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Kiyoshi Nishikawa
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Quantum Systems in Chemistry and Physics

Progress in Methods and Applications

Springer

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PTCP Aim and Scope

Progress in Theoretical Chemistry and Physics

A series reporting advances in theoretical molecular and material sciences, including theoretical, mathematical and computational chemistry, physical chemistry and chemical physics and biophysics.

Aim and Scope

Science progresses by a symbiotic interaction between theory and experiment: theory is used to interpret experimental results and may suggest new experiments; experiment helps to test theoretical predictions and may lead to improved theories. Theoretical Chemistry (including Physical Chemistry and Chemical Physics) provides the conceptual and technical background and apparatus for the rationalisation of phenomena in the chemical sciences. It is, therefore, a wide ranging subject, reflecting the diversity of molecular and related species and processes arising in chemical systems. The book series *Progress in Theoretical Chemistry and Physics* aims to report advances in methods and applications in this extended domain. It will comprise monographs as well as collections of papers on particular themes, which may arise from proceedings of symposia or invited papers on specific topics as well as from initiatives from authors or translations.

The basic theories of physics – classical mechanics and electromagnetism, relativity theory, quantum mechanics, statistical mechanics, quantum electrodynamics – support the theoretical apparatus which is used in molecular sciences. Quantum mechanics plays a particular role in theoretical chemistry, providing the basis for the valence theories, which allow to interpret the structure of molecules, and for the spectroscopic models, employed in the determination of structural information from spectral patterns. Indeed, Quantum Chemistry often appears synonymous with Theoretical Chemistry; it will, therefore, constitute a major part of this book series. However, the scope of the series will also include other areas of theoretical

chemistry, such as mathematical chemistry (which involves the use of algebra and topology in the analysis of molecular structures and reactions); molecular mechanics, molecular dynamics and chemical thermodynamics, which play an important role in rationalizing the geometric and electronic structures of molecular assemblies and polymers, clusters and crystals; surface, interface, solvent and solid state effects; excited-state dynamics, reactive collisions, and chemical reactions.

Recent decades have seen the emergence of a novel approach to scientific research, based on the exploitation of fast electronic digital computers. Computation provides a method of investigation which transcends the traditional division between theory and experiment. Computer-assisted simulation and design may afford a solution to complex problems which would otherwise be intractable to theoretical analysis, and may also provide a viable alternative to difficult or costly laboratory experiments. Though stemming from Theoretical Chemistry, Computational Chemistry is a field of research in its own right, which can help to test theoretical predictions and may also suggest improved theories.

The field of theoretical molecular sciences ranges from fundamental physical questions relevant to the molecular concept, through the statics and dynamics of isolated molecules, aggregates and materials, molecular properties and interactions, to the role of molecules in the biological sciences. Therefore, it involves the physical basis for geometric and electronic structure, states of aggregation, physical and chemical transformations, thermodynamic and kinetic properties, as well as unusual properties such as extreme flexibility or strong relativistic or quantum-field effects, extreme conditions such as intense radiation fields or interaction with the continuum, and the specificity of biochemical reactions.

Theoretical Chemistry has an applied branch (a part of molecular engineering), which involves the investigation of structure-property relationships aiming at the design, synthesis and application of molecules and materials endowed with specific functions, now in demand in such areas as molecular electronics, drug design or genetic engineering. Relevant properties include conductivity (normal, semi- and super-), magnetism (ferro- and ferri-), optoelectronic effects (involving nonlinear response), photochromism and photoreactivity, radiation and thermal resistance, molecular recognition and information processing, biological and pharmaceutical activities, as well as properties favouring self-assembling mechanisms and combination properties needed in multifunctional systems.

Progress in Theoretical Chemistry and Physics is made at different rates in these various research fields. The aim of this book series is to provide timely and in-depth coverage of selected topics and broad-ranging yet detailed analysis of contemporary theories and their applications. The series will be of primary interest to those whose research is directly concerned with the development and application of theoretical approaches in the chemical sciences. It will provide up-to-date reports on theoretical methods for the chemist, thermodynamician or spectroscopist, the atomic, molecular or cluster physicist, and the biochemist or molecular biologist who wish to employ techniques developed in theoretical, mathematical and computational chemistry in their research programs. It is also intended to provide the graduate student with a readily accessible documentation on various branches of theoretical chemistry, physical chemistry and chemical physics.

Preface

This volume collects 33 selected papers from the scientific contributions presented at the Sixteenth International Workshop on *Quantum Systems in Chemistry and Physics* (QSCP-XVI), which was organized by Pr. Kiyoshi Nishikawa at the Ishikawa Prefecture Museum of Art in Kanazawa, Ishikawa, Japan, from September 11 to 17, 2011. Close to 150 scientists from 30 countries attended the meeting. Participants of QSCP-XVI discussed the state of the art, new trends, and future evolution of methods in molecular quantum mechanics, as well as their applications to a wide range of problems in chemistry, physics, and biology.

The particularly large attendance to QSCP-XVI was partly due to its coordination with the VIIth Congress of the *International Society for Theoretical Chemical Physics* (ISTCP-VII), which was organized by Pr. Hiromi Nakai at Waseda University in Tokyo, Japan, just a week earlier, and which gathered over 400 participants. These two reputed meetings were therefore exceptionally successful, especially considering that they took place barely five months after the Fukushima disaster. As a matter of fact, they would have both been cancelled if it wasn't for the courage and resilience of our Japanese colleagues and friends as well as for the wave of solidarity of both QSCP-XVI and ISTCP-VII faithful attendees.

Kanazawa is situated in the western central part of the Honshu island in Japan, and the Ishikawa Prefecture Museum of Art (IPMA) sits in the heart of the city centre – which offers a variety of museums including the 21st Century Museum of Contemporary Art – and next to the Kenrokuen Garden, one of most beautiful gardens in Japan. IPMA is the main art gallery of Ishikawa Prefecture and its collection includes a National Treasure and various important cultural properties in its permanent exhibition halls.

Details of the Kanazawa meeting including the scientific program can be found on the website: http://qscp16.s.kanazawa-u.ac.jp. Altogether, there were 24 morning and afternoon sessions, where 12 key lectures, 50 plenary talks and 28 parallel talks were given, and 2 evening poster sessions, each with 25 flash presentations of posters which were displayed in the close Shiinoki Cultural Complex. We are grateful to all the participants for making the QSCP-XVI workshop such a stimulating experience and great success.

The QSCP-XVI workshop followed traditions established at previous meetings:

QSCP-I, organized by Roy McWeeny in 1996 at San Miniato (Pisa, Italy)
QSCP-II, by Stephen Wilson in 1997 at Oxford (England)
QSCP-III, by Alfonso Hernandez-Laguna in 1998 at Granada (Spain)
QSCP-IV, by Jean Maruani in 1999 at Marly le Roi (Paris, France)
QSCP-V, by Erkki Brändas in 2000 at Uppsala (Sweden)
QSCP-VI, by Alia Tadjer in 2001 at Sofia (Bulgaria)
QSCP-VII, by Ivan Hubac in 2002 at Bratislava (Slovakia)
QSCP-VIII, by Aristides Mavridis in 2003 at Spetses (Athens, Greece)
QSCP-IX, by Jean-Pierre Julien in 2004 at Les Houches (Grenoble, France)
QSCP-X, by Souad Lahmar in 2005 at Carthage (Tunisia)
QSCP-XI, by Oleg Vasyutinskii in 2006 at Pushkin (St Petersburg, Russia)
QSCP-XII, by Stephen Wilson in 2007 near Windsor (London, England)
QSCP-XIII, by Piotr Piecuch in 2008 at East Lansing (Michigan, USA)
QSCP-XIV, by Gerardo Delgado-Barrio in 2009 at El Escorial (Spain)
QSCP-XV, by Philip Hoggan in 2010 at Cambridge (England)

The lectures presented at QSCP-XVI were grouped into seven areas in the field of *Quantum Systems in Chemistry and Physics*:

1. Concepts and Methods in Quantum Chemistry and Physics
2. Molecular Structure, Dynamics, and Spectroscopy
3. Atoms and Molecules in Strong Electric and Magnetic Fields
4. Condensed Matter; Complexes and Clusters; Surfaces and Interfaces
5. Molecular and Nano Materials, Electronics, and Biology
6. Reactive Collisions and Chemical Reactions
7. Computational Chemistry, Physics, and Biology

The breadth and depth of the scientific topics discussed during QSCP-XVI are reflected in the contents of this volume of proceedings of *Progress in Theoretical Chemistry and Physics*, which includes six parts:

I. Fundamental Theory (three chapters)
II. Molecular Processes (nine chapters)
III. Molecular Structure (six chapters)
IV. Molecular Properties (three chapters)
V. Condensed Matter (six chapters)
VI. Biosystems (six chapters)

In addition to the scientific program, the workshop had its share of cultural activities. There was an impressive traditional drum show on the spot. One afternoon was devoted to a visit in a gold craft workshop, where participants had a chance to test gold plating. There was also a visit to a zen temple, where they could discuss with zen monks and practice meditation for a few hours. The award ceremony of the CMOA Prize and Medal took place in the banquet room of the Kanazawa Excel Hotel Tokyu.

The Prize was shared between three of the selected nominees: Shuhua Li (Nanjing, China); Oleg Prezhdo (Rochester, USA); and Jun-ya Hasegawa (Kyoto, Japan). The CMOA Medal was awarded to Pr Hiroshi Nakatsuji (Kyoto, Japan). Following an established tradition at QSCP meetings, the venue of the following (XVIIth) workshop was disclosed at the end of the banquet: Turku, Finland.

We are pleased to acknowledge the support given to QSCP-XVI by the Ishikawa Prefecture, Kanazawa City, Kanazawa University, the Society DV-Xα, Quantum Chemistry Research Institute, Inoue Foundation of Science, Concurrent Systems, HPC SYSTEMS, FUJITSU Ltd, HITACHI Ltd, Real Computing Inc., Sumisho Computer System Corporation, and CMOA. We are most grateful to all members of the Local Organizing Committee (LOC) for their work and dedication, which made the stay and work of the participants both pleasant and fruitful. Finally, we would like to thank the Honorary Committee (HC) and International Scientific Committee (ISC) members for their invaluable expertise and advice.

We hope the readers will find as much interest in consulting these proceedings as the participants had in attending the meeting.

The Editors

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Part I
Fundamental Theory

Chapter 1
The Relativistic Kepler Problem and Gödel's Paradox

Erkki J. Brändas

Abstract Employing a characteristic functional model that conscripts arrays of operators in terms of energy and momentum adjoined with their conjugate operators of time and position, we have recently derived an extended superposition principle compatible both with quantum mechanics and Einstein's laws of relativity. We have likewise derived a global, universal superposition principle with the autonomous choice to implement, when required, classical or quantum representations. The present viewpoint amalgamates the microscopic and the macroscopic domains via abstract complex symmetric forms through suitable operator classifications including appropriate boundary conditions. An important case in point comes from the theory of general relativity, i.e. the demand for the proper limiting order at the Schwarzschild radius. In this example, one obtains a surprising relation between Gödel's incompleteness theorem and the proper limiting behaviour of the present theory at the Schwarzschild singularity. In the present study, we will apply our theoretical formulation to the relativistic Kepler problem, recovering the celebrated result from the theory of general relativity in the calculation of the perihelion movement of Mercury.

1.1 Introduction

In this chapter, we will focus on some irreconcilable viewpoints in physical and mathematical sciences. In particular, we will concentrate on the problem to unify quantum mechanics with classical theories like special and general relativity as

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well as the assertion of the inherent limitations of nontrivial axiomatic systems, the latter known as Gödel's inconsistency theorem(s) [1]. A surprising result is the interconnection between the two problems above, which also leads to reverberating consequences for the biological evolution [2, 3]. A crucial property of the derivations is the extension of the dynamical equations to the evolution of open (dissipative) systems, corresponding to specific biorthogonal formulations of general complex symmetric forms [2] or alternatively operator equations including non-positive metrics [3]. To display the generality of the formulation, we will apply the functional model to recover the correct solution of the relativistic Kepler problem. The conventional idea expresses the empirical Kepler laws as derivable from classical Newton gravity. There is, however, a relativistic extension that accounts for the famous rosette orbit, experimentally confirmed as the perihelion motion of the planet Mercury, see e.g. Refs. [4–6]. The latter writes under the name of the "relativistic Kepler problem", see e.g. Ref. [4] for an approximate derivation within the theory of special relativity. Along these lines, we will portray the explicit connection between Gödel's paradox and the imperative limiting condition at the Schwarzschild boundary intrinsic to the present operator derivation of the theory of general relativity.

Since we will especially focus on the relativistic problem, we will not say anything more on the actual connections to condensed matter or rather to complex enough systems like biological order and microscopic self-organisation [2, 3]. In doing so, we have already referred to Löwdin's pedagogical and very intriguing analysis of the Kepler problem demonstrating some rather surprising properties of special relativity. The difficulties to analyse experimental conditions and predictions in comparing Newton's and Einstein's theories [5] have been excellently described already in the mid-1980s [6]. For a modern appraisal of Einstein's legacy, where the evolution of science, as unavoidably intertwined by the master's illustrious mistakes, is magnificently portrayed, see e.g. Ref. [7]. The consensus so far is that Einstein is essentially right.

In Sects. 1.2 and 1.3, we will give the background facts for the mathematical procedures used for (i) merging classical and quantum approaches, including relativity with quantum theory, (ii) including a global superposition principle combining abstract operations with materialistic notions and (iii) (see also the conclusion) the interrelation between the Schwarzschild peripheral boundary limit and Gödel's (in)famous incompleteness theorem.

In Sect. 1.4, we will demonstrate the validity of the method by analysing the relativistic Kepler problem by computing the perihelion motion of the planet Mercury, followed by Sect. 1.5, displaying the explicit connection between the Schwarzschild singularity and Gödel's theorem. The final conclusion summarises the *modus operandi* and its subsequent consequences.

1.2 Extended Operator Equations and Global Superposition Principles

In order to consider the positions mentioned above, we will revisit our general theoretical development founded on complex symmetric forms [2]. Our operator formulation is very general, yet comparatively simple, simultaneously regulating straightforwardly space-time degrees of freedom with the corresponding conjugate energy-momentum four-vector. For example, we will consider abstract kets in terms of the coordinate $\vec{x}$ and linear momentum $\vec{p}$

$$\left|\vec{x}, ict\right\rangle, \quad \left|\vec{p}, \frac{iE}{c}\right\rangle \tag{1.1}$$

cf. the general scalar product for a free particle

$$\left\langle \vec{x}, -ict|\vec{p}, \frac{iE}{c}\right\rangle = (2\pi\hbar)^{-2} e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{x}-Et)} \tag{1.2}$$

In Eq. (1.2), we refer to a more general scalar product including all four dimensions. In view of the fact that the construction should be complex symmetric, see e.g. Refs. [2, 3], we have appended a minus sign before *ict* in the bra-position. In general our biorthogonal construction should read

$$\left\langle (\vec{x}, ict)^*|\vec{p}, \frac{iE}{c}\right\rangle \tag{1.3}$$

which will be particularly important in connection with the so-called complex scaling method [8, 9] and more generally when analytic continuation is achieved via one or several parameters being made complex. The scalar product Eq. (1.3) contains operators and their conjugate partners (in terms of time and coordinate derivatives and Planck's constant divided by 2π) related as usual, e.g.

$$E_{\text{op}} = i\hbar\frac{\partial}{\partial t}; \quad \vec{p} = -i\hbar\vec{\nabla} \tag{1.4}$$

and

$$\tau = T_{\text{op}} = -i\hbar\frac{\partial}{\partial E}; \quad \vec{x} = i\hbar\vec{\nabla}_p \tag{1.5}$$

Our objective is to find a complex symmetric formulation that contains the seed of the relativistic frame invariants. The trick is to entrench an apposite matrix of operators whose characteristic equation mimics the Klein–Gordon equation (or in general the Dirac equation). Intuitively, one might infer that we have realised the feat of obtaining the negative square root of the aforementioned operator matrix. Thus, the entities of the formulation are operators and furthermore since they permit

more general characterisations, compared to standard self-adjoint ones, they must be properly extended. We will not at present devote more time on the mathematical background except referring to relevant work in the past [2, 3, 10]. Making use of the operator construction allocated above, the formulation becomes ($E = mc^2$)

$$\hat{\mathcal{H}} = |m, \bar{m}\rangle \begin{pmatrix} m & \frac{-i\,\vec{p}}{c} \\ \frac{-i\,\vec{p}}{c} & -m \end{pmatrix} \begin{vmatrix} m^* \\ \bar{m}^* \end{vmatrix} \tag{1.6}$$

with $|m\rangle = \left|\vec{p}, iE/c\right\rangle$ and $|\bar{m}\rangle = \left|\vec{p}, -iE/c\right\rangle$ (note the complex conjugation in the bra-position, required to characterise a complex symmetric form, see e.g. [2]) and references therein, and

$$\hat{\mathcal{T}} = |\tau, \bar{\tau}\rangle \begin{pmatrix} c\tau & -i\,\vec{x} \\ -i\,\vec{x} & -c\tau \end{pmatrix} \begin{vmatrix} \tau^* \\ \bar{\tau}^* \end{vmatrix} \tag{1.7}$$

with $|\tau\rangle = \left|\vec{x}, ict\right\rangle$ and $|\bar{\tau}\rangle = \left|\vec{x}, -ict\right\rangle$. Note that the entities presented in Eqs. (1.6) and (1.7) are general (vector) operators in both the matrix and in the bra-ket. Furthermore, we have separated the formulation of the energy-momentum and the space-time; notwithstanding they are coupled via Eqs. (1.4) and (1.5). This relationship compels that space-time develops concurrently with energy-momentum dynamics and vice versa.

It is quite simple, see Refs. [2, 3, 10], to solve the biorthogonal characteristic equation corresponding to $\hat{\mathcal{H}}, \hat{\mathcal{T}}$, defining the eigenvalues $\lambda_\pm = \pm m_0$ and $\gamma_\pm = \pm\tau_0$ from

$$\begin{aligned} \lambda^2 = m_0^2 = m^2 - p^2c^{-2} \\ \gamma^2 = \tau_0^2 = \tau^2 - x^2c^{-2} \end{aligned} \tag{1.8}$$

with $\vec{p}\cdot\vec{p} = p^2;\ \vec{x}\cdot\vec{x} = x^2$. The problems engendered by the vectorial components in the operator matrices in Eqs. (1.6, 1.7) are easily solved as follows: the secular determinant gives way to expressions in terms of p^2 and x^2; decomposing the kinetic energy operator for instance into one of the eleven sets of orthogonal coordinate systems in which the Helmholtz equation separates, one may hence substitute the "vector entity" with the appropriate degrees of freedom being in accordance with the conditions under study. When applied to gravitational interactions, to be detailed below, polar coordinates will be preferable. To develop the formulation in correspondence with (classical) special relativity, we must distinguish the proper operator that in classical terminology goes with the velocity υ, cf. the customary parameter $\beta = p/mc =$ ("classical particles") $= \upsilon/c$, $\upsilon = |\vec{\upsilon}|$ being the group velocity of the particle/wave. Via the plane wave, see Eq. (1.2), we obtain basically for the latter

$$\vec{\upsilon} = \frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \frac{\mathrm{d}E}{\mathrm{d}\vec{p}} \tag{1.9}$$

Even though Eq. (1.9) obtains from classical (Newton) dynamics, it is not hard to prove that the relation $\mathrm{d}E = \mathrm{d}(mc^2) = \vec{\upsilon}\,\mathrm{d}\vec{p}$ is valid also in the theory of special relativity as well, see e.g. Löwdin [4]. From Eqs. (1.6–1.8), we obtain the general result (using $\vec{x} = \vec{\upsilon}\tau$)

$$m = \frac{m_0}{\sqrt{1-\beta^2}}; \quad \tau = \frac{\tau_0}{\sqrt{1-\beta^2}}; \quad x = \frac{x_0}{\sqrt{1-\beta^2}} \tag{1.10}$$

The solutions, Eq. (1.10), correspond each to a root of the characteristic equation Eqs. (1.6–1.8). Although the general setting of the complex symmetric forms ensures biorthogonality, the eigenvectors for $\hat{\mathcal{H}}$ (and similarly for $\hat{\mathcal{T}}$) obtain simply as

$$\begin{aligned} |m_0\rangle &= c_1\,|m\rangle + c_2\,|\bar{m}\rangle\,; \quad \lambda_+ = m_0 \\ |\bar{m}_0\rangle &= -\,c_2\,|m\rangle + c_1\,|\bar{m}\rangle\,; \quad \lambda_- = -m_0 \\ |m\rangle &= c_1\,|m_0\rangle - c_2\,|\bar{m}_0\rangle \\ |\bar{m}\rangle &= c_2\,|m_0\rangle + c_1\,|\bar{m}_0\rangle \end{aligned} \tag{1.11}$$

$$c_1 = \sqrt{\frac{1+X}{2X}}; \quad c_2 = -i\sqrt{\frac{1-X}{2X}}; \quad X = \sqrt{1-\beta^2}; \quad c_1^2 + c_2^2 = 1.$$

Note that the formal superposition, Eq. (1.11), reproduces a physical attribute, yielding the present derivation of special relativity a tangible conception outside a purely abstract understanding. Another important observation, associated with the biorthogonal setting of the system, entails that the analysis shows that the formulation turns out to be nonstatistical. We notice moreover that the description for a zero rest mass particle (photon) corresponds to a degenerate singularity of the equations since

$$\begin{aligned} \hat{\mathcal{H}}_u = |m,\bar{m}\rangle \begin{pmatrix} \frac{p}{c} & \frac{-ip}{c} \\ \frac{-ip}{c} & -\frac{p}{c} \end{pmatrix} \begin{pmatrix} m \\ \bar{m} \end{pmatrix} &= |0,\bar{0}\rangle \begin{pmatrix} 0 & \frac{2p}{c} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \bar{0} \end{pmatrix} \\ |m_0\rangle \to |0\rangle &= \tfrac{1}{\sqrt{2}}\,|m\rangle - i\,\tfrac{1}{\sqrt{2}}\,|\bar{m}\rangle\,; \\ |\bar{m}_0\rangle \to |\bar{0}\rangle &= \tfrac{1}{\sqrt{2}}\,|m\rangle + i\,\tfrac{1}{\sqrt{2}}\,|\bar{m}\rangle\,. \end{aligned} \tag{1.12}$$

In Eq. (1.12), we have chosen a momentum p in an arbitrary direction with the mass consistently given by p/c. We also note another detail. The operator matrix and its representation must, as we have demonstrated above, have a complex conjugate in the bra-position. However, since we here encounter a degeneracy with the Segrè characteristic equal to two, we have attained a so-called Jordan block "in disguise". To display the more familiar canonical (triangular) form of the description, we

must find the proper similitude by turning to the conventional description in terms of unitary transformation in the standard Hilbert space. Hence, we signify the operator with the subscript "u". There is in fact an entrenched point here, *viz.* that the unitary formalism of standard quantum mechanics via analytic continuation – to account e.g. for so-called unstable states [2, 9] – by necessity presupposes a biorthogonal picture, which then permits the mapping of the co- and contravariant formulation of the global superposition principle of classical legitimacy. It is within this epitomised picture that we have made the statement that we advocate non-probabilistic formulations of our universe including biological organisation and immaterial evolution [2, 3, 10].

It is thus not surprising that the transformation which brings the matrix to the Jordan canonical form is unitary for the degenerate situation corresponding to a Jordan block, a degenerate eigenvalue ($m_0 = 0$) with Segrè characteristic equal to two (the dimension of the block). The unitarity of the transformation implies that the canonical representation contains an equal amount of particle-antiparticle character (charge neutral) and that orthonormality between the base vectors is conserved. This behaviour, Eq. (1.12), signifies that zero rest mass particles here cannot be separated into particle-antiparticle pairs, yet the dimensionality of the singularity is two corresponding to the (linearly independent) base vectors $|0\rangle$; $|\bar{0}\rangle$, cf. the two linearly independent solutions of Maxwell's equation. Although one would sometimes say that the photon is its own antiparticle, this is consequently not correct. As can be seen from Eq. (1.12), the corresponding expansion coefficients of the orthogonal vectors are simply related by complex conjugation. A further difference, comparing particles with and without rest mass, comes from the limiting procedure in the case of the former, i.e. of letting $\upsilon \to c$, for more details see e.g. [2, 3] and references therein. In the next section, we will give the crucial extension to incorporate gravitational interactions in order to demonstrate its efficacy and accuracy by determining the perihelion motion of Mercury.

1.3 Operator Algebra and the Theory of General Relativity

In analogy with the aforementioned formulation, the general structure sets up a characteristic operator equation in terms of energy and momenta, see e.g. Refs. [2, 3], and their conjugate operators, i.e. the time and the position. The interrelated forms of the operators and the associated conjugates include in principle the specific tensor properties of gravitational interactions. As displayed before [2, 3], we will not only re-establish Einstein's laws of relativity but we will also benefit from the option of selecting separate classical and/or a quantum representations. Thus, with the proper choice of appropriate operator realisations, e.g. the present perspective of uniting the microscopic and the macroscopic views, various representations of reality maps out. In this connection, one may mention related issues [2, 3], e.g. the idea of decoherence, or protection thereof, referring to classical reality, or the law of light deflection, the gravitational redshift and the time delay in Einstein general relativity.

With this proviso, incorporating gravity is quite easy. The main problem will be to augment the conjugate pair formulation with the dynamics by appending, to our previous model in the generalised basis $|m, \bar{m}\rangle$, the interaction

$$m\kappa(r) = \frac{m\mu}{r}; \quad \mu = \frac{G \cdot M}{c^2} \tag{1.13}$$

thereby supporting a modified Hamiltonian (operator) matrix initially for the case $m_0 \neq 0$

$$\hat{\mathcal{H}} = |m, \bar{m}\rangle \begin{pmatrix} m(1-\kappa(r)) & \frac{-i\,\vec{p}}{c} \\ \frac{-i\,\vec{p}}{c} & -m(1-\kappa(r)) \end{pmatrix} \begin{vmatrix} m^* \\ \bar{m}^* \end{vmatrix} \tag{1.14}$$

where μ is the gravitational radius, G the gravitational constant and M a spherically symmetric nonrotating mass distribution (which does not change sign when $m \rightarrow -m$). The fundamental nature of M and the materialisation of black hole-like objects are discussed in some detail in Ref. [10].

To sum up, we find that the operator $\kappa(r) \geqslant 0$ depends formally on the operator r of the particle m, which represents the distance to the mass object M. The conjugate operators $\vec{x}$ and τ, corresponding to the energy and the momentum, will, all things considered, restore the curved space-time scales indicative of classical theories. Continuing further, one might in principle use the formulas obtained above by incorporating the $p' = p(1-\kappa(r))^{-1}$ instead of p, or alternatively solving for the proper values of Eq. (1.14) in analogy with Eq. (1.11), one obtaining

$$\begin{aligned} \lambda^2 &= m^2(1-\kappa(r))^2 - \frac{p^2}{c^2} \\ \lambda_{\pm} &= \pm m_0(1-\kappa(r)) \end{aligned} \tag{1.15}$$

It is important to emphasise that the relations obtained from Eq. (1.15) do not lead to a unique relation between the mass and the rest mass. The reason is quite deep since it involves two principal problems. First, one needs to account for the commensuration between the conjugate operators and second to unite the formulation with respect to particles with rest mass $m_0 \neq 0$ and $m_0 = 0$. The latter is a blessing in disguise since, as we know, Einstein's law of general relativity predicts that a photon deviates twice as much as estimated by Newton's classical theory.

In order to make a slight detour suitable for our final goal, i.e. the determination of the perihelion motion of Mercury, we will consider the following model; see below and also Refs. [2, 10]. First, we will portray Mercury as a particle, with nonzero rest mass m, orbiting a gravitational source, the Sun being represented as a spherical black hole-like object with mass M, $M \gg m$. Second, assuming a nonrotating object M, one derives, since the angular momentum is a constant of motion, the relation $m\upsilon r = m\mu c$, by postulating a limit velocity c at the limiting distance at the gravitational radius μ. Actually, we are measuring the distance between the particle (Mercury) m from M (the Sun), in units of μ, i.e. $N\mu$, where N is a large number,

interpreting the condition as $m\upsilon r = mN\mu c/N$. In the last relation, m is the mass operator (nonzero eigenvalue!), r the radial distance in "gravitational units", while the velocity is given in fractions of c. Consequently, the constant angular momentum in, e.g. the z-direction prompted by the velocity υ in the x-y plane, with unit vector $\vec{n}$, acquiesces the given condition specified as Eq. (1.17) below.

It is interesting to note the boundary condition derived above, depending on the large difference in the masses between m and M and subject to distances down to microscopic dimensions, makes for a circular trajectory in a plane perpendicular to the direction of the angular momentum. Nevertheless, as we will see, the boundary condition to be obtained below will be commensurate with the perihelion shift of Mercury, see also Ref. [10]. In general, one obtains in the macroscopic domain

$$\vec{\upsilon} = \frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \frac{\mathrm{d}\vec{x}}{\mathrm{d}\varphi}\frac{D}{r^2}; \quad \frac{\mathrm{d}}{\mathrm{d}t} = \frac{D}{r^2}\frac{\mathrm{d}}{\mathrm{d}\varphi} \tag{1.16}$$

where the area velocity D is a constant of motion in classical dynamics and D multiplied by m is a constant of motion in the case of special relativity [4]. Here, we will also derive an analogous condition for the general case, see more below.

To sum up, we have derived a boundary condition for a bound (quasi-) stationary trajectory using the proper polar representation $|r, ict\rangle\,;\,|p_r, iE/c\rangle$

$$\upsilon = \kappa(r)c = \frac{\mu c}{r} \tag{1.17}$$

Accordingly the complex symmetric representation, with $\upsilon/c = \kappa(r)$, becomes

$$\hat{\mathcal{H}} = |m, \bar{m}\rangle \begin{pmatrix} m(1-\kappa(r)) & -im\kappa(r)\vec{n} \\ -im\kappa(r)\vec{n} & -m(1-\kappa(r)) \end{pmatrix} \begin{vmatrix} m^* \\ \bar{m}^* \end{vmatrix} \tag{1.18}$$

leading to the formal scaling relation, where we have removing the vector $\vec{n}$ in the matrix for simplicity (in the actual calculation in the next section, it will of course be preserved!)

$$m \begin{pmatrix} (1-\kappa(r)) & -i\kappa(r) \\ -i\kappa(r) & -(1-\kappa(r)) \end{pmatrix} \to m \begin{pmatrix} \sqrt{(1-2\kappa(r))} & 0 \\ 0 & -\sqrt{(1-2\kappa(r))} \end{pmatrix} \tag{1.19}$$

The diagonal part in Eq. (1.19) reveals the scaling property of the mass ($m_0 \neq 0$). However, the most interesting point is the divulgence of a Jordan block singularity at $r = 2\mu$ at the celebrated Schwarzschild radius representing the canonical form at the degenerate point $\kappa(r) = \frac{1}{2}$

$$m \begin{pmatrix} \frac{1}{2} & -i\frac{1}{2} \\ -i\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \to \begin{pmatrix} 0 & m \\ 0 & 0 \end{pmatrix} \tag{1.20}$$

under the unitary transformation, see the analogy with the previous section,

$$\begin{aligned} |m_0\rangle \to |0\rangle &= \frac{1}{\sqrt{2}}|m\rangle - i\frac{1}{\sqrt{2}}|\bar{m}\rangle\,; \\ |\bar{m}_0\rangle \to |\bar{0}\rangle &= \frac{1}{\sqrt{2}}|m\rangle + i\frac{1}{\sqrt{2}}|\bar{m}\rangle\,. \end{aligned} \tag{1.21}$$

Returning to the conjugate problem, we see a more complex situation compared to the case of special relativity. As already pointed out, photons or particles of zero rest mass ($m_0 = 0$), exhibit a different gravitational law compared to particles with $m_0 \neq 0$. The latter, i.e. the well-known prediction and the experimentally confirmed fact of the light deviation in the Sun's gravitational field, measured during a solar eclipse, instantly boosted Einstein to international fame. Therefore, we need to account for this "inconsistency" for zero rest mass particles, by introducing the notation $\kappa_0(r) = G_0 \cdot M/(c^2 r)$. Hence, one obtains ($m_0 = 0$) that

$$m(1 - \kappa_0(r)) = \frac{p}{c} \tag{1.22}$$

where $\kappa_0(r)$ is to be uniquely determined below. From the fact that $\hat{\mathcal{H}}$ is singular, cf. Eq. (1.12), and one obtains

$$\begin{pmatrix} \frac{p}{c} & \frac{-ip}{c} \\ \frac{-ip}{c} & -\frac{p}{c} \end{pmatrix} \to \begin{pmatrix} 0 & \frac{2p}{c} \\ 0 & 0 \end{pmatrix} \tag{1.23}$$

cf. the analogous unitary transformation in the previous section. As expected from the special theory, light particles in the complex symmetric formulation correspond to Jordan blocks for all values of r. To be consistent, we require Eq. (1.22) to be compatible with the boundary condition Eq. (1.17) and the relations, Eqs. (1.19, 1.20). Hence, in order to be commensurate with the case $m_0 \neq 0$, we impose zero average momentum, Eq. (1.22), at the Schwarzschild radius $r = 2\mu = R_{LS}$, i.e. that $\bar{p} = 0$ at $\kappa(r) = 1/2$ and hence that $G_0 = 2G$ or

$$\kappa_0(r) = 2\kappa(r) \tag{1.24}$$

Equation (1.24) is nothing but Einstein's famous law of light deflection, i.e. that photons deflect twice the amount predicted by Newton's gravity law for nonzero rest mass particles.

Returning to the conjugate problem, we have previously, see Refs. [2, 3, 10], proved that the renowned Schwarzschild gauge obtains from the similarity

$$\begin{pmatrix} cds & 0 \\ 0 & -cds \end{pmatrix} \propto \begin{pmatrix} cAd\tau & -iBd\vec{x} \\ -iBd\vec{x} & -\mathrm{c}Ad\tau \end{pmatrix} \tag{1.25}$$

where the conjugate operator, defined by Eqs. (1.4, 1.5), now becomes

$$i\hbar\frac{\partial}{\partial t} = E_{\mathrm{op}}(t) = i\hbar\frac{\partial}{\partial s}\frac{\partial s}{\partial t} = E_{\mathrm{op}}(s)\sqrt{1-2\kappa(r)}$$

$$E_s\sqrt{1-2\kappa(r)} = E_t; \frac{\partial s}{\partial t} = \sqrt{1-2\kappa(r)}; s = -i\hbar\frac{\partial}{\partial E_s} \tag{1.26}$$

From Eq. (1.26), we conclude that E_s and E_t represent the energy of the system at the space-time "point" s and (t,r) respectively, where the system consists of a "particle-antiparticle" configuration and the black hole system denoted by M. Note that E_s includes also the rest mass energy and appropriate kinetic energy ($m_0 \neq 0$). As mentioned, the result is compatible with the Schwarzschild metric, see [2, 3, 10] and further below.

Deriving the apposite gauge, one finds that

$$A = B^{-1} = (1-2\kappa(r))^{\frac{1}{2}} \tag{1.27}$$

and, thus, the celebrated line element expression (in the spherical case) becomes

$$-c^2\mathrm{d}s^2 = -c^2\mathrm{d}t^2(1-2\kappa(r)) + \mathrm{d}r^2(1-2\kappa(r))^{-1} \tag{1.28}$$

First, we notice that the relations between the quantities dependent on s and t, as given in Eq. (1.26), are compatible with Eq. (1.25). This leads, see e.g. [3], directly to the renowned Einstein laws, the gravitational redshift and the gravitational time delay. Second, we observe that the area velocity multiplied by the mass is a constant of motion. In analogy with the special case [4], where

$$mD = m_0A_0; \quad m = \frac{m_0}{\sqrt{1-\beta^2}}; \quad D = A_0\sqrt{1-\beta^2} \tag{1.29}$$

one obtains

$$mD = m_sA_s; m = m_s\sqrt{1-2\kappa(r)}; A_s = D\sqrt{1-2\kappa(r)} \tag{1.30}$$

where depending on the actual situation m_sA_s can be further decomposed according to Eq. (1.29).

In order to prepare for the computation of the perihelion movement of planet Mercury, we need to discuss a final point. As is well-known, see standard physics texts or [4], the force law, the momentum law and the energy law are not compatible in the relativistic domain. For instance, from

$$E = mc^2(1-\kappa(r)); \mathrm{d}E = 0 \tag{1.31}$$

follows that

$$\boldsymbol{f} = \boldsymbol{n}G\left(\frac{mM}{r^2}\right)(1-\kappa(r))^{-1}; \quad \boldsymbol{n} = -\frac{\boldsymbol{r}}{r} \tag{1.32}$$

i.e. that the force gets modified by the extra factor $(1-\kappa(r))^{-1}$. The reason for this discrepancy lies clearly in the inability of the Eqs. (1.31, 1.32) to account for the conjugate problem as well as the boundary condition at the Schwarzschild radius.

To cope with this inconsistency, we introduce the modified Hamiltonian (operator) matrix for the case $m_0 \neq 0$, cf. Eq. (1.14),

$$\widehat{\mathcal{H}}_{\text{mod}} = |m, \bar{m}\rangle \begin{pmatrix} m & \frac{-i\bar{p}}{c} \\ \frac{-i\bar{p}}{c} & -m \end{pmatrix} \begin{vmatrix} m^* \\ \bar{m}^* \end{vmatrix} \tag{1.33}$$

where $\bar{p} = p/(1-\kappa(r))$obtaining

$$E = E_s\sqrt{1-2\kappa(r)} = (1-\kappa(r))E_{\text{mod}} \tag{1.34}$$

Note that $E = mc^2$, $E_s = m_s c^2$ and $E_{\text{mod}} = m_{\text{mod}}c^2$ appearing in Eq. (1.34) contain appropriate rest mass and kinetic energies commensurate with our present relativity theory. Alternatively, one might propose the classical ansatz

$$\begin{aligned} \upsilon' &= \frac{\upsilon}{(1-\mu/r)}; \quad \upsilon = \frac{\mathrm{d}r}{\mathrm{d}t}; \quad \upsilon' = \frac{\mathrm{d}\tilde{r}}{\mathrm{d}t} = \frac{\mathrm{d}r}{\mathrm{d}t}\left\{\frac{r}{(r-\mu)}\right\} \\ \tilde{r} &= h(r) = \int h'(r)\mathrm{d}r; \quad h'(r) = \frac{r}{(r-\mu)} \\ \tilde{r} &= \int_{2\mu}^{r} \frac{u}{(u-\mu)}\mathrm{d}u = r - 2\mu + \mu\log\left\{\frac{(r-\mu)}{\mu}\right\} \end{aligned} \tag{1.35}$$

which yields the converse connection

$$\begin{aligned} \frac{r}{\mu-1} &= f\left(\frac{\tilde{r}}{\mu+1}\right); \; f(x) = x - \log\{f(x)\} \\ f'(x) &= \frac{f(x)}{1+f(x)}; \end{aligned} \tag{1.36}$$

and the corresponding links $\tilde{r} = 0 \leftrightarrow r = 2\mu$ and $r \approx \tilde{r}$ for $r >> \mu$. We observe that these natural (classical) gravitational coordinates impart an apt spectral range for the operator r since $\tilde{r}$ is zero inside the Schwarzschild radius. Furthermore, the consistency relations Eqs. (1.31, 1.32), albeit not exact in the general case, agrees to first order of $\kappa(r)$. (In fact, an exact relationship for the force can be found if

the variations above are carried out in the coordinates $\overline{r}; \mathrm{d}\overline{r} = \mathrm{d}r\,(1-\kappa(r)))$ In analogy, one obtains for

$$E = mc^2\sqrt{1-2\kappa(r)}; \quad \mathrm{d}E = 0 \tag{1.37}$$

and getting similarly

$$\boldsymbol{f} = \boldsymbol{n}G\left(\frac{mM}{r^2}\right)(1-2\kappa(r))^{-1} = \boldsymbol{n}G\left(\frac{m_sM}{r^2}\right)\left(\sqrt{1-2\kappa(r)}\right)^{-1} \tag{1.38}$$

Consequently, since we will carry out the calculation in the next section in terms of covariant energies and masses, we will use the following equations

$$E = mc^2\sqrt{1-2\kappa(r)} = m_sc^2(1-2\kappa(r))$$
$$\boldsymbol{f} = \boldsymbol{n}G\left(\frac{m_sM}{r^2}\right)\left(\sqrt{1-2\kappa(r)}\right)^{-1} = \boldsymbol{n}m_sc^2\frac{\kappa(r)}{r}\,(1+\kappa(r)+\ldots) \tag{1.39}$$

which together with Eqs. (1.29, 1.30) will serve as constants of motion in the determination of the perihelion rosette orbit. In passing, we note that zero rest mass particles, e.g. the photons, will follow the law

$$E = mc^2(1-2\kappa(r))$$
$$\boldsymbol{f} = \boldsymbol{n}2G\left(\frac{mM}{r^2}\right)(1-2\kappa(r))^{-1} = \boldsymbol{n}2mc^2\frac{\kappa(r)}{r}\,(1+2\kappa(r)+\ldots) \tag{1.40}$$

in analogy with Eqs. (1.37, 1.38) and in accordance with Eqs. (1.22, 1.24).

1.4 The General Kepler Problem

Since this will primarily be a "classical" computation, it is important to realise that our global formalism, combining the classical and the quantum interpretation, incorporates boundary conditions as obtained from the present picture thrown as a characteristic operator array formulation. Using simple generalisations of the so-called Binet's formulas in classical mechanics, we will consider the computation in the following way, see e.g. any textbook on classical mechanics or Ref. [4] for details. First, we give a summarising documentation of the essential steps of the classical Kepler problem (m the mass of Mercury and M the mass of the Sun); then we will proceed by the corresponding extension to the relativistic case in particular pointing out the relevant alterations enforced by the boundary conditions derived above, see particularly Eq. (1.39).

Using the area velocity D, see Eq. (1.16), which is a constant of motion, $D = A$ in the classical case of the central force problem, one derives straightforwardly the following relations in standard polar coordinates r, φ (here, the particle motion is in a plane perpendicular to the angular momentum vector $\boldsymbol{L}$)

$$\begin{aligned} \upsilon_r &= \frac{\mathrm{d}r}{\mathrm{d}t} = -D\frac{\mathrm{d}u}{\mathrm{d}\varphi}; \upsilon_\varphi = -Du \\ \upsilon^2 &= (\upsilon_r)^2 + (\upsilon_\varphi)^2 = D^2\left\{\left(\frac{\mathrm{d}u}{\mathrm{d}\varphi}\right)^2 + u^2\right\} \end{aligned} \tag{1.41}$$

where for convenience the variable $u = 1/r$ has been introduced. In addition to the velocity formulas, one obtains for the acceleration

$$\begin{aligned} a_r &= -\frac{\mathrm{d}D}{\mathrm{d}t}\frac{\mathrm{d}u}{\mathrm{d}\varphi} - D^2u^2\left\{\frac{\mathrm{d}^2u}{\mathrm{d}\varphi^2} + u\right\} \\ a_\varphi &= -u\frac{\mathrm{d}D}{\mathrm{d}t} \end{aligned} \tag{1.42}$$

From Eqs. (1.41, 1.42) and $a_\varphi = 0$, one obtains straightforwardly (G being the gravitational constant as before)

$$-\left(\frac{A^2}{r^2}\right)\left\{\frac{\mathrm{d}^2u}{\mathrm{d}\varphi^2} + u\right\} = -G\frac{M}{r^2} \tag{1.43}$$

or simply

$$\frac{\mathrm{d}^2u}{\mathrm{d}\varphi^2} + u = \alpha; \quad \alpha = G\frac{M}{A^2} \tag{1.44}$$

Note that Eq. (1.44) has the standard solution $u = \alpha + \beta\cos(\varphi - \varphi_0)$, which for simplicity we can take $\varphi_0 = 0$. As is well-known, the conic intersections in polar coordinates take the form

$$u = \alpha + \beta\cos\varphi \tag{1.45}$$

In the present context, we realise that $\alpha > |\beta|$ yields an elliptic orbit, where β can be expressed in terms of E and α via

$$\begin{aligned} E &= \frac{1}{2}m\upsilon^2 - GmMu = \frac{1}{2}mA^2\left\{\left(\frac{\mathrm{d}u}{\mathrm{d}\varphi}\right)^2 + u^2\right\} - GmMu \\ E &= \frac{1}{2}mA^2(\beta^2 - \alpha^2) \end{aligned} \tag{1.46}$$

Incidentally, we note that the deviation of a particle with mass m passing a large sphere with mass M gives a hyperbolic orbit ($\alpha < |\beta|$) yielding the exact formula (considering the point $u = 0$)

$$2\theta = 2\arcsin\left(\frac{\alpha}{\beta}\right); \quad \theta = \varphi - \frac{\pi}{2} \tag{1.47}$$

and finally, to complete the picture, a parabolic orbit obtains for $\alpha = |\beta|$.

In order to generalise this description to the relativistic domain, we will, see also previous section, represent Mercury as a particle, with a nonzero rest mass m, orbiting the gravitational source, the Sun, the latter being characterised as a nonrotating spherical black hole-like object with mass M. Furthermore, we assume $M \gg m$, so that the Schwarzschild radius of Mercury is negligible compared to that of the Sun. Noting that we have a central force, one gets

$$\left(\frac{\mathrm{d}m}{\mathrm{d}t}\right)\upsilon_\varphi + ma_\varphi = 0 \tag{1.48}$$

from which, using Eqs. (1.41, 1.42), it follows that $mD = m_\mathrm{s}A_\mathrm{s}$ is a constant of motion, cf. Eqs. (1.16, 1.29, 1.30) above. Employing further the energy law and the force law, where the total energy also is a constant of motion, Eq. (1.39) yields, introducing the parameters $q = m_\mathrm{s}/m_0$ and the energy quotient $\lambda = E_\mathrm{s}/E_0$ (note that we are expressing the mass and the area velocity with the subindex "s")

$$\begin{aligned} q &= \frac{m_\mathrm{s}}{m_0} = \frac{1}{\sqrt{1-\beta^2}}; \alpha = G\frac{M}{A_\mathrm{s}^2} \\ \lambda &= \frac{E_\mathrm{s}}{m_0c^2} = q\,(1-2\mu u))\,; \quad \mu = G\frac{M}{c^2} \end{aligned} \tag{1.49}$$

It is important to note that Eq. (1.49) contains a factor 2μ in the expression for λ above while the force still is given by Eq. (1.39). In analogy with Eq. (1.41), we find that

$$\upsilon^2 = D^2\left\{\left(\frac{\mathrm{d}u}{\mathrm{d}\varphi}\right)^2 + u^2\right\} = \left(\frac{A_\mathrm{s}^2}{q^2}\right)\left\{\left(\frac{\mathrm{d}u}{\mathrm{d}\varphi}\right)^2 + u^2\right\} \tag{1.50}$$

which with the definitions given in Eq. (1.49)

$$q = \frac{\lambda}{(1-2\mu u)}; \quad \upsilon^2 = c^2\left(1 - \frac{1}{q^2}\right) \tag{1.51}$$

yields

$$\left(\frac{\mathrm{d}u}{\mathrm{d}\varphi}\right)^2 + u^2 = \left(\frac{c^2}{A_\mathrm{s}^2}\right)(q^2 - 1) \tag{1.52}$$

Expressing the differential equation in terms of the parameters α and λ in Eq. (1.49), one obtains after taking the derivative with respect to φ and dividing by $2\,(\mathrm{d}u/\mathrm{d}\varphi)$

$$\frac{\mathrm{d}^2u}{\mathrm{d}\varphi^2} + u = \frac{\alpha\lambda^2}{(1-2\mu u)^3} \tag{1.53}$$

This is a differential equation separable in the classical variables u and φ. Note also the difference between this study and the one using the theory of special relativity, where the factor 2 in front of μ is missing in Eq. (1.53), see Ref. [4] for more details.

An approximate solution to Eq. (1.53) can be derived by expanding the right-hand side in a power series in $\kappa(u) = \mu u$ which gives

$$\frac{\mathrm{d}^2u}{\mathrm{d}\varphi^2} + u\left(1 - 6\alpha\mu\lambda^2\right) = \alpha\lambda^2 + 24\mu^2u^2\lambda^2 + \ldots \tag{1.54}$$

To first order in μu, Eq. (1.53) generates the formula, cf. the classical case

$$\begin{aligned} u &= \alpha_1 + \beta\cos\varphi_1 \\ \varphi_1 &= \varphi\left(1 - 6\alpha\mu\lambda^2\right)^{\frac{1}{2}} \\ \alpha_1 &= \alpha\lambda^2\left(1 - 6\alpha\mu\lambda^2\right)^{-1} \end{aligned} \tag{1.55}$$

where β can be obtained in analogy with the classical case above, i.e. from the quotient λ in Eq. (1.49), Eq. (1.52) gives

$$\left(\frac{\mu}{\alpha}\right)\left\{\left(\frac{\mathrm{d}u}{\mathrm{d}\varphi}\right)^2 + u^2\right\} = \frac{\lambda^2}{(1-\mu u)^2} - 1 \tag{1.56}$$

Finding optimum values for u, i.e. for which $\frac{\mathrm{d}u}{\mathrm{d}\varphi} = 0$, yields

$$\lambda^2 = \left(1 - \frac{\mu}{R}\right)^2\left\{1 + \left(\frac{\mu}{\alpha}\right)\left(\frac{1}{R^2}\right)\right\}; \quad R = (\alpha_1 + \beta)^{-1} \tag{1.57}$$

To first order of μ/R, neglecting higher orders, Eq. (1.57) yields the wanted result for $(\beta^2 - \alpha_1^2)$, i.e.

$$\lambda^2 = 1 + \frac{\mu}{\alpha_1}(\beta^2 - \alpha_1^2) \tag{1.58}$$

Using the energy quotient $\lambda = E_s/E_0$, it follows that for $|\beta| > \alpha_1$ $(\lambda > 1)$, one obtains a hyperbolic type orbit, for $|\beta| = \alpha_1$ $(\lambda = 1)$ a parabolic orbit and for $|\beta| < \alpha_1$

($\lambda < 1$) an elliptic type orbit, cf. the classical case. The latter condition corresponds to a *rosette orbit* comprising an ellipse with a perihelion motion matching maximum values, for the angles $\varphi_1 = 2\pi n$ or $\varphi = 2\pi n\left(1 - 6\alpha\mu\lambda^2\right)^{-\frac{1}{2}} = 2\pi n(1 + 3\alpha\mu\lambda^2 + \cdots)$, of $u = 1/r$, indicating that for each rotation the perihelion moves an angle

$$\Delta\varphi = 6\pi\alpha\mu\lambda^2 \tag{1.59}$$

which on account of Eq. (1.58) or $\lambda \approx 1$ writes $\Delta\varphi = 6\pi\alpha\mu$. In terms of the eccentricity, e, of the ellipse, Eq. (1.59) can be written

$$\Delta\varphi = \frac{6\pi\mu}{a(1-e^2)} \tag{1.60}$$

with $e = d/a$ and the ellipse, Eq. (1.55), has been expressed in Cartesian coordinates

$$\frac{(x-d)^2}{a^2} + \frac{y^2}{b^2} = 1$$

We may also consider the deviation of a particle with nonzero rest mass passing a large sphere with mass M. Approximately one obtains in analogy with the classical case when $r = \infty$ or $u = 0$ giving the condition $\cos\varphi_1 = -\alpha_1/\beta$ (real solution in the hyperbolic case). Using Eqs. (1.50, 1.55, 1.57) one obtains for small values of α_1/β, cf. Eq. (1.47), introducing the angle $\theta = \varphi - \pi/2$

$$2\theta \approx 2\frac{\alpha_1}{\beta} = 2\frac{\mu}{R}\left(\frac{c}{\upsilon_0}\right)^2 \tag{1.61}$$

where υ_0 is the value of υ at $u = 0$. Here, we observe that for photons using Eq. (1.40) and $\upsilon_0 = c$ that

$$2\theta \approx 4\frac{\alpha_1}{\beta} = 4\frac{\mu}{R} \tag{1.62}$$

Equations (1.59, 1.60, 1.62) agree with the results of Einstein's theory of general relativity for the perihelion movement of Mercury and the law that a photon deviates in a gravitational field twice the amount as predicted by Newton's gravitational law.

1.5 Relation Between the Schwarzschild Singularity and Gödel's Theorem

In order to discuss the relation between the singularity (Jordan block) occurring at $r = 2\mu = R_{LS}$, where R_{LS} is the renowned Schwarzschild radius, and Gödel's paradox, we will return to the discussion in connection with Eq. (1.19), i.e., considering the matrix $m\mathcal{G}$ where

$$\mathcal{G} = \begin{pmatrix} 1-\kappa(r) & -i\kappa(r) \\ -i\kappa(r) & 1-\kappa(r) \end{pmatrix} \tag{1.63}$$

obtained from the operator ansatz in terms of energy and momenta for the gravitational problem. Before adjusting to the conjugate problem, we recapitulate that the matrix $\mathcal{G}$ results from the requirement of the boundary condition given by Eq. (1.17). In particular, we emphasise the occurrence of Jordan blocks (dimension 2) as being the consequence at the degenerate point at the Schwarzschild radius.

To convey the unexpected relation with the Gödelian theorem, we refer to our procedure to convert the exegesis of a truth-functional proposition calculus to a linear algebra terminology, see e.g. for details and further references [3, 11]. In brief, we consider two propositions P and $Q = \neg P$ as expressed in the following table, where $\neg$ is the operation of logical negation

$$\text{Truth Table} = \begin{matrix} \\ \text{true} \\ \text{false} \end{matrix} \begin{matrix} \begin{matrix} \text{true} & \text{false} \end{matrix} \\ \begin{pmatrix} P(x) & Q(x) \\ \neg Q(x) & \neg P(x) \end{pmatrix} \end{matrix} \tag{1.64}$$

The table will be understood as follows: "the first row" is true when P is true and Q is false, and the second row reads false if Q is true and P is false. The map entails the translation of the truth table, Eq. (1.64), into a truth matrix $\mathcal{P}$ by means of probability operators/functions p and $q = (I - p)$ referring to a basis in Dirac notation $|\text{true}\rangle$ and $|\text{false}\rangle$ allocating a negative signature to the negation row:

$$\mathcal{P} = \begin{matrix} \\ |\text{true}\rangle \\ |\text{false}\rangle \end{matrix} \begin{matrix} \begin{matrix} |\text{true}\rangle & |\text{false}\rangle \end{matrix} \\ \begin{pmatrix} p & (1-p) \\ -(1-p) & -p \end{pmatrix} \end{matrix} \tag{1.65}$$

Note that $\mathcal{P}$ by definition relates to the so-called bias operator since it conveys classical probability information through the system operators $\Gamma_\pm = \frac{1}{2}(I \pm \mathcal{P}^2)$ through (I is the unit matrix)

$$\frac{1}{2}(I + \mathcal{P}^2) = pI; \frac{1}{2}(I - \mathcal{P}^2) = (1-p)I$$

The matrix, Eq. (1.65), is easy to diagonalise (if $p \neq \frac{1}{2}$), i.e.

$$\mathcal{P} = \begin{pmatrix} p & (1-p) \\ -(1-p) & -p \end{pmatrix} \rightarrow \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}$$
$$\lambda^2 = p^2 - (1-p)^2;\ \lambda_\pm = \pm\sqrt{2p-1} \tag{1.66}$$

for more details, see e.g. Refs. [3, 11]. It easy to see what happens when $p = \frac{1}{2}$, i.e. when the bias is zero and neither P nor $Q = \neg P$ can be true (or false) since

$$\widehat{\mathcal{P}} = (|\text{true}\rangle, |\text{false}\rangle) \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} \langle\text{true}| \\ \langle\text{false}| \end{pmatrix} = |\overline{\text{true}}\rangle\langle\overline{\text{false}}| \tag{1.67}$$

or

$$\widehat{\mathcal{P}} = \left(|\overline{\text{true}}\rangle, |\overline{\text{false}}\rangle\right) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \langle\overline{\text{true}}| \\ \langle\overline{\text{false}}| \end{pmatrix}$$

$$|\overline{\text{true}}\rangle = \frac{1}{\sqrt{2}}\{|\text{true}\rangle - |\text{false}\rangle\}$$

$$|\overline{\text{false}}\rangle = \frac{1}{\sqrt{2}}\{|\text{true}\rangle + |\text{false}\rangle\} \tag{1.68}$$

or in terms of the truth table, Eq. (1.64)

$$\mathcal{P} = \begin{matrix} \\ |\text{true}\rangle \\ |\text{false}\rangle \end{matrix} \begin{matrix} \begin{matrix} |\text{true}\rangle & |\text{false}\rangle \end{matrix} \\ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \end{matrix} = \begin{matrix} \\ |\overline{\text{true}}\rangle \\ |\overline{\text{false}}\rangle \end{matrix} \begin{matrix} \begin{matrix} |\overline{\text{true}}\rangle & |\overline{\text{false}}\rangle \end{matrix} \\ \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \end{matrix} \tag{1.69}$$

The result, Eqs. (1.68, 1.69), reveals an exceptional interpretation of the degenerate situation, since it charts a self-referential statement, see more below, as a Jordan block (Segrè characteristic equal to two) in the present general (quantum) logical framework. Thus choosing $P = G$, where G is the famous Gödel arithmetical proposition with neither G nor $\neg G$ provable within the given set of axioms of elementary arithmetic [1]. The paradox epitomises a *singularity*, since $\mathcal{P}$ is non-diagonal, while simultaneously the truth table conveys that G is not true and $\neg G$ is not false or both G and $\neg G$ are false. The fundamental conclusion is that decoherence of classical truth values (cf. the wave-function collapse in quantum mechanics) is forbidden at the degenerate point $p = \frac{1}{2}$. Nevertheless, we recover the classical result since $\mathcal{P}^2 = 0$, i.e. without some bias at hand our information is zero, i.e. $p = (1 - p) = \frac{1}{2}$.

As discussed earlier, the present interpretation of the truth table can be obtained from conventional representations with the use of a non-positive definite metric Δ; $\Delta_{11} = -\Delta_{22} = 1$; $\Delta_{12} = \Delta_{12} = 0$. In this picture, we can use conventional bra-ket nomenclature, while for another selection of Δ, leading e.g. to a complex symmetric choice, it would require complex symmetric realisations. In both cases, the formulation is biorthogonal. With this realisation, we can make an identification between Eqs. (1.63) and (1.66), making the replacement $q = \kappa(r)$, where q is related to the probability function/operator of the simple proposition $Q = \neg P$. Hence, we realise a probabilistic origin combined with the nonclassical, self-referential character of gravitational interactions. Note also the analogy between the formulations, i.e. that the result of a classical measurement, i.e. the truth or

falsity of the statement Q, entails that either $q = 1$ or that $q = 0$. The (in)famous Gödel proposition (neither provable right nor wrong within the given axiomatic system) is logically formulated here as a special point singularity, see Eqs. (1.67–1.69). Similarly, decoherence to a particle or antiparticle is impossible at $\kappa(r) = \frac{1}{2}$ attributing via the self-referentiability property of gravitation, an automatic code protection principle at the Schwarzschild fringe. This relationship prompts the label "Gödelian time arrow" as combining the cosmological expansion with the gravitational collapse at the black hole boundary; see more in Ref. [11].

1.6 Conclusion

In conclusion, we emphasise the following points: (i) we have re-derived a previously obtained operator array formulation, which in its complex symmetric form permits a viable map of gravitational interactions within a combined quantum-classical structure; (ii) the choice of representation allows the implementation of a global superposition principle valid both in the classical as well as the quantum domain; (iii) the scope of the presentation has focused on obtaining well-known results of Einstein's theory of general relativity particularly in connection with the correct determination of the perihelion motion of the planet Mercury; (iv) finally, we have obtained a surprising relation with Gödel's celebrated incompleteness theorem.

In particular, we have considered the exacting determination of perihelion motions as acquired commensurate with the theory of general relativity. We also noted and explained that the theory of special relativity yields half the correct perihelion shift since it does not take account of the proper background dependence. In this chapter, we have emphasised that in order to recover the relativistic Kepler problem correctly, one must set up and explicitly prepare the precise boundary condition at the Schwarzschild boundary. The interconnection, alluded to in the title, ensues from the simple fact that the condition, Eq. (1.17), together with Eqs. (1.18–1.20), yields a singularity in Eq. (1.63). The latter is trivially formulated as an analogue of Gödel's incompleteness theorem via the translation of the conventional truth-functional proposition calculus to regular linear algebra generalised to include general non-positive definite metrics.

In a separate contribution [11], we have analysed within the present framework an assessment of the various arrows of time and the possible symmetry violations instigated by gravitation including the fundamental problem of molecular chirality [12]. Other related developments involve Penrose's concept of objective reduction (OR), i.e. gravity's role in quantum state reduction and decoherence as a fundamental concept that relates micro-macro domains including theories of human consciousness [13], see also Ref. [3] for more details. Note also efforts to derive quantum mechanics from general relativity [14].

There are finally many consequences that follow from the present formulation, i.e. fundamental symmetry violations, scale invariance and the non-probabilistic traits of evolution due to the regulation of self-reference [11]. In principle, the

present analogy supports the derivation of the gravitational law from the viewpoint of a general truth-functional proposition calculus. The functional behaviour for $\kappa(r)$ then drives from a quotient between the 2D surface surrounding a 3D sphere at the point "s" and the 3D surface surrounding a 4D volume, the latter by instigating an extra dimension from $c\mathrm{d}t = \mathrm{d}r(1-2\kappa(r))^{-1}$.

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Chapter 2
The Dirac Electron: Spin, *Zitterbewegung*, the Compton Wavelength, and the Kinetic Foundation of Rest Mass

Jean Maruani

Abstract The Dirac equation, which was derived by combining, in a consistent manner, the relativistic invariance condition with the quantum superposition principle, has shown its fecundity by explaining the electron spin, predicting antimatter, and enabling Schrödinger's trembling motion (*Zitterbewegung*). It has also yielded as expectation value for the electron speed the velocity of light. But the question has hardly been raised as to the effect of this intrinsic motion on the electron mass. In this chapter, we conjecture that the internal structure of the electron should consist of a massless charge describing, at light velocity, a vibrating motion in a domain defined by the Compton wavelength, the measured rest mass being generated by this very internal motion.

> Around 1950, I had the rare opportunity of meeting Albert Einstein .... The professor addressed my colleague: '*Vot* are you studying?' 'I'm doing a thesis on quantum theory'. '*Ach*!' said Einstein, 'a *vaste* of time!'
>
> He turned to me: 'And *vot* are you doing?' I was more confident: 'I'm studying experimentally the properties of pions'. 'Pions, pions! *Ach*, *vee* don't understand *de* electron! *Vy* bother *mit* pions?' ...
>
> Leon Lederman: *Life in Physics and the Crucial Sense of Wonder*, CERN Courier, 10 September 2009

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2.1 Introduction

The atomic theory of matter, which was conjectured on qualitative empirical grounds as early as the sixth century BC, was shown to be consistent with increasing experimental and theoretical developments since the seventeenth century AD, and definitely proven by the quantitative explanation of the Brownian motion by Einstein and Perrin early in the twentieth century [1]. It then took no more than a century between the first measurements of the electron properties in 1896 and of the proton properties in 1919 and the explosion of the number of so-called elementary particles – and their antiparticles – observed in modern accelerators to several hundred (most of which are very short lived and some, not even isolated). Today, the 'standard model' assumes all particles to be built from three groups of four basic fermions – some endowed with exotic characteristics – interacting through four basic forces mediated by bosons – usually with zero charge and mass and with integer spin [2].

In this zoo of particles, only the *electron*, which was discovered even before the atomic theory was proven and the atomic structure was known, is really unsecable, stable, and isolatable. The *proton* also is stable and isolatable, but it is made up of two quarks *up* (with charge +2/3) and one quark *down* (with charge −1/3). As for the *quarks*, while expected to be stable, they have not been isolated. The other particle constitutive of the atomic nucleus, the *neutron*, is also made up of three quarks, one *up* and two *down*, but it is not stable when isolated, decaying into a proton, an electron, and an antineutrino (with a 15-min lifetime). The fermions in each of the higher two classes of the *electron* family (*muon* and *tau*) and of the two *quark* families (*strange*/*charmed* and *bottom*/*top*) are unstable (and not isolatable for the quarks). Only the elusive *neutrinos* in the three classes, which were postulated to ensure conservation laws in weak interaction processes, are also considered as being unsecable, stable, and isolatable.

Although quantum chromodynamics has endeavoured to rationalize the world of quarks, gluons, the strong interaction, and composite particles [2], it is not as in a developed stage as quantum electrodynamics, where electrons, photons, the electromagnetic interaction, and the whole domain of chemical physics are unified in a refined manner [3, 4]. This latter theory is but an extension of the Dirac theory [5, 6], which treated the electron in a *consistent* quantum-relativistic manner while its interaction with the electromagnetic field was considered semi-classically, to a full quantum-relativistic treatment of charged particles interacting with each other and with a *quantized* electromagnetic field by exchanging virtual photons.

Traditional attributes of matter are opacity (to light), resistance (to penetration), inertia (to motion), and weight. A transparent glass has no opacity (to visible light), but it requires a very hard material (a diamond cutter) to be penetrated. Pure air also shows transparency, but it shows resistance to penetration only at very high speeds (blasts, storms, planes, parachutes). These two attributes are well understood today as quantum effects due to the interactions of molecules with electromagnetic fields and with other molecules.

The attribute of inertia was identified by Galileo as being a resistance to acceleration/deceleration (rather than to uniform linear motion), while the attribute of weight (also investigated by Galileo) was related by Newton to the attraction by a massive body (as expressed in Kepler's rules). These two attributes were later correlated in general relativity theory by Einstein. But the quantum theory has not been directly involved in either inertia or weight until Dirac's attempt to bring together quantum and relativistic conditions in a matrix linear equation for the electron, using the total energy mc^2 rather than the kinetic energy $p^2/2m_0$ in his Hamiltonian operator.

In this chapter, we shall reassess some of the physical implications of the Dirac equation [5, 6], which were somehow overlooked in the sophisticated formal developments of quantum electrodynamics. We will conjecture that the *internal structure* of the electron should consist of a *massless charge* describing at *light velocity* an oscillatory motion (*Zitterbewegung*) in a small domain defined by the *Compton wavelength*, the observed *spin momentum* and *rest mass* being jointly generated by this very internal motion.

2.2 Compton Wavelength and de Broglie Wavelength

Although the corpuscular aspect of electromagnetic radiation, which was surmised by Newton in the seventeenth century, was used by Planck in 1900 to explain Wien's black body radiation law and by Einstein in 1905 to explain Lenard's photoelectric effect, its most spectacular demonstration was Compton's explanation in 1923 of the anomalous scattering of X-rays by bound electrons.

If an incident photon ($\boldsymbol{p}_1$, $E_1 = p_1 c$) hits an electron considered as nearly at rest (0, $m_0 c^2$), producing an electron recoil ($\boldsymbol{p}_0$, E_0), the direction of the scattered photon ($\boldsymbol{p}_2$, $E_2 = p_2 c$) makes an angle θ with that of the incident photon. Applying the laws of conservation of energy and momentum to the scattering process:

$$\boldsymbol{p}_1 = \boldsymbol{p}_2 + \boldsymbol{p}_0, \quad p_1 c + m_0 c^2 = p_2 c + \left(m_0^2 c^4 + p_0^2 c^2\right)^{\frac{1}{2}}, \tag{2.1}$$

one derives

$$m_0 c(p_1 - p_2) = p_1 p_2 (1 - \cos\theta). \tag{2.2}$$

Using the incident and scattered photon wavelengths, $\lambda_1 = h/p_1$, $\lambda_2 = h/p_2$, and introducing the electron *Compton wavelength*, $\lambda_C = h/m_0 c$, one obtains

$$\lambda_2 - \lambda_1 = \lambda_C (1 - \cos\theta). \tag{2.3}$$

This expression is rigorous with the relativistic treatment we have used. But the occurrence of the Compton wavelength λ_C is not a relativistic effect since Eq. (2.2)

also holds (to first order, except around $\theta = 0°$) if one uses the classical formula, $E_0 = p_0^2/2m_0$, for the kinetic energy of the ejected electron. In fact, the occurrence of this electron wavelength stems from the assumption that light is made of particles endowed with kinetic momentum, $p = h/\lambda$, as well as with energy, $E = p\,c$.

The question remains as to how the electron interacts, at the subquantum level, to scatter the photon. One could speculate on the fact that for $\theta = \pi/2$ (orthogonal scattering) the Compton wavelength adds to the photon wavelength while the electron recoils along $\phi \sim -\pi/4$ (as would a tiny mirror inclined at $\pi/4$), while for $\theta = 0$ (no scattering) the photon wavelength remains unchanged and the electron unmoved. Adding the electron *Compton wavelength* to the *orthogonally scattered* photon wavelength reduces the photon energy by the amount used for the electron ejection.

The *Compton wavelength*, $\lambda_C = h/m_0c$, is different from the *de Broglie wavelength*, $\lambda_B = h/m_0v$, in that it is unrelated to the particle velocity but solely depends on its rest mass (and light velocity). The larger the rest mass, the smaller the wavelength or, one could say, *the larger the Compton wavelength, the smaller the particle rest mass*.

2.3 The Dirac Equation

It will be useful to recall the Lorentz transformation equations of the space and time coordinates of a free particle between two inertial frames S and S':

$$x' = \gamma(x - \beta ct) \tag{2.4a}$$

$$ct' = \gamma(-\beta x + ct) \tag{2.4b}$$

where $\beta = v/c$ and $\gamma = (1 - \beta^2)^{-1/2}$, v being the velocity of frame S' relative to frame S and c, the velocity of light. In similar transformation equations for the electromagnetic field (ruled by Maxwell's equations), the electric field components play the role of space coordinates and the magnetic field's that of a time coordinate.

It can be seen that, while the space and time coordinates depend on the reference frame, the combination

$$x_0^2 \equiv (ct)^2 - \underline{r}^2 \equiv x_4^2 - x_1^2 - x_2^2 - x_3^2 \tag{2.5a}$$

is relativistically invariant under any change of frame (its square root is Minkowski's *proper interval*). This formula can alternatively be written as

$$x_4^2 = x_0^2 + x_1^2 + x_2^2 + x_3^2. \tag{2.5b}$$

The dependence of the measured time on the inertial frame (the $-\beta x$ term in Eq. 2.4b), which entails $\gamma \neq 1$, stems from the invariance of c with respect to the frame. Einstein's equivalence relation $E = mc^2$ arises from the resulting intrication of space and time. One of the clues that led de Broglie to the idea of matter waves (and to the explanation of quantization rules in atomic spectra by assuming standing waves in electron orbits) was a comparison of this relation with that expressing the quantization of light, $E = h\,c/\lambda$, which yields $m = h/\lambda\,c$ for photons and, by analogy, $\lambda = h/mv$ for particles with non-zero rest mass.

The Dirac equation was derived in several steps [5, 6], starting with the time-dependent wave equation for a free particle in the Schrödinger representation:

$$i\hbar\,\frac{\partial \Psi}{\partial t} = H\;\Psi, \quad \text{or} \quad i\hbar\,\frac{\partial \Psi}{\partial (ct)} = mc\;\Psi, \tag{2.6}$$

where the Hamiltonian operator was given the relativistic form: $H = mc^2$. The term expressing the external motion is embedded in the relativistic formula for the mass: $m = m_0\gamma$. In order to unveil this term, H is transformed to the form

$$\begin{aligned} H = mc^2 = \left[\frac{m_0^2c^6}{(c^2 - v^2)}\right]^{1/2} &= \left[m_0^2c^4 + \frac{m_0^2c^4v^2}{(c^2 - v^2)}\right]^{1/2} = \\ &= \left(m_0^2c^4 + p^2c^2\right)^{1/2} = \left(m_0^2c^2 + p^2\right)^{1/2}c, \\ \text{or} \quad mc &= \left(m_0^2c^2 + p^2\right)^{1/2}, \end{aligned} \tag{2.7a}$$

with $p = m_0\gamma v = mv = p_0\gamma$. When $v \ll c$, H reduces to the usual form: $H_0 = (m_0c^2 +)\; p_0^2/2m_0\;(+\ldots)$.

In Eq. (2.7a), $p^2 = p_1^2 + p_2^2 + p_3^2$ with $p_i = mv_i$ along x_i, and from Eqs. (2.5) and (2.6) one can define an *additional 'momentum'* $\boldsymbol{p_4 \equiv mc}$, corresponding to the *time 'coordinate'* $\boldsymbol{x_4 \equiv ct}$, and an *invariant 'momentum'* $\boldsymbol{p_0 \equiv m_0c}$, for a *particle at rest*. Equation (2.7a) can then be written as

$$p_4^2 = p_0^2 + p_1^2 + p_2^2 + p_3^2. \tag{2.7b}$$

Comparing Eqs. (2.7b) and (2.5b) shows that the *relativistically invariant 'momentum'* p_0 corresponds to the *relativistically invariant 'coordinate'* x_0. To the 'Pythagorean relation' between the *generalized coordinates*, $x_4^2 = x_0^2 + \underline{r}^2$, corresponds a similar relation between the *generalized momenta*, $p_4^2 = p_0^2 + \underline{p}^2$.

By analogy with the non-relativistic case, one can write

$$p_1 \rightarrow -i\hbar\,\frac{\partial}{\partial x},\; p_2 \rightarrow -i\hbar\,\frac{\partial}{\partial y},\; p_3 \rightarrow -i\hbar\,\frac{\partial}{\partial z},\; p_4 \rightarrow i\hbar\,\frac{\partial}{\partial (ct)}, \tag{2.8}$$

the last expression being introduced to bring time on the same footing as the space coordinates. At this stage, the operator associated with p_0 is just p_0. Equation (2.6) can then be written as

$$\left[p_4 - \left(p_0^2 + p_1^2 + p_2^2 + p_3^2\right)^{1/2}\right]\Psi = 0, \tag{2.9}$$

which is linear in p_4 but not in the other p_i's and, therefore, not fully satisfactory from the relativistic point of view.

The *second step* was thus to multiply this equation on the left side by $\left[p_4 + \left(p_0^2 + p_1^2 + p_2^2 + p_3^2\right)^{1/2}\right]$, yielding the more symmetric form

$$\left[p_4^2 - \left(p_0^2 + p_1^2 + p_2^2 + p_3^2\right)\right]\Psi = 0, \tag{2.10}$$

where only those solutions belonging to positive values of p_4 are also solutions of Eq. (2.9). This is the so-called Klein-Gordon equation, which reduces to the wave equation for $m_0 = 0$ and is suitable for the description of zero-spin free particles.

Although Eq. (2.10) fulfils the relativistic condition of space-time equivalence, it does not fulfil the quantum requirement of linearity so that the superposition principle, probability density formula and uncertainty principle could apply [5, 6].

The *third step* was to look for an analogous equation *linear* in all p_μ's, that is,

$$\left[p_4 - \left(\boldsymbol{\alpha}_0 p_0 + \boldsymbol{\alpha}_1 p_1 + \boldsymbol{\alpha}_2 p_2 + \boldsymbol{\alpha}_3 p_3\right)\right]\Psi = 0, \tag{2.11}$$

where the $\boldsymbol{\alpha}_\mu$'s must be matrices independent of the p_μ's and of the x_μ's in free space. Multiplying to the left side by $[p_4 + (\boldsymbol{\alpha}_0 p_0 + \boldsymbol{\alpha}_1 p_1 + \boldsymbol{\alpha}_2 p_2 + \boldsymbol{\alpha}_3 p_3)]$ yields

$$\left[p_4^2 - \left(\boldsymbol{\alpha}_0 p_0 + \boldsymbol{\alpha}_1 p_1 + \boldsymbol{\alpha}_2 p_2 + \boldsymbol{\alpha}_3 p_3\right)^2\right]\Psi = 0. \tag{2.12}$$

This coincides with Eq. (2.10) only if one has, for $\mu, \nu = 0, 1, 2, 3$:

$$\boldsymbol{\alpha}_\mu^2 = 1, \quad \boldsymbol{\alpha}_\mu \boldsymbol{\alpha}_\nu + \boldsymbol{\alpha}_\nu \boldsymbol{\alpha}_\mu = 0. \tag{2.13}$$

In addition to being normalized and anticommutative, these matrices, of course, must be Hermitian. These conditions are similar to those for the three components σ_x, σ_y, σ_z of the spin operator $\boldsymbol{\sigma}$ and of their Pauli representations as 2D matrices:

$$\sigma_x \sim \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y \sim \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} \quad \sigma_z \sim \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.14}$$

But now we have four components for the four-vector (p_1, p_2, p_3, p_0), and the four $\boldsymbol{\alpha}_\mu$ matrices fulfil the above requirements only if they possess at least four dimensions; e.g. [5, 6], using the 2D Pauli matrices as off-diagonal elements of the 4D Dirac matrices relative to the p_μ's:

$$\boldsymbol{\alpha}_1 \equiv \begin{pmatrix} 0 & \boldsymbol{\sigma}_x \\ \boldsymbol{\sigma}_x & 0 \end{pmatrix} \quad \boldsymbol{\alpha}_2 \equiv \begin{pmatrix} 0 & \boldsymbol{\sigma}_y \\ \boldsymbol{\sigma}_y & 0 \end{pmatrix} \quad \boldsymbol{\alpha}_3 \equiv \begin{pmatrix} 0 & \boldsymbol{\sigma}_z \\ \boldsymbol{\sigma}_z & 0 \end{pmatrix} \quad \boldsymbol{\alpha}_0 \equiv \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.15}$$

A result is that for a vector to be representative of the wave function Ψ it must have four components or, alternatively, that Ψ must contain a variable taking on four values. Dirac has explained why the electron has spin, which was known as requiring the wave function Ψ to have two components, and that this number must be doubled because the quasi-linear Eq. (2.11), which is equivalent to the quadratic Eq. (2.10) under the conditions (2.13), has additional, negative-energy solutions, which he assigned to an antielectron having opposite charge [5].

As expected, Eq. (2.11) is invariant under Lorentz transformations [5, 6]. It was noticed by de Broglie [6] that the process leading from Eq. (2.10) to (2.11) is similar to that leading from the second-order equations for the electric and magnetic fields $\underline{E}$ and $\underline{B}$ of electromagnetic radiation to the four coupled, first-order, Lorentz-invariant Maxwell equations.

Although spin was first introduced phenomenologically (see Sect. 2.4) and shown to require only 2D matrices for its representation (Eq. 2.14), the theoretical proof for its existence required a four-component wave vector, yielding additional negative-energy states. This hints that *spin*, as well as *Zitterbewegung* (see Sect. 2.4), must be related to these states. This appears in the entanglement of the four components of Ψ when Eq. (2.11) is written explicitly in the form of four coupled equations [6].

One may notice that the matrices $\boldsymbol{\alpha}_i$ multiplying the components p_i of the momentum that describe the *external trajectory* of the particle are off-diagonal, whereas the matrix $\boldsymbol{\alpha}_0$ multiplying the momentum p_0 related to the rest mass energy m_0c^2 is diagonal. This suggests there is some *internal motion* orthogonal to the external trajectory, as hinted in Eq. (2.7b) where the generalized momentum $\boldsymbol{mc}$ appears as a *Pythagorean sum* of the two orthogonal momenta $\boldsymbol{m}_0\boldsymbol{c}$ and $\boldsymbol{p}$.

Indeed, three internal motions (which have been shown to be related) have been discussed by Dirac from his equation. One involves the well-established *spin* angular momentum, which gives rise to the *measured* magnetic moment; another is the *Zitterbewegung* (proper oscillatory motion) derived by Schrödinger from Dirac's equation; and finally there is an internal motion adding to that defining the external trajectory of the particle to give it the *computed* velocity c. We shall comment on these three motions.

2.4 The Electron Internal Motion: Spin, *Zitterbewegung*, and Light Velocity

The electron spin entered quantum mechanics in two different ways. The first was the explanation, by Goudsmit and Uhlenbeck (1925), of the Zeeman splitting of the spectral lines of atoms by a magnetic field (1896) and of the Stern and Gerlach deflection of the trajectory of atoms by an inhomogeneous field (1922). The electron

was endowed with an *intrinsic* magnetic moment and, since it has electric charge, with a *rotational* internal motion adding to its quantized motion around a nucleus. This electron property was later shown to be responsible for most of materials' magnetism, known for long: ferro (and anti) and ferri (and anti), as well as para (but not dia). Electron paramagnetic resonance (EPR) spectroscopy and related techniques [7] are based on this property, and on a similar property proposed by Pauli for nuclei [1924], which is at the basis of nuclear magnetic resonance (NMR).

Various models have been designed to account for the magnetic properties of the electron [6]. In the simple model of a loop with radius r described by a point charge $-e$, the *measured* magnitude of the induced magnetic moment $\underline{\mu}$ orthogonal to the loop can be used to derive the *rotational* velocity v:

$$\begin{aligned} \mu = I.S = \left(\frac{-e.v}{2\pi r}\right).\pi r^2 &= -\frac{e.v\ r}{2} \\ &= -\left(\frac{1}{2}\right)\frac{e\ \hbar}{2m_0} \rightarrow v = \frac{\hbar}{2m_0 r}. \end{aligned} \tag{2.16}$$

If one identifies r with the *measured* Compton radius, $r_C = \hbar/2\,m_0 c$ (Sect. 2.2 and Eq. 2.34), this formula yields: $v = c$!

The second intrusion of the electron spin came through a non-energetic, symmetry requirement, the so-called Fermi-Dirac statistics for systems of identical, half-integer spin particles, which results in total antisymmetry of the Schrödinger wave function in a combined space and spin coordinate domain. This entails the Pauli exclusion principle (1925) in the framework of the independent-particle, Slater-determinantal model. The expression of atomic and molecular wave functions as linear combinations of Slater determinants has been the basis of most of the subsequent methodologies of quantum chemistry, thermodynamics, and spectroscopy.

These two aspects of the electron spin, that of an internal dynamical variable introduced to satisfy a symmetry requirement and that related to an intrinsic magnetic moment interacting with an external field, were elucidated by Dirac from his quantum-relativistic equation. But it also yielded an electron moving at the speed of light!

To have the electron magnetic moment show up, it is necessary to make it interact with an external magnetic field; and to have its spin momentum appear, it has to be combined with an orbital momentum. Equation (2.11) was thus extended to include interactions with an electromagnetic field. Let us call A_4 and $\underline{A}$ the scalar and vector potentials in *MKSA* units (in earlier formulations of the Dirac equation [5, 6], $\underline{A}$ was divided by c due to the use of *cgs* units). We can write

$$\left[\left(p_4 + \frac{e\ A_4}{c}\right) - \boldsymbol{\alpha}_0 p_0 - \underline{\boldsymbol{\alpha}}.\left(\underline{p} + e\ \underline{A}\right)\right]\Psi = 0. \tag{2.17}$$

It can be noticed that the *internal* momentum p_0 remains *unchanged* in the presence of a field. In the Heisenberg picture, which is more suitable to make comparisons

between classical and quantum mechanics, the equations of motion are determined by the Hamiltonian

$$H = c\ p_4 = -e\ A_4 + c\boldsymbol{\alpha}_0 p_0 + c\underline{\boldsymbol{\alpha}}.(\underline{p} + e\ \underline{A})]. \tag{2.18}$$

This gives, using the forms and properties of the $\boldsymbol{\alpha}_\mu$ matrices (Eqs. 2.13, 2.14, and 2.15), especially the fact that $\boldsymbol{\alpha}_0$ is normalized and anticommutes with $\boldsymbol{\alpha_i}$ ($i = 1, 2, 3$) while commuting with $(\underline{p} + e\underline{A})$:

$$\left(p_4 + \frac{e\ A_4}{c}\right)^2 = \left[\boldsymbol{\alpha}_0 p_0 + \underline{\boldsymbol{\alpha}}.(\underline{p} + e\ \underline{A})\right]^2 = p_0^2 + \left[\underline{\boldsymbol{\sigma}}.(\underline{p} + e\ \underline{A})\right]^2. \tag{2.19}$$

If one uses the general relation for any two 3D vectors $\underline{C}$ and $\underline{D}$ commuting with the $\boldsymbol{\sigma_i}$'s, which results from the properties of the Pauli matrices (Eqs. 2.14),

$$(\underline{\boldsymbol{\sigma}}.\underline{C}).(\underline{\boldsymbol{\sigma}}.\underline{D}) - \underline{C}.\underline{D} = i\ \underline{\boldsymbol{\sigma}}.\underline{C}\times\underline{D},$$

one obtains for $\underline{C} = \underline{D} = (\underline{p} + e\underline{A})$, substituting $\underline{p} = -i\,\hbar\underline{\nabla}$ then $\underline{B}\,(\underline{r},\, t) = \underline{\nabla}\times\underline{A}\,(\underline{r},\, t)$,

$$\left[\underline{\boldsymbol{\sigma}}.(\underline{p} + e\ \underline{A})\right]^2 - (\underline{p} + e\ \underline{A})^2 = i\,e\,\underline{\boldsymbol{\sigma}}.\ (\underline{p}\times\underline{A} + \underline{A}\times\underline{p}) =$$

$$= \hbar\,e\,\underline{\boldsymbol{\sigma}}.\ \underline{\nabla}\times\underline{A} = \hbar\ e\ \underline{\boldsymbol{\sigma}}.\underline{B}.$$

Equation (2.19) then becomes

$$\left(p_4 + \frac{e\ A_4}{c}\right)^2 = p_0^2 + (\underline{p} + e\ \underline{A})^2 + e\ \hbar\ \underline{\boldsymbol{\sigma}}.\underline{B}. \tag{2.20}$$

In order to compare this expression with the non-relativistic one, H is written in the perturbative form: $H = m_0c^2 + H'$. To first order, this yields

$$H' = -e\ A_4 + \frac{(\underline{p} + e\ \underline{A})^2}{2m_0} + \left(\frac{e\ \hbar}{2m_0}\right)\underline{\boldsymbol{\sigma}}.\underline{B}. \tag{2.21}$$

In addition to the potential and kinetic energy terms of the classical Hamiltonian for a slow electron, there appears an extra term, which can be seen as expressing the interaction of the electron with a magnetic field $\underline{B}$ through an *intrinsic magnetic moment*, $\underline{\mu} = -(e\ \hbar/2m_0)\ \underline{\boldsymbol{\sigma}}$, in agreement with Eq. (2.16). This extra term arises naturally from the factor $\underline{\boldsymbol{\sigma}}$ embedded in Eq. (2.19).

The spin angular momentum itself does not give rise to any *potential* energy. To show its existence, Dirac computed the angular momentum integrals for an electron moving in a central electric field, that is, from Eq. (2.18):

$$H = -e\ \underline{A}_4(r) + c\ \boldsymbol{\alpha}_0 p_0 + c\ \underline{\boldsymbol{\alpha}}.\underline{p}. \tag{2.22}$$

In the Heisenberg picture, one obtains, for the l_1 component, say, of the orbital angular momentum $\underline{l} = -i\,\hbar \underline{r} \times \underline{\nabla}$,

$$\begin{aligned} i\hbar\,\frac{\partial l_1}{\partial t} &= [l_1, H] = c\,[l_1.(\underline{\boldsymbol{\alpha}}\,\underline{p}) - (\underline{\boldsymbol{\alpha}}\,\underline{p}).l_1] = \\ &= c\,\underline{\boldsymbol{\alpha}}(l_1.\underline{p} - \underline{p}.\,l_1) = -i\hbar\,c(\boldsymbol{\alpha}_3.p_2 - \boldsymbol{\alpha}_2.p_3) \neq 0; \end{aligned} \tag{2.23}$$

similarly, for the corresponding component of the Pauli matrix operator,

$$\begin{aligned} i\hbar\,\frac{\partial \sigma_1}{\partial t} &= [\sigma_1, H] = c\,[\sigma_1.(\underline{\boldsymbol{\alpha}}\,\underline{p}) - (\underline{\boldsymbol{\alpha}}\,\underline{p}).\sigma_1] = \\ &= c\,(\sigma_1\underline{\boldsymbol{\alpha}} - \underline{\boldsymbol{\alpha}}\sigma_1).\underline{p} = 2\,i\,c\,(\boldsymbol{\alpha}_3.p_2 - \boldsymbol{\alpha}_2.p_3) \neq 0. \end{aligned} \tag{2.24}$$

From Eq. (2.23) it is seen that l_1 is *not* a constant of the motion, but from Eq. (2.24) it is seen that

$$\frac{\partial l_1}{\partial t} + \left(\frac{\hbar}{2}\right)\frac{\partial \sigma_1}{\partial t} = 0. \tag{2.25}$$

Dirac interpreted this as the electron having a *spin* angular momentum, $\underline{s} = (\hbar/2)\,\underline{\boldsymbol{\sigma}}$, that has to be *added* to the *orbital* angular momentum $\underline{l}$ to get a constant of the motion. It is the same matrix/operator vector $\underline{\boldsymbol{\sigma}}$ that fixes the direction of $\underline{s}$ and that of the magnetic moment $\underline{\boldsymbol{\mu}}$ derived from Eq. (2.21), and this justifies the simple model leading to Eq. (2.16).

Following considerations developed by Bohr, Darwin, and Pauli, de Broglie [6] showed that it is not possible to separate the electron spin momentum from its orbital momentum because, in any direct measurement, the uncertainties on the components of the orbital momentum would be larger than the spin momentum. This is due to the electron having a finite size, defined by the Compton radius.

Equations (2.25) and (2.21) do not tell us *at which velocity* the electron 'rotates' to acquire kinetic and magnetic spin momenta. This is provided by another computation by Dirac [5]. He used a Heisenberg picture with a field-free Hamiltonian (but the conclusion would also hold with a field present):

$$H = c\,(\boldsymbol{\alpha}_0 p_0 + \boldsymbol{\alpha}_1 p_1 + \boldsymbol{\alpha}_2 p_2 + \boldsymbol{\alpha}_3 p_3). \tag{2.26}$$

The *linear momentum* $\underline{p}$ obviously commutes with H and thus is a *constant of the motion*. Making use of the properties of the $\boldsymbol{\alpha}_k$'s (Eqs. 2.13), one can further write, for an arbitrary component v_k ($k = 1, 2, 3$) of the electron velocity,

$$\begin{aligned} i\hbar\,\frac{\partial x_k}{\partial t} &= [x_k, H] = c\,(x_k\,\underline{\boldsymbol{\alpha}}.\underline{p} - \underline{\boldsymbol{\alpha}}.\underline{p}\,x_k) = c\,\boldsymbol{\alpha}_k\,(x_k p_k - p_k x_k) \\ &= i\hbar\,c\,\boldsymbol{\alpha}_k \rightarrow v_k = \left|\frac{\partial x_k}{\partial t}\right| = \pm c, \end{aligned} \tag{2.27}$$

showing the electron moves at light velocity! If we used the classical expression for the energy of a free particle, $H = p^2/2\,m_0$, in Eq. (2.26), we would recover, through Eq. (2.27), the classical relation between velocity and momentum, $v_k = p_k/m_0$, which we expect also to hold in the relativistic case.

The paradox was elucidated through the 'trembling motion' (*Zitterbewegung*) discovered by Schrödinger [8] while investigating the velocity operators $\boldsymbol{\alpha}_k$ introduced by Dirac to linearize his equation. The equation of motion of a velocity component, $v_k = c\boldsymbol{\alpha}_k$, can be written as

$$i\hbar\,\frac{\partial \alpha_k}{\partial t} = \alpha_k H - H\alpha_k .$$

Since $c\,\boldsymbol{\alpha}_k$ anticommutes with all the terms in Eq. (2.26) except $c\,\boldsymbol{\alpha}_k p_k$, one also has

$$\boldsymbol{\alpha}_k H + H\boldsymbol{\alpha}_k = \boldsymbol{\alpha}_k (c\;\boldsymbol{\alpha}_k\, p_k) + (c\;\boldsymbol{\alpha}_k\, p_k)\;\boldsymbol{\alpha}_k = 2c\, p_k .$$

These two equations together yield

$$i\hbar\,\frac{\partial \boldsymbol{\alpha}_k}{\partial t} = 2\boldsymbol{\alpha}_k H - 2c\, p_k .$$

Since H and p_k are time independent, this entails

$$i\hbar\,\frac{\partial^2 \boldsymbol{\alpha}_k}{\partial t^2} = 2\left(\frac{\partial \boldsymbol{\alpha}_k}{\partial t}\right) H .$$

This differential equation in $\partial\boldsymbol{\alpha}_k/\partial t$ can be integrated twice, yielding the explicit time dependence of the velocity, then position, operators. One first obtains

$$v_k = c\;\boldsymbol{\alpha}_k = c^2 p_k H^{-1} + \left(\frac{i\hbar c}{2}\right)\gamma_k^0 e^{-i\omega t} H^{-1}, \tag{2.28}$$

where $\omega = 2H/\hbar$ and $\gamma_k^0 = \partial\boldsymbol{\alpha}_k/\partial t$ at $t = 0$. As $H = mc^2$, the first term is a constant of the order of p_k/m, the classical relation between momentum and velocity. But there is an extra term, here also, oscillating at the frequency:

$$\nu' = \frac{2mc^2}{h}, \tag{2.29}$$

which stems mainly from the rest mass energy m_0c^2 in the power expansion of H following Eq. (2.7a).

Only the *constant part* is observed in a practical measurement, which gives the *average velocity* through a time interval much larger than ν^{-1}; whereas the *oscillatory part* explains why the *instantaneous velocity* has eigenvalues $\pm c$ [5, 6]. Further integration yields the time dependence of the electron coordinate x_k, and it is seen that the *amplitude* of the oscillatory motion is of the order of $\hbar/2m_0c$, the Compton radius of the relativistic electron (Sect. 2.2 and Eq. 2.34).

Zitterbewegung vanishes when one takes expectation values over wave packets made up solely of positive (or negative) energy states [8], which are not full solutions of the wave equation because of the coupling of the four components of Ψ in Eq. (2.11). This motion was interpreted as being due to a *wave beat* between the states with energies $\pm mc^2$, the beat frequency being the difference of the two wave frequencies: $\pm mc^2/h$ [6]. It was also shown (e.g. [9]) that transitions between positive and negative energy states are possible whenever the electron potential energy undergoes variations of at least m_0c^2 over distances of at most h/m_0c. This is another clue that the Compton wavelength, internal motion, and negative energy states are deeply related. Recently [10] it has been shown that *Zitterbewegung* can affect harmonic generation by strong laser pulse and that stimulated *Zitterbewegung* can be generated by laser-induced transitions between positive and negative energy states.

Comparing the preceding results with those expressed in Eqs. (2.16) and (2.21) makes it clear that the *internal motion* giving rise to the kinetic and magnetic *spin momenta* is nothing but *Zitterbewegung*. A classical relativistic model was proposed [11] in which *spin* appears as the *orbital* angular momentum of *Zitterbewegung*. Moreover, the quantum-relativistic relation of the *Zitterbewegung frequency* to the *inertial mass* together with the general-relativistic equivalence of this latter to the *gravitational mass* establish a link between *spin* and *gravitation*. In a stochastic electrodynamics (SED) model [12], *Zitterbewegung* arises from the *electromagnetic interaction* of a semi-classical particle with the *vacuum zero-point field*, and the *van der Waals* force generated by this oscillatory motion is identified with the *Newtonian* gravitational field. More generally, there have been various attempts to involve general relativity into quantum mechanics (e.g. [13, 14]) or to derive one from the other (e.g. [15, 16]).

In his detailed analysis of Dirac's theory [6], de Broglie pointed out that, in spite of his equation being Lorentz invariant and its four-component wave function providing tensorial forms for all physical properties in space-time, it does not have space and time playing full symmetrical roles, in part because the condition of hermiticity for quantum operators is defined in the space domain while time appears only as a parameter. In addition, space-time relativistic symmetry requires that Heisenberg's uncertainty relations,

$$\Delta p_i . \Delta x_i \sim \hbar \quad (i = 1, 2, 3), \tag{2.30}$$

be completed by a similar relation for the energy, the 'time component' of the four-vector momentum whose space components are the p_i's. This did not seem to be consistent with the energy corresponding to the Hamiltonian H rather than to the operator $i\hbar\, \partial/\partial t$. However, consistency can be recovered by writing

$$\Delta H . \Delta t = \Delta(mc^2) . \Delta t = \Delta(mc) . \Delta(ct) = \Delta(p_4) . \Delta(x_4) \sim \hbar, \tag{2.31}$$

assigning the *full* momentum $p_4 = mc$ to the *time* component $x_4 = ct$, the corresponding operator being $i\hbar\, \partial/\partial(ct)$, in accordance with Eq. (2.8).

If, in Eq. (2.31), mc is replaced by $m_0\gamma c$ (with γ defined in Eqs. 2.4), it comes

$$\Delta(m_0\gamma c).\Delta(ct) = \Delta(m_0 c).\Delta(ct\gamma) = \Delta(m_0 c).\Delta(c\tau_0) \sim \hbar, \tag{2.32}$$

where τ_0 is the *proper time* of the electron, which defines its *internal clock*. To the *internal* time coordinate $c\tau_0 = x_0$ is associated the *rest* mass momentum $m_0 c = p_0$. If one removes the Δ's, one obtains

$$m_0 c.c\tau_0 \sim \hbar \rightarrow \tau_0 \sim \frac{\hbar}{m_0 c^2} = \frac{1}{2\pi\nu_0}, \tag{2.33}$$

where ν_0 is half the *Zitterbewegung* frequency for the electron *at rest*. For this latter, $p_i = 0$ $(i = 1, 2, 3)$ and, using the expression for $\boldsymbol{\alpha}_0$ in Eq. (2.15) and the vector form for Ψ, Eq. (2.11) reduces to

$$i\hbar\,\frac{\partial\Psi_j}{\partial t} = +\,m_0 c^2\Psi_j \rightarrow \Psi_j = \Psi_{j0}\exp\left(-2\pi i\,\nu_0 t\right) = \Psi_{j0}\exp\left(-\frac{i}{\tau_0}\,t\right),$$

$$i\hbar\,\frac{\partial\Psi_k}{\partial t} = -\,m_0 c^2\Psi_k \rightarrow \Psi_k = \Psi_{k0}\exp\left(+2\pi i\,\nu_0 t\right) = \Psi_{k0}\exp\left(+\frac{i}{\tau_0}\,t\right),$$

where $j = 1, 2$; $k = 3, 4$; and $\nu_0 = m_0 c^2/h$. The difference (beat) frequency $\nu_0' = 2\nu_0$ of the positive and negative energy states is the *Zitterbewegung* frequency for the electron *at rest*. In the complex exponential argument, $\tau_0 \sim 1.29 \times 10^{-21}$ s defines the *time scale* of the electron internal motion.

2.5 The Electron Radii

The spin angular momentum and associated magnetic moment of the electron emerged naturally from Dirac's quantum-relativistic treatment. What also came out from the Dirac equation is that the oscillatory motion (*Zitterbewegung*) giving rise to these momenta involves negative energy states and takes place at light velocity. As the rest masses of both electron and positron are non-zero, one may wonder why they do not go to infinity at that velocity. A first clue is that, since the electron and positron 'rest masses' are opposite and since the 'trembling motion' involves both positive and negative energy states, the 'vibrating entity' has zero average mass, departures from this value being allowed by Heisenberg's uncertainty principle.

There have been a number of speculations on the foundations of inertia, gravitation, and mass (e.g. [15–17]). In the following, we present a novel conjecture based on the previous discussion.

Let us consider again the simple classical picture of a particle endowed with charge e and mass m_0 moving at velocity c around a loop of radius r_C. In this picture, the intrinsic angular momentum would be $s = m_0 c.r_C = r_C.2\pi\hbar/\lambda_C$, from

the definition of λ_C in Eq. (2.3). As in the Bohr model for the orbital motion of an electron around a nucleus, the spin $s/\hbar$ of the electron takes a (half) integer value if the loop circumference $2\pi r_C$ involves a (half) integer number of wavelengths λ_C (the 'half' stemming from the loop being actually a sphere in space-time). This 'loop' could then be considered as some kind of 'intrinsic orbit' with radius $r_C = \lambda_C/4\pi$. From the definition of the Compton wavelength (Eq. 2.3), one may express the rest mass as a function of the inverse of this 'orbit radius':

$$m_0 = \frac{\hbar}{2c\ r_C}, \quad r_C = \frac{\lambda_C}{4\pi}. \tag{2.34}$$

One may then say that this ***intrinsic orbit*** (which defines the 'internal structure' of the particle) is described at velocity c (as results from the Dirac equation), while the ***external orbit*** (in an atom for instance) is described at velocity v. However, this makes it necessary to consider that the charged entity describing the intrinsic orbit has ***zero rest mass***. This suggests that the ***rest mass observed*** with respect to an external body (such as an atomic nucleus) arises from the very intrinsic motion of the charged entity at velocity c.

The above picture should, of course, be amended to account for the contraction of the loop radius with this fast motion. In fact, if a charged entity describes a spherical motion at light velocity it should look as punctual to an external observer (or a nucleus). But this would violate Heisenberg's uncertainty principle. The quantization condition of the 'intrinsic orbit' can actually be recovered from the relation: $\Delta p.\Delta r \sim \hbar/2$ (the quotient 2 being due to the half-integer value of the spin). If one replaces Δr by r_C and Δp by $m_0 c$ then r_C can be written as $r_C \sim \hbar/2\, m_0 c$, yielding $4\pi r_C \sim h/m_0 c = \lambda_C$, the *Compton wavelength*. This derivation is similar to that of the *Bohr radius* a_0 (which expresses the non-collapse of the electron onto the nucleus) by substituting Δr by a_0 and Δp by p in the quantum condition, $\Delta p.\Delta r \sim \hbar$, and using the balance condition: $p^2/m\ a_0 = e^2/4\pi\varepsilon_0 a_0^2$.

It should be noted, however, that, while we know what holds the electron in a confined region around the *Bohr radius*, the *attraction* by the nucleus, we do not know what holds the conjectured, massless charged entity in a confined region around the *Compton radius*. One may think of a *pressure* generated by interactions with virtual particles of the Dirac sea, yielding a kind of Brownian motion at the subquantum level, the *Zitterbewegung*. However, contrary to the Brownian motion, the electron internal motion is not random, since it gives rise to observable spin momentum and magnetic moment.

Another property of the electron is the so-called *classical radius* r_0, which is the size that the electron would need to have its rest mass m_0 entirely due to its electric potential energy E_0. According to classical electrostatics, the energy required to assemble a sphere of radius r_0 and charge e is given by $E_0 = k\ e^2/4\pi\varepsilon_0 r_0$, where $k = ½$ if the charge is evenly distributed on the surface and grows larger for a density increasing towards the centre. Assuming all the rest mass energy $m_0 c^2$ is of electrostatic origin yields, for $k = 1$, $r_0 = e^2/4\pi\varepsilon_0 m_0 c^2$ (Table 2.1). This is the length scale at which renormalization becomes important in quantum electrodynamics.