, \mathbf{b}) = \cos (-\pi/4) = 1/\sqrt{2}, \qquad (10a)$$

$$E\left[A(\lambda,\mathbf{a})B(\lambda,\mathbf{b}')\right] = \cos 2(\mathbf{a},\mathbf{b}') = \cos\left(-3\pi/4\right) = -1/\sqrt{2}, \qquad (10b)$$

$$E\left[A(\lambda, \mathbf{a}')B(\lambda, \mathbf{b})\right] = \cos 2(\mathbf{a}', \mathbf{b}) = \cos(\pi/4) = 1/\sqrt{2}, \qquad (10c)$$

and $E[A(\lambda, \mathbf{a}')B(\lambda, \mathbf{b}')] = \cos 2(\mathbf{a}', \mathbf{b}') = \cos(-\pi/4) = 1/\sqrt{2}$, (10d) then apparently yielding

$$E[s(\lambda)] = 1/\sqrt{2} - (-1/\sqrt{2}) + 1/\sqrt{2} + 1/\sqrt{2} = 4/\sqrt{2} = 2\sqrt{2}.$$

Voila! The expected value of *s* apparently equals $2\sqrt{2} \approx 2.8284$, a real number outside of the interval [-2,+2], defying Bell's inequality! What could be more simple, direct, and stunning?

The answer is seen most simply by constructing and then examining a matrix, which in the jargon of the operational subjective theory of probability is called "the realm matrix of possible observation values" that could result from the performance of the gedankenexperiment in CHSH form. I will display this entire matrix on the next page, in a partitioned form of its full extension as it pertains to every aspect of the problem we shall discuss. Then we shall discuss it, piece by piece. I should mention here that while the name "realm matrix of possibilities" has arisen from within the operational subjective construction of the theory of probability, the matrix itself is merely a well-defined matrix of numbers that can be understood and appreciated by any experimentalist, no matter what may be your personal views about the foundations of probability. In the jargon of quantum physics it might be called the ensemble matrix of possible observation vectors.

6. A Neglected Functional Dependence

In specifying the QM motivated expectation $E[s(\lambda)]$ as they do in our Equation (8), Aspect/Bell fail to recognize a *symmetric functional dependence* among the values of the four proposed polarization products composing $s(\lambda)$ as defined in Equation (7), when it is meant to correspond to the result of the 4-ply thought-experiment on the same pair of photons. Perhaps surprisingly, the achieved values of any three *products* of the paired polarization indicators imply a unique value for the fourth product. We now engage to substantiate this claim.

6.1. The Realm Matrix of Experimental Quantities

Consider the realm matrix of all quantities relevant to the observations that might be made in the proposed 4-ply gedankenexperiment on a pair of photons under investigation. On the left side of the realm equation is written the name $\mathbf{R}(\mathbf{X})$, where \mathbf{X} is a partitioned vector of names of every quantity that will be relevant to the outcome of the experiment and what quantum theory asserts about it. You will already recognize those appearing in the first two partitioned sections. On the right side of the realm equation appears a matrix whose columns exhaustively identify the values of these partitioned quantities that could possibly result from conducting the gedankenexperiment. We shall discuss them in turn.

($(A(\mathbf{a}))$		(1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1)
	$B(\mathbf{b})$		(1 1	1	1	1					1		1					
	$A(\mathbf{a}')$		-	-	1	1	1	1			-1							
	$B(\mathbf{b}')$		1	1	-1		1	1		-1	1			-1	1		-1	
	****		I	-1	1	-1	I	-1	I	-1	I	-1	1	-1	I	-1	1	-1
	$A(\mathbf{a})B(\mathbf{b})$																	
	$A(\mathbf{a})B(\mathbf{b}')$		1	1	1						-1				1	1	1	1
	$A(\mathbf{a}')B(\mathbf{b})$		1	-1	1	-1	-1	1	-1	1	1	-1	1	-1	-1	1	-1	1
			1	1	-1	-1	1	1	-1	-1	-1	-1	1	1	-1	-1	1	1
	$A(\mathbf{a}')B(\mathbf{b}')$		1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1
_	****																	
R	$\mathcal{A}(\mathbf{a}')\mathcal{B}(\mathbf{b}')$	=	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1
	* * * * *																	
	$\Sigma_{/\left(a,b\right)}$		3	-1	-1	-1	1	1	-3	1	1	-3	1	1	-1	-1	-1	3
	$\Sigma_{/(a,b')}$		3	1	-1	1	1	-1	-3	-1	-1	-3	-1	1	1	-1	1	3
	$\Sigma_{/(\mathbf{a}',\mathbf{b})}$		3	-1	1	1	-1	-1	-3	1	1	-3	-1	-1	1	1	-1	3
	$\Sigma_{/\left(\mathbf{a}',\mathbf{b}' ight)}$		3	1	1	-1	-1	1	-3	-1	-1	-3	1	-1	-1	1	1	3
	* * * * *																	ł
	$s(\lambda)$		2	_	-2	2	2				-2			2	2	_	2	2
	$S_{\mathcal{A}/\mathcal{B}(\mathbf{a}',\mathbf{b}')}$		2	4	0	2	2	0	0	-2	-4	-2	-2	0	0	-2	2	0
			1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1)
1			-															,

The sixteen columns of four-dimensional vectors in the first partitioned block exhaustively list all the speculative 4×1 vectors of observation values that could possibly arise among the four experimental detections of photons at the four angles of polarizer pairings. In order to observe the detection *products* at the four relative angles $A(\mathbf{a})B(\mathbf{b}), A(\mathbf{a})B(\mathbf{b}'), A(\mathbf{a}')B(\mathbf{b})$, and $A(\mathbf{a}')B(\mathbf{b}')$, we would surely have to observe each of the four *multiplicands* involved in their specification: $A(\mathbf{a}), B(\mathbf{b}), A(\mathbf{a}')$, and $B(\mathbf{b}')$. Since each of these observation values might equal only either -1 or +1, there are sixteen possibilities of the 4-dimensional result of the 4-ply experiment. There are no presumptions made about these prospective quantity values: neither whether they "exist" or not prior to the conduct of the experiment at all, nor even whether they exist in any form after the experiment is conducted. We have merely made a list of what we could possibly observe if indeed we were capable of conducting the proposed gedankenexperiment on the same pair of photons. The observation vector would have to equal one of the 16 columns appearing in the top bank of the partitioned realm matrix.

Every other component quantity in the columns displayed in subsequent blocks of the realm matrix is computed via some function of these possibilities. Notice once again that the "exhaustiveness" of this list presupposes the principle of local realism, specifying for example that the value of $A(\mathbf{a})$ identifying whether the photon passes through the polarizer at A or not, would be the same no matter whether the polarizer at which the paired photon engages station B is set at direction \mathbf{b} or at \mathbf{b}' .

To begin the completion of the realm matrix, the second block of components identifies the four designated *products* of the paired polarization indicators that yield the value of the quantity s as it is simply defined in Equation (6). The first row of this second block, identifying the product $A(\mathbf{a})B(\mathbf{b})$, is the componentwise product of the first two rows of the first block. The second row of this block, identifying the product $A(\mathbf{a})B(\mathbf{b}')$, is the componentwise product of the first block, and so on. This second block lists exhaustively all the combinations of polarization products that we could possibly observe in the conduct of our gedankenexperiment. Examine any one of these columns of products, checking that in fact the value of each product in that column is equal to the product of the corresponding multiplicands appearing in the column directly above it.

The first item to notice about this realm matrix is that, whereas the sixteen columns of the first block of polarization observations are distinct, the second block contains only *eight* distinct column vectors. Columns 9 through 16 in block two of the realm matrix reproduce columns 1 through 8 in reverse order. Moreover, examining the first three rows of this second block more closely, it can be recognized that the first eight columns of these rows exclusively exhaust the simultaneous measurement possibilities for the three product quantities they identify. These are the eight vectors of the cartesian product $\{+1, -1\}^3$, which are repeated in columns nine through sixteen in reverse order. Together, what these two observations mean is that the fourth product quantity in this second block of vector components is derivable as a function of the first three. What is more, any one of the product quantities identified in block two is determined by the same computational function of the other three! This is what I meant earlier when alluding that the photon detection products in the gedankenexperiment have embedded within them four symmetric functional relations. This can be seen by examining the columns of the *fourth* block of the matrix, which we shall do shortly.

The third block of the realm matrix contains only a single row, corresponding to a quantity we designate as $\mathcal{A}(\mathbf{a}')\mathcal{B}(\mathbf{b}')$. This quantity takes values only of

 ± 1 , but it is logically independent of the product quantities appearing in the first three rows of block two. This is the quantity that Aspect/Bell think they are assessing when they freely specify the quantum expectations for all four angle settings as they do, seemingly defying Bell's inequality. We denote its name with calligraphic type to distinguish it from the actual polarization product

 $A(\mathbf{a}')B(\mathbf{b}')$ whose functional relation to the other three products we are now identifying. Peculiar, this singular component of the fourth partition block is not an "Alice and Bob" observation quantity, but rather an "Aspect/Bell" imagined quantity. It is logically independent of the first three "Alice and Bob" products. This is to say that whatever values these products may be, the value of $\mathcal{A}(\mathbf{a}')\mathcal{B}(\mathbf{b}')$ may equal +1 in the appropriate row among the first eight columns, or it may equal -1 in the corresponding column among the second eight. However, it does *not* represent the photon detection product $A(\mathbf{a}')B(\mathbf{b}')$ in the four imagined experiments on a single photon pair.

6.2. Specifying the Functional Form via Block Four

Quantities in the fourth block of the realm matrix are designated with the names $\Sigma_{/(\mathbf{a},\mathbf{b})}$, $\Sigma_{/(\mathbf{a},\mathbf{b}')}$, $\Sigma_{/(\mathbf{a}',\mathbf{b})}$, and $\Sigma_{/(\mathbf{a}',\mathbf{b}')}$. These quantities are defined by sums of column elements in *those rows of the second block* that are *not marked* behind the slash in the notational subscript. For examples,

$$\Sigma_{/(\mathbf{a},\mathbf{b})} \equiv A(\mathbf{a})B(\mathbf{b}') + A(\mathbf{a}')B(\mathbf{b}) + A(\mathbf{a}')B(\mathbf{b}'), \text{ and}$$

$$\Sigma_{/(\mathbf{a},\mathbf{b}')} \equiv A(\mathbf{a})B(\mathbf{b}) + A(\mathbf{a}')B(\mathbf{b}) + A(\mathbf{a}')B(\mathbf{b}').$$

The quantities $\Sigma_{/(\mathbf{a}',\mathbf{b})}$ and $\Sigma_{/(\mathbf{a}',\mathbf{b}')}$ are defined similarly.

Next to notice is that the fourth row of the *second* matrix block, corresponding to $A(\mathbf{a}')B(\mathbf{b}')$, has an entry of 1 if and only if the fourth row of the *fourth* block, corresponding to $\Sigma_{/(\mathbf{a}',\mathbf{b}')}$, has an entry of -1 or +3 in the same column. When that entry is +1 or -3, the corresponding entry of the second block is -1. What this recognition does is to identify the functional relation of the fourth polarization product to the first three polarization products, viz.,

$$A(\mathbf{a}')B(\mathbf{b}') = \mathbf{G}\left[A(\mathbf{a})B(\mathbf{b}), A(\mathbf{a}')B(\mathbf{b}), A(\mathbf{a})B(\mathbf{b}')\right]$$

$$\equiv \left(\Sigma_{/(\mathbf{a}',\mathbf{b}')} = -1 \text{ or } +3\right) - \left(\Sigma_{/(\mathbf{a}',\mathbf{b}')} = +1 \text{ or } -3\right).$$
 (11)

Here and throughout this note I am using indicator notation in which parentheses surrounding a mathematical statement that might be true and might be false signifies the number 1 when the interior statement is true, and signifies 0 when it is false.

Some eyeball work is required to recognize the functional relationship (11) by examining the final row of block two and of block four together. It may take even more concentration to recognize that this very same functional rule identifies each of the other three polarization products as a function of the other three as well! The four product quantities $A(\cdot)B(\cdot)$ are related by four symmetric functional relationships, each of them being calculable via the same functional

rule applied to the other three! This surprising recognition identifies the source of the Aspect/Bell error in assessing the QM-motivated expectation for $s(\lambda)$ in the way they do.

It is surely true that $E[s(\lambda)]$ equals a linear combination of four expectations of polarization products, as specified in Equation (8). Moreover, if the definition of $s(\lambda)$ in Equation (6) were understood to represent the combination of observed products from experiments on four distinct pairs of photons, then the possible values of $s(\lambda)$ would span the integers $\{-4, -2, 0, 2, 4\}$; the expectation of each product $E[A(\mathbf{a}^*)B(\mathbf{b}^*)]$ would equal $-1/\sqrt{2}$ or $+1/\sqrt{2}$ as appropriate to the angle $(\mathbf{a}^*, \mathbf{b}^*)$; and $E[s(\lambda)]$ would equal $2\sqrt{2}$ as proposed by Aspect/Bell. This involves no violation of any probabilistic inequality at all, and there is no suggestion of mysterious activity of quantum mechanics.

However, when it is proposed that the paired polarization experiments at all four considered angles pertain to the same photon pair, then each of the products is restricted to equal the specified function value of the other three that we identified explicitly for $A(\mathbf{a}')B(\mathbf{b}')$ in Equation (11) as $\Sigma_{/(\mathbf{a}',\mathbf{b}')}$ via the function $\mathbf{G}[A(\mathbf{a})B(\mathbf{b}), A(\mathbf{a}')B(\mathbf{b}), A(\mathbf{a})B(\mathbf{b}')]$. In this context, Aspect's expected quantity would be representable equivalently by any of the following equations:

$$E[s(\lambda)] = E[A(\mathbf{a})B(\mathbf{b})] - E[A(\mathbf{a})B(\mathbf{b}')] + E[A(\mathbf{a}')B(\mathbf{b})]$$

+ $E\{G[A(\mathbf{a})B(\mathbf{b}), A(\mathbf{a})B(\mathbf{b}'), A(\mathbf{a}')B(\mathbf{b})]\}$
= $E[A(\mathbf{a})B(\mathbf{b})] - E[A(\mathbf{a})B(\mathbf{b}')] + E[A(\mathbf{a}')B(\mathbf{b}')]$
+ $E\{G[A(\mathbf{a})B(\mathbf{b}), A(\mathbf{a})B(\mathbf{b}'), A(\mathbf{a}')B(\mathbf{b}')]\}$
= $E[A(\mathbf{a})B(\mathbf{b})] + E[A(\mathbf{a}')B(\mathbf{b})] + E[A(\mathbf{a}')B(\mathbf{b}')]$
- $E\{G[A(\mathbf{a})B(\mathbf{b}), A(\mathbf{a}')B(\mathbf{b}), A(\mathbf{a}')B(\mathbf{b}')]\}$
= $-E[A(\mathbf{a})B(\mathbf{b}')] + E[A(\mathbf{a}')B(\mathbf{b})] + E[A(\mathbf{a}')B(\mathbf{b}')]\}$
= $-E[A(\mathbf{a})B(\mathbf{b}')] + E[A(\mathbf{a}')B(\mathbf{b})] + E[A(\mathbf{a}')B(\mathbf{b}')]\}$ (12)
+ $E\{G[A(\mathbf{a})B(\mathbf{b}'), A(\mathbf{a}')B(\mathbf{b}), A(\mathbf{a}')B(\mathbf{b}')]\}$

The symmetries imposed on this problem would yield an identical result in each case, which would surely *not* yield $2\sqrt{2}$ at all. *This is the mathematical error of neglect to which the title of this current exposition alludes.* What might the symmetries yield?

The functional relation we have exposed in Equation (11) is *not* linear. If it were, then the specification of an expectation for its arguments would imply the expectation value for the function value. As it is not, the specification of expectation values for the arguments only imply *bounds* on any cohering expectation value for the fourth. These numerical bounds can be computed using a theorem due to Bruno de Finetti which he first presented at his famous lectures at the Institute Henri Poincaré in 1935. He named it only in his swansong text [21]. It was first characterized in the form of a linear programming problem by Bruno and Gilio [22], and has appeared in various forms in recent decades. Among them are presentations in dual form by Whittle [23] [24] using standard formalist notation and objectivist concepts. We shall review the content of de Finetti's

theorem shortly, and then examine its relevance to assessing the expectation of $s(\lambda)$ motivated by considerations of quantum mechanics. We need first to air some further brief remarks about the final block of the realm matrix.

6.3. The Remaining Block of Quantities and Their Realm Components

The first row of block five of the realm matrix merely identifies the values of $s(\lambda)$ associated with the polarization observation possibilities enumerated in the columns of block one. Each component of this row is computed from the corresponding column of block two according to the defining Equation (1). It is evident that every entry of this row is either -2 or +2. This corresponds to the argument we have made following the factorization Equation (9) in Section 5. The second row of this block pertains to a quantity denoted as $s_{A/B(\mathbf{a}',\mathbf{b}')}$. Its value is defined similarly to Equation (6), but its final summand is specified as the Aspect/Bell quantity $\mathcal{A}(\mathbf{a}')\mathcal{B}(\mathbf{b}')$ rather than the actual polarization product quantity $A(\mathbf{a}')B(\mathbf{b}')$ that appears in this equation defining $s(\lambda)$. Again peculiar, its realm can be seen to include the elements $\{-4, -2, 0, 2, 4\}$ whereas the realm of $s(\lambda)$ includes only $\{-2, 2\}$. The fact that the possibilities for $s_{\mathcal{A}/\mathcal{B}(\mathbf{a}',\mathbf{b}')}$ include both -4 and +4 is what makes it not surprising that the expectation of *this quantity* is $2\sqrt{2}$ as pronounced by proponents of the Aspect/Bell analysis.

The third row of block five is merely an accounting device, denoting that the "sure" quantity, 1, is equal to 1 no matter what the observed results of the four imagined optic experiments of Aspect/Bell might be. Its relevance will become apparent when the need arises to apply de Finetti's fundamental theorem to quantum assertions.

It is time for a rest and an interlude. It is a mathematical interlude whose complete understanding relies only on your knowledge of some basic methods of linear algebra. If you would like a slow didactic introduction to the subject, my best suggestion is to look at Chapter 2.10 of my book [25]. You may even wish to start in Section 2.7. Another purely computational presentation appears in the article of Capotorti *et al.* [26], Section 4. I will make another attempt here in a brief format, merely to keep this current exposition self-contained. What does the fundamental theorem of probability say?

7. The Relevance of the Fundamental Theorem of Probability

In brief, the fundamental theorem says that if you can specify expectation values for any vector of quantities whatsoever, then the rules of probability provide numerical bounds on a cohering expectation for any other quantity you would like to assess. These can be computed from the compilation of a linear programming routine. If the expectations you have specified are incoherent (meaning self-contradictory) among themselves, then the linear programming problems they motivate have no solution. This theorem is immediately relevant to our situation here in which we have identified quantum-theory-motivated expectations for any three of the four detection products that determine the value of s for the gedankenexperiment. We wish to find the bounds on the cohering expectation for the fourth detection product which is restricted to equal a function value determined by these three. A discursive pedagogical introduction is available in Lad [[25], Section 2.10]. In brief, here is how the theorem works.

Suppose you have identified the expectations for N quantities, and you are wondering what you might assert as the expectation for another one, call it the $(N+1)^{st}$. What you should do to assess your sensible possibilities is firstly to construct the realm matrix of possible values for the vector of all (N+1) quantities. Let's call the vector $\mathbf{X}_{N+1} = (X_1, X_2, \dots, X_N, X_{N+1})^T$, and call its realm matrix then $\mathbf{R}(\mathbf{X}_{N+1})$. In general it will look something like the realm matrix we have just constructed for various aspects of our gedankenexperiment. It will have N+1 rows, and some number K columns. Just as an example, the realm matrix we have already constructed happens to have (N+1)=16 rows and K=16 columns. (Mind you, we have not yet specified expectation for the first N components of the quantity vector to which this realm applies, but let's not let that deter us. I am merely suggesting here an example of a realm matrix that could be considered to have (N+1) rows. Let's continue with the general abstract specification.)

Now any such vector of quantities can be expressed as the product of its realm matrix with a particular vector of events. The matrix equation, displayed in a form that partitions the final row, would look like this:

$\begin{pmatrix} X_1 \end{pmatrix}$		$\int x_{1,1}$	<i>x</i> _{1,2}	•••	$x_{1,(K-1)}$	$x_{1,K}$	$\left(\begin{array}{c} \left(\mathbf{X}_{N+1} = \mathbf{x}_{1} \right) \end{array} \right)$
		x _{2,1}	<i>x</i> _{2,2}	•••	$x_{2,(K-1)}$	<i>x</i> _{2,<i>K</i>}	$\left(\mathbf{X}_{N+1}=\mathbf{x}_{2}\right)$
X ₃		x _{3,1}	<i>x</i> _{3,2}	•••	$x_{3,(K-1)}$	<i>x</i> _{3,<i>K</i>}	$\left(\mathbf{X}_{N+1}=\mathbf{x}_{3}\right)$
:	=	:	÷	·.	:	:	: .
X_N		<i>x</i> _{<i>N</i>,1}	$x_{N,2}$		$x_{N,(K-1)}$	$x_{N,K}$	
***		***	* *	* *	* *	**	$\left \left(\mathbf{X}_{N+1} = \mathbf{x}_{(K-1)} \right) \right $
$\left(X_{N+1}\right)$		$(x_{(N+1),1})$	$x_{(N+1),2}$	•••	$x_{(N+1),(K-1)}$	$x_{(N+1),K}$	$\left(\left(\mathbf{X}_{N+1} = \mathbf{x}_{K} \right) \right)$

On the left of this equation is the column vector of the quantity observations under consideration. To the right of the equality comes firstly the $(N+1) \times K$ realm matrix whose *K* columns list all the possible columns of numbers that could possibly result as the observation vector. These *K* columns, each of which has (N+1) components, correspond to vectors denoted as $\mathbf{x}_{.1}, \mathbf{x}_{.2}, \mathbf{x}_{.3}, \dots, \mathbf{x}_{.(K-1)}$, and $\mathbf{x}_{.K}$. (The initial subscripted dot denotes that this is a whole column of numbers. The number that follows the dot denotes which of the columns of the matrix it is we are talking about.) This matrix is multiplied by the final $K \times 1$ column vector of events that identify whether the quantity vector \mathbf{X}_{N+1} turns out upon observation to be the first, the second,..., or the K^{th} of these listed columns. We shall denote this vector by $\mathbf{Q}(\mathbf{X}_{N+1})$, and call it "the partition vector generated by \mathbf{X}_{N+1} ". One and only one of its component events will equal 1 and the rest will equal 0. But we do not know which of them is the 1, because we do not know which column of possibilities in the realm matrix will be the one that represents the observed outcome of the vector of quantities \mathbf{X}_{N+1} .

We can represent this matrix equation more concisely and in a useful form by writing it in an abbreviated partitioned form:

$$\begin{pmatrix} \mathbf{X}_{N} \\ X_{N+1} \end{pmatrix} = \mathbf{R} \begin{pmatrix} \mathbf{X}_{N} \\ X_{N+1} \end{pmatrix} \mathbf{Q} \left(\mathbf{X}_{(N+1)} \right).$$

The payoff from constructing this matrix structure is that now every row of this partitioned equation has on its left-hand side the unknown value of a quantity, X_i . On the right-hand side in that row appears a list of the possible values of that quantity, each multiplied in a linear combination with the events that denote whether each of them is indeed the value of this quantity (in the context of the observed values of the other quantities shown in that column as well). Each row of this equation specifies how a different one of the quantities under consideration equals a linear combination of events. We have heard of that before. The expectation of a linear combination equals the same linear combination of expectations for those events, which would be their probabilities if we could specify values for them. This tells us that we can evaluate an expectation operator on this partitioned equation to yield the result that

$$E\begin{pmatrix} \mathbf{X}_{N} \\ X_{N+1} \end{pmatrix} = \mathbf{R}\begin{pmatrix} \mathbf{X}_{N} \\ X_{N+1} \end{pmatrix} P \Big[\mathbf{Q} \Big(\mathbf{X}_{(N+1)} \Big) \Big].$$

Well, we have not mentioned anything about probability specifications appearing in the vector $P\left[\mathbf{Q}\left(\mathbf{X}_{(N+1)}\right)\right]$ on the right-hand side of this equality. The only restrictions of probability are that these must be non-negative numbers that sum to 1, since the vector $\mathbf{Q}\left(\mathbf{X}_{(N+1)}\right)$ constitutes a partition. We have mentioned only that expectations have been identified for the first *N* components of the vector on the left-hand side, $E(\mathbf{X}_N)$. Yet we can compute something important on the basis of this realization. The linearity of this equation ensures that the implied value for the expectation of the final unspecified component $E(X_{N+1})$ must lie within a specific interval. It is computable as the

minimum and maximum values of $\mathbf{R}(X_{N+1})\mathbf{q}_{K}$

subject to the linear restrictions $\mathbf{R}(\mathbf{X}_N)\mathbf{q}_K = E(\mathbf{X}_N)$,

as required of the expectations that we have presumed to be specified,

and where the components of \mathbf{q}_{K} must be non-negative and must sum to 1.

Such a computation is provided by the procedures of a linear programming problem. The "solutions" to these linear programming problems are the vectors \mathbf{q}_{\min} and \mathbf{q}_{\max} that yield these minimum and maximum values for $E(X_{N+1})$ subject to these constraints. The final row vector identifying $E(X_{N+1})$ whose extreme values we seek is called "the objective function" of the problems. Its coefficients are the partitioned final row of the general realm matrix we identify as $\mathbf{R}(X_{N+1})$. Notice that that X is not bold. It represents merely the final quan-

tity in the column vector \mathbf{X}_{N+1} . The coefficients vector of the objective function is the final row vector of the realm matrix.

Here are the specific details appropriate to our gedankenexperiment.

I have listed the order of the quantities in the vector at left to begin with the sure quantity, 1, which equals 1 no matter what happens in the gedankenexperiment. There follow the four summands of the CHSH quantity s, of which we have noticed that each one of them is restricted in the gedankenexperiment to equal a function value of the other three. That is why there are only eight columns in their realm matrix, as opposed to sixteen columns in the expansive realm matrix we have already examined. As to the components of the vector \mathbf{q}_{s} at the right of the right-hand side, notice that quantum theory says nothing at all about these, individually. Each of them would equal the probability that the 4-ply gedankenexperiment would yield detection products designated by a specific column of the realm matrix. However, these would involve the joint detection of photon products in four distinct measurements that are known to be incompatible. On account of the generalised uncertainty principle, quantum theory eschews specification of such probabilities. Nonetheless, for any individual photon detection product in a specific experimental design, denoted on the left-hand side of the equation, quantum theory does specifies an expectation value of either $1/\sqrt{2}$ or $-1/\sqrt{2}$, as we have recognized. Since these four products are not all free to equal +1 or -1 at the same time, we may assert expectation values for any three of them, and use linear programming computations to find the cohering bounds on the expectation of the fourth that would accompany them, yielding bounds on the expectation Equation (13).

7.1. The Result: Quantum Theory Identifies Restrictions on the Valuation of q_8

This is what we find. The columns of the matrix below display the computed results of the paired \mathbf{q}_{\min} and \mathbf{q}_{\max} vectors corresponding to four linear programming problems. Each of them determines a bound on an expected function value that appears in one of the four forms of the expectation value $E[s(\lambda)]$ which we displayed in Equation (12). The first pair of columns, for example, identify the fifth row of the matrix in Equation (13) as the objective function, $E[A(\mathbf{a}',\mathbf{b}')]$, constrained by QM-specified values of the expectations of the first four rows. The second pair of columns identify the fourth row of (13) as the objective function constrained by QM specifications of expectations for rows 1, 2, 3, and 5, and display the appropriate solution vectors; and so on.

ſ	$_{\min} \left(a', b' ight)$	$_{\max}(\mathbf{a}',\mathbf{b}')$	$_{\min}(\mathbf{a'},\mathbf{b})$	$_{\max}(\mathbf{a}',\mathbf{b})$	$_{\min}(\mathbf{a},\mathbf{b}')$	$_{\max}(\mathbf{a},\mathbf{b}')$	$_{\min}(\mathbf{a},\mathbf{b})$	$_{\max}(\mathbf{a},\mathbf{b})$
q_1	0	0.1464	0	0.1464	0.5607	0.7803	0	0.1464
q_2	0.7803	0.5607	0	0.1464	0.1464	0	0	0.1464
q_3	0.0732	0	0.0732	0	0	0.0732	0	0
q_4	0	0.1464	0.7803	0.5607	0.1464	0	0	0.1464
q_5	0	0.1464	0	0.1464	0.1464	0	0.7803	0.5607
q_6	0.0732	0	0	0	0	0.0732	0.0732	0
$ q_7 $	0.0732	0	0.0732	0	0	0	0.0732	0
q_8	0	0	0.0732	0	0	0.0732	0.0732	0)

Each of these column vectors resides in 8-dimensional space, providing a coherent assessment of probabilities for the constituent event vector $\mathbf{Q}(\mathbf{X}_{s})$, without specifying precise probabilities for any of them. In fact, quantum theory denies itself the capability of identifying such probabilities precisely. We will discuss this feature further, below. However the results of the linear programming computations can and do specify possibilities for what might be specified in a way that would cohere with what quantum theory can and does tell us. The columns of this matrix identify some of them. In fact, these columns display extreme values of what are possible. Any convex (linear) combination of them would cohere with quantum theory as well. Thus, geometrically the columns constitute vertices of a polytope of quantum-theory-supported possibilities for $P[\mathbf{Q}(\mathbf{X}_8)]$. This polytope is called "the convex hull" of these vectors. However, although we have found eight of them, the rank of the matrix of all of them is only four! That is, these eight-dimensional vectors all reside within a four-dimensional subspace of a unit-simplex. Why is quantum theory not more specific in specifying the expectation of Bell's quantity E(s)? We shall delay this discussion until we have clarified what we have learned from these results of $\mathbf{q}_{\min}\left(\mathbf{a}^{*},\mathbf{b}^{*}\right)$ and $\mathbf{q}_{\max}\left(\mathbf{a}^{*},\mathbf{b}^{*}\right)$.

7.2. Implied Bounds on Expected Detection Products and on $E(s) \in (1.1213, 2]$

According to the prescription of Equation (12), each of these \mathbf{q}_8 vectors appearing in Section 7.1 would identify a vertex of another polytope of cohering expectation vectors for the components of the CHSH quantity *s*. Followed at bottom by the expectation values E(s) they imply, these are

$\int E[A(\mathbf{a})B(\mathbf{b})]$	0.7071	0.7071	0.7071	0.7071	0.7071	0.7071	-1.0000	-0.1213
$E[A(\mathbf{a})B(\mathbf{b}')]$	-0.7071	-0.7071	-0.7071	-0.7071	0.1213	1.0000	-0.7071	-0.7071
$E[A(\mathbf{a}')B(\mathbf{b})]$	0.7071	0.7071	-1.0000	-0.1213	0.7071	0.7071	0.7071	0.7071 .
$E[A(\mathbf{a}')B(\mathbf{b}')]$	-1.0000	-0.1213	0.7071	0.7071	0.7071	0.7071	0.7071	0.7071
$\begin{bmatrix} E[s] \end{bmatrix}$	1.1213	2.0000	1.1213	2.0000	2.0000	1.1213	1.1213	2.0000

In any of these columns appear three values of $E\left[A(\mathbf{a}^*)B(\mathbf{b}^*)\right]$ specifications supported by quantum theory, and a fourth value which is either a lower

bound or upper bound on any cohering expectation for the fourth. (By the way, 0.7071 is the value of $1/\sqrt{2}$ to four decimal places.) At the bottom of the column is the value of E(s) that would correspond to these four. The vectors of the four $E\left[A(\mathbf{a}^*)B(\mathbf{b}^*)\right]$ values are the vertices of the four-dimensional space of QM-supported expectation values of the gedankenexperiment, and the value of E(s) listed at bottom would be a quantum-theory-permitting assessment of E(s), Bell's quantity. All of their convex combinations lie within Bell's reputed bounds of $\left[-2, +2\right]$. There is more to be said about this, but let us first address now the question of why quantum theory leaves four dimensions of freedom unaccounted for in its prescriptions.

7.3. Why are There Four Free Dimensions to the QM Specification of E(s)?

Let's just get down to it, without any prelude. Quantum theory specifies precise values for outcome probabilities of the photon pair detections at any choice of three angle settings of the gedankenexperiment. Consider for example the polarization detection probabilities at the angles (\mathbf{a}, \mathbf{b}) , $(\mathbf{a}, \mathbf{b}')$, and $(\mathbf{a}', \mathbf{b})$. These have been identified in our Equation (1), while the corresponding expectations of detection products appeared in Equation (2). If quantum theory were to specify a complete distribution for the outcome of this gedankenexperiment, it would have to specify eight probabilities. These would involve three corresponding to detection events at any one of the polarization angles, also jointly at any two of the three detection angles, and also at all three of the detection angles. But according to the uncertainty principle discussed in Section 3, the theory eschews commitments regarding the latter four of these probabilities: neither

$$P\left\{\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}') = +1\right)\right]\right\}, \text{ nor } P\left\{\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\left[\left(A(\mathbf{a}') = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\right\}, \text{ nor } P\left\{\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\left[\left(A(\mathbf{a}') = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\right\}, \text{ nor } P\left\{\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\right\}, \text{ nor } P\left\{\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}') = +1\right)\right], \left[\left(A(\mathbf{a}') = +1\right)\left(B(\mathbf{b}') = +1\right)\right]\right\}, \text{ nor } P\left\{\left[\left(A(\mathbf{a}') = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\right\}\right\}$$

For each of these would amount to claims regarding the joint outcomes of incompatible measurements, characterised by Hermitian matrix operators that do not commute. Quantum theory explicitly avoids such claims. That leaves four dimensions of the eight-dimensional pmf over the four detection products unspecified... explicitly! That is why quantum theory allows four unspecified dimensions to the expectations it provides regarding the four polarization products on the same pair of photons.

Perhaps this comment does need a little bit more explication. You will need to

view Equation (13) while reading the following remarks. They concern assertions that quantum theory does allow us to make, and those that it doesn't. Recall that we are considering a linear programming problem in which quantum expectations are asserted for the polarization products at the angle settings (\mathbf{a}, \mathbf{b}) , $(\mathbf{a}, \mathbf{b}')$, and $(\mathbf{a}', \mathbf{b})$, and investigating coherent bounds for expectation of the product at the setting $(\mathbf{a}', \mathbf{b}')$. Notice firstly that quantum theory does allow us to, and indeed insists that we assert

$$E[A(\mathbf{a})B(\mathbf{b})] = q_1 + q_2 + q_3 + q_4 - q_5 - q_6 - q_7 - q_8$$

= $1/\sqrt{2}$

Examining the corresponding columns of the realm matrix seen in (13), it is evident that these involve assertions regarding the outcomes of $(A(\mathbf{a})B(\mathbf{b}) = +1)$ and $(A(\mathbf{a})B(\mathbf{b}) = -1)$ irrespective of the values of $A(\mathbf{a})B(\mathbf{b}')$ and $A(\mathbf{a}')B(\mathbf{b})$. For each of these events involve an outcome of the product $A(\mathbf{a})B(\mathbf{b})$ summed over all four possible joint outcomes of the products $A(\mathbf{a})B(\mathbf{b}')$ and $A(\mathbf{a}')B(\mathbf{b})$. So these latter two incompatible observations would be irrelevant to the assertion of this expectation. The same feature would pertain to the required assertions of $E[A(\mathbf{a})B(\mathbf{b}')]$ and $E[A(\mathbf{a}')B(\mathbf{b})]$ which are involved in the first LP problem. Neither of these involves any concomitant assertions regarding observations incompatible with them. On the other hand, an assertion of a probability for the joint occurrence of two pairs of polarization observations, such as

 $P\left\{\left[\left(A(\mathbf{a}) = +1\right)\left(B(\mathbf{b}') = +1\right)\right]\left[\left(A(\mathbf{a}') = +1\right)\left(B(\mathbf{b}) = +1\right)\right]\right\}$ for example, would require specifications of the sum $q_1 + q_3$. Examining Equation (13) makes clear that it is only columns 1 and 3 of the matrix in which this joint event is instantiated. Asserting a specific value for the sum $q_1 + q_3$ would necessarily entail assessments of joint probabilities for incompatible events. The same would be true of any of the other three probabilities regarding joint events for which quantum theory eschews assessment.

If one were to claim, as do the reigning proponents of Bell violations, that the probabilities of quantum theory support the valuation of $E[s(\lambda)] = 2\sqrt{2}$ according to the derivation that concluded our Section 5, that would be just plain wrong. Full stop.

Our next project is an amusing one, of actually envisaging the 4-dimensional polytope of quantum probabilities relevant to the gedankenexperiment. This will be achieved by passing the 4-dimensional quantum polytope we have identified through the 3-dimensional space in which we live. By this method we can view it, just as the inhabitants of 2-dimensional space in Abbott's amusing story of *Flatland* [27] viewed the sphere passing through their lower dimensional world. It suddenly appeared as a point, which gradually expanded to circles of increasing diameter, and then diminished until they suddenly disappeared again. Let's view what we can of our 4-dimensional quantum polytope in this way.

7.4. Transforming the Expectation Polytope into Quantum Probabilities

0.2197 0.4268

 $P_{\perp}(\mathbf{a}',\mathbf{b}')$

0

The expected photon detection products displayed in Section 7.2 can be transformed into P_{++} probabilities by applying the transformation $P_{++}(\mathbf{a}^*, \mathbf{b}^*) = \left[E(\mathbf{a}^*, \mathbf{b}^*) + 1 \right] / 4$ of Equation (3) to the eight vertices. This yields the vertices of another polytope in the space of the probability vector $\left[P_{++}(\mathbf{a}, \mathbf{b}), P_{++}(\mathbf{a}, \mathbf{b}'), P_{++}(\mathbf{a}', \mathbf{b}), P_{++}(\mathbf{a}', \mathbf{b}') \right]$ displayed below: $P_{++}(\mathbf{a}, \mathbf{b})$ 0.4268 0.4268 0.4268 0.4268 0.4268 0.4268 0.4268 0 0.2197 $P_{++}(\mathbf{a}, \mathbf{b}')$ 0.0732 0.0732 0.0732 0.0732 0.2803 0.5000 0.0732 0.0732 $P_{++}(\mathbf{a}', \mathbf{b})$ 0.4268 0.4268 0.4268 0 0.2197 0.4268 0.4268 0.4268 0.4268 0.4268

7.5. And Now Viewing It !... as It Passes through Our Space

The convex hull of the 4-D column vectors shown in Section 7.4 can be visualized through a sequence of 3-D intersections it affords with slices perpendicular to any one of its axes. **Figure 3** displays such a sequence of slices perpendicular to the $P_{++}(\mathbf{a}', \mathbf{b}')$ axis at values increasing from 0 to 0.4268. When

0.4268 0.4268

0.4268

0.4268

0.4268

 $P_{++}(\mathbf{a}',\mathbf{b}') = 0$, the intersection of the slice identifies only a single vertex point (0.0732, 0.4268, 0.4268) which appears in the subplot (1,1). See also column one of the matrix in Section 7.4. As the value of $P_{++}(\mathbf{a}',\mathbf{b}')$ for the slice level increases to a 0.1098 in subplot (2,1), the intersection appears as a tetrahedron. The size of the intersecting tetrahedron increases further at the probability level 0.2197 in subplot (3,1). The tetrahedrons continue to increase in size as the level of the $P_{++}(\mathbf{a}',\mathbf{b}')$ increases still further to 0.2561 in subplot (1, 2), but a corner of their intersections begins to be cut off there. This clipped portion is cut more severely from the enlarging polytope as $P_{++}(\mathbf{a}',\mathbf{b}')$ increases further, displayed in subplots (2,2) through (3,2) which is our view of the polytope when it suddenly disappears.

The symmetry of the configuration implies that slices along the other axes would create identical intersection sequences.

8. What to Make of Aspect's and Subsequent Empiricism

Taken in by the alluring derivation of Section 5.3 which ignores the symmetric functional relations among the polarization products of the gedankenexperiment, Aspect and followers were convinced that Bell's inequality has been defied, and that the theory of hidden variables must be rejected. This conclusion would support the assertion that quantum theory has identified the structure of randomness which supposedly inheres in Nature at its finest resolution. The behaviour of the photons is considered to be governed purely by a probability distribution. It remained only to devise some physical experiments that could verify the defiance of the inequality.

According to the tenets of objective probability theory and its statistical programme, probabilities are not observable quantities. What are observable are

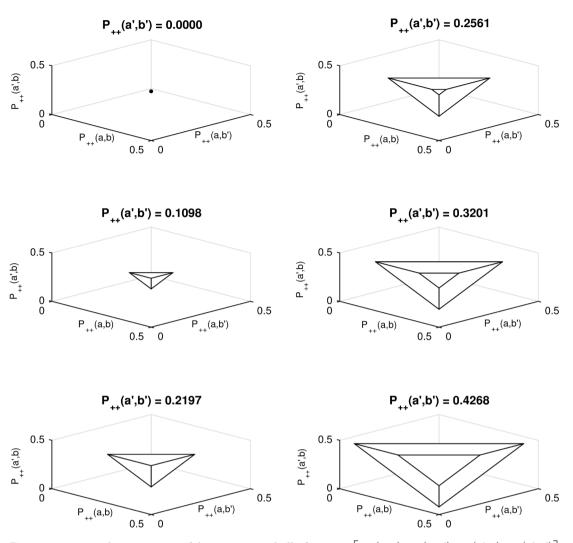


Figure 3. Sequential intersections of the 4-D convex hull of vectors $[P_{++}(\mathbf{a},\mathbf{b}), P_{++}(\mathbf{a}',\mathbf{b}), P_{++}(\mathbf{a}',\mathbf{b}), P_{++}(\mathbf{a}',\mathbf{b}')]$ with slices perpendicular to the $P_{++}(\mathbf{a}',\mathbf{b}')$ axis, at levels increasing from 0 to 0.4268 as designated in the heading of each component figure. Read the display sequentially down the first column and then down the second column.

outcomes of random variables which are generated by them. It is a matter of statistical theory to devise methods for estimating the unobservable probabilities and their implied expectations from carefully observed outcomes of the random variables they generate. Understood in this way, Equation (8) which I repeat here constitutes a structure requiring estimation if the violation of Bell's inequality is to be verified:

$$E[s(\lambda)] = E[A(\mathbf{a})B(\mathbf{b})] - E[A(\mathbf{a})B(\mathbf{b}')]$$
$$+ E[A(\mathbf{a}')B(\mathbf{b})] + E[A(\mathbf{a}')B(\mathbf{b}')] + E[A(\mathbf{a}')B(\mathbf{b}')]$$

Resorting to long respected statistical procedures, the unobservable expectations of detection products on the right-hand-side of this equation can be estimated by the generally applicable non-parametric method of moments. Supported by the probabilistic law of large numbers, its validity as an estimating procedure stems from the 1930's.

The programme for estimating Equation (8) would proceed as follows. To estimate the first component of $E[s(\lambda)]$, which is $E[A(\mathbf{a})B(\mathbf{b})]$, one would conduct *N* independent polarization experiments at the angle setting (\mathbf{a}, \mathbf{b}) , and record the value of the polarization products $A(\mathbf{a})B(\mathbf{b})$ observed in each case, these being either -1 or +1. The average of these values would provide a method of moments estimate of the expectation $E[A(\mathbf{a})B(\mathbf{b})]$ which is common to all of these random experiments. A similar programme would be followed in estimating the other three components of $E[s(\lambda)]$.

Using the notation of Aspect [14] we would conduct N repetitions of the CHSH/Bell experiment with the relative polarizing angles set at (\mathbf{a}, \mathbf{b}) , resulting in $N_{++}(\mathbf{a}, \mathbf{b})$ observations of $(A(\mathbf{a}), B(\mathbf{b})) = (+, +)$, $N_{+-}(\mathbf{a}, \mathbf{b})$ observations of (+, -), $N_{-+}(\mathbf{a}, \mathbf{b})$ observations of (-, +), and $N_{--}(\mathbf{a}, \mathbf{b})$ observations of (-, -). An estimated version of equation (8) would then be expressed as

$$\hat{E}[s(\lambda)] \equiv \hat{E}[A(\mathbf{a})B(\mathbf{b})] - \hat{E}[A(\mathbf{a})B(\mathbf{b}')] + \hat{E}[A(\mathbf{a}')B(\mathbf{b})] + \hat{E}[A(\mathbf{a}')B(\mathbf{b}')],$$
(14)

where the component estimator $\hat{E}[A(\mathbf{a})B(\mathbf{b})]$ is defined by

$$\hat{E}\left[A\left(\mathbf{a}\right)B\left(\mathbf{b}\right)\right] = \frac{\left[N_{++}\left(\mathbf{a},\mathbf{b}\right) - N_{+-}\left(\mathbf{a},\mathbf{b}\right) - N_{-+}\left(\mathbf{a},\mathbf{b}\right) + N_{--}\left(\mathbf{a},\mathbf{b}\right)\right]}{\left[N_{++}\left(\mathbf{a},\mathbf{b}\right) + N_{+-}\left(\mathbf{a},\mathbf{b}\right) + N_{-+}\left(\mathbf{a},\mathbf{b}\right) + N_{--}\left(\mathbf{a},\mathbf{b}\right)\right]}, \quad (15)$$

with a similar specification for the components of $\hat{E}[s(\lambda)]$ pertaining to the relative angles $(\mathbf{a}', \mathbf{b})$, $(\mathbf{a}, \mathbf{b}')$, and $(\mathbf{a}', \mathbf{b}')$. The denominator of (15) is equal to N, the number of experiments run at this angle, merely displayed as the sum of its four component counts of $N_{\pm\pm}(\mathbf{a}, \mathbf{b})$.

The momentous results were published by Aspect *et al.* [11] [12], confirming the apparent defiance of Bell's inequality to several decimal places. Through the following three decades the experimental setup was embellished so to account for a variety of various possible loopholes tendered as an explanation.

8.1. Examining and Reassessing Aspect's Empirical Results

What are we to make of Aspect's and subsequent empirical results?

Aspect [[14], p.15], and [12] reports the estimation $\hat{E}[s(\lambda)]$ from experimental data, using the method of moments as defined in Equations (14) and (15). Of course actually, it is impossible to conduct an experiment on a single pair of photons at all four angle settings, much less conduct a sequence of such experiments. Instead, experimental sequences of observations using different photon pairs were generated at each of four angle settings. These were presumed to provide independent estimates of the four expectations as they appear in Equation (15). These independent estimates were then inserted into Equation (14), yielding Aspect's touted estimate $\hat{E}[s(\lambda)]$ near to $2\sqrt{2}$.

Although experimentation protocols have subsequently been improved to account for the challenges of possible loopholes during the following thirty years, the estimation procedures using the improved data have been the same. Results from several of the improved protocols have been reported only in the form of so-called p-values of significance for hypothesis tests posed as to whether

 $E[s(\lambda)]$ exceeds 2 or not. The results have been lionized, apparently quite impressive, and deemed to be decisive.

We can now recognize the fault in Aspect's estimation procedure which allows complete liberty in all four polarization product estimations $\hat{E} \left[A(\mathbf{a}^*) B(\mathbf{b}^*) \right]$, using experimental incidence values of $N_{\pm\pm}(\mathbf{a}^*, \mathbf{b}^*)$ from many experimental runs with different photon pairs. Each of his experimental observations may be whatever value it happens to be at its experimental angle setting, identifying whatever value of polarization product that it does. However, if the estimation were meant to apply to the ontological understanding of $s(\lambda)$ in the gedankenexperiment within which he and Bell couch their theoretical claims, he would have to adjust this methodology. One might well pick experimental runs using three different photon pairs at any three angles one wishes, to simulate the behaviours $A(\mathbf{a}^*)B(\mathbf{b}^*)$ for any three polarization products of a single pair of photons. However, to be consistent with the Aspect/Bell problem as posed for this single pair of photons at all four relative angle settings, one then would need to compute the implied value of the polarization product observation for the fourth angle according to the functional form that we have identified in Equation (11). The same functional form connects the detection product at any one of the four angle settings to the other three.

Statistical estimation values reported by Aspect as well as those by subsequent research groups over the past thirty years have no relevance to the estimation of $E[s(\lambda)]$ as it is understood to pertain to four spin products on a single pair of photons. It is perfectly reasonable to find estimation values exceeding the bounds of [-2,+2] as they have. For although these results *could reasonably pertain* to an estimate of $E[s(\lambda)]$ with $s(\lambda)$ defined as a combination of polarization products on *four different pairs of photons*, they *do not pertain* to Bell's inequality which is relevant to a 4-ply gedankenexperiment on the same pair of photons at all four angle settings. In the context to which their experimental results are appropriate, $E[s(\lambda)]$ is not bound by the Bell bounds of [-2,+2], but rather by the interval [-4,+4] which is unchallenged in this context.

Nonetheless, Aspect's empirical estimation programme might be adjusted to account for the symmetric functional relations that would necessarily characterise the imagined results of the gedankenexperiment. In the next subsection I shall display the unsurprising results of such an adjusted methodology. They do not suggest any defiance of Bell's inequality at all. The simulation I construct will mimic the way Aspect's data needs to be treated, recognizing his data as the result of conditionally independent experiments on distinct pairs of photons at each of the four relative angle settings of the polarizers.

8.2. Exposition by Simulation

Because Aspect's experimental observation data is not available in full, a method

for correcting his estimation procedure shall now be displayed using simulated data based on quantum theoretic specifications, along with a presentation of its numerical implications. To begin, four columns of one million (10⁶) pseudo random numbers, uniform on [0,1], were generated with a MATLAB routine. These were then transformed into simulated observations of paired photon polarization experiments at the four relative angles we have been studying. These transformations were performed using the QM probabilities based on calculations of $\frac{1}{2}\cos^2(\mathbf{a}^*, \mathbf{b}^*)$ and $\frac{1}{2}\sin^2(\mathbf{a}^*, \mathbf{b}^*)$ as described in our Equations (1). Each resulting simulated polarization pair was then multiplied together to yield a polarization product. In this way were created four columns of simulated observations corresponding to polarization products from one million experiments at each of the four angles: $(\mathbf{a}', \mathbf{b}'), (\mathbf{a}, \mathbf{b}'), (\mathbf{a}', \mathbf{b})$. We shall refer to this matrix of simulated polarization products below as the SIMPROD matrix.

Aspect's estimation Equation (15) was applied to each of these columns, yielding estimates of the expected polarization product pertinent to that column, $\hat{E} | A(\mathbf{a}^*) B(\mathbf{b}^*) |$. These appear in the first row of **Table 1**. These four estimates were then inserted into Equation (14) appropriately to yield an Aspect estimate $\hat{E}[s(\lambda)] = 2.827738$, appearing in the second row of the Table under *each* of these columns. This number is quite near to $2\sqrt{2} \approx 2.828427$, as was Aspect's reported empirical estimate, proposed as an evidential violation of Bell's inequality. As we now know, the problem is that when the product observations are supposed to apply to *the same* photon pair, the observed value of the polarization product at any angle is required to be related to the product at the other three angles via the functional equation we specified in our Equation (11). The four of them may not all range freely in a gedankenexperiment, as they may in real experiments on *different* pairs of photons. Rather, they are required to be bound by the symmetric functional relation $G(\cdot, \cdot)$ that we have identified. The rows of the matrix SIMPROD do not respect this requirement, so the Aspect estimate $\hat{E}[s(\lambda)]$ which they produce cannot be used to estimate the expected value of $s(\lambda)$ for the gedanken experiment. We shall now endeavor to correct this error.

The third row of **Table 1** has been generated then by first applying the function $G(\cdot, \cdot)$ to each choice of three components of the rows of the SIMPROD matrix. Each result was entered into the same row of a companion matrix of the

Table 1. Corrections to Aspect's estimate of	Ε	5	$[\lambda]$)	
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$\left(\mathbf{a}^{*},\mathbf{b}^{*} ight)$	(\mathbf{a},\mathbf{b})	$\left(a,b'\right)$	(\mathbf{a}',\mathbf{b})	$\left(a',b'\right)$
$\hat{E} \Big[A ig(\mathbf{a}^* ig) B ig(\mathbf{b}^* ig) \Big]$	0.707232	-0.706186	0.706840	0.707480
Aspect $\hat{E}[s]$	2.827738	2.827738	2.827738	2.827738
Functional $\hat{E}\left[A\left(\mathbf{a}^{*}\right)B\left(\mathbf{b}^{*}\right)\right]$	-0.353078	0.354348	-0.354766	-0.353934
Corrected $\hat{E}[s]$	1.767180	1.767204	1.765740	1.766964

same size, but placed into the column corresponding to the column entry that was *not* used in the evaluation of the *G* function. Let's call this matrix by the name SIMGEN. Next, Aspect's estimation Equation (15) was applied to each of the four columns of SIMGEN, and the result is printed in the third row of **Table 1**, labeled "Functional $\hat{E}[A(\mathbf{a}^*)B(\mathbf{b}^*)]$ ". These display estimates of

E[G(,,)] required for estimation of the four alternative expectation equations (12). In this way we can be considered to have generated 4 times 10⁶ simulated versions of the Aspect/Bell gedankenexperiment. Their component results can be taken to be any three simulation results from a row of SIMPROD along with the fourth result being the functionally generated result found in the same row and the appropriate fourth column of SIMGEN. Finally, the last row of Ta**ble 1** presents the estimated values of $E[s(\lambda)]$ deriving from these simulated experiments. They appear as "corrected estimates", column by column, for each of which the $\hat{E} | G(\cdot, \cdot) |$ is the one appropriate to that column while the other three expected polarization products are those appropriate to the other three columns of row 1 of the Table. The elements of this row display corrected estimates of $E[s(\lambda)]$ as they should be calculated with the simulated Aspect data. Each of these four estimates is slightly different from the others. Averaging them over the four ways of generating a column of polarization products from the other three columns of simulated products would yield a "Corrected estimate" of $E[s(\lambda)]$ as 1.766772, well within the Bell bounds of [-2, +2].

Based on Aspect's report of his experimental data, I feel quite sure that applying this same estimation procedure to his experimental data, considered as a simulation of the impossible gedankenexperiment, would yield a similar result.

Results on the order of this peculiar number are quite stable over repeated runs of this simulation as described. Since the theoretical analysis reported in this article yields only an interval of cohering possibilities for $E[s(\lambda)]$, this simulation leaves us with a tantalizing problem of how to account for this stable result, which is quite near to $\left[3/\sqrt{2}-1/(2\sqrt{2})\right] \approx 1.767766952966369$. This specific result is a construct of the gratuitous independence feature embedded in the simulation results across each of the three angle pairings used to generate the function-bound simulation results. Such a feature would be highly suspect in Nature, given what we know now about quantum entanglement itself in a single experiment. I should mention that among all distributions in the polytope cohering with the prescriptions of quantum theory, the maximum entropy distribution inheres an expectation value of E(s) = 1.1522. Discussion of its assessment and related issues must await another forum. However, there can be no real empirical evidence on the issue, since it is impossible in principle to activate the setup of the four imagined simultaneous experiments on a single pair of photons. Thus, the physicists' long interest in the fabled gedankenexperiment.

8.3. A Comment on Empirical Work and Statistical Estimation

While Aspect's conception of statistical estimates appropriate to the photon de-

tection problem is understandable, and corrections can be made to improve its relevance to the Aspect/Bell problem, developments of statistical theory and practice during the past fifty years have surely generated superior methods for evaluating the physical theory of quantum behavior. These rely on the subjective theory of probability which, under the leadership of Bruno de Finetti and researchers adhering to his viewpoint, has gained substantial credibility from the past half-century of research in the foundations of probability and statistics. There are even some prominent physicists among its proponents, though not many. Proclaimers of inherent randomness in the physics of quantum behaviour have won the day for now, largely on the basis of the mistaken violation of Bell's inequality that we have debunked in this article. In the very least, it is apparent that calls for open access to raw data [28] from several well-known research programs that publish summary results, usually in the form of discredited p-values, need to be heeded.

9. Concluding Comments

The mathematical structure of the Aspect/Bell problem and its resolution align well with the theory of subjective probability. This viewpoint is in keeping with Einstein's interpretation of quantum mechanics, known by his famous adage that the old one does not roll dice. However, readers more comfortable with the standard realist interpretation of quantum mechanics may also consider the probabilities as ontic properties of the photons themselves without disturbing the mathematical issues we have engaged. Anyone who professes uncertain knowledge about the possible values of a quantum optical gedankenexperiment may assert whatever probabilities are deemed appropriate for the sixteen possible observation vectors displayed in block one of our experimental realm matrix. This may involve as many or as few expectations as one wishes, whether based on the accepted theory of quantum mechanics or not. These of course need to be assessed scientifically in the light of what evidence can be brought to bear. Similarly, realist proponents of quantum theory may hypothesize whatever probability values they think it prescribes. However, since the sixteen vectors of possible polarization observations listed in the realm matrix provide an exclusive and exhaustive list of possible gedankenexperiment results, the sum of these probabilities must equal 1 for anyone who makes coherent assertions. This understanding is what resolves the conundrum posed by apparent violations of Bell's inequality.

As to the characterization of the theory of hidden variables, this is another endeavour that has been misconstrued in accepted literature, largely on the basis of the mistaken understanding of the defiance of Bell's inequality which we have corrected here. I have examined this matter in a separate manuscript entitled "Resurrection of the principle of local realism and the prospects for supplementary variables." Along with a manuscript on my reassessment of Mermin's "quantum mysteries" [29], it is currently available only on my ResearchGate page. For now I shall merely state that mathematically, the theory of supplementary variables specifies the form of a mixing density $\rho(\lambda)$ that can be made isomorphic to *any* coherent distribution over the empirical observations of polarization experiments whatsoever. It matters not whether they are the prescriptions of quantum theory or not. At any rate, no coherent distribution over observable quantities supports the defiance of Bell's inequality, whether considered to be a formalization of hidden variables theory or not.

Virtually all discussion of quantum probabilities since the original work of Bell has supported the conclusion that probabilities pertinent to quantum behaviour can violate the seemingly innocuous inequality that he identified. The mathematical error that has been discovered and reported here substantiates the end of an era of accepting this conclusion. The results we have aired will have ramifications for many published estimations based on more sophisticated experimentation as well. There are further consequences for a host of theoretical issues that have been studied and discussed in the context of a mistaken understanding. These include related notions of hidden variables, entangled particles, and information transfer. Discussions of these topics do require philosophical attention to a variety of conceptual constructs in which they are imbedded. However, the analysis of Aspect/Bell presented here has nothing to do with philosophical distinctions. It has identified a mathematical error in accepted work that must be recognized no matter what might be the philosophical positions of interested parties. Probabilistic forecasts motivated by quantum theory do not violate any laws of probability theory.

Discussions of related issues proceeding henceforth will need to begin with this new recognition. Interestingly, this resolution was suspected in some way by Bell himself, though not the analytical detail. This was clearly evident in his musings on the hidden variables question in Bell [10] which he himself had reprinted in a collection of his publications, Bell [30]. My discovery of the functional relations involved among the components of the 4-ply gedanken quantity S and the 4-D polytope of their cohering quantum theoretic distributions is truly novel.

A final reference relevant to this analysis is the article of Romano Scozzafava [31] on the role of probability in statistical physics. He discusses several issues that clarify fundamental matters in the context of the constructive mathematics of Bruno de Finetti's operational subjective statistical method.

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Conflicts of Interest

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

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A Notable Quasi-Relativistic Wave Equation and Its Relation to the Schrödinger, Klein-Gordon, and Dirac Equations

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Abstract

An intriguing quasi-relativistic wave equation, which is useful between the range of applications of the Schrödinger and the Klein-Gordon equations, is discussed. This equation allows for a quantum description of a constant number of spin-0 particles moving at quasi-relativistic energies. It is shown how to obtain a Pauli-like version of this equation from the Dirac equation. This Pauli-like quasi-relativistic wave equation allows for a quantum description of a constant number of spin-1/2 particles moving at quasi-relativistic energies and interacting with an external electromagnetic field. In addition, it was found an excellent agreement between the energies of the electron in heavy Hydrogen-like atoms obtained using the Dirac equation, and the energies calculated using a perturbation approach based on the quasi-relativistic wave equation discussed in this work provides interesting pedagogical opportunities for a fresh approach to the introduction to relativistic effects in introductory quantum mechanics courses.

Keywords

Quantum Mechanics, Schrödinger Equation, Klein-Gordon Equation, Dirac Equation, Relativistic Quantum Mechanics

1. Introduction

Most physicists are familiar with the Schrödinger equation, which describes the movement of a spin-0 particle with mass (m) moving at speeds much smaller than the speed of light (c) [1] [2] [3] [4] [5]. The one-dimensional Schrödinger equation corresponding to a free particle is given by the following expression [1]

[2] [3] [4] [5]:

$$i\hbar\frac{\partial}{\partial t}\psi_{Sch}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_{Sch}(x,t).$$
(1)

In Equation (1), \hbar is the Plank constant (*h*) divided by 2π and ψ_{Sch} is the (scalar) wavefunction. Most Physics Ph.D. graduates know about the Klein-Gordon equation, which describes the movement of a spin-0 particle with mass moving at relativistic speeds [6] [7]. The one-dimensional Klein-Gordon equation corresponding to a free particle is given by the following expression [6] [7]:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_{KG}(x,t) = \frac{\partial^2}{\partial x^2}\psi_{KG}(x,t) - \frac{m^2c^2}{\hbar^2}\psi_{KG}(x,t).$$
(2)

In Equation (2), ψ_{KG} is also a scalar wavefunction. Equation (2) is not a Schrödinger-like equation because in contrast to the Schrödinger equation, Equation (2) includes a second order temporal derivative. Introductory Quantum Mechanics courses often cover the Schrödinger equation [1] [2] [3] [4] [5]. More advance Quantum Mechanics courses often cover the Klein Gordon equation [6] [7]. This is done for introducing the readers to the consequences for quantum mechanics of taking seriously the concepts and ideas of Einstein's Special Theory of Relativity [8] [9].

Historically, while looking in 1926 for the right quantum equation, Erwin Schrödinger first explored, but did not publish, the equation that we today call the Klein-Gordon equation, which was also published in 1926 by Oskar Klein and Walter Gordon. Schrödinger was well-aware of the special theory of relativity; thus, he was looking for a Lorentz invariant wave equation [6] [7] [8] [9] [10]. The Schrödinger equation is not Lorentz invariant but Galilean invariant [10] [11]; therefore, a relativistic quantum mechanics cannot be based on the Schrödinger equation.

A fully relativistic quantum theory requires to be founded on equations like the Klein-Gordon equation, which is valid for any two observers moving respect to each other at constant velocity [6] [7]. However, judging by its popularity among present physicists, Schrödinger took the correct decision. The solutions of the Klein-Gordon equation are plagued with several unwanted properties that made Equation (2) less easy to work with than using Equation (1) [6] [7]. Equation (1) describes a particle of mass (*m*), linear momentum (*p*), and kinetic energy (*K*) related by the classical relation $K = p^2/2m$, which is not valid at relativistic speeds [6] [7] [11].

Fortunately for Schrödinger, he was able to reproduce the results previously obtained by Bohr for the energies of the bounded states of the electron in the Hydrogen atom [1] [2] [3] [4] [5]. This was possible because the electron in the Hydrogen atom has non-relativistic energies [1] [2] [3] [4] [5]. However, electrons are not spin-0 particles but spin-1/2 particles.

Electrons moving at low velocities respect to c, can be approximately described by a two-component vector wavefunction (spinor) [2] [6] [7]. The spinor

nature of the electron wavefunction produces experimentally detectable results when the electron interacts with an external electromagnetic field [4] [6] [7]. The Pauli equation, which was discovered by Wolfgang Ernst Pauli in 1927, is a Schrödinger-like equation; therefore, it is not a Lorentz-invariant. The Pauli equation describing the interaction of a free electron with a constant magnetic field, with magnitude B_{ext} pointing in the *z* direction, can be written in the following way [4]:

$$i\hbar\frac{\partial}{\partial t}\psi_{P}(\boldsymbol{r},t) = -\frac{\hbar^{2}}{2m}\nabla^{2}\psi_{P}(\boldsymbol{r},t) - \mu_{B}B_{ext}\sigma_{z}\psi_{P}(\boldsymbol{r},t).$$
(3)

In Equation (3), ∇^2 is the Laplace operator [1] [2] [3] [4] [5],

 $\mu_{B} = e\hbar/(2mc)$ is the Bohr magneton [4], *e* is the electron charge, and σ_{z} is the 2 × 2 Pauli matrix [2]:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

 $\psi_{\scriptscriptstyle P}$ is not a scalar wavefunction but the two-component spinor wavefunction:

$$\psi_{P}(\mathbf{r},t) = \begin{pmatrix} \psi_{P+}(\mathbf{r},t) \\ \psi_{P-}(\mathbf{r},t) \end{pmatrix}.$$
(5)

Consequently, Equation (3) is equivalent to a system of two independent Schrödinger equations for ψ_{P_+} and ψ_{P_-} that are only different in the sign of the last term in the right side of the equations. When $B_{ext} = 0$, both equations are equal to the three-dimensional version of Equation (1) [1] [2] [3] [4] [5]. The exact description of electrons moving at relativistic velocities requires a fourcomponent (biespinor) wavefunction, and the solution of the Lorentz invariant Dirac equation [6] [7]. The Dirac equation of a free electron is given by the following equation [2] [6] [7] [12]:

$$i\hbar\frac{\partial}{\partial t}\psi_{D}(\boldsymbol{r},t) = C[\hat{\boldsymbol{\alpha}}\cdot\hat{\boldsymbol{p}}]\psi_{D}(\boldsymbol{r},t) + mc^{2}\hat{\beta}\psi_{D}(\boldsymbol{r},t).$$
(6)

In Equation (6), each of the three components of the vector operator α and the operator β are 4 × 4 Dirac's matrices [2] [6] [7] [14]. Each of the tree components of the linear momentum operator p is the differential operator [2] [6] [7] [12].

$$\hat{p}_{j} = -i\hbar \frac{\partial}{\partial j}, \ j = x, y, z.$$
(7)

Consequently, the Dirac equation is not a Schrödinger-like equation because only includes spatial derivatives of first order, while Equations (1) and (3) include spatial derivatives of second order. The bispinor ψ_D has four components; therefore, it can be represented using two spinors in the following way [2] [12]:

$$\psi_D(\mathbf{r},t) = \begin{pmatrix} \varphi(\mathbf{r},t) \\ \chi(\mathbf{r},t) \end{pmatrix}.$$
(8)

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Clearly, a price in mathematical complexity is paid for improving the relativistic description of quantum particles. Consequently, from a purely pedagogical point of view, it would be convenient to be able to have a Schrödinger-like equation capable to describe quantum-particles at relativistic energies. Unfortunately, this is not in general possible [6] [7]. Nevertheless, it was recently found a Schrödinger-like equation capable to describe quantum-particles at quasi-relativistic energies [11] [13] [14] [15] [16].

Rigorously, the number of particles may not be constant in a fully relativistic quantum theory [6] [7]. This is because when the sum of the kinetic and the potential (*U*) energy of a particle with mass *m* doubles the energy associate to the mass of the particle, *i.e.*, $E' = K + U = 2mc^2$, then a pair particle-antiparticle could be created from E' [2] [6] [7]. Consequently, the number of particles is constant at quasi-relativistic energies, *i.e.*, when $E' = K + U < 2mc^2$. At quasi-relativistic energies close to mc^2 , the Schrödinger equation does not provide a good description of the states of the quantum particle because it assumes that $K = p^2/2m$, while at relativistic speeds the correct relation between *K*, *p*, and the square of the velocity of the particle (v^2) is given by the following equation [8] [9] [11] [13] [14] [15] [16]:

$$K = \frac{p^2}{(\gamma_v + 1)m}, \ \gamma_v = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}.$$
 (9)

A free spin-0 particle can be (approximately) described by the following quasi-relativistic wave equation, which was first proposed by one of the authors of this work [11] [13] [14] [15] [16]:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_v + 1)m}\frac{\partial^2}{\partial x^2}\psi(x,t).$$
 (10)

Clearly, Equation (10) is a Schrödinger-like equation. Like in Equation (1), ψ is a scalar wavefunction. Moreover, Equation (10) coincides with Equation (1) at low velocities when $\gamma_v \sim 1$. However, Equation (10) describes a particle at quasi-relativistic energies because it implies the relation between *K*, *p*, and v^2 given by Equation (9) [11] [13] [14] [15] [16]. Consequently, from a purely pedagogical point of view, the quasi-relativistic wave equation (Equation (10)) is very interesting.

Moreover, the quasi-relativistic wave equation can be solved following the same mathematical steps required for solving the Schrödinger equation in most of the problems often included in Introductory Quantum Mechanics courses. This includes a free particle [11], confinement of a quantum particle in box [11] [14] [15], reflection by a sharp quantum potential [15], tunnel effect [15], and the quasi-relativistic description of Hydrogen-like atoms [14] [15] [16]. Therefore Equation (10) allows for a smooth introduction of special relativity concepts and ideas in Introductory Quantum Mechanics courses.

The quasi-relativistic wave equation also enriches the accumulated physics

knowledge, and open new ways to tackle quantum problems involving particles at quasi-relativistic energies. Because Equation (10) is a Schrödinger-like equation, it permits to calculate probabilities like it is done for Equation (1) [11]. Moreover, Equation (10) allows for a quasi-relativistic description of multi-particle systems where the number of particles is constant [17]. This includes all problems in Chemistry where the number of electrons is constant and $E' < 2mc^2$. The energy of the most energetic electrons in heavy elements is quasi-relativistic. Therefore, often their description either involves a perturbative theory based on the Schrödinger equation [2] [4] [5], or a more precise but much more complicate quantum electrodynamic description [18].

The quasi-relativistic wave equation potentially represents a novel non-perturbative approach for tackling such problems without having to pay a heavy price in mathematical complexity, thus helping to grasp the essence of the consequences of introducing the ideas and concepts of spatial theory of relativity in quantum mechanics.

In this work, first, for completeness, the connection between Equation (10) and the Klein-Gordon equation will be summarized. Then, for the first time, a quasi-relativistic version of Equation (3) will be directly obtained from the Dirac equation. Finally, also for the first time, an equation giving the quasi-relativistic energies of the bound states of the electron in Hydrogen-like atoms will be obtained using a perturbative approach based on the quasi-relativistic wave equation. The quasi-relativistic energies calculated in this way have a much better correspondence, with the energies calculated using the Dirac equation, than the energies calculated using a perturbative theory based on the Schrödinger equation.

2. Relationship between the Klein-Gordon and the Quasi-Relativistic Wave Equations

From the following well-known relativistic equations [8] [9] [15]:

$$E^{2} - m^{2}c^{4} = p^{2}c^{2} \Leftrightarrow \left(E + mc^{2}\right)\left(E - mc^{2}\right) = p^{2}c^{2}.$$
(11)

And:

$$E = \gamma_{v}mc^{2}, \ p = \gamma_{v}mV, \ E = K + mc^{2}.$$
 (12)

One can formally obtain Equation (2) by substituting E and p in Equation (11) by the following energy and momentum quantum operators [1] [2] [3] [4] [6] [7]:

$$\hat{E} = i\hbar \frac{\partial}{\partial t}, \ \hat{p} = -i\hbar \frac{\partial}{\partial x}.$$
(13)

The factor $(E + mc^2)$ in Equation (11) is always different than zero for E > 0; consequently, Equation (11) and the following algebraic equation are equivalents for E > 0:

$$K = (E - mc^{2}) = \frac{p^{2}}{(\gamma_{v} + 1)m}.$$
 (14)

1

Then from Equations (13) and (14) follow the following differential equation [13] [14] [15]:

$$\hbar \frac{\partial}{\partial t} \psi_{KG+}(x,t) = -\frac{\hbar^2}{(\gamma_v + 1)m} \frac{\partial^2}{\partial x^2} \psi_{KG+}(x,t) + mc^2 \psi_{KG+}(x,t).$$
(15)

A simple substitution in Equations (2) and (15) shows that the following plane wave is a solution of both equations for E > 0:

$$\psi_{KG+}(x,t) = \mathrm{e}^{\frac{t}{\hbar}(px-Et)}.$$
(16)

Moreover, the following wavefunction is a solution of Equation (10):

$$\psi(x,t) = \psi_{KG+} e^{iw_m t}, \ w_m = \frac{mc^2}{\hbar}.$$
 (17)

Therefore, Equation (17) allows finding a solution of Equation (2) with E > 0 from a solution of Equation (10). This is the relationship between the freeparticle Klein-Gordon and quasi-relativistic wave equations. This relationship is also valid when the particle is moving through a potential U[11] [13] [14] [15] [19]. For instance, the quasi-relativistic wave equation for a particle moving at quasi-relativistic energies through piecewise constant potentials is given by the following equation [15]:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_v + 1)m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t).$$
(18)

Looking for a solution of Equation (18) of the form:

$$\psi(x,t) = X(x) e^{-\frac{i}{\hbar}Kt}, \quad K = E' - U.$$
(19)

It is obtained the time-independent quasi-relativistic wave equation [15]:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} X(x) + \kappa^2 X(x) = 0,$$

$$\kappa = \frac{p}{\hbar} = \frac{1}{\hbar} \sqrt{(\gamma_v + 1)mK} = \frac{1}{\hbar} \sqrt{(\gamma_v + 1)m(E' - U)}.$$
(20)

At low velocities, when $\gamma_{\nu} \sim 1$, Equation (1) coincides with the time-independent Schrödinger equation for the same problem [1] [2] [3] [4]. The allowed values of κ are determined by the boundary conditions of the problem. From Equations (12) and (14) follows that [15] [17]:

$$\gamma_{\nu}^{2} = 1 + \left(\frac{\hbar k}{mc}\right)^{2} \Longrightarrow K = \frac{\hbar^{2} \kappa^{2}}{\left[1 + \sqrt{1 + \frac{\hbar}{mc}k}\right]m}.$$
(21)

At low velocities, when $\gamma_v \sim 1$ and $\hbar\kappa \ll mc$, Equation (21) gives $K = \hbar^2 \kappa^2 / 2m$, which is the non-relativistic relation between K and κ [1] [2] [3] [4]. It is worth noting that Equations (10) and (18) are not linear equations [11] [13] [14] [15]. This may rise some objections due to the importance of the superposition principle in quantum mechanics [1]-[7] [11] [13] [14] [15]. How-

ever, it should be noted that, if X_1 and X_2 are two solutions of the time-independent quasi-relativistic wave equation (Equation (20)), respectively corresponding to different kinetic energies K_1 and K_2 , then the following wavefunction is a solution of the Klein-Gordon equation:

$$\psi_{KG+}(x,t) = X_1(x) e^{-\frac{i}{\hbar}(K_1 + mc^2)t} + X_2(x) e^{-\frac{i}{\hbar}(K_2 + mc^2)t}.$$
(22)

From this point of view, the time-independent relativistic wave equation should not be considered a fundamental equation, but a useful auxiliar equation for finding solutions of a fundamental Lorentz invariant wave equation satisfying the superposition principle [14].

3. The Quasi-Relativistic Wave Equation of a Free Electron

The wavefunction in Equations (1), (2), (10), and (18) are scalars, thus describe the state of a spin-0 particle with mass. However, electrons are not spin-0 particles but spin-1/2 particles. Equation (6) gives the correct relativistic equation of a free electron. However, as it is shown below, a spinor quasi-relativistic wave equation can be obtained when E > 0. Proposing a solution of Equation (6) of the following form [2]:

$$\psi_D(\mathbf{r},t) = \begin{pmatrix} \varphi(\mathbf{r}) \\ \chi(\mathbf{r}) \end{pmatrix} e^{-\frac{i}{\hbar}Et}.$$
(23)

Substituting Equation (23) in Equation (6), and considering that for a free electron $E = K + mc^2$, allows for rewriting Equation (6) as the following system of two time-independent spinor equations [2]:

$$c[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}]\chi = (E - mc^2)\varphi = K\varphi, \ c[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}]\varphi = (E + mc^2)\chi.$$
(24)

In Equation (24), each of the three components of the vector operator σ is a 2 × 2 Pauli's matrix [2] [6] [7] [14]. $E + mc^2 > 0$ when E > 0, thus when E > 0, the second equation of Equation (24) can be rewritten in the following way:

$$\chi = \frac{c[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}]}{\left(E + mc^2\right)} \varphi = \frac{[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}]}{\left(\gamma_v + 1\right)mc} \varphi$$
(25)

Substituting Equation (25) in the first equation of Equation (24) results in the following equation:

$$\frac{\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\right]^2}{(\gamma_v+1)m}\boldsymbol{\varphi} = -\frac{\hbar^2}{(\gamma_v+1)m}\nabla^2\boldsymbol{\varphi} = K\boldsymbol{\varphi}.$$
(26)

Therefore, when E > 0, each one of the two components of φ exactly satisfies the same time-independent quasi-relativistic wave equation, which corresponds to a free spin-0 particle with kinetic energy K. Consequently, when E > 0, the three-dimensional version of Equation (10) is the time-dependent quasi-relativist wave equation corresponding to each component of φ in Equation (26).

4. The Pauli-Like Quasi-Relativistic Wave Equation

The Schrödinger-like Pauli equation given by Equation (3) can be obtained from the Dirac equation for an electron interacting with an external electromagnetic field [2]. Following the same procedure, a quasi-relativistic version of Equation (3) can be obtained. When an external electromagnetic field interact with the electron, Equation (24) should be modified in the following way [2]:

$$c\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}-\frac{e}{c}\boldsymbol{A}\right]\boldsymbol{\chi}=\left(\boldsymbol{E}-\boldsymbol{m}\boldsymbol{c}^{2}-\boldsymbol{e}\boldsymbol{A}_{o}\right)\boldsymbol{\varphi},\ c\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}-\frac{e}{c}\boldsymbol{A}\right]\boldsymbol{\varphi}=\left(\boldsymbol{E}+\boldsymbol{m}\boldsymbol{c}^{2}-\boldsymbol{e}\boldsymbol{A}_{o}\right)\boldsymbol{\chi}.$$
(27)

In Equation (27), $-eA_o$ is the electron electrostatic energy and the vector potential *A* is associated to an external magnetic field [2] [8]. When

 $(E + mc^2 - eA_o) > 0$, the second equation of Equation (27) can be rewritten in the following way:

$$\chi = \frac{c \left[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} - \frac{e}{c} \boldsymbol{A} \right]}{\left(\boldsymbol{E} + mc^2 - e\boldsymbol{A}_o \right)} \boldsymbol{\varphi}.$$
 (28)

The Schrödinger-like Pauli equation can be obtained doing $E = E' + mc^2$ and assuming $|E' - eA_o| \ll mc^2$. Therefore, the fraction $c/(E' - eA_o + 2mc^2)$ in Equation (28) can be developed in powers of $(E' - eA_o)$ and Equation (28) can be approximated by the following expression [2]:

$$\chi \approx \frac{1}{2m} \left[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} - \frac{e}{c} \boldsymbol{A} \right] \boldsymbol{\varphi}.$$
 (29)

Substituting Equation (29) in the first equation of Equation (27) allows obtaining the Schrödinger-like time-independent Pauli equation [2]:

$$\left\{\frac{\left[\hat{\boldsymbol{p}} - \frac{\boldsymbol{e}}{c}\boldsymbol{A}\right]^{2}}{2m} + \boldsymbol{e}\boldsymbol{A}_{o} - \boldsymbol{\mu}_{B}\left(\hat{\boldsymbol{\sigma}}\cdot\vec{B}\right)\right\}\boldsymbol{\varphi} = \boldsymbol{E}'\boldsymbol{\varphi}.$$
(30)

For a free electron moving through a constant magnetic field, with magnitude B_{ext} pointing in the *z* direction, Equation (30) can be approximated as:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\mathbf{r}) - \mu_B B_{ext}\sigma_z\varphi(\mathbf{r}) = E'\varphi.$$
(31)

Which is the time-independent Pauli-equation corresponding to Equation (3). However, if one assumed that $|-eA_o| \ll E + mc^2$, then the fraction $c/(-eA_o + E' + 2mc^2)$ in Equation (28) can be developed in powers of $-eA_o$ and Equation (28) can be approximated by the following expression:

$$\chi \approx \frac{1}{(\gamma_{\nu} + 1)mc} \left[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} - \frac{e}{c} \boldsymbol{A} \right] \boldsymbol{\varphi}.$$
 (32)

Substituting Equation (32) in the first equation of Equation (27) allows obtaining the following time-independent Pauli-like quasi-relativistic wave equation:

$$\left\{ \frac{\left[\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right]^{2}}{(\gamma_{v} + 1)m} + e\boldsymbol{A}_{o} - \frac{2\mu_{B}}{(\gamma_{v} + 1)} (\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{B}) \right\} \varphi = E'\varphi.$$
(33)

For a free electron moving through a constant magnetic field, with magnitude B_{ext} pointing in the *z* direction, Equation (33) can be approximated as:

$$-\frac{\hbar^2}{(\gamma_v+1)m}\nabla^2\varphi(\mathbf{r}) - \frac{2\mu_B}{(\gamma_v+1)}B_{ext}\sigma_z\varphi(\mathbf{r}) = E'\varphi.$$
(34)

Equation (34) is the quasi-relativistic version of Equation (31). When the electron moves slowly, $\gamma_{\nu} \sim 1$, thus Equation (34) coincides with Equation (31). Equation (34) includes two corrections to Equation (3). First, includes the correct relativistic relation between *K* and *p*. Second, as shown in **Figure 1**, the energy difference corresponding to the two components of φ is not independent of *K*, as suggested by Equation (31), but decreases by a factor of twice $2/(\gamma_{\nu} + 1)$ at quasi-relativistic energies. This relevant result could be easily tested experimentally.

5. Relativistic Corrections to the Energies of the Bounded States in Hydrogen-Like Atoms

For Hydrogen-like atoms, we can assume the vector potential in Equation (27) is null, and:

$$eA_o = U_C(r) = -\frac{e^2}{4\pi\varepsilon_o} \frac{Z}{r}.$$
(35)

In Equation (35), U_c is the Coulombic electrostatic energy, Z is the atomic number, and ε_o is the electric permittivity of vacuum [2] [4] [13] [15]. The exact Dirac's energies of the bound states of the electron in Hydrogen-like atoms are given by the following equation [2]:

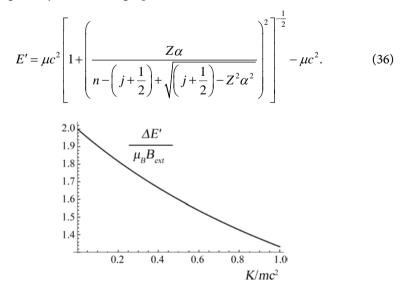


Figure 1. Plot of twice $2/(\gamma_v + 1)$ as a function of K in mc^2 units.

In Equation (36), $n = 1, 2, \dots; l = 0, 1, \dots, (n-1); j = l \pm 1/2,$ $\alpha = (1/4\pi\varepsilon_o) \times (e^2/\hbar c) \approx 1/137$ is the fine structure constant, $\mu = (m_e m_n)/(m_e + m_n)$ is the reduced mass of the electron in a Hydrogen-like atom with a nucleus of mass m_n , and m_e is the electron mass [2]. Often the following approximation to Equation (36), which is valid when $E' \ll mc^2$, is obtained using a perturbative approach based in the Schrödinger equation [2] [12]:

$$E' = E_{Sch} \left(1 + \Delta E_{K,Sch} + \Delta E_{D,Sch} + \Delta E_{SO,Sch} \right).$$
(37)

In Equation (37), E_{Sch} gives the values, of the bounded energies of the electron in Hydrogen-like atoms, obtained using the Schrödinger equation [1] [2] [3] [4] [5] [14]:

$$E_{Sch} = -\left[\frac{\mu}{2\hbar^{2}} \left(\frac{e^{2}}{4\pi\varepsilon_{o}}\right)^{2}\right] \frac{Z^{2}}{n^{2}} = -\frac{\mu c^{2}}{4} \frac{\alpha^{2} Z^{2}}{n^{2}}.$$
 (38)

 $\Delta E_{K,Sch}$ is the relativistic correction to the kinetic energy, which is given by the following expression [2] [11] [12] [13] [14]:

$$\Delta E_{K,Sch} = -E_{Sch} \frac{\alpha^2 Z^2}{n^2} \left(\frac{3}{4} - \frac{n}{l + \frac{1}{2}} \right).$$
(39)

 $\Delta E_{D,Sch}$ is the so-called the Darwin correction, which is only not null when l = 0 [2] [12]:

$$\Delta E_{D,Sch} = -E_{Sch} \frac{\alpha^2 Z^2}{n^2}.$$
(40)

Finally, $\Delta E_{SO,Sch}$ is the so-called spin-orbit correction, which is only not null when $l \neq 0$ [2] [12]:

$$\Delta E_{D,Sch} = -E_{Sch} \frac{\alpha^2 Z^2}{2n} \frac{j(j+1) - l(l+1) + 3/4}{l\left(l+\frac{1}{2}\right)(l+1)}.$$
(41)

From Equations (38) to (41) follows the relativistic corrections are much smaller that E_{sch} when $(\alpha Z/n)^2 \ll 1$. One should expect the energies calculated using Equation (37) sensibly differ from the exact Dirac's energies for the lowest energy states (smallest *n*-values) of heavy Hydrogen-like atoms. At this point, however, no one should be surprised by the fact that following a similar procedure than the used for obtaining Equation (37), but using a perturbative approach based in the quasi-relativistic wave equation (details shown in the **Appendix**), one can find a much better approximation to Equation (36), which is valid until quasi-relativistic energies:

$$E' = E_{QR} \left(1 + \Delta E_{D,QR} + \Delta E_{SO,QR} \right). \tag{42}$$

In Equation (42), E_{QR} gives the energies of the bounded states obtained using the quasi-relativistic wave equation for Hydrogen-like atoms [15]:

$$E_{QR} = -\frac{\mu c^2}{\Xi} \left[\Xi - (2n + \Delta)\sqrt{\Xi} \right].$$
(43)

In Equation (43), $\Delta = \Delta(l, Z)$ and Ξ are given by the following equations [15]:

$$\Xi = 4n^2 + 4\alpha^2 Z^2 + 4n\Delta + \Delta^2.$$
(44)

And:

$$\Delta(l,Z) = \left[\left(1 + \sqrt{(1+2l)^2 - 4\alpha^2 Z^2} \right) - 2(l+1) \right],$$

$$\sqrt{(1+2l)^2 - 4\alpha^2 Z^2} \approx (1+2l) - \frac{2\alpha^2 Z^2}{(1+2l)} - \frac{2\alpha^4 Z^4}{(1+2l)^3}.$$
(45)

In some cases, for heavy Hydrogen-like atoms with $Z \gg 1$, the term inside the square root in Equation (45) could be negative; in these cases, the approximation to the square root included in Equation (45) should be used. As should be expected, $E_{QR} \approx E_{Sch} (1 + \Delta E_{K,Sch})$ when $E' \ll mc^2$ [15]. It is worth noting that E_{QR} is identical to the positive energies calculated for the Hydrogen atom using the Klein-Gordon equation [19]. $\Delta E_{D,QR}$ is the new Darwin correction, which also is only not null when l = 0:

$$\Delta E_{D,QR} = -k_D E_{QR} \frac{\alpha^2 Z^2}{n}, \ k_D = (\gamma_v + 1)^{\frac{n}{n+1}}.$$
 (46)

 $\Delta E_{SO,QD}\,$ is the new spin-orbit correction, which also is only not null when $l\neq 0$:

$$\Delta E_{D,Sch} = -k_{SO} E_{QR} \frac{\alpha^2 Z^2}{2n} \frac{j(j+1) - l(l+1) + \frac{3}{4}}{l(l+\frac{1}{2})(l+1)}, \ k_{SO} = \left(\frac{\gamma_V + 1}{2}\right)^{-(n-l+1)^{5/2}}.$$
 (47)

The energies of the ground state (n = 1, l = 0, j = 1/2) of the Hydrogen atom (Z = 1) calculated using Equations (36), (37), (38), (42), and (43) are E' = -13.6022, -13.6022, -13.6020, -13.6019, and -13.6029 eV, respectively. All these values are within a 0.005% error respect to the exact Dirac's energy. This is because $E' \ll mc^2$ when Z = 1. A comparison between the calculated values of the energy difference between two emission lines (ΔE_L) of the Hydrogen atom are shown in Table 1. ΔE_L was calculated using the following equation:

$$\Delta E_{L} = \left[E' \left(n_{2}, l_{2}, j_{2} = l_{2} + \frac{1}{2} \right) - E' \left(n_{1}, l_{1}, j_{1} = l_{1} + \frac{1}{2} \right) \right]$$

$$- \left[E' \left(n_{2}, l_{2}, j_{2} = l_{2} - \frac{1}{2} \right) - E' \left(n_{1}, l_{1}, j_{1} = l_{1} + \frac{1}{2} \right) \right].$$
(48)

E' was evaluated using Equations (36), (37), and (42). For the *a*-Lyman doublet, we used $n_2 = 2$, $l_2 = 1$ and $n_1 = 1$, $l_1 = 0$ [2] [12]. For the *a*-Balmer doublet, we used $n_2 = 3$, $l_2 = 1$ and $n_1 = 2$, $l_1 = 0$ [2] [12]. The last column of **Table 1** corresponds to $n_2 = 3$, $l_2 = 2$ and $n_1 = 2$, $l_1 = 1$. It was chosen as an instance where both l_2 and l_1 are not zero. In all instances in **Table 1**, there is an excellent correspondence between the calculated values. Again, this is because $E' \ll mc^2$ when Z = 1.

Z

$\Delta E_L ({ m meV})$	<i>a</i> -Lyman	<i>a</i> -Balmer	Other
Equation (36)	0.0452718	0.0134139	0.00447118
Equation (37)	0.0452703	0.0134134	0.00447114
Equation (42)	0.0452715	0.0134138	0.00447119
ΔE_{1} (meV)		ΔE_t (meV)	
7×10^{6} 6×10^{6} 5×10^{6} 4×10^{6} 3×10^{6} 1×10^{6} (a)		2.0×10° 1.5×10° 1.0×10° 500 000	2
ΔE_{L} (me)	60 80 100 500 000 400 000 V) 300 000 200 000 100 000	(c)	60 80 100

Table 1. Calculated values of ΔE_L (in meV) for the Hydrogen atom obtained using Equations (36), (37), and (42) for (a) *a*-Lyman doublet, (b) *a*-Balmer doublet, and (c) corresponding to the energy difference between two others emission lines.

Figure 2. Dependence on Z of ΔE_L (in meV) calculated using (red, continuous) Equation (36), (black, dot-dashed,) Equation (37), and (blue, dashed) Equation (42) for (a) *a*-Lyman doublet, (b) *a*-Balmer doublet, (c) another example corresponding to the last column of **Table 1**.

More importantly, Equation (42) provides a better approximation than Equation (37) to the values of ΔE_L calculated using Equation (36). This is confirmed by the plots shown in **Figure 2** showing the dependence on Z of ΔE_L . Clearly, as expected, at quasi-relativistic energies ($Z \gg 1$), Equation (42) (dashed blue curve) provides a much better approximation than Equation (37) (dot-dashed black curve) to the values of ΔE_L calculated using the exact Dirac's energies (continuous red curve).

6. Conclusion

It was shown that the time dependent Equations (1) and (18), and the time-independent Equation (20) are very useful equations which are directly related to the Klein-Gordon equation, thus allowing a quantum description of a constant number of spin-0 particles moving at quasi-relativistic energies. It was presented and discussed, for the first time, a Pauli-like quasi-relativistic wave equation which is directly related to the Dirac equation, thus allowing for a quantum description of a constant number of spin-1/2 particles moving at quasi-relativistic energies and interacting with an external electromagnetic field. Finally, using a perturbative approach based on the quasi-relativistic wave equations discussed in this work, it was found and validated, also for the first time, an equation giving the energies of the bounded states in Hydrogen-like atoms. The authors hope we have been able to motivate the curiosity of the readers. Undoubtedly, the equations and methods discussed here enrich the accumulated physics knowledge, and open new ways to tackle quantum problems involving a constant number of particles at quasi-relativistic energies. This also provides interesting pedagogical opportunities for a fresh approach to the introduction of relativistic effect in introductory quantum mechanics courses.

Conflicts of Interest

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

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Appendix

Equations (37) and (42) can both be obtained from Equation (27) with a null vectorial potential (*A*) and eA_o given by Equation (35). For obtaining Equation (37), Equation (28) should be approximated in the following way [2]:

$$\chi \approx \frac{1}{2mc} \left(1 - \frac{E' - U_c}{2mc^2} \right) [\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}] \boldsymbol{\varphi}.$$
(A1)

Then, substituting Equation (A1) in the first equation of Equation (27) results [2]:

$$\frac{1}{2m} \left[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \right] \left(1 - \frac{E' - U_C}{2mc^2} \right) \left[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \right] \varphi = \left[E' - U_C(r) \right] \varphi.$$
(A2)

Or:

$$\left[-\frac{\hbar^2}{2m}\nabla^2\varphi + U_C(r)\right]\varphi - \left\{\frac{1}{2m}\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\right]\left[\frac{E'-U_C(r)}{2mc^2}\right]\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\right]\right\}\varphi = E'\varphi. \quad (A3)$$

The time-independent Schrödinger equation for Hydrogen-like atoms is equal to Equation (A3) after excluding the term between curls in the left size of Equation (A3) [1] [2] [3] [4] [5]; therefore, the relativistic corrections to the energies calculated using the Schrödinger equation are contained in this term [2]. However, if Equation (28) is approximated in the following way:

$$\chi \approx \frac{1}{(\gamma_{v}+1)mc} \left(1 + \frac{U_{C}}{(\gamma_{v}+1)mc^{2}}\right) [\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}] \varphi.$$
(A4)

Then, substituting Equation (A4) in the first equation of Equation (27) results:

$$\frac{1}{(\gamma_{\nu}+1)m} \left[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \right] \left(1 + \frac{U_{C}}{(\gamma_{\nu}+1)mc^{2}} \right) \left[\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \right] \varphi \left[E' - U_{C}(r) \right] \varphi.$$
(A5)

Or:

$$\left[-\frac{\hbar^{2}}{(\gamma_{\nu}+1)m}\nabla^{2}\varphi+U_{c}(r)\right]\varphi+\left\{\frac{1}{(\gamma_{\nu}+1)m}\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\right]\left[\frac{U_{c}(r)}{(\gamma_{\nu}+1)mc^{2}}\right]\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\right]\right\}\varphi=E'\varphi.$$
(A6)

The time-independent quasi-relativistic wave equation for Hydrogen-like atoms is equal to Equation (A6) after excluding the term between curls in the left size of Equation (A6) [12]; therefore, the relativistic corrections to the energies calculated using the quasi-relativistic wave equation are contained in this term. In Equation (A3), the term between curls produces three relativistic corrections to the energy, which are given by Equations (39) to (41) [2]. It can be shown, following the same procedure [2], but using the wavefunctions satisfying the quasi-relativistic wave equation for Hydrogen-like atoms [14] [16], that the term between curls in Equation (A6) produces two relativistic corrections to the energy, which are given by Equations (46) and (47).



Erratum to "Various Empirical Equations to Unify between the Gravitational Force and the **Electromagnetic Force**" [Journal of Modern Physics 12 (2021) 859-869]

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Abstract

The original online version of this article (Miyashita, T. (2021) Various Empirical Equations to Unify between the Gravitational Force and the Electromagnetic Force, Journal of Modern Physics, Vol. 12, 859-869. https://doi.org/10.4236/jmp.2021.127054) unfortunately contains the very important mistakes. The author discovered the possible problem in Equation (26) shown in Appendix. To fix the problem, the author wishes to change Equation (2) and make it more accurate.

Keywords

Erratum

1) Page 2 Equation (2) should be revised to the following:

$$\frac{Gm_p^2}{\frac{e^2}{4\pi\varepsilon_0}} = \frac{4.5}{2\pi} \times \frac{m_e}{e} \times hc \times \left(1\frac{C}{J \cdot m} \times \frac{1}{1 \text{ kg}}\right)$$
(2)

where *h* is the Planck constant.

2) So, the following Equation (12) cannot be used.

$$\hbar c = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^{\frac{1}{2}} \left(\frac{q_m^2}{\mu_0\pi}\right)^{\frac{1}{2}}$$
(12)

Then,

$$\frac{Gm_p^2}{e^2} = \frac{1.8672 \times 10^{-64}}{2.3071 \times 10^{-28}} = 8.0936 \times 10^{-37}$$
(A)

$$\frac{m_e}{e} \times hc = \frac{9.1094 \times 10^{-31}}{1.6022 \times 10^{-19}} \times 1.9864 \times 10^{-25} = 1.1294 \times 10^{-36}$$
(B)

Regarding the factor of 9/2, we used 4.48870 instead of 4.5. Regarding the factor of π , we used 3.13189 instead of 3.14159. So,

$$\frac{4.5}{2\pi} = \frac{4.48870}{2 \times 3.13189} = 0.71661$$
 (C)

$$\frac{4.5}{2\pi} \times \frac{m_e}{e} \times hc = 0.71661 \times 1.1294 \times 10^{-36} = 8.0936 \times 10^{-37}$$
(D)

Equation (D) is equal to Equation (A). Therefore, the compensation method is perfect.

Equation (2) should be changed, but any other equations can be unchanged.



Frontier Orbitals, Combustion and Redox Transfer from a Fermionic-Bosonic Orbital Perspective

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Abstract

Oxygenations are highly exergonic, yet combustion of organic matter is not spontaneous in an atmosphere that is 21% O2. Electrons are fermions with a quantum spin number s of $1/2\hbar$. An orbital containing a single electron with s= 1/2 is fermionic. Orbitals can contain a maximum of two electrons with antiparallel spins, *i.e.*, spin magnetic quantum numbers m_c of 1/2 and -1/2. An orbital filled by an electron couple has s = 0 and bosonic character. The multiplicity of a reactant is defined as |2(S)| + 1 where S is the total spin quantum number. The Wigner spin conservation rules state that multiplicity is conserved. The transmission coefficient κ of absolute reaction rate theory also indicates the necessity for spin conservation. Burning is fermionic combustion that occurs when sufficient energy is applied to a bosonic molecule to cause homolytic bond cleavage yielding fermionic products capable of reaction with the bifermionic frontier orbitals of triplet multiplicity O₂. Neutrophil leucocytes kill microorganisms by bosonic combustion and employ two mechanisms for changing the multiplicity of O₂ from triplet to singlet. Microorganisms, composed of bosonic singlet multiplicity molecules, do not directly react with bifermionic O2, but are highly susceptible to electrophilic attack by bosonic electronically excited singlet molecular oxygen $({}^{1}O_{2}^{*})$. Hydride ion (H⁻) transfer is the common mode of cytoplasmic redox metabolism. Bosonic transfer of an orbital electron couple protects from damage by obviating fermionic reaction with bifermionic O₂. Bosonic coupled electron transfer raises the consideration that quantum tunneling might be involved in facilitating such redox transfer.

Keywords

Fermion, Boson, Orbital, Spin, Combustion, Redox Transfer, Tunneling

1. Introduction and Background

A wavefunction (ψ) defines a quantum system. An orbital is described by ψ_{n,l,m_l} where *n* is the principle quantum number, *l* is the azimuthal or angular momentum quantum number, and m_l is the magnetic quantum number. An electron occupying an orbital is described by the wave function ψ_{n,l,m_l,s,m_s} where the electron-spin quantum number *s* describes the total spin and the spin magnet quantum number m_s describes each electron spin as 1/2 or -1/2 [1] [2].

According to the exchange principle, a pair of particles, *a* and *b*, can be described by a wavefunction $\psi(a, b)$. Exchanging the particles generates a new wavefunction $\psi(b, a)$. If particles are identical and indistinguishable, their probability distributions will be identical, $\psi^2(a, b) = \psi^2(b, a)$, regardless of the orientation of the particles. When the square roots of the probability distributions yield the wavefunctions $\psi(a, b) = \psi(b, a)$, exchange is symmetric and the particles are bosons. When the wavefunctions $\psi(a, b) = -\psi(b, a)$, exchange is antisymmetric and the particles are fermions. Bosons obey ordinary commutation. Rotating a boson through 360 degrees returns it to its original state, $\psi = \frac{360^{\circ}}{2} \psi$. Bosons are symmetric particles with integral spin. Photons are bosons with zero mass and integer spin, fermions anti-commute, Rotating a fermion through 360 degrees, $\psi = \frac{360^{\circ}}{2} - \psi$, changes the sign or phase of the fermion, but does not return the particle to its original state. An additional 360 degrees rotation, $-\psi = \frac{360^{\circ}}{2} \psi \psi$, is required to return the antisymmetric particle to its original state. Electrons, protons and neutrons are fermions with mass.

Bosons differ from fermions with regard to quantum spin. The natural unit of quantum spin is the reduced Planck's constant (*h*-bar or \hbar), where $\hbar = h/(2\pi)$. Bosons have spins with integer values. Photons are bosons with a spin value of $1\hbar$. Fermions have spins that are 1/2 integers. Electrons are fermions with a spin of $1/2\hbar$. Electrons possess intrinsic spin described by the quantum number *s*. Such spin is independent of orbital motion and is without analogy in classical physics. The spin magnetic quantum number *m_s* has two spin possibilities: 1/2 (spin up, \uparrow) or -1/2 (spin down, \downarrow). The multiplicity of an atom or molecule equals |2(S)| + 1 where *S* is the total spin.

2. Fermionic and Bosonic Orbitals

Fermions can combine to yield a wavefunction with bosonic character. An alpha particle made up of four fermions is bosonic [3]. An electron is a fermion. As such, an orbital filled by a single electron has an s = 1/2 and fermionic character [4] [5]. An orbital filled by an antisymmetric electron couple has s = 0 and bosonic character. The frontier orbitals of atoms and molecules are directly involved in reaction chemistry and include the lowest unoccupied (LU(A)MO), the highest occupied (HO(A)MO), and the single electron occupied (SO(A)MO) atomic (A) or molecular (M) orbitals [6].

The vast majority of reactions observed in organic and biochemistry involve singlet multiplicity reactants. Reactions involve frontier LUMO and HOMO are

bosonic. Free radical reactions involve fermionic frontier orbitals, *i.e.*, SO(A)MO. Reaction chemistry can be approached from a fermionic-bosonic orbital perspective.

Consistent with the fermion nature of electrons, Pauli's exclusion principle limits an orbital to a maximum of two antiparallel electrons, *i.e.*, m_s of 1/2 (\uparrow) and -1/2 (\downarrow). In Figure 1, note that the lower energy 1s and 2s orbitals of atomic N each contain two antiparallel electrons, *i.e.*, an orbital couple with s = 0. These orbitals are closed to reaction chemistry. The frontier orbitals of atomic N include the three 2p orbitals. These 2p orbitals are degenerate, *i.e.*, each orbital has the same energy. Each 2p orbital contains a single fermionic electron. Hund's maximum multiplicity rule states that the electrons in degenerate singly occupied orbitals will have parallel spins [7]. As such, each of the three 2p frontier orbitals of N have an s = 1/2 and the S of N is 3(1/2). The spin multiplicity, *i.e.*, |2(S)| + 1, for N is thus |2(3/2)| + 1 = 4. Stated differently, atomic nitrogen is a triradical with quartet spin multiplicity. Each 2P orbital of N is a SOAO, and as such, atomic N is trifermionic. As depicted in Figure 1 and stated in Table 1, the product of reacting two quartet multiplicity N atoms is singlet multiplicity N₂.

The lower energy 1s and 2s orbitals of N all contain coupled antiparallel electrons with s = 0. These non-frontier bosonic orbitals do not participate in reaction. Likewise, the sigma bonding (σ) and antibonding (σ) orbitals of N₂, derived from the 1s and 2s orbitals of the atomic N's, are bosonic and closed to reaction chemistry. The frontier π bonding orbitals of N₂ are both filled by an electron couple with s = 0 and have bosonic character. In its ground state, N₂ is singlet multiplicity, triple bonded and bosonic.

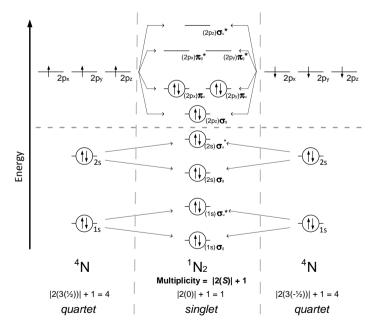


Figure 1. Orbital diagrams for atomic nitrogen (N), shown on left and right sides of the figure and separated by dashed vertical lines. The resulting molecular orbital diagram for N₂ is shown in the center. The filled σ_g and π_u bonding orbitals, shown above the dashed horizontal line, are responsible for the triple bond of N₂.

Reactant B	Reaction Complex
Singlet bosonic	Singlet bosonic
Doublet fermionic	Doublet fermionic
Triplet bifermionic	Triplet bifermionic
Quartet trifermionic	Quartet trifermionic
Doublet fermionic	Singlet bosonic
Triplet bifermionic	Doublet fermionic
Quartet trifermionic	Triplet bifermionic
Triplet bifermionic	Singlet bosonic
Quartet trifermionic	Doublet fermionic
Quartet trifermionic	Singlet bosonic
	Singlet bosonic Doublet fermionic Triplet bifermionic Quartet trifermionic Doublet fermionic Triplet bifermionic Quartet trifermionic Quartet trifermionic

 Table 1. Conservation of spin multiplicity from a fermionic-bosonic orbital perspective.

3. Spin Conservation

3.1. Transmission Coefficient of Absolute Reaction Rate Theory

Absolute reaction rate theory states that the rate of a chemical reaction requires that reactants first combine to form an activated complex,

$$k = \kappa (kT/h) K$$

where k is the rate, κ is the transmission coefficient, kT/h has the dimensions of frequency and K is the equilibrium constant for the activated complex. The transmission coefficient, κ , for typical reactions approximates unity, *i.e.*, each activated complex yields product, but not every activated complex at the potential-energy barrier will cross over to product [8]. The value of κ decreases by several orders of magnitude in reactions involving change in spin state [8].

3.2. Wigner Spin Conservation from a Fermionic-Bosonic Perspective

The Wigner spin conservation rules state that a reacting system resists any change in spin angular momentum, *i.e.*, multiplicity [9] [10]. The total spin number, *S*, of an atom or molecule defines its multiplicity; *i.e.*, |2S| + 1 = multiplicity. When S = 0, the multiplicity is singlet, when S = 1/2, the multiplicity is doublet, when S = 1/2 + 1/2, the multiplicity is triplet, et cetera. Reactions involving change in multiplicity have transmission coefficient, κ , values of less than 10^{-4} . The spin states or multiplicities of the reactants determine the spin state or multiplicity of the activated complex, and are conserved in the spin states or multiplicities of the resulting product or products. For example, if the impossibility of orbital overlap is ignored and reaction is assumed to involve a bosonic singlet multiplicity molecule and a bifermionic triplet multiplicity, and bifermionic triplet multiplicity must be conserved in the product or products. These and other possibilities are described in **Table 1**.

With regard to multiplicity, singlet-singlet reactions are allowed and yield singlet products. From a frontier orbital perspective, bosonic HOMO-LUMO interactions are allowed and yield bosonic products. For example, reaction of singlet multiplicity hypochlorite (OCl⁻) with singlet multiplicity hydrogen peroxide (H₂O₂) yields singlet multiplicity water (H₂O), singlet multiplicity chloride (Cl⁻) and electronically excited singlet multiplicity molecular oxygen (${}^{1}O_{2}^{*}$). Singlet multiplicity reactants produce singlet multiplicity products. Spin conservation requires ${}^{1}O_{2}^{*}$, not triplet multiplicity ${}^{3}O_{2}$, as the product of the H₂O₂-OCl⁻ reaction. Production of ${}^{1}O_{2}^{*}$ is required for spin conservation, but violates Hund's maximum multiplicity rule [11], and as such, ${}^{1}O_{2}^{*}$ is electronically excited with a lifetime of about a microsecond [12]. As illustrated in Figure 2, ${}^{1}O_{2}^{*}$ relaxes to its triplet ground state by emitting a near infrared photon [13].

Bosonic frontier orbital interactions make up the vast majority of organic and biochemical reaction. Reactions involving a singlet with either a doublet, triplet or quartet multiplicity molecule must conserve spin. If bosonic-fermionic reaction occurs, the reaction product will retain the multiplicity of the fermionic reactant. Relative to frontier orbital considerations, such reactions require highly improbable LUMO-SOMO interaction. However, reactions involving doublet-doublet, triplet-triplet and quartet-quartet multiplicity reactants all yield singlet multiplicity products. Based on frontier orbital considerations, these fermion-fermion, bifermion-bifermion, and trifermion-trifermion reactions involve SOMO-SOMO interactions and produce bosonic products. The unfavourability of singlet-triplet, *i.e.*, bosonic-bifermionic, reaction is well illustrated by considering the reaction of ground state triplet multiplicity (S = 1/2 + 1/2 or -1/2 + -1/2) molecular oxygen (${}^{3}O_{2}$) with a singlet multiplicity (S = 0) substrate molecule.

As illustrated in **Figure 2**, ${}^{3}O_{2}$ has two singly occupied frontier orbitals. As defined by Hund's maximum multiplicity rule, the lowest energy or ground state of ${}^{3}O_{2}$ is achieved when both of its pi antibonding (π_{g}^{*}) frontier orbitals have one electron, *i.e.*, each π_{g}^{*} orbital has the same m_{g} *i.e.*, 1/2 + 1/2 or -1/2 + -1/2 [11]. Since the two frontier orbitals of ${}^{3}O_{2}$ are both fermionic, ${}^{3}O_{2}$ is described as bifermionic. Oxygen is the second most electronegative element, and as such, organic oxygenation reactions are highly exergonic, but frontier orbital interaction are highly improbable, and combustion is not spontaneous.

Radicals react with radicals. Frontier orbital interactions involving SOMO-SOMO reactants are easily conceived. The products of such doublet-doublet reactions are singlet. In SOMO-SOMO reaction, the fermionic electrons of each SOMO couple to produce a bosonic product. For example, frontier orbital interaction of the fermionic π_g^* SOMO of doublet multiplicity hydroperoxyl radical (²HO₂) with the fermionic π_g^* SOMO orbital of doublet multiplicity superoxide radical (²O₂⁻) yields singlet multiplicity hydrogen peroxide (H₂O₂) and electronically excited singlet multiplicity molecular oxygen (¹O₂^{*}) [14].

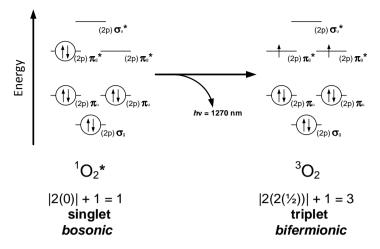


Figure 2. The frontier orbitals of electronically excited ${}^{1}O_{2}^{*}$ violate Hund's maximum multiplicity rule (left) and has a microsecond life time relaxing to ground state ${}^{3}O_{2}$ (right) by near-infrared photon (1270 nm) emission.

The role of ${}^{3}O_{2}$ in quenching the phosphorescence from relaxation of electronically excited triplet multiplicity dye (${}^{3}dye^{*}$) is explained by triplet-triplet annihilation yielding bosonic products. This same triplet-triplet quenching is responsible for photodynamic action. Reaction of the electronically excited triplet dye (${}^{3}dye^{*}$) with ${}^{3}O_{2}$ returns the dye to its ground state (${}^{1}dye$) and photodynamically generates ${}^{1}O_{2}^{*}$ [15] [16].

4. Combustion

Combustion, defined as an act or instance of burning, requires fuel and molecular oxygen, and produces heat and light. The organic molecules that serve as fuel are of singlet multiplicity and present bosonic frontier orbitals that are unreactive with the bifermionic frontier orbitals of ${}^{3}O_{2}$. Consistent with absolute reaction rate theory and the spin conservation rules, such reactions are not spontaneous.

4.1. Fermionic Combustion

To initiate burning, a sufficient amount of energy, e.g., a flame, must be applied to cause homolytic bond cleavage of the singlet multiplicity fuel molecule. Each homolytic cleavage yields two doublet multiplicity SOMO products. These fermionic products can directly react with the bifermionic frontier orbitals of ${}^{3}O_{2}$. Radicals react with radicals. As described in **Table 1**, reaction of a doublet multiplicity (*i.e.*, S = 1/2) radical with triplet multiplicity (*i.e.*, S = -1/2 + -1/2) molecular oxygen yields doublet multiplicity (S = -1/2) product, heat and light. In turn, the doublet multiplicity (S = -1/2) product can now react with another triplet multiplicity (S = 1/2 + 1/2) ${}^{3}O_{2}$, et cetera, resulting in reaction propagation, *i.e.*, burning. Note that fermionic-fermionic reaction yields bosonic product, and that fermionic-multifermionic reaction yields the least fermionic product.

4.2. Bosonic Combustion

The neutrophil leukocyte, a phagocytic white blood cell, is tasked with defending the host animal against a vast variety of pathogenic microorganisms [17]. Fifty years ago, I pondered the possibility that phagocytic leukocytes kill microbes by changing the multiplicity of molecular oxygen from triplet to singlet [18]. From a frontier orbital perspective, changing bifermionic ${}^{3}O_{2}$ to bosonic ${}^{1}O_{2}^{*}$ opens the possibilities for bosonic electrophilic reaction with the bosonic molecular composition of microbes, i.e., bosonic combustion. Conventional fermionic combustions involve highly exergonic oxygenation reactions that generate electronically excited carbonyls that relax by emitting photons in the visible spectrum. The bosonic combustions of neutrophil leukocyte microbicidal action also involve highly exergonic oxygenations that generate electronically excited carbonyls with relaxation by photon emission. Light is emitted when neutrophil leukocytes phagocytose and kill opsonized microbes, and the photon emission or chemiluminescence is proportional to ³O₂ consumption and to glucose metabolism via the hexose monophosphate metabolic (HMP) shunt. As described in the section below, neutrophil leukocytes employ two mechanisms for the conversion of bifermionic ${}^{3}O_{2}$ to bosonic ${}^{1}O_{2}^{*}$. The first involves fermionic-fermionic annihilation, and the second involves myeloperoxidase-mediated bosonic-bosonic reaction.

4.3. Neutrophil Combustive Microbicidal Metabolism

Neutrophil reduced nicotinamide adenine dinucleotide phosphate (NADPH) oxidase controls HMP metabolism by accepting two reducing equivalents from NADPH thus liberating the oxidized NADP+ that is required for glucose-6-phosphate (G-6-P) dehydrogenase metabolism of glucose. Biochemical dehydrogenations involve hydride (H⁻) transfer. The bosonic character of such redox exchange will be considered subsequently. The riboflavin prosthetic group of NADPH oxidase facilitates decoupling of the bosonic electron pair. Riboflavin mediated separation allows fermionic expression of the separated electrons and results in reactive electron capture by bifermionic ³O₂ [14]. The product of such univalent reduction is the doublet multiplicity hydroperoxyl radical (²HO₂). $^{2}\text{HO}_{2}$ is an acid with a pKa of 4.8 that dissociates yielding a proton (H⁺) and doublet multiplicity superoxide radical $(^{2}O_{2}^{-})$. The reaction of fermionic $^{2}HO_{2}$ and fermionic ²O₂⁻ is a radical-radical annihilation yielding bosonic singlet multiplicity hydrogen peroxide (¹H₂O₂) and bosonic electronically excited singlet multiplicity molecular oxygen $({}^{1}O_{2}^{*})$ [19]. As described in Table 1, reactions of fermions yield bosonic products.

Neutrophils contain abundant myeloperoxidase (MPO). The haloperoxidase action of MPO provides an additional mechanism for generation of bosonic ${}^{1}O_{2}^{*}$. MPO consumes the $H_{2}O_{2}$ and acid (H⁺) products of NADPH oxidase ac-

tivity to oxidize chloride (Cl⁻) to hypochlorous acid (HOCl) or its conjugate base hypochlorite (OCl⁻). All of the reactants and products of MPO haloperoxidase action are singlet multiplicity and present bosonic frontier orbitals. The HOCl/OCl⁻ produced can further react non-enzymatically with additional H_2O_2 producing Cl⁻ and ${}^{1}O_{2}^{*}$ [20]. MPO can catalyze classical peroxidase activity involving radials, but such activity is distinct from the acid haloperoxidase action involved in microbicidal action [17].

Generation of ¹O₂^{*} violates Hund's maximum multiplicity rule; *i.e.*, the electronic configuration with highest multiplicity has the lowest energy. The greater the number of wave functions possible for a system, the lower the energy. Higher multiplicity states produce greater nuclear-electron attraction and are of lower energy [11]. As such, ${}^{1}O_{2}^{*}$ is metastable with a lifetime of about a microsecond. This lifetime restricts its potent electrophilic reactivity to within a radius of about 0.2 microns (µm) [12]. Upon phagocytosis, the microbe becomes the locus of neutrophil microbe killing. Generation of the bosonic reactant ${}^{1}O_{2}^{*}$ within the phagolysosome space of the neutrophil directly focuses its potent electrophilic reactivity to the target microbe and minimizes collateral damage. Purified MPO selectively binds all gram-negative bacteria tested and can bind and inactivate endotoxin even in the absence of haloperoxidase function [21]. Selective MPO binding to microbes correlates with selective MPO-mediated microbicidal action. Bosonic combustion is limited by the lifetime of ¹O₂^{*}. Such reactive restrictions have the advantage of selectively focusing and confining combustive action to the microbe while avoiding bystander injury to host cells [22].

5. Bosonic Transfer of Reducing Equivalents

Cytoplasmic redox transfers, *i.e.*, pre-cytochrome electron transfers, typically involve the movement of two reducing equivalents from one singlet multiplicity molecule to another, and is described as H⁻ transfer. Such hydride transfer involves the movement of a proton plus an orbital couple of antiparallel electrons. The orbital couple has a s = 0, and as such, transfer is singlet multiplicity and bosonic.

Biological systems are exposed to an atmosphere with abundant O_2 . The bosonic character of biochemical systems provides protection against direct reaction with bifermionic O_2 . As previously considered, any biologic transfer involving a single fermionic electron would open the possibility for direct fermionic reaction with O_2 . The resulting fermionic-bifermionic reaction would produce a fermionic product and the possibility for further fermionic-bifermionic propagation.

Redox transfer of a bosonic orbital electron couple might offer additional advantage. The bosonic nature of the alpha particle facilitates quantum tunneling from the nucleus [23]. The bosonic nature of a Cooper pair of electrons facilitates superconductivity [24]. Alpha particle radiation and Cooper pairing in superconductivity are very different from each other, and both phenomena are very different from biochemical redox electron transfer. However, the commonality of bosonic pairing in quantum tunneling raises suppositions with regard to a possible role in facilitating biological redox transfer.

6. Summary and Conclusion

Reaction chemistry involves frontier orbital interactions. An orbital is fermionic if occupied by a single electron, and bosonic if occupied by an electron pair. With regard to orbital reactivity, bosonic orbitals react with bosonic orbitals generating bosonic products, fermionic orbitals react with fermionic orbitals generating bosonic products, and fermionic orbitals react with bifermionic molecules generating less fermionic products. Fermionic-bosonic reactions are improbable, but the products of any such reaction must conserve the fermionic character of the reaction complex. As a general observation, all reactions favor bosonic products. Burning or fermionic combustion is initiated by homolytic bond cleavage producing fermionic products that react with bifermionic triplet O2: The bosonic combustion of neutrophil leukocytes is initiated by changing the multiplicity of O₂ from triplet to singlet allowing bosonic electrophilic dioxygenation. With the exception of cytochrome chain transfer, intermolecular redox reactions involve transfer of an orbital electron pair and are bosonic. Such transfer obviates the possibility for fermionic reaction with bifermionic O2 and additional fermionic propagation. As a supposition, quantum tunneling might facilitate intermolecular redox transfer of a bosonic orbital electron couple.

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Conflicts of Interest

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

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Calculation of *G* Gravity Constant from the Mass and Electron Charge, and Fine Structure Constant

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Abstract

This study proposes, from the theoretical point of view, the calculation of the gravitational constant G, made starting from the charge and the electron mass, taking the constant of the Fine Structure into examination. In the empty space, couples of virtual positron electrons dematerialize, giving virtual photon origin. They, at their time, will become electrons, positrons and so on. These transformations are made keeping the board of their "amount of movement" and when they meet the matter, these couples come, reissued depending on the field and on the matter mass. The matter is the change of the trend of their gyromagnetic movement relationship which puts under pressure. In presence of two masses, this gyromagnetic movement relationship is already partially oriented towards the other mass. From here a force is established between these two masses that give as calculated constant equal to 6.678532. This value of G, obtained leaving from the charge and the electron mass, is very near the experimental values estimated in these last decades regard the value of the gravitational constant of G.

Keywords

Electron, Positron, Gravitational Constant, String Theory, Theory of Everything, Fine Structure Constant

1. Introduction

This study stems from a reflection on the quantum vacuum. The vacuum field, according to the quantum concept, can have no null energy states. The question is to answer, at a theoretical level, what is the mechanism and what are the possible causes that generate energy. The real nature of the physical vacuum is a debated topic and is the basis of modern cosmology and represents a tool to understand the foundations of physics. In this study, it is believed that the energy produced in the vacuum field comes from pairs of electrons and positrons. The electron-positron dipoles, in addition to interacting with each other producing virtual photons, affect neighboring dipoles by transferring to them "amount of motion". The contribution of this study is that, when electron and positron pairs meet particles of matter, they exert a pressure on it transferring energy that, hypothetically, is manifested as electromagnetic fluctuation. Keeping a holistic view of the physical phenomena discussed in this study and combining electron-positron electromagnetic interactions with Newtonian dynamics, it has come to the calculation of the gravitational constant *G*, resulted close to modern values calculated in the laboratory.

The Law of Universal Gravitation represents a milestone of scientific knowledge to the main thread of this study is represented by the calculation of the Gravitational Constant G, starting from the interaction between electron and positron. The calculation of G was carried out on an atomic scale, instead of considering the large masses predicted by Newton's equation. We wonder if this constant can represent a common denominator between the behavior of particles, the structure of matter and the dynamics of celestial masses and if, at theoretical level, the constant G can be considered a "mediator" between General Relativity, the forces of the Standard Model of particles and String Theory. The Law of Universal Gravitation represents a milestone of scientific knowledge to interpret celestial mechanics and a cornerstone of predictive science. In Newton's formulation and in the field equation of general relativity appears the proportionality coefficient G, independent of the physical location and masses used to determine it experimentally. In the last two and a half centuries, there have been experiments for the approximate calculation of G, from the eighteenth century to the present with increasingly refined methods and instruments [1] [2]. Recently, a team of quantum physicists from the University of Vienna and the Austrian Academy of Sciences realized for the first time in the laboratory a miniature version of the Cavendish experiment using millimeter-order masses. A result that opens new perspectives for the possible connection between gravitational and quantum physics [3] [4] [5] [6]. In this study, contrary to the techniques used in the past, such as the torsion balance or based on the principle of the pendulum, is proposed the calculation of the constant of gravitation G starting from the charge and the electron mass. The calculation, expressed in theoretical form, was conducted by the Belgian physicist Fernand Léon Van Rutten, and presented posthumously, having disappeared in 2016. This is a written memoir that Belgian Physicist left to his daughter as a scientific testament. The calculation of the constant of G, in the Van Rutten point of view, originates from the "bricks" of the matter rather than start her big masses of the celestial bodies, according to the Newtonian concept. A universal constant being of G, his estimated value, leaving from the electron positron interaction with respect to the big masses, therefore represents a point of connection among the concept of "micro" and "macro" cosmos, and nominates himself as unifying element between the fine matter and the gravity. The costing of gravitational or constant universal gravitation strength of G, is in fact the same one for all the bodies equipped with mass, be they as big as the stars or as little as sand grains. And, in the universe everything reduces himself to particles. Studying the world at smaller scales, on the order of the Angstrom, provides an opportunity to understand what we observe at larger scales. Of course, for each of these scales the behavior of matter is different.

The idea of a "hierarchy of universes" is not new. It, in fact, was already alive in Democritus of Abdera, understood as "scale factors", while new concepts were taken up in 1761 by J.H. Lambert and gradually developed until today, through H. Alfvén, O. Klein, D.D. Ivanenko and others [7]. Over the centuries, the need of physicists to find a formula or mechanism that brings together the four forces that interact on matter, gravity, electromagnetism, strong interaction and weak interaction, has been a common thread and an ambitious goal in the world of Physics. Recently, the study of gravity has been extended to include antimatter [8]. A holistic approach that associates physical structures, apparently different as gravity and electromagnetism, had been studied in the beginning by Michael Faraday (1849-1950) and then resumed, after about half a century by Weyl (1918) [9] and from the '20s by Albert Einstein with the "Unified Field Theory". But, after the innovations of the late 1800s and early 1900s, the search for a universal theory that encompassed the four forces that interact on matter became an insistent goal in the scientific world and among Physicists. The goal was, and is, to conceive a new theory, the "Theory of Everything", initially coined by J. Ellis (1986) [10] and pursued by Stephen Hawking [11]. Among the best-known empirical observations, the relationship between the gravitational universe and the universe of elementary particles stands out, the result of which concurs to hypothesize the existence of a similarity in a geometric and physical sense between macro universes and strong micro universes [12]. The adjective "strong" must be however contextualized in the scale physics, where the strong nuclear force that helps to keep together the matter is far superior to the other three fundamental forces: gravity, electromagnetism and weak nuclear forces. The calculation of G, leaving from the electron-positron analysis proposed in this study, reaches the surprising result to combine the electromagnetism with the gravity, Fine Structure with the String Theory, through a deterministic physical principle and not a mathematical formulation with the limit already highlighted by the Gödel's Theorem of Incompleteness [13]. A question, that of unifying the fundamental interactions of physics, which does not cease to arouse interest in research, also discussed in recent publications [14] [15] [16].

2. Constants and Variables

Etymologically and conceptually, the term "constant" ensures that some quantities remain so over time. However, in spite of their current use, the origin of "constants" is still an open question, not only in the world of Physics. Their importance cannot certainly be neglected, since different values of physical constants would radically change the knowledge of physical phenomena known up to now. In this study, the value of the Constant G has been deduced using other physical constants, such as the speed of light, mass, the fine structure constant [17] [18], Plank's constant, the inverse of the fine structure constant multiplied by 0.75, and fundamental quantities such as the electron charge. Unlike the constants used for the calculation of this work, as known validated by observation and experiment, the Gravitational Constant G derived from the interaction between electron-positron, is instead theoretical in nature. Its value, however, was found to be very close to both G of Newton's gravity, and to that recently calculated in the laboratories.

The variables in the calculation, however, are represented by the gyromagnetic orientation of the dipole electron-positron, which exerts pressure on matter when it intercepts it, and the distance electron-positron, which in this case must be much greater than the wavelength. From the outcome of this study, the value of the constant G can be considered for the different scales of mass magnitude, from the subatomic to the cosmic universe and vice versa and, in perspective, contribute to a better definition of the value of the constant G in the International System.

3. Method

The Method used to calculate the *G* constant is based on the concept of the "circumstantial paradigm" [19] associated with the deductive method, *i.e.*, guiding the logical procedure from hypothesis to conclusion. In this case, the "clue" coincides with the hypothesis that there exists a particle responsible for gravity, produced due to the interaction between electron-positron and their formation and destruction processes over time.

The procedure to realize the calculation of the constant G involves the use of other physical constants and is divided into two phases. The first considers an electromagnetic interaction in the electron-positron pairs; the second phase concatenates, through the gyromagnetic ratio of dipole, electromagnetic interactions with Newtonian dynamics, from which it is possible to obtain the value of gravitational constant G.

4. Discussion

In this study, we will try to show that the gravitational constant of *G* could be the result of a relationship between other physics constants. To explain the Universal Attraction Law, it was often assumed that a particle called graviton exists [20] [21] [22] [23]. In this study, we will show that a particle responsible for the gravity exists indeed. The space is not completely empty, it contains neutrinos, electromagnetic waves and fields, like the electromagnetic field and the gravitational field. The importing thing more, according to the cosmologists, is that the space contains most of the energy of the cosmos [24]. In this study we will show, as he says A.V. Rykov [25], that this energy could be formed by virtual couples of the

electron and positron that arise and, they disappear, forming photons immediately [26] [27] [28]. These couples [29] could be the Strings of the last approaches to physics [30] [31] [32]. In fact, Heisemberg's uncertainty principle states that the uncertainty of energy of a particle multiplied by the uncertainty of its lifetime must be greater or equal to the Plank constant divided by 4π , because these particles to be measurable.

- Below this value, these particles are imperceptible and so-called virtual.
- The encounter of virtual particles is not new.

Already the Lamb effect [33] can only be explained by a process in which a nucleon issues a virtual meson which interacts electromagnetically with the atomic electron and is subsequently reabsorbed by the nucleus [34].

These mesons are virtual electron-positron couples or photons to high energy. We will afterwards do the following hypotheses:

1) The space is height of these virtual couples or dipoles.

2) These virtual electron and positron couples do not disappear, but are annihilated giving virtual photon which, at their time, rematerialize in electrons and positrons origin and so away, giving the appearance of a movement of the electron and positron couple which travels in the space.

3) During their short life duration, these dipoles affect the near dipoles, transmitting them part of their "Momentum". These interactions between dipoles determine, hypothetically, electromagnetic fluctuations in the empty space.

4) But above all, when they meet a matter particle, are sent to following the particle field back and therefore exercise a pressure on the matter itself.

We will say that these pairs form and destroy sinusoidally over time. Therefore, the segment which joins these two charges is crossed by a current I and in complex notation, will have in Equation (1):

ρ

$$I = I/j\omega \tag{1}$$

e, it is the electron charge and $\omega = 2\pi v$, dove v it is the oscillation frequency.

In a distant r point from the dipole, the delayed potential is express as in Equation (2):

$$A = \frac{\Gamma \mu I}{4\pi r} e^{-\frac{j\omega r}{c}}$$
(2)

(μ , is the magnetic permeability of the medium, Γ the distance between the electron and the positron, *c* the light speed).

This takes, cross the classical reasoning [35], to the average flow of the vector of Poynting in direction of the dipole. If we integrate between 0 and π we get in Equation (3):

$$\frac{\Gamma^2 I^2 \int \sin^2 \theta d\Omega}{8\varepsilon c \lambda^2 \int \sin \theta d\Omega} = \left(\frac{\Gamma}{\lambda}\right)^2 I^2 4/(3\pi c)$$
(3)

(Ω is the solid angle, $d\Omega = 2\pi \sin \theta d\theta$, and λ is the wavelength of the oscillation, $\varepsilon = 1/4\pi$).

This relation is only valid if the distance is large, that is for $r \gg \lambda$.

If we substitute l^2 for its value $\dot{r}\omega^2 e^2$ in Equation (4), we get the energy radiated during the lifetime of the dipole, that is, a time equal to $1/\nu$.

$$E = \left(\frac{\Gamma}{\lambda}\right)^2 \frac{\nu 4\pi e^2}{3c} \nu 4\pi e^2 = 2h\nu \tag{4}$$

Because, after its short life, the dipole transforms into two photons hv so we get in Equation (5):

$$\alpha = \left(\frac{\Gamma}{\lambda}\right)^2 = \frac{3hc}{8\pi e^2} \tag{5}$$

a is a constant, the inverse of the constant of Fine Structure, multiplied by 0.75. Max Born insists on the importance of this constant: the only one which can be formed from e, while c and h indicate a deeper relation between electro-dynamics and quantum theory [36].

Now we find out what the gyromagnetic ratio g_0 of the dipole will be. Since the current in the dipole is $I = ej\omega$, the magnetic moment will be $e\omega\Gamma^2$ and λ being the wavelength of the oscillation, its angular momentum will be $m\omega\lambda^2$ and the gyromagnetic ratio becomes $g_0 = \pm (e/m)\alpha = \pm \gamma_0 \alpha$.

The orientation of these γ_0 is determined by the direction from which they come, and we will say that, whatever their sign, these γ_0 exert pressure on the particles of matter they encounter.

If we take a reference axis, with respect to this axis, each of these electrified particles arrives to an angle θ , the projection of their gyromagnetic on this axis relationships will be: $\gamma \alpha \cos \theta$, and the variations on this axis will be in Equation (6):

$$d\gamma = \gamma \alpha \sin \vartheta d\vartheta \tag{6}$$

If we integrate between γ_0 and γ we get: γ in Equation (7)

$$\log(\gamma_0/\gamma) = -\alpha \cos \vartheta + \text{constant}$$
(7)

If we place the constant = 0, γ becomes in Equation (8):

z

$$\gamma = \gamma_0 e^{-\alpha \cos \theta} \tag{8}$$

We take now in Equation (9) a particle of mass M and we will say that the number of electrons positrons received with a solid angle d Ω at any time is proportional to:

$$A e^{-\alpha \cos \theta} d\Omega \tag{9}$$

A is determined by the total number of electrons positrons present. *y* in the solid angle it will be in Equation (10):

$$A\gamma_0 e^{-\alpha\cos\vartheta} d\Omega \tag{10}$$

If we integrate the ratio of these two relations we obtain $\gamma = \gamma_0$.

So, in relation to a given axis, on a half-face because of γ_0 dipole coming from all directions, seen from this face, this mass M will be subjected to a pressure that tries to push it back and its force applied will be described in Equation (11):

$$f_1 = M \gamma_0 E \tag{11}$$

E, has the dimensions of an electric field. This field may be due to the virtual electrons and positrons surrounding the mass *M*, and we will not make any other assumptions about this field.

Following the reaction action principle, for two particles at a distance r, on the invisible faces of the other particles, the force that tends to bring them together will be in Equation (12):

$$f_2 = \left(M_1 M_2 / r^2\right) \gamma_0^2$$
 (12)

On the other faces, that is, those of the other mass, γ_0 of the dipole coming from this other mass undergoes an average orientation perpendicular to the surface of this other mass.

Their orientation is no longer anisotropic and because, in relation to their size, these masses are very distant from each other. In first approximation, y_0 is affected by the other particle, it can simply be multiplied by $\cos \theta$.

So, we'll have for the force that tries to repel these particles, described in Equation (13):

$$f_{3} = \left(M_{1}M_{2}/r^{2}\right)\gamma_{0}^{2}\frac{\int\cos\theta \cdot e^{-\alpha\cos\theta}d\Omega}{\int e^{-\alpha\cos\theta}d\Omega}$$
(13)

If we integrate f_3 between 0 and $\pi/2$, in Equation (14) we obtain for average γ^2 of the force that moves away the two particles:

$$\gamma_2 = \frac{1 - \alpha \cdot \left(1 + \frac{1}{\alpha}\right) e^{-\alpha}}{1 - e^{-\alpha}} \gamma_0^2 \tag{14}$$

in Equation (15) as $e^{-\alpha} \ll 1$ we can neglect it to the denominator and doing $f_2 - f_3$, we get the force both between the two masses, and for the gravitational constant of *G*:

$$G = e^2 / m^2 \left[1 - 1 + \alpha \left(1 + \frac{1}{\alpha} \right) e^{-\alpha} \right]$$
(15)

If we take $e^2/m^2 = 2.7801987 \text{ E}32$ and a = 102.7770278 we obtain the gravitational constant of $G = 6.678532 \times 10^{-11} \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-2}$.

This gravitational constant of *G* is very close value the experimental values obtained in these last decades. In a conference about the value of *G* in the 1998, the average not weighed up on 10 results is [37]: $6.6772 \times 10^{-11} \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-2}$.

Jan Gundlach and Stephen Merkowitz [38] found in 2000:

$$(6.674215 \pm 0.000092) \times 10^{-11} \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-2}$$

In Zurich the professor Schlamminger [39] found:

$$G = (6.67404 \pm 0.00021) \times 10^{-11} \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-2}$$

More recently, Rosi and colleagues found the value [40]: $G = 6.67191(99) \times 10^{-11} \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-2}$ [Relative uncert.: 150 ppm] While Mohr, Newell, and Taylor, proposed the value of *G* equal to [41]: CODATA (2014) $G = 6.67408(31) \times 10^{-11} \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-2}$ [Relative std. uncert.: 4.7×10^{-5}].

5. Conclusions

We conclude that the calculation of G is revealed to be compatible with other experimental measures of the gravitational constant of G, obtained by other authors with theoretical and experimental methods.

We advanced various hypotheses with this work:

- The Strings are virtual electrons positrons dipoles.
- These dipoles pressing the matter.
- The validity to add the three quarters of the constant of the Fine Structure in the projection calculation of yon axis.

The hypothesis formulated in this study has our permission to make a first fine approach to calculate the constant of gravitation G to leave only from the charge and the mass of the electron and from the Fine Structure constant. The calculation of G, made leaving from the mass and from the electron charge, avoids making instrumental mistakes for his determination. This study clearly shows the relationship between gravity and the electromagnetism and the Fine Structure, besides to offer, at hypothesis level, also a reflection on the antimatter and add the new pieces to the complex mosaic of "Theory of Everything".

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