CHAPTER FIVE : THE UNIFICATION OF QUANTUM MECHANICS AND GENERAL RELATIVITY

The standard physics has completely failed to unify quantum mechanics and general relativity, notably because of indeterminacy, a non Baconian idea introduced at the Solvay Conference of 1927. The current attempts of the standard physics at unification revolve around hugely expensive particle colliders, and these attempts are limited to the unification of the electromagnetic and weak and strong nuclear fields, leaving out gravitation completely. So it is reasonable to infer that the standard physics will never be able to produce a unified field theory. In great contrast ECE theory has succeeded with unifying all four fundamental fields with a well known geometry due to Cartan as described in foregoing chapters of this book.

Towards the end of the nineteenth century the classical physics evolved gradually into special relativity and the old quantum theory. The experiments that led to this great paradigm shift in natural philosophy are very well known, so need only a brief description here. There were experiments on the nature of broadband (black body) radiation leading to the Rayleigh Jeans law, the Steffan Boltzmann distribution and similar. The failure of the Rayleigh Jeans law led to the Planck distribution and his inference of what was later named the photon. The photoelectric effect could not be explained using the classical physics, the Brownian motion needed a new type of stochastic physics indicating the existence of molecules, first proposed by Dalton. The specific heats of solids could not be explained adequately with classical nineteenth century physics. Atomic and molecular spectra could not be explained with classical methods, notably the anomalous Zeeman effect.

The Michelson Morley experiment gave results that could not be explained with the classical Newtonian physics, so that Fitzgerald in correspondence with Heaviside suggested a radically new physics that came to be known as special relativity. The mathematical framework for special relativity was very nearly inferred by Heaviside but was developed by Lorentz and Poincaré. Einstein later made contributions of his own. The subjects of special relativity and quantum theory began to develop rapidly. The many contributions of Sommerfeld are typically underestimated in the history of science, those of his students and post doctorals are better known. The old quantum theory evolved into the Schroedinger equation after the inference by de Broglie of wave particle dualism. Peter Debye asked his student Schroedinger to try to solve the puzzle posed by the fact that a particle could be a wave and vice versa, and during this era Compton gave an impetus to the idea of photon as particle by scattering high frequency electromagnetic radiation from a metal foil - Compton scattering.

The Schroedinger equation proved to be an accurate description of for example spectral phenomena in the non relativistic limit. In the simplest instance the Schroedinger equation quantizes the classical kinetic energy of the free particle, and does not attempt to incorporate special relativity into quantum mechanics. Sommerfeld had made earlier attempts but the main problem remained, how to quantize the Einstein energy equation of special relativity. The initial attempts by Klein and Gordon resulted in negative probability, so were abandoned for this reason. Pauli had applied his algebra to the Schroedinger equation, but none of these methods were successful in describing the g factor, Landé factor or Thomas precession in one unified framework of relativistic quantum mechanics.

Dirac famously solved the problem with the use of four by four matrices and Pauli algebra but in so doing ran in to the problem of negative energies. Dirac suggested tentatively that negative energies could be eliminated with the Dirac sea, but this introduced an unobservable, the Dirac sea still has not been observed experimentally. Unobservables began to proliferate in twentieth century physics, reducing it to dogma. However, Dirac was famously successful in explaining within one framework the g factor of the electron, the Landé factor, the Thomas factor and the Darwin term, and in producing a theory free of negative probabilities. The Dirac sea seemed to give rise to antiparticles which were observed. The Dirac sea itself cannot be observed, and the problem of negative energies was not solved by Dirac.

It is not clear whether Dirac ever accepted indeterminacy, a notion introduced by Bohr and Heisenberg and immediately rejected by Einstein, Schroedinger, de Broglie and others as anti Baconian and unphysical. The Dirac equation reduces to the Schroedinger and Heisenberg equations in well defined limits, but indeterminacy is pure dogma. It is easily disproven experimentally and has taken on a life of its own that cannot be described as science. Heisenberg described the Dirac equation as an all time low in physics, but many would describe indeterminacy in the same way. In this chapter, indeterminacy is disproven straightforwardly with the use of higher order commutators. Heisenberg's own methods are used to disprove the Heisenberg Uncertainty Principle, a source of infinite confusion for nearly ninety years. One of the major outcomes of ECE theory is the rejection of the Heisenberg Uncertainty Principle in favour of a quantum mechanics based on geometry.

The negative energy problem that plagued the Dirac equation is removed in this chapter by producing the fermion equation of relativistic quantum mechanics. This equation is not only Lorentz covariant but also generally covariant because it is derived from the tetrad postulate of a generally covariant geometry - Cartan geometry. All the equations of ECE theory are automatically generally covariant and Lorentz covariant in a well defined limit of general covariance. So the fermion equation is the first equation of quantum mechanics unified with general relativity. It has the major advantages of producing rigorously positive energy levels and of being able to express the theory in terms of two by two matrices. The fermion equation produces everything that the Dirac equation does, but with major advantages. So it should be viewed as an improvement on the deservedly famous Dirac equation, an improvement based on geometry and the ECE unified field theory.

The latter also produces the d'Alembert and Klein Gordon equations, and indeed all of the valid wave equations of physics. Some of these are discussed in this chapter.

5.1 THE FERMION EQUATION

The structure of ECE theory is the most fundamental one known in physics at present, simply because it is based directly on a rigorously correct geometry. The fermion equation can be expressed as in UFT 173 on www.aias.us in a succinct way:

$$\Pi_\mu \phi \sigma^\mu = mc \sigma^1 \phi \quad -(1)$$

where the fermion operator in covariant representation is defined as:

$$\Pi_\mu = (\Pi_0, \Pi_1, \Pi_2, \Pi_3). \quad -(2)$$

Here:

$$\Pi_0 = \sigma^0 p_0, \quad \Pi_i = \sigma^3 p_i \quad -(3)$$

where p_μ is the energy momentum four vector:

$$p_\mu = (p_0, p_1, p_2, p_3). \quad -(4)$$

The Pauli matrices are defined by:

$$\sigma^\mu = (\sigma^0; \sigma^1, \sigma^2, \sigma^3) \quad -(5)$$

where:

$$\sigma^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad -(6)$$

The eigenfunction of Eq. (1) is the tetrad {1 - 10}:

$$\phi = \begin{bmatrix} \phi_1^R & \phi_2^R \\ \phi_1^L & \phi_2^L \end{bmatrix} \quad -(7)$$

whose entries are defined by the right and left Pauli spinors:

$$\phi^R = \begin{bmatrix} \phi_1^R \\ \phi_2^R \end{bmatrix}, \phi^L = \begin{bmatrix} \phi_1^L \\ \phi_2^L \end{bmatrix}. \quad -(8)$$

This eigenfunction is referred to as "the fermion spinor".

The position representation of the fermion operator is defined by the symbol δ and is:

$$\delta_\mu = -\frac{i}{\hbar} \pi_\mu . \quad -(9)$$

Therefore the fermion equation is the first order differential equation:

$$i\hbar \delta_\mu \phi \sigma^\mu = mc\sigma^1 \phi. \quad -(10)$$

For purposes of comparison, the covariant format of the Dirac equation in chiral representation {13} is:

$$\gamma^\mu \partial_\mu \phi_D = mc\,\phi_D \quad -(11)$$

where:

$$\phi_D = \begin{bmatrix} \phi^R \\ \phi^L \end{bmatrix} \quad -(12)$$

is a column vector with four entries, and where the Dirac matrices in chiral representation {13} are:

$$\gamma^\mu = (\gamma^0, \gamma^1, \gamma^2, \gamma^3). \quad -(13)$$

The complete details of the development of Eq. (1) are given in Note 172(8) accompanying UFT 172 on www.aias.us The ordering of terms in Eq. (1) is important because matrices do not commute and ϕ is a 2 x 2 matrix. The energy eigenvalue of Eq. (1) is rigorously positive, never negative. The complex conjugate of the adjoint matrix of the fermion spinor is referred to as the "adjoint spinor" of the fermion equation, and is defined by:

$$\phi^+ = \begin{bmatrix} \phi_1^{R*} & \phi_1^{L*} \\ \phi_2^{R*} & \phi_2^{L*} \end{bmatrix}. \quad -(14)$$

The adjoint equation of Eq. (1) is defined as:

$$-i\hbar\, \partial_\mu \phi^+ \sigma^\mu = mc\, \sigma^1 \phi^+ \quad -(15)$$

where the complex conjugate of $i\hbar$ has been used. These equations have well known counterparts in the Dirac theory {1 - 10, 13} but in that theory the 4 x 4 gamma matrices are used and the definition of the adjoint spinor is more complicated.

The probability four-current of the fermion equation is defined as:

$$j^\mu = \frac{1}{2}\mathrm{Tr}\left(\phi\sigma^\mu\phi^+ + \phi^+\sigma^\mu\phi\right) \quad -(16)$$

and its Born probability is:

$$j^0 = \phi_1^R\phi_1^{R*} + \phi_2^R\phi_2^{R*} + \phi_1^L\phi_1^{L*} + \phi_2^L\phi_2^{L*} \quad -(17)$$

which is rigorously positive as required of a probability. It is the same as the Born probability of the chiral representation {1 - 10, 13} of the Dirac equation. In the latter the four current is defined as:

$$j_D^\mu = \overline{\phi}_D\gamma^\mu\phi_D \quad -(18)$$

and the adjoint Dirac spinor is a four entry row vector defined by:

$$\overline{\phi}_D = \phi_D^+\gamma^0. \quad -(19)$$

It is shown as follows that the probability four-current of the fermion equation is conserved:

$$\partial_\mu j^\mu = 0. \quad -(20)$$

To prove this result multiply both sides of Eq. (1) from the right with ϕ^+:

$$i\hbar\partial_\mu\phi\sigma^\mu\phi^+ = mc\sigma^1\phi\phi^+. \quad -(21)$$

Multiply both sides of Eq. (15) from the right with ϕ

$$-i\hbar\partial_\mu\phi^+\sigma^\mu\phi = mc\sigma^1\phi^+\phi \quad -(22)$$

and subtract Eq. (22) form Eq. (21):

$$i\hbar\partial_\mu\left(\phi\sigma^\mu\phi^+ + \phi^+\sigma^\mu\phi\right) = mc\sigma^1\left(\phi\phi^+ - \phi^+\phi\right) \quad -(23)$$

By definition:

$$\phi\phi^+ - \phi^+\phi = \begin{bmatrix}\phi_1^R & \phi_2^R \\ \phi_1^L & \phi_2^L\end{bmatrix}\begin{bmatrix}\phi_1^{R*} & \phi_1^{L*} \\ \phi_2^{R*} & \phi_2^{L*}\end{bmatrix} - \begin{bmatrix}\phi_1^{R*} & \phi_1^{L*} \\ \phi_2^{R*} & \phi_2^{L*}\end{bmatrix}\begin{bmatrix}\phi_1^R & \phi_2^R \\ \phi_1^L & \phi_2^L\end{bmatrix} \quad -(24)$$

so

$$\mathrm{Trace}\left(\phi\phi^+ - \phi^+\phi\right) = 0. \quad -(25).$$

Therefore:

$$\mathrm{Trace}\left(\partial_\mu\left(\phi\sigma^\mu\phi^+ + \phi^+\sigma^\mu\phi\right)\right) = 0 \quad -(26)$$

and

$$\partial_\mu j^\mu = 0 \quad -(27)$$

Q. E. D.

The fermion equation (1) may be expanded into two simultaneous equations:

$$\left(E + c\underline{\sigma}\cdot\underline{p}\right)\phi^L = mc^2\phi^R \quad -(28)$$

$$\left(E - c\underline{\sigma}\cdot\underline{p}\right)\phi^R = mc^2\phi^L \quad -(29)$$

in which E and p are the operators of quantum mechanics:

$$E = i\hbar \frac{\partial}{\partial t}, \quad \underline{p} = -i\hbar \underline{\nabla} \qquad -(30)$$

Eqs. (28) and (29) may be developed as:

$$(E - c\underline{\sigma} \cdot \underline{p})(E + c\underline{\sigma} \cdot \underline{p})\phi^L = m^2 c^4 \phi^L \qquad -(31)$$

$$(E + c\underline{\sigma} \cdot \underline{p})(E - c\underline{\sigma} \cdot \underline{p})\phi^R = m^2 c^4 \phi^R \qquad -(32)$$

from which there emerge equations such as:

$$\left(E^2 - c^2 \underline{\sigma} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{p}\right) \phi^R = m^2 c^4 \phi^R \qquad -(33)$$

Using the quantum postulates this becomes the wave equation:

$$\left(\square + \left(\frac{mc}{\hbar}\right)^2 \right) \phi^R = 0 \qquad -(34)$$

and it becomes clear that the fermion equation is a factorization of the EEC wave equation:

$$\left(\square + \left(\frac{mc}{\hbar}\right)^2 \right) \phi = 0 \qquad -(35)$$

whose eigenfunction is the tetrad (ϕ).

Therefore the fermion equation is obtained from the tetrad postulate and Cartan geometry. The tetrad is defined by:

$$\begin{bmatrix} V^R \\ V^L \end{bmatrix} = \begin{bmatrix} \phi_1^R & \phi_2^R \\ \phi_1^L & \phi_2^L \end{bmatrix} \begin{bmatrix} V^1 \\ V^2 \end{bmatrix} \qquad -(36)$$

i.e. as a matrix relating two column vectors.

The parity operator P acts on the fermion spinor as follows:

$$\underline{P}\psi = \begin{bmatrix} \psi_1^L & \psi_2^L \\ \psi_1^R & \psi_2^R \end{bmatrix} \quad -(37)$$

and the anti fermion is obtained straightforwardly from the fermion equation by operating on each term with P as follows:

$$\underline{P}(E) = E, \ \underline{P}(\underline{p}) = -\underline{p}, \ \underline{P}\begin{bmatrix} \psi_1^R & \psi_2^R \\ \psi_1^L & \psi_2^L \end{bmatrix} = \begin{bmatrix} \psi_1^L & \psi_2^L \\ \psi_1^R & \psi_2^R \end{bmatrix}. \quad -(38)$$

Note carefully that the eigenstates of energy are always positive, both in the fermion and anti fermion equations. The anti fermion is obtained from the fermion by reversing helicity:

$$\underline{P}(\underline{\sigma}\cdot\underline{p}) = -\underline{\sigma}\cdot\underline{p} \quad -(39)$$

and has opposite parity to the fermion, the same mass as the fermion, and the opposite electric charge. The static fermion is indistinguishable from the static anti fermion {13}. So CPT symmetry is conserved as follows form fermion to anti fermion:

$$C\underline{P}T \rightarrow (-C)(-\underline{P}) \quad -(40)$$

where C is the charge conjugation operator and T the motion reversal operator. Note carefully that there is no negative energy anywhere in the analysis.

The pair of simultaneous equations (28) and (29) can be written as:

$$(E - c\underline{\sigma}\cdot\underline{p})(E + c\underline{\sigma}\cdot\underline{p})\phi^L = m^2c^4\phi^L \quad -(41)$$

an equation which can be re arranged as:

$$(E^2 - m^2c^4)\phi^L = c^2\,\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p}\,\phi^L. \quad -(\cancel{35}\ 42)$$

and factorized to give:

$$(E - mc^2)(E + mc^2)\phi^L = c^2\,\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p}\,\phi^L. \quad -(\cancel{36}\ 43)$$

If $\underline{p}$ is real valued, Pauli algebra means that:

$$\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p} = p^2 \quad -(\cancel{37}\ 44)$$

so if E and $\underline{p}$ are regarded as functions, not operators, Eq. (~~38~~ 43) becomes the Einstein energy equation:

$$E^2 - m^2c^4 = c^2p^2 \quad -(\cancel{38}\ 45)$$

multiplied by ϕ^L on both sides. It si well known {1 - 10} that the Einstein energy equation is a way of writing the relativistic energy and momentum:

$$E = \gamma mc^2, \quad -(\cancel{39}\ 46)$$

$$\underline{p} = \gamma m\underline{v}. \quad -(\cancel{40}\ 47)$$

Realizing this, Eq. (~~36~~ 43) can be linearized as follows. First, express it as:

$$(E - mc^2)\phi^L = \frac{c^2\,\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{p}}{E + mc^2}\phi^L \quad -(48)$$

and approximate the total energy:

$$E = \gamma mc^2 \quad -(\cancel{42}\ 49)$$

by the rest energy:

$$E \sim mc^2 \qquad (\cancel{43})\ 50$$

then Eq. (48) becomes:

$$\left(E - mc^2\right)\phi^L = \frac{1}{2m}\,\underline{\sigma}\cdot\underline{p}\;\underline{\sigma}\cdot\underline{p}\;\phi^L \qquad (\cancel{43})\ 51$$

which has the structure of the free particle Schroedinger equation:

$$E_{NR}\,\phi^L = \frac{p^2}{2m}\,\phi^L \qquad (\cancel{44})\ 52$$

in which the non relativistic limit of the kinetic energy is defined in the limit v << c by:

$$E_{NR} = E - mc^2 = (\gamma - 1)\,mc^2 \rightarrow \frac{p^2}{2m}. \qquad (\cancel{45})\ 53$$

So the fermion equation reduces correctly to the non relativistic Schroedinger equation for the free particle, Q. E. D.

The great importance of the fermion equation to chemical physics emerges from the fact that it can describe the phenomena for which the Dirac equation is justly famous while at the same time eliminating the problem of negative energy as we have just seen. In quantum field theory this leads to a free fermion quantum field theory. This aim is very difficult to achieve {13} in the standard quantum field theory because methods have to be devised to deal with the negative energy. The latter is due simply to Dirac's choice of gamma matrices.

The way in which the fermion equation describes the g factor of the electron, the Landé factor, the Thomas factor and Darwin term is described in the following section.

5.2 INTERACTION OF THE ECE FERMION WITH THE ELECTROMAGNETIC FIELD.

The simplest and most powerful way of describing this interaction for each polarization index a of ECE theory is through the minimal prescription

$$p^\mu \rightarrow p^\mu - eA^\mu \quad - (\cancel{46}\ 54)$$

where a negative sign is used {13} because the charge on the electron is -e. Eq. ($\cancel{46}$ 54) can be written as:

$$E \rightarrow E - e\phi \quad - (\cancel{47}\ 55)$$

and:

$$\underline{p} \rightarrow \underline{p} - e\underline{A} \quad - (\cancel{48}\ 56)$$

Using Eqs. ($\cancel{47}$ 55) and ($\cancel{48}$ 56) in the Einstein energy equation ($\cancel{38}$ 45) gives:

$$(E - e\phi)^2 = c^2(\underline{p} - e\underline{A})^2 + m^2c^4 \quad - (\cancel{49}\ 57)$$

which can be factorized as follows:

$$(E - e\phi - mc^2)(E - e\phi + mc^2) = c^2(\underline{p} - e\underline{A})^2 \quad - (\cancel{50}\ 58)$$

and written as:

$$E = mc^2 + e\phi + c^2(\underline{p} - e\underline{A})(E - e\phi + mc^2)^{-1}(\underline{p} - e\underline{A}) \quad - (59)$$

in a form ready for quantization. The latter is carried out with:

$$\underline{p} \rightarrow -i\hbar\underline{\nabla} \quad - (\cancel{52}\ 60)$$

and produces many well known effects and new effects of spin robit coupling described in papers of ECE theory such as UFT 248 ff on www.aias.us.

The most famous result of the Dirac equation, and its improved version, the ECE fermion equation, is electron spin resonance, which depends on the use of the Pauli matrices as is very well known. In this section the various intricacies of this famous derivation are explained systematically. Electron spin resonance occurs in the presence of a static magnetic field, so the scalar potential can be omitted from consideration leaving hamiltonians such as:

$$H_2 \phi = \frac{1}{2m}\left(\underline{\sigma}\cdot\left(-i\hbar\underline{\nabla} - e\underline{A}\right)\underline{\sigma}\cdot\left(-i\hbar\underline{\nabla} - e\underline{A}\right)\right)\phi \quad -\left(\overset{61}{\cancel{53}}\right)$$

Note carefully that the operator $\underline{\nabla}$ acts on the wave function, which is denoted ϕ for ease of notation. The following type of Pauli algebra:

$$\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{W} = \underline{\nabla}\cdot\underline{W} + i\underline{\sigma}\cdot\underline{\nabla}\times\underline{W} \quad -\left(\overset{62}{\cancel{54}}\right)$$

leads to:

$$H_2\phi = \frac{1}{2m}\Big(ie\hbar\left(\underline{\nabla}\cdot\underline{A} + i\underline{\sigma}\cdot\underline{\nabla}\times\underline{A}\right) - \hbar^2\left(\nabla^2 + i\underline{\sigma}\cdot\underline{\nabla}\times\underline{\nabla}\right)$$
$$+ e^2\left(A^2 + i\underline{\sigma}\cdot\underline{A}\times\underline{A}\right) + ie\hbar\left(\underline{A}\cdot\underline{\nabla} + i\underline{\sigma}\cdot\left(\underline{A}\times\underline{\nabla}\right)\right)\Big)\phi \quad -\left(\overset{63}{\cancel{55}}\right)$$

Assuming that $\underline{A}$ is real valued, then:

$$\underline{A}\times\underline{A} = \underline{0}. \quad -\left(\overset{64}{\cancel{56}}\right)$$

Also:

$$\underline{\nabla}\times\underline{\nabla} = \underline{0} \quad -\left(\overset{65}{\cancel{57}}\right)$$

so:

$$H_2\phi = \frac{1}{2m}\Big(-\hbar^2\nabla^2\phi + e^2A^2\phi + ie\hbar\,\underline{\nabla}\cdot(\underline{A}\phi) - e\hbar\,\underline{\sigma}\cdot\underline{\nabla}\times(\underline{A}\phi) + ie\hbar\,\underline{A}\cdot\underline{\nabla}\phi - e\hbar\,\underline{\sigma}\cdot\underline{A}\times\underline{\nabla}\phi\Big) \qquad -(66\ \cancel{58})$$

It can be seen that the fermion equation produces many effects in general, all of which are experimentally observable. So it is a very powerful result of geometry and ECE unified field theory. Gravitational effects can be considered through the appropriate minimal prescription as in papers such as UFT 248 ff. Many of these effects remain to be observed.

Electron spin resonance is given by the term:

$$H_2\phi = -\frac{e\hbar}{2m}\,\underline{\sigma}\cdot\left(\underline{\nabla}\times(\underline{A}\phi) + \underline{A}\times\underline{\nabla}\phi\right) + \dots$$

$$= -\frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B} + \dots \qquad -(67\ \cancel{59})$$

where the standard relation between B and A has been used to illustrate the argument:

$$\underline{B} = \underline{\nabla}\times\underline{A} \qquad -(68)$$

In the rigorous ECE theory the spin connection enters into the analysis. A vast new subject area of chemical physics emerges because electron spin resonance (ESR) and nuclear magnetic resonance (NMR) dominate the subjects of chemical physics and analytical chemistry.

Use of a complex valued potential such as that in an electromagnetic field rather than a static magnetic field produces many more effects through the equation:

$$\Big((E-e\phi)+c\underline{\sigma}\cdot(\underline{p}-e\underline{A})\Big)\Big((E-e\phi)-c\underline{\sigma}\cdot(\underline{p}-e\underline{A}^*)\Big)\phi^R$$

$$= m^2c^4\phi^R, \qquad -(69)$$

$$\phi := \phi^R,$$

i.e.

$$(E-e\phi-mc^2)(E-e\phi+mc^2)\phi = c^2\underline{\sigma}\cdot(\underline{p}-e\underline{A})\,\underline{\sigma}\cdot(\underline{p}-e\underline{A}^*)\phi + ec(E-e\phi)\,\underline{\sigma}\cdot(\underline{A}^*-\underline{A})\phi \quad -(69b)$$

where * denotes "complex conjugate". Eq. (69b) can be linearized as:

$$(E-e\phi-mc^2)\phi = \left(\frac{c^2\underline{\sigma}\cdot(\underline{p}-e\underline{A})\,\underline{\sigma}\cdot(\underline{p}-e\underline{A}^*)}{E-e\phi+mc^2}\right)\phi + \left(\frac{ec(E-e\phi)}{E-e\phi+mc^2}\right)\underline{\sigma}\cdot(\underline{A}^*-\underline{A})\phi \quad -(\cancel{62})(70)$$

and re arranged as follows:

$$E\phi = (e\phi+mc^2)\phi + \frac{1}{2m}\underline{\sigma}\cdot(\underline{p}-e\underline{A})\left(1-\frac{e\phi}{2mc^2}\right)^{-1}\underline{\sigma}\cdot(\underline{p}-e\underline{A}^*)\phi \quad \cancel{(63)}$$
$$+\frac{e}{2mc}(mc^2-e\phi)\left(1-\frac{e\phi}{2mc^2}\right)^{-1}\underline{\sigma}\cdot(\underline{A}^*-\underline{A})\phi \quad -(71)$$

In the approximation:

$$e\phi \ll mc^2. \quad -(\cancel{64}\ 72)$$

Eq. ($\cancel{63}$ 71) gives:

$$E\phi = (H_1+H_2+H_3)\phi \quad -(\cancel{65}\ 73)$$

where the three hamiltonians are defined as follows:

$$H_1 = e\phi+mc^2, \quad -(\cancel{66}\ 74)$$

$$H_2 = \frac{1}{2m}\underline{\sigma}\cdot(\underline{p}-e\underline{A})\left(1+\frac{e\phi}{2mc^2}\right)\underline{\sigma}\cdot(\underline{p}-e\underline{A}^*), \quad -(\cancel{67}\ 75)$$

$$H_3 = \frac{1}{2}ec\left(1+\frac{e\phi}{2mc^2}\right)\underline{\sigma}\cdot(\underline{A}^*-\underline{A}), \quad -(\cancel{68}\ 76)$$

leading to many new fermion resonance effects using the electromagnetic field rather than the static magnetic field.

For example the H_2 hamiltonian can be developed as:

$$
\begin{aligned}
H_{21}\phi = \frac{1}{2m}\Big(& ie\hbar\left(\underline{\nabla}\cdot\underline{A}^* + i\underline{\sigma}\cdot\underline{\nabla}\times\underline{A}^*\right) \\
& -\hbar^2\left(\nabla^2 + i\underline{\sigma}\cdot\underline{\nabla}\times\underline{\nabla}\right) \\
& + e^2\left(\underline{A}\cdot\underline{A}^* + i\underline{\sigma}\cdot\underline{A}\times\underline{A}^*\right) \\
& + ie\hbar\left(\underline{A}\cdot\underline{\nabla} + i\underline{\sigma}\cdot\left(\underline{A}\times\underline{\nabla}\right)\right)\Big)\phi \qquad -(\cancel{69}\ 77)
\end{aligned}
$$

an equation that can be written as:

$$
\begin{aligned}
H_{21}\phi = \frac{1}{2m}\Big(& ie^2\underline{\sigma}\cdot\underline{A}\times\underline{A}^*\phi - e\hbar\,\underline{\sigma}\cdot\underline{A}\times\underline{\nabla}\phi \\
& - e\hbar\,\underline{\sigma}\cdot\underline{\nabla}\phi\times\underline{A}^* - e\hbar\,\underline{\sigma}\cdot\left(\underline{\nabla}\times\underline{A}^*\right)\phi + \ldots\Big) \qquad -(78)
\end{aligned}
$$

giving four out of many terms that can give novel fermion resonance effects. Using for the sake of argument:

$$\underline{B}^* = \underline{\nabla}\times\underline{A}^* \qquad -(79)$$

then the hamiltonian reduces to:

$$H_{211} = -\frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B}^{*} \quad -(\cancel{72}\ 80)$$

and a term due to the conjugate product of the electromagnetic field:

$$H_{212} = i\frac{e^{2}}{2m}\,\underline{\sigma}\cdot\underline{A}\times\underline{A}^{*} \quad -(81\ \cancel{73})$$

which defines the B(3) field introduced in previous chapters:

$$\underline{B}^{(3)*} = -ig\,\underline{A}\times\underline{A}^{*} = -ig\,\underline{A}^{(1)}\times\underline{A}^{(2)} \quad -(82\ \cancel{74})$$

Eq. (81 ~~73~~) is the hamiltonian that defines radiatively induced fermion resonance (RFR), extensively discussed elsewhere {1 - 10} but derived here in a rigorous way from the fermion equation or chiral representation of the Dirac equation.

$$H_{211} = -\frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B}^{*} \quad -(80)$$

and a term due to the conjugate product of the electromagnetic field:

$$H_{212} = \frac{ie^2}{2m}\,\underline{\sigma}\cdot\underline{A}\times\underline{A}^{*} \quad -(81)$$

which defines the B(3) field introduced in previous chapters:

$$\underline{B}^{(3)*} = -ig\,\underline{A}\times\underline{A}^{*} = -ig\,\underline{A}^{(1)}\times\underline{A}^{(2)} \quad -(82)$$

Eq. (81) is the hamiltonian that defines radiatively induced fermion resonance (RFR), extensively discussed elsewhere {1 - 10} but derived here in a rigorous way from the fermion equation or chiral representation of the Dirac equation.

Spin orbit coupling and the Thomas factor can be derived from the H_{22} hamiltonian defined as follows:

$$-H_{22}\phi = \frac{e}{4m^2c^2}\left(\underline{\sigma}\cdot(\underline{p}-e\underline{A})\,\phi\;\underline{\sigma}\cdot(\underline{p}-e\underline{A})\right)\phi \quad -(83)$$

This hamiltonian has its origins in the following equation:

$$E\phi = \left(mc^2 + e\phi + c^2(\underline{p}-e\underline{A})(E-e\phi+mc^2)^{-1}\cdot(\underline{p}-e\underline{A})\right)\phi \quad -(84)$$

in the approximation:

$$E = \gamma mc^2 \sim mc^2. \quad -(85)$$

In this approximation. Eq. (84) becomes:

$$E\phi = \left(mc^2 + e\phi + \frac{1}{2m}\left(\underline{p} - e\underline{A}\right)\left(1 - \frac{e\phi}{2mc^2}\right)^{-1} \cdot \left(\underline{p} - e\underline{A}\right)\right)\phi \quad -(86)$$

and in the approximation:

$$e\phi << 2mc^2 \quad -(87)$$

the H_{22} hamiltonian is recovered as the last term on the right hand side.

In the derivation of the spin orbit coupling term several assumptions are made, but not always made clear in textbooks. The vector potential $\underline{A}$ is not considered in the derivation of spin orbit interaction, so that only electric field effects are considered. Therefore the relevant hamiltonian reduces to:

$$H_{22}\phi = \frac{e}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\phi\,\underline{\sigma}\cdot\underline{p}\,\phi. \quad -(88)$$

It is assumed that the first $\underline{p}$ is the operator:

$$\underline{p} = -i\hbar\underline{\nabla} \quad -(89)$$

but that the second $\underline{p}$ is a function. This point is rarely if ever made clear in the textbooks. This assumption can be justified only on the grounds that it seems to succeed in describing the experimental data. When this assumption is made Eq. (88) reduces to:

$$H_{22}\phi = -\frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\,\phi\,\underline{\sigma}\cdot\underline{p}\,\phi \quad -(90)$$

The $\underline{\nabla}$ operator acts on $\phi\,\underline{\sigma}\cdot\underline{p}\,\psi$, so by the Leibnitz Theorem :

$$\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{p}\,\psi\right) = \underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\right)\phi\psi + \underline{\sigma}\cdot\underline{p}\;\underline{\nabla}\left(\phi\psi\right) \quad -(91)$$

and the spin orbit interaction term emerges from:

$$H_{22}\psi = -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\left(\phi\psi\right)\underline{\sigma}\cdot\underline{p}\right). \quad -(92)$$

In this equation the Leibnitz Theorem asserts that:

$$\underline{\nabla}\left(\phi\psi\right) = \left(\underline{\nabla}\phi\right)\psi + \phi\left(\underline{\nabla}\psi\right) \quad -(93)$$

so the spin orbit interaction term is:

$$H_{22}\psi = -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\phi\,\underline{\sigma}\cdot\underline{p}\right)\psi \quad -(94)$$
$$+ \;\ldots$$

It is seen Eq. (94) is only one out of many possible effects that emerge from the fermion equation and which should be systematically investigated experimentally.

In the development of the spin orbit term the obsolete standard physics is used as follows:

$$\underline{E} = -\underline{\nabla}\phi \quad -(95)$$

so the spin orbit hamiltonian becomes:

$$H_{22}\psi = -\frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p}\,\psi. \quad -(96)$$

Now use the Pauli algebra:

$$\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p} = \underline{E}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{E}\times\underline{p} \quad -(97)$$

so the real part of the hamiltonian from these equations becomes:

$$H_{22}\phi = \frac{e\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\times\underline{p}\,\phi \quad -(98)$$

in which $\underline{p}$ is regarded as a function, and not an operator. If this second $\underline{p}$ is regarded as an operator, then new effects appear.

Note carefully that in the derivation of the Zeeman effect, ESR, NMR and the g factor of the electron, both $\underline{p}$'s are regarded as operators, but in the derivation of spin orbit interaction, only the first $\underline{p}$ is regarded as an operator, the second $\underline{p}$ is regarded as a function.

Finally in the standard derivation of spin orbit interaction, the Coulomb potential of electrostatics is chosen for the scalar potential:

$$\phi = -\frac{e}{4\pi r\epsilon_0} \quad -(99)$$

so the electric field strength is:

$$\underline{E} = -\underline{\nabla}\phi = -\frac{e}{4\pi\epsilon_0 r^3}\,\underline{r}\,. \quad -(100)$$

The relevant spin orbit hamiltonian becomes:

$$H_{22}\phi = -\frac{e^2\hbar}{8\pi c^2\epsilon_0 m^2 r^3}\,\underline{\sigma}\cdot\underline{r}\times\underline{p}\,\phi \quad -(101)$$

in which the orbital angular momentum is:

$$\underline{L} = \underline{r}\times\underline{p}\,. \quad -(102)$$

Therefore the spin orbit hamiltonian is:

$$H_{22}\phi = -\frac{e^2\hbar}{8\pi c^2\epsilon_0 m^2 r^3}\,\underline{\sigma}\cdot\underline{L}\,\phi \quad -(103)$$

In the description of atomic and molecular spectra, the spin angular momentum operator is defined as:

$$\underline{S} = \frac{1}{2}\hbar\,\underline{\sigma} \quad -(104)$$

and the orbital angular momentum also becomes an operator. So:

$$H_{22}\phi = -\gamma\,\underline{S}\cdot\underline{L}\,\phi = -\frac{e^2}{8\pi c^2\epsilon_0 m^2 r^3}\,\underline{S}\cdot\underline{L}\,\phi \quad -(105)$$

and the Thomas factor of two is contained in Eq. (105) as part of the denominator. The derivation of the Thomas factor is one of the strengths of the fermion equation, which as we have argued does not suffer from the negative energy problem of the Dirac equation.

Consider again the H_{22} hamiltonian:

$$H_{22}\phi = \frac{e}{4m^2c^2}\,\underline{\sigma}\cdot\left(\underline{p}-e\underline{A}\right)\phi\,\underline{\sigma}\cdot\left(\underline{p}-e\underline{A}\right)\phi \quad -(106)$$

and assume that:

$$\underline{A} = \underline{0} \quad -(107)$$

so:

$$H_{22}\phi = \frac{e}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\phi\,\underline{\sigma}\cdot\underline{p}\,\phi. \quad -(108)$$

In the derivation of spin orbit coupling and the Thomas factor the first $\underline{p}$ is regarded as an operator and the second $\underline{p}$ as a function. In the derivation of the Darwin term both $\underline{p}$'s are regarded as operators, defined by:

$$-i\hbar\underline{\nabla}\phi = \underline{p}\phi \quad -(109)$$

with expectation value:

$$\langle \underline{p} \rangle = \int \phi^* \underline{p} \phi \, d\tau \quad -(110)$$

Therefore the Darwin term is obtained from:

$$H_{22}\phi = \frac{e}{4m^2c^2}\left(\underline{\sigma}\cdot(-i\hbar\underline{\nabla})\phi\,\underline{\sigma}\cdot(-i\hbar\underline{\nabla})\right)\phi \quad -(111)$$

and is a quantum mechanical phenomenon with no classical counterpart.

From Eq. (111):

$$H_{22}\phi = -\frac{e\hbar^2}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\,\phi\,\underline{\sigma}\cdot\underline{\nabla}\right)\phi \quad -(112)$$

and the fist del operator $\underline{\nabla}$ operates on all that follows it, so:

$$H_{22}\phi = -\frac{e\hbar^2}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{\nabla}\phi\right). \quad -(113)$$

The Leibnitz Theorem is used as follows:

$$\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{\nabla}\phi\right) = \left(\underline{\nabla}\phi\right)\left(\underline{\sigma}\cdot\underline{\nabla}\phi\right) + \phi\,\underline{\nabla}\left(\underline{\sigma}\cdot\underline{\nabla}\phi\right). \quad -(114)$$

Therefore:

$$H_{22}\phi = -\frac{e\hbar^2}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\phi\,\underline{\sigma}\cdot\underline{\nabla}\phi + \underline{\sigma}\cdot\phi\,\underline{\nabla}\left(\underline{\sigma}\cdot\underline{\nabla}\phi\right)\right) \quad -(115)$$

Usually the Darwin term is considered to be:

$$H_{Darwin}\,\phi = -\frac{e\hbar^2}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\phi\,\underline{\sigma}\cdot\underline{\nabla}\phi \quad -(116)$$

and the second term in Eq. (115) can be developed as:

$$\underline{\sigma}\cdot\underline{\nabla}\left(\underline{\sigma}\cdot\underline{\nabla}\phi\right) = \left(\underline{\sigma}\cdot\underline{\nabla}\right)\left(\underline{\sigma}\cdot\underline{\nabla}\right)\phi \quad -(117)$$

so:

$$H_{22}\phi = -\frac{e\hbar^2}{4m^2c^2}\left(\underline{\nabla}\phi\cdot\underline{\nabla}\phi + \phi\,\nabla^2\phi\right) \quad -(118)$$

5.3 NEW ELECTRON SPIN ORBIT EFFECTS FROM THE FERMION EQUATION

On the classical standard level consider the kinetic energy of an electron of mass m and linear momentum $\underline{p}$:

$$H = \frac{p^2}{2m} \quad -(119)$$

and use the minimal prescription (56) to describe the interaction of an electron with a vector potential $\underline{A}$. The interaction hamiltonian is defined by:

$$\bar{H} = \frac{1}{2m}\left(\underline{p} - e\underline{A}\right)\cdot\left(\underline{p} - e\underline{A}\right)$$

$$= \frac{p^2}{2m} - \frac{e}{2m}\left(\underline{p}\cdot\underline{A} + \underline{A}\cdot\underline{p}\right) + \frac{e^2A^2}{2m} \quad -(120)$$

As discussed in earlier chapters the vector potential can be defined by:

$$\underline{A} = \frac{1}{2}\underline{B} \times \underline{r} . \quad -(121)$$

Now consider the following tem of the hamiltonian:

$$H_1 = -\frac{e}{2m}\left(\underline{p}\cdot\underline{A} + \underline{A}\cdot\underline{p}\right) = -\frac{e}{4m}\left(\underline{p}\cdot\underline{B}\times\underline{r} + \underline{B}\times\underline{r}\cdot\underline{p}\right) \quad -(122)$$

where the orbital angular momentum can be defined as follows:

$$\underline{p}\cdot\left(\underline{B}\times\underline{r}\right) = \underline{B}\cdot\underline{r}\times\underline{p} = \underline{B}\cdot\underline{L} . \quad -(123)$$

This analysis gives the well known hamiltonian for the interaction of a magnetic dipole moment with the magnetic flux density:

$$H_1 = -\frac{e}{2m}\underline{L}\cdot\underline{B} = -\underline{m}_D\cdot\underline{B} . \quad -(124)$$

The classical hamiltonian responsible for Eq. (124) is:

$$H_1 = -\frac{e}{2m}\left(\underline{p}\cdot\underline{A} + \underline{A}\cdot\underline{p}\right) \quad -(125)$$

which can be written in the SU(2) basis as:

$$H_1 = -\frac{e}{2m}\left(\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A} + \underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p}\right) . \quad -(126)$$

Using Pauli algebra:

$$\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A} = \underline{p}\cdot\underline{A} + i\,\underline{\sigma}\cdot\underline{p}\times\underline{A} \quad -(127)$$

$$\underline{\sigma} \cdot \underline{A}\, \underline{\sigma} \cdot \underline{p} = \underline{A} \cdot \underline{p} + i\underline{\sigma} \cdot \underline{A} \times \underline{p} \quad -(128)$$

and the same result is obtained because:

$$i\underline{\sigma} \cdot (\underline{p} \times \underline{A} + \underline{A} \times \underline{p}) = 0. \quad -(129)$$

However, as discussed for example by H. Merzbacher in "Quantum Mechanics" (Wiley, 1970):

$$\underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \left(\underline{r} \cdot \underline{p} + i\underline{\sigma} \cdot \underline{L} \right) \quad -(130)$$

$$\underline{\sigma} \cdot \underline{A} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \left(\underline{r} \cdot \underline{A} + i\underline{\sigma} \cdot \underline{r} \times \underline{A} \right). \quad -(131)$$

in which:

$$\frac{1}{r^2} \underline{\sigma} \cdot \underline{r}\, \underline{\sigma} \cdot \underline{r} = 1. \quad -(132)$$

Therefore:

$$\underline{\sigma} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{A} = \frac{1}{r^2} \Big(\underline{r} \cdot \underline{p}\, \underline{r} \cdot \underline{A} + i\underline{\sigma} \cdot \underline{L}\, \underline{r} \cdot \underline{A} + i\underline{r} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{r} \times \underline{A} - \underline{\sigma} \cdot \underline{L}\, \underline{\sigma} \cdot \underline{r} \times \underline{A} \Big). \quad -(133)$$

From comparison of the real and imaginary parts of Eqs (127) and (133):

$$\underline{p} \cdot \underline{A} = \frac{1}{r^2} \left(\underline{r} \cdot \underline{p}\, \underline{r} \cdot \underline{A} - \underline{\sigma} \cdot \underline{L}\, \underline{\sigma} \cdot \underline{r} \times \underline{A} \right) \quad -(134)$$

in which:

$$\underline{\sigma} \cdot \underline{p} \times \underline{A} = \underline{\sigma} \cdot \underline{L}\, \underline{r} \cdot \underline{A} + \underline{r} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{r} \times \underline{A} \quad -(135)$$

$$\underline{r} \cdot \underline{A} = \frac{1}{2} \underline{r} \cdot \underline{B} \times \underline{r} = \frac{1}{2} \underline{B} \cdot \underline{r} \times \underline{r} = 0 . \quad -(136)$$

Therefore we obtain the important identities:

$$\underline{p} \cdot \underline{A} = -\frac{1}{r^2} \underline{\sigma} \cdot \underline{L} \, \underline{\sigma} \cdot \underline{r} \times \underline{A}, \quad -(137)$$

$$\underline{\sigma} \cdot \underline{p} \times \underline{A} = \underline{r} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{r} \times \underline{A} . \quad -(138)$$

The hamiltonian (125) can therefore be written as:

$$H_1 = -\frac{e}{m} \underline{p} \cdot \underline{A} = \frac{e}{mr^2} \underline{\sigma} \cdot \underline{L} \, \underline{\sigma} \cdot \underline{r} \times \underline{A} = -\underline{m}_B \cdot \underline{B} . \quad -(139)$$

Finally use eqs. (121) and (139) to find:

$$H_1 = \frac{e}{2m} \underline{\sigma} \cdot \underline{L} \left(\underline{\sigma} \cdot \underline{B} - \frac{\underline{\sigma} \cdot \underline{r}}{r^2} \underline{B} \cdot \underline{r} \right) \quad -(140)$$

$$= -\underline{m}_D \cdot \underline{B}$$

It can be seen that the well known hamiltonian responsible for the Zeeman effect has been developed into a hamiltonian that gives electron spin resonance of a new type, a resonance that arises from the interaction of the Pauli matrix with the magnetic field as in Eq. (140). If the magnetic field is aligned in the Z axis then:

$$\sigma_Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad -(141)$$

and the electron spin orbit (ESOR) resonance frequency is:

$$\omega = \frac{eB}{m\hbar} \underline{\sigma} \cdot \underline{L} \quad -(142)$$

This compares with the usual ESR frequency:

$$\omega = \frac{eB}{m} \quad -(143)$$

from the hamiltonian derived already in this chapter from the fermion equation.

The ESOR hamiltonian contains a novel spin orbit coupling when quantized:

$$H_1 \phi = \frac{e}{2m} \underline{\sigma} \cdot \underline{B} \; \underline{\sigma} \cdot \underline{L} \, \phi . \quad -(144)$$

Defining the spin angular momentum as:

$$\underline{S} = \frac{1}{2} \hbar \underline{\sigma} \quad -(145)$$

gives {1 - 10}:

$$\underline{L} \cdot \underline{S} \phi = \frac{1}{2} \left(J^2 - L^2 - S^2 \right) \phi$$
$$= \frac{1}{2} \hbar^2 \left(J(J+1) - L(L+1) - S(S+1) \right) \phi \quad -(146)$$

so the energy levels of the ESOR hamiltonian operator are:

$$E = \frac{e\hbar}{2m} \left(J(J+1) - L(L+1) - S(S+1) \right) \underline{\sigma} \cdot \underline{B} \quad -(147)$$

giving the ESOR frequency:

$$\omega = \frac{e\hbar}{2m} \left(J(J+1) - L(L+1) - S(S+1) \right) \quad -(148)$$

in which the total angular momentum J is defined by the Clebsch Gordan series:

$$J = L + S, L + S - 1, \ldots, |L - S| \quad -(149)$$

Eq. (144) was first derived in UFT 249 and is different from the well known ESR spin hamiltonian:

$$H_{ESR} = -\frac{e}{2m}\underline{L}\cdot\underline{B} + \lambda\underline{S}\cdot\underline{L} - \frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B} = -g_{spin}\,\underline{\sigma}\cdot\underline{B}. \quad -(150)$$

It was derived using well known Pauli algebra together with the fermion equation and potentially gives rise to many useful spectral effects.

For chemical physicists and analytical chemists therefore the most useful format of the fermion equation is:

$$E\phi = \left(mc^2 + e\phi + \frac{1}{2m}\underline{\sigma}\cdot(\underline{p} - e\underline{A})\left(1 + \frac{e\phi}{2mc^2}\right)\underline{\sigma}\cdot(\underline{p} - e\underline{A})\right)\phi \quad -(151)$$

and a few examples have been given in this chapter of its usefulness. In ECE theory Eq. (151) has been derived from Cartan geometry and by using the minimal prescription. The fermion equation as argued is the chiral Dirac equation without the problem of negative energy, which to chemists was never of much interest. In chemistry the subject is approached as follows. Consider one term of the complete equation (151):

$$H_1\phi = -\frac{e}{2m}\left(\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p} + \underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A}\right)\phi. \quad -(152)$$

By regarding $\underline{\sigma}$ as a function rather than an operator this term can be developed using Pauli algebra as follows:

$$H_1 \phi = -\frac{e}{2m}\left(\underline{A}\cdot\underline{p} + \underline{p}\cdot\underline{A} + i\underline{\sigma}\cdot\left(\underline{A}\times\underline{p} + \underline{p}\times\underline{A}\right)\right) \quad -(153)$$

For a uniform magnetic field:

$$\underline{A} = \frac{1}{2}\underline{B}\times\underline{r} \quad -(154)$$

so:

$$H_1 \phi = -\frac{e}{4m}\left(\underline{B}\times\underline{r}\cdot\underline{p} + \underline{p}\cdot\underline{B}\times\underline{r} + i\underline{\sigma}\cdot\left((\underline{B}\times\underline{r})\times\underline{p} + \underline{p}\times(\underline{B}\times\underline{r})\right)\right)\phi \quad -(155)$$

By regarding $\underline{p}$ as a function:

$$\underline{B}\times\underline{r}\cdot\underline{p} = \underline{B}\cdot\underline{r}\times\underline{p} = \underline{B}\cdot\underline{L} \quad -(156)$$

so the hamiltonian becomes:

$$H_1 \phi = -\frac{e}{2m}\underline{L}\cdot\underline{B}\phi + \left(i\underline{\sigma}\cdot\underline{A}\times\underline{p} + i\underline{\sigma}\cdot\underline{p}\times\underline{A}\right)\phi \quad -(157)$$

At this stage $\underline{p}$ is regarded as an operator so the second term on the right hand side of eq. (157) does not vanish. The use of $\underline{p}$ and $\underline{\sigma}$ as functions or operators is arbitrary, and justified only by the final comparison with experimental data. From Eqs. (157) and (154) the hamiltonian can be written in the format used in chemistry

$$H_1 \phi = \left(-\frac{e}{2m}\underline{L}\cdot\underline{B} - \frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B}\right)\phi \quad -(158)$$
$$= -\frac{e}{2m}\left(\underline{L} + 2\underline{S}\right)\phi$$

The total angular momentum is conserved so Eq. (158) can be written as:

$$H_1 \phi = -\frac{e}{2m} g_L \underline{J} \cdot \underline{B} \phi \quad -(159)$$

where:

$$J = L + S, \ldots, |L - S| \quad -(160)$$

from the Clebsch Godan series.

The conventional spin orbit term emerges as described earlier in this chapter from another term of the hamiltonian:

$$H_{so} \phi = \frac{e}{4mc^2} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \phi \, \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \phi \quad -(161)$$

in which the first $\underline{p}$ is described as an operator but in which the second $\underline{p}$ is a function, giving the spin orbit term:

$$H_{so} \phi = -\frac{ie\hbar}{4m^2c^2} \underline{\sigma} \cdot \underline{\nabla} \phi \, \underline{\sigma} \cdot \underline{p} \phi \quad -(162)$$

So the complete ESR hamiltonian is:

$$H \phi = \left(-\frac{e}{2m} \underline{L} \cdot \underline{B} - \frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B} - \xi \underline{S} \cdot \underline{L} \right) \phi \quad -(163)$$

in which the spin orbit coupling constant is:

$$\xi = \frac{e}{4\pi c^2 \epsilon_0 m^2 r^3} \quad -(164)$$

Finally both S and L are operators, so:

$$\underline{S} \cdot \underline{L}\, \psi = \frac{\hbar^2}{2} \left(J(J+1) - L(L+1) - S(S+1) \right) \psi . \quad -(165)$$

The above is the very well known conventional description of ESR in the language used by chemists, and is a description based in ECE theory on geometry. In ECE theory it can be developed in many ways because it is generally covariant while the obsolete standard description is Lorentz covariant.

However, several new spectroscopies can be developed using a well known Pauli algebra but one which seems never to have been applied to fermion resonance spectroscopies:

$$\underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \left(\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L} \right) \quad -(166)$$

$$\underline{\sigma} \cdot \underline{A} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \left(\underline{r} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{r} \times \underline{A} \right) . \quad -(167)$$

For a uniform magnetic field:

$$\underline{r} \cdot \underline{A} = 0 \quad -(168)$$

so:

$$\underline{p} \cdot \underline{A} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{L}\, \underline{\sigma} \cdot \underline{A} \times \underline{r} \quad -(169)$$

and

$$\underline{\sigma} \cdot \underline{p} \times \underline{A} = \frac{1}{r^2} \underline{r} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{r} \times \underline{A} \quad -(170)$$

as in note 250(7) accompanying UFT 250 on www.aias.us. Using these results it is found that:

$$H_1 \phi = -\frac{e}{2m}\left(\underline{p}\cdot\underline{A} + \underline{A}\cdot\underline{p}\right)\phi$$

$$= -\frac{e}{mr^2}\,\underline{\sigma}\cdot\underline{A}\times\underline{r}\;\underline{\sigma}\cdot\underline{L}\,\phi. \quad -(171)$$

Using Eq. (171) for a uniform magnetic field gives:

$$\underline{A}\times\underline{r} = \frac{1}{2}\left(\underline{B}\times\underline{r}\right)\times\underline{r} = \frac{1}{2}\left(\underline{r}\left(\underline{r}\cdot\underline{B}\right) - r^2\underline{B}\right) \quad -(172)$$

giving a novel spin orbit hamiltonian in the useful form:

$$H_1\phi = \frac{e}{\hbar m}\,\underline{\sigma}\cdot\left(\underline{B} - \frac{\underline{r}}{r^2}\left(\underline{r}\cdot\underline{B}\right)\right)\underline{S}\cdot\underline{L}\,\phi. \quad -(173)$$

Its expectation value is:

$$\langle H_1 \rangle = \frac{e}{\hbar m}\int \phi^* H_1 \phi \, d\tau \quad -(174)$$

with the normalization:

$$\int \phi^* \phi \, d\tau = 1. \quad -(175)$$

Using the result:

$$\underline{S}\cdot\underline{L}\,\phi = \frac{\hbar^2}{2}\left(J(J+1) - L(L+1) - S(S+1)\right)\phi \quad -(176)$$

the energy eigenvalues of the hamiltonian are:

$$E = \frac{e\hbar}{2m}\left(J(J+1) - L(L+1) - S(S+1)\right)\left(\underline{\sigma}\cdot\underline{B} - \int \psi^* \frac{\underline{\sigma}\cdot\underline{r}}{r^2}\,\underline{r}\cdot\underline{B}\,\psi\, d\tau\right) \quad -(177)$$

as in note 250(9) accompanying UFT 250 on www.aias.us.

In spherical polar coordinates:

$$\begin{aligned} X &= r\sin\theta\cos\phi \\ Y &= r\sin\theta\sin\phi \\ Z &= r\cos\theta \end{aligned} \quad -(178)$$

and integration of a function over all space means:

$$\int f\, d\tau = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_0^{\infty} f\, r^2 \sin\theta\, dr\, d\theta\, d\phi. \quad -(179)$$

If the magnetic field is aligned in the Z axis then in Cartesian coordinates:

$$\frac{\underline{\sigma}\cdot\underline{r}}{r^2}\,\underline{r}\cdot\underline{B} = \sigma_Z B_Z\left(\frac{Z^2}{X^2+Y^2+Z^2}\right) \quad -(180)$$

and if it is assumed on average that:

$$\left\langle \frac{Z^2}{X^2+Y^2+Z^2} \right\rangle = \frac{1}{3} \quad -(181)$$

the Eq. (177) reduces to:

$$E = \frac{1}{3}\frac{e\hbar}{m}\sigma_Z B_Z\left(J(J+1) - L(L+1) - S(S+1)\right) \quad -(182)$$

and electron spin orbit resonance occurs at:

$$\omega = \frac{2}{3}\frac{e}{m}B_Z\left(J(J+1) - L(L+1) - S(S+1)\right). \quad -(183)$$

In spherical coordinates:

$$\frac{Z^2}{X^2+Y^2+Z^2} = \cos^2\theta \quad -(184)$$

so:

$$\int \phi^* \frac{\underline{\sigma}\cdot\underline{r}}{r^2}\, \underline{r}\cdot\underline{B}\,\phi\, d\tau = B_Z \sigma_Z \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \phi^* \cos^2\theta\, \phi\, r^2 \sin\theta\, dr\, d\theta\, d\phi \quad -(185)$$

It is seen that this part of the hamiltonian is r dependent and must be evaluated for each wave function ϕ. The only analytical wave functions are those of atomic H, so computational methods can be used to evaluate the energy levels of Eq. (185) for the H atom. The results are given in UFT 250 on www.aias.us and summarized later in this chapter.

Consider now the hamiltonian:

$$H = -\frac{e}{2m}\left(\underline{\sigma}\cdot\underline{p}\;\underline{\sigma}\cdot\underline{A} + \underline{\sigma}\cdot\underline{A}\;\underline{\sigma}\cdot\underline{p}\right) \quad -(186)$$

in its quantized form:

$$H\phi = -\frac{e}{2m}\frac{\hbar}{i}\left(\underline{\sigma}\cdot\underline{\nabla}\;\underline{\sigma}\cdot\underline{A} + \underline{\sigma}\cdot\underline{A}\;\underline{\sigma}\cdot\underline{\nabla}\right)\phi \quad -(187)$$

Note that:

$$\underset{\sim}{r}\cdot\underset{\sim}{p} = \frac{\hbar}{i}\, r\, \underline{e}_r\cdot\underline{\nabla} = \frac{\hbar}{i}\, r \frac{\partial}{\partial r} \quad -(188)$$

where the radial unit vector is defined as:

$$\underline{e}_r = \frac{\underset{\sim}{r}}{r} \quad -(189)$$

From Pauli algebra:

$$\underline{\sigma} \cdot \underline{A} = \frac{\underline{\sigma} \cdot \underset{\sim}{r}}{r^2} \left(\underset{\sim}{r} \cdot \underline{A} + i \underline{\sigma} \cdot \underset{\sim}{r} \times \underline{A} \right) \quad - (190)$$

and for a uniform magnetic field

$$\underline{A} = \frac{1}{2} \underline{B} \times \underline{r} \quad - (191)$$

in which:

$$\underset{\sim}{r} \cdot \underline{A} = 0 \quad - (192)$$

it follows that:

$$\underline{\sigma} \cdot \underline{A} = i \frac{\underline{\sigma} \cdot \underline{r}}{r^2} \underline{\sigma} \cdot \underline{r} \times \underline{A} \quad - (193)$$

As in note 251(1) accompanying UFT 251 on www.aias.us it follows that:

$$\left(\underline{\sigma} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{A} \right) \phi = \frac{\hbar}{r} \left(\underline{\sigma} \cdot \underline{r} \times \underline{A} \frac{\partial \phi}{\partial r} + \frac{\partial}{\partial r} \left(\underline{\sigma} \cdot \underline{r} \times \underline{A} \right) \phi \right.$$
$$\left. - \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \times \underline{A}\, \underline{\sigma} \cdot \underline{L} \phi \right) \quad - (194)$$

Using Eq. (191) it follows that:

$$\frac{1}{r} \underset{\sim}{r} \times \underline{A} = \frac{r}{2} \left(\underline{B} - \underline{e}_r \left(\underline{B} \cdot \underline{e}_r \right) \right) \quad - (195)$$

and that:

$$\frac{1}{r}\frac{\partial}{\partial r}\underline{r}\times\underline{A} = \underline{B} - \frac{1}{2r}\frac{\partial}{\partial r}\left(r^2\underline{e}_r(\underline{e}_r\cdot\underline{B})\right)$$

$$= \underline{B} - \underline{e}_r(\underline{e}_r\cdot\underline{B}) \quad -(196)$$

so:

$$\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A}\,\phi = \underline{\sigma}\cdot\underline{B}_1\left(\hbar\phi + \frac{1}{2}r\frac{\partial\phi}{\partial r} - \frac{1}{2}\underline{\sigma}\cdot\underline{L}\,\phi\right) \quad -(197)$$

in which the modified magnetic flux density is:

$$\underline{B}_1 = \underline{B} - \underline{e}_r(\underline{e}_r\cdot\underline{B}) \quad -(198)$$

The hamiltonian (187) can therefore be developed as:

$$H\phi = -\frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B}_1\left(\phi + r\frac{\partial\phi}{\partial r}\right) + \frac{e}{2m}\underline{\sigma}\cdot\underline{B}_1\,\underline{\sigma}\cdot\underline{L}\,\phi. \quad -(199)$$

Recall that the conventional development of the hamiltonian is well known:

$$H\phi = \frac{ie\hbar}{2m}\left(\underline{\nabla}\cdot(\underline{A}\phi) + \underline{A}\cdot\underline{\nabla}\phi\right) \quad -(200)$$

$$-\frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{\nabla}\times(\underline{A}\phi) + \underline{A}\times\underline{\nabla}\phi$$

$$= -\frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B} + \frac{ie\hbar}{2m}\left((\underline{\nabla}\cdot\underline{A})\phi + 2\underline{\nabla}\phi\cdot\underline{A}\right)$$

and misses the information given in Eq. (199).

As in note 251(2) on www.aias.us It is possible to define three novel types of hamiltonian:

$$H_1 \phi = -\frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B}_1 \phi \quad -(201)$$

$$H_2 \phi = -\frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B}_1 \, r \frac{\partial \phi}{\partial r} \quad -(202)$$

$$H_3 \phi = \frac{e}{2m} \underline{\sigma} \cdot \underline{B}_1 \, \underline{\sigma} \cdot \underline{L} \, \phi \quad -(203)$$

whose energy expectation values are:

$$E_1 = -\frac{e\hbar}{2m} \int \phi^* \underline{\sigma} \cdot \underline{B}_1 \phi \, d\tau \quad -(204)$$

$$E_2 = -\frac{e\hbar}{2m} \int \phi^* \underline{\sigma} \cdot \underline{B}_1 \, r \frac{\partial \phi}{\partial r} \, d\tau \quad -(205)$$

$$E_3 = \frac{e}{2m} \int \phi^* \underline{\sigma} \cdot \underline{B}_1 \, \underline{\sigma} \cdot \underline{L} \, \phi \, d\tau \quad -(206)$$

with the Born normalization:

$$\int \phi^* \phi \, d\tau = 1 \quad -(207)$$

These are developed in UFT 251 for the hydrogenic wavefunctions, giving many novel results of usefulness to analytical chemisty.

The use of well known Pauli algebra in a new way is illustrated on the simplest level in UFT 252 with the kinetic energy hamiltonian itself:

$$H \phi = \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{p} \, \phi \quad -(208)$$

in which the Pauli algebra is:

$$\underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} (\underset{\sim}{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L}) \quad -(209)$$

Therefore:

$$\underline{\sigma} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} (\underset{\sim}{r} \cdot \underset{\sim}{p} + i \underline{\sigma} \cdot \underline{L}) (\underset{\sim}{r} \cdot \underset{\sim}{p} + i \underline{\sigma} \cdot \underline{L})$$

$$= \frac{1}{r^2} \left(\underset{\sim}{r} \cdot \underset{\sim}{p} \, \underset{\sim}{r} \cdot \underset{\sim}{p} + i (\underset{\sim}{r} \cdot \underset{\sim}{p} \, \underline{\sigma} \cdot \underline{L} + \underline{\sigma} \cdot \underline{L} \, \underset{\sim}{r} \cdot \underline{p}) - L^2 - i \underline{\sigma} \cdot \underline{L} \times \underline{L} \right) \quad -(210)$$

which can be quantized using:

$$\underset{\sim}{r} \cdot \underline{p} \, \phi = \frac{\hbar}{i} r \frac{\partial \phi}{\partial r} \quad -(211)$$

$$L^2 \phi = \hbar^2 l(l+1) \phi, \quad \underline{L} \times \underline{L} \phi = i \hbar \phi,$$

$$\underline{S} \cdot \underline{L} \phi = \frac{\hbar^2}{2} (j(j+1) - l(l+1) - s(s+1)) \phi.$$

Therefore there are results such as the following which are instructive in the use of operators in quantum mechanics:

$$\underset{\sim}{r} \cdot \underline{p} (\underset{\sim}{r} \cdot \underline{p} \phi) = \frac{\hbar}{i} r \left(\frac{\partial}{\partial r} \left(\left(\frac{\hbar}{i} r \frac{\partial}{\partial r} \right) \phi \right) \right) \quad -(211)$$

As shown in detail in UFT 252 the hamiltonian (208) can be developed as:

$$-\frac{\hbar^2}{2m}\,\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{\nabla}\,\phi$$

$$= -\frac{\hbar^2}{2m}\nabla^2\phi + \frac{1}{m}\left(\frac{\underline{S}\cdot\underline{L}}{r}\left(2\frac{\partial\phi}{\partial r} + \frac{\phi}{r}\right)\right) \quad -(212)$$

where the wavefunctions are the spherical harmonics:

$$\phi = Y_l^m \quad -(213)$$

The analysis gives two novel classes of energy expectation values:

$$E_1 = \frac{\hbar^2}{m}\left(j(j+1) - l(l+1) - s(s+1)\right)\int \phi^* \frac{1}{r}\frac{\partial\phi}{\partial r}\,d\tau \quad -(214)$$

and

$$E_2 = \frac{\hbar^2}{2m}\left(j(j+1) - l(l+1) - s(s+1)\right)\int \phi^* \frac{1}{r^2}\phi\,d\tau \quad -(215)$$

which are evaluated by computer in UFT 252.

Similarly the hamiltonian quadratic in the potential:

$$H_5 = \frac{e^2}{2m}\,\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{A}\,\phi \quad -(216)$$

can be developed as in UFT 252 using Eq. (191) as:

$$H_5 \phi = \frac{e^2 B_Z^2}{8m} r^2 (1 - \cos^2\theta) \phi \quad -(217)$$

again giving novel types of spectroscopy.

The hamiltonian:

$$H_7 \phi = \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \left(1 + \frac{e\phi}{2mc^2} \right) \underline{\sigma} \cdot \underline{p} \phi \quad -(218)$$

from the fermion equation gives the spin orbit component:

$$H_8 \phi = \frac{e}{4m^2c^2} \underline{\sigma} \cdot \underline{p} \, \phi \, \underline{\sigma} \cdot \underline{p} \phi \quad -(219)$$

as we have seen and Eq. (219) can also be developed using Eq. (209) to give:

$$H_8 \phi = \frac{e}{4m^2c^2} (\underset{\sim}{r} \cdot \underset{\sim}{p} + i \underline{\sigma} \cdot \underline{L}) \frac{\phi}{r^2} (\underset{\sim}{r} \cdot \underset{\sim}{p} + i \underline{\sigma} \cdot \underline{L}) \quad -(220)$$

There are several terms in this equation that can be developed as in UFT 252. For example:

$$H_9 \phi = \frac{e}{4m^2c^2} \underset{\sim}{r} \cdot \underset{\sim}{p} \left(\frac{\phi}{r^2} \underset{\sim}{r} \cdot \underset{\sim}{p} \phi \right) \quad -(221)$$

in which:

$$\underset{\sim}{r} \cdot \underset{\sim}{p} \phi = -i\hbar r \frac{\partial \phi}{\partial r} \quad -(222)$$

So the hamiltonian gives:

$$H_9 \phi = \frac{e^2 \hbar^2}{16 m^2 c^2 \pi \epsilon_0} \left(j(j+1) - l(l+1) - s(s+1) \right) \frac{1}{r^3} \left(3\phi - r \frac{\partial \phi}{\partial r} \right) \quad -(223)$$

and two types of energy expectation values:

$$E_{q1} = \frac{3 e^2 \hbar^2}{16 \pi \epsilon_0 m^2 c^2} \left(j(j+1) - l(l+1) - s(s+1) \right) \int \frac{\phi \phi^*}{r^3} d\tau \quad -(224)$$

and

$$E_{q2} = \frac{- e^2 \hbar^2}{16 \pi \epsilon_0 m^2 c^2} \left(j(j+1) - l(l+1) - s(s+1) \right) \int \frac{\phi \phi^*}{r^2} d\tau \quad -(225)$$

which give observable new fermion resonance spectra.

The main spin orbit hamiltonian (220) can be developed into the following four hamiltonians:

$$H_{10} \phi = \frac{e}{4 m^2 c^2} \underline{\sigma} \cdot \underline{p} \left(\frac{\phi}{r^2} \underline{\sigma} \cdot \underline{p} \, \phi \right) \quad -(226)$$

$$H_{11} \phi = \frac{i e}{4 m^2 c^2} \underline{\sigma} \cdot \underline{L} \left(\frac{\phi}{r^2} \underline{\sigma} \cdot \underline{p} \, \phi \right) \quad -(227)$$

$$H_{12} \phi = \frac{i e}{4 m^2 c^2} \underline{\sigma} \cdot \underline{p} \left(\frac{\phi}{r^2} \underline{\sigma} \cdot \underline{L} \, \phi \right) \quad -(228)$$

$$H_{13} \phi = -\frac{e}{4 m^2 c^2} \underline{\sigma} \cdot \underline{L} \left(\frac{\phi}{r^2} \underline{\sigma} \cdot \underline{L} \, \phi \right) \quad -(229)$$

and these are evaluated systematically in UFT 252 giving many new results.

Finally in this section the effect of gravitation on fermion resonance spectra can be evaluated as in UFT 253 using the gravitational minimal prescription:

$$E \rightarrow E + m \Phi \quad -(230)$$

where the gravitational potential is:

$$\Phi = -\frac{GM}{r} \quad (231)$$

where G is Newton's constant and where Φ is the gravitational potential. Here M is a mass that is attracted to the mass of the electron m. Vriosu effects of gravitaton are developed in UFT 253.

5.4 REFUTATION OF INDETERMINACY

5.4 REFUTATION OF INDETERMINACY: QUANTUM HAMILTON AND FORCE EQUATIONS

The methods used to derive the fermion equation can be used as in UFT 175 to UFT 177 on www.aias.us can be used to derive the Schroedinger equation from differential geometry. The fundamental axioms of quantum mechanics can be derived from geometry and relativity. These methods can be used to infer the existence of the quantized equivalents of the Hamilton equations of motion, which Hamilton derived in about 1833 without the use of the lagrangian dynamics. It is very well known that the Hamilton equations use position (x) and momentum (p) as conjugate variables in a well defined classical sense {1 - 10} and so x and p are "specified simultaneously" in the dense Copenhagen jargon of the twentieth century.. Therefore, by quantum classical equivalence, x and p are specified simultaneously in the quantum Hamilton equations, thus refuting the Copenhagen interpretation of quantum mechanics based on the commutator of operators of position and momentum . The quantum Hamilton equations were derived for the first time in UFT 175 in 2011, and are described in this section. They show that x and p are specified simultaneously in quantum mechanics, a clear illustration of the confusion caused by the Copenhagen interpretation.

The anti commutator $\{\hat{x}, \hat{p}\}$ is used in this section to derive further refutations of Copenhagen, in that $\{\hat{x}, \hat{p}\}$ acting on a wavefunctions that are exact solutions of Schroedinger's equation produces expectation values that are zero for the harmonic oscillator, and non zero for atomic H. The anti commutator $\{\hat{x}, \hat{p}\}$ is shown to be proportional to $[x^2, p^2]$, whose expectation values for the harmonic oscillator are all zero, while for atomic H they are all non-zero. For the particle on a ring, combinations can be zero, while individual commutators of this type are non-zero. For linear motion self inconsistencies in the Copenhagen interpretation are revealed, and for the particle on a sphere the commutator is again non-zero. The hand calculations in fifteen additional notes accompanying UFT 175 are checked with computer algebra, as are all calculations in UFT theory to which computer algebra may be applied. Tables were produced in UFT 175 of the relevant expectation values. The Copenhagen interpretation is completely refuted because in that interpretation it makes no sense for the expectation value of a commutator of operators to be both zero and non-zero for the same pair of operators. One of the operators would be absolutely unknowable and the other precisely knowable if the expectation value were non zero, and both precisely knowable if it were zero. These two interpretations refer respectively to non zero and zero commutator expectation values, and both interpretations cannot be true for the same pair of operators. Prior to the work in UFT 175 in 2011, commutators of a given pair of operators were thought to be zero or non zero, never both zero and non zero, so a clear refutation of Copenhagen was never realized. In ECE theory, Copenhagen and it unscientific, anti Baconian, jargon are not used, and expectation values are straightforward consequences of the fundamental operators introduced by Schroedinger. The latter immediately rejected Copenhagen, as did Einstein and de Broglie.

The Schroedinger equation is derived in ECE from the tetrad postulate of Cartan geometry, which is reformulated as the ECE wave equation:

$$(\square + R)\, q^a_{\ \nu} = 0 \qquad -(232)$$

where:

$$R := q^{\nu}_{\ a}\, \partial^{\mu}\left(\omega^a_{\ \mu\nu} - \Gamma^a_{\ \mu\nu}\right) \qquad -(233)$$

as discussed earlier in this book. The fermion equation in its wave format is the limit:

$$R \to \left(\frac{mc}{\hbar}\right)^2 \quad -(234)$$

and for the free particle reduces to:

$$-\frac{\hbar^2}{2m}\nabla^2\phi = (E - mc^2)\phi. \quad -(235)$$

This equation reduces to the Schroedinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\phi = E_{NR}\phi \quad -(236)$$

where:

$$E_{NR} = E - mc^2. \quad -(237)$$

In the presence of potential energy the Schroedinger equation becomes:

$$-\frac{\hbar^2}{2m}\nabla^2\phi = (E_{NR} + V)\phi. \quad -(238)$$

In this derivation, the fundamental axiom of quantum mechanics follows from the wave equation (232) and from the necessity that the classical equivalent of the hamiltonian operator H is the hamiltonian in classical dynamics, the sum of the kinetic and potential energies:

$$H = E_{NR} + V. \quad -(239)$$

So in ECE physics, quantum mechanics can be derived from general relativity in a straightforward way that can be tested against experimental data at each stage. For example earlier in this chapter the method resulted in many new types of spin orbit spectroscopies.

The two quantum Hamilton equations are derived respectively using the well known position and momentum representations of quantum mechanics. In the position representation the Schroedinger axiom is:

$$\hat{p}\phi = -i\hbar\frac{\partial\phi}{\partial x}, \quad (\hat{p}\phi)^* = i\hbar\frac{\partial\phi}{\partial x} \quad -(240)$$

from which it follows that:

$$[\hat{x}, \hat{p}]\phi = i\hbar\phi. \quad -(241)$$

So the expectation value of the commutator is:

$$\langle[\hat{x}, \hat{p}]\rangle = i\hbar. \quad -(242)$$

In the position representation the expectation value, <x>, of x is x. It follows that:

$$\frac{d}{dx}\langle\hat{x}\rangle = -\frac{i}{\hbar}\langle[\hat{x}, \hat{p}]\rangle = 1. \quad -(243)$$

Note that this tautology can be derived as follows from the equation:

$$\frac{d}{dx}\langle\hat{x}\rangle = \frac{d}{dx}\int\phi^*\hat{x}\phi\, d\tau \quad -(244)$$

which can be proven as follows. First use the Leibnitz Theorem to find that:

$$\frac{d}{dx}\int\phi^*\hat{x}\phi\, d\tau = \left(\int\frac{d\phi^*}{dx}\hat{x}\phi\, d\tau + \int\phi^*\hat{x}\frac{d\phi}{dx}\, d\tau\right). \quad -(245)$$

In quantum mechanics the operators are hermitian operators defined as follows:

$$\int\phi_n^*\hat{A}\phi_n\, d\tau = \left(\int\phi_n^*\hat{A}\phi_m\, d\tau\right)^* = \left(\int\hat{A}^*\phi_m^*\phi_n\, d\tau\right) \quad -(246)$$

Therefore it follows that that Eq. (245) is:

$$\frac{d}{dx}\langle \hat{x} \rangle = 1 = -\frac{i}{\hbar}\int \psi^* (\hat{p}\hat{x} - \hat{x}\hat{p})\psi \, d\tau \quad -(247)$$

which is Eq. (243), Q. E. D.

The first quantum Hamilton equation is obtained by generalizing x to any hermitian operator A of quantum mechanics:

$$\hat{x} \rightarrow \hat{A} \quad -(248)$$

so one format of the first quantum Hamilton equation is:

$$\frac{d}{dx}\langle \hat{A} \rangle = \frac{i}{\hbar}\langle [\hat{p}, \hat{A}] \rangle . \quad -(249)$$

In the special case:

$$\hat{A} = \hat{H} \quad -(250)$$

then:

$$\frac{d}{dx}\langle \hat{H} \rangle = \frac{i}{\hbar}\langle [\hat{p}, \hat{H}] \rangle . \quad -(251)$$

However, it is known that:

$$\frac{d}{dt}\langle \hat{p} \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{p}] \rangle \quad -(252)$$

so from Eqs. (251) and (252) the quantum Hamilton equation is:

$$\frac{d}{dx}\langle \hat{H} \rangle = -\frac{d}{dt}\langle \hat{p} \rangle . \quad -(253)$$

The expectation values in this equation are:

$$H = \langle \hat{H} \rangle, \quad p = \langle \hat{p} \rangle \quad -(254)$$

so the first Hamilton equation of motion of 1833 follows, Q. E. D.:

$$\frac{dH}{dx} = -\frac{dp}{dt} \,. \quad -(255)$$

The second quantum Hamilton equation follows from the momentum representation:

$$\hat{x}\phi = -\frac{\hbar}{i}\frac{\partial\phi}{\partial p}, \quad \hat{p}\phi = p\phi \quad -(256)$$

from which the following tautology follows:

$$\frac{d}{dp}\langle \hat{p} \rangle = \frac{\hbar}{i}\left[\langle \hat{x}, \hat{p} \rangle\right] = 1 \quad -(257)$$

This tautology can be obtained from the equation:

$$\frac{d}{dp}\langle \hat{p} \rangle = \frac{d}{dp}\int \phi^* \hat{p}\phi \, d\tau . \quad -(258)$$

Now generalize p to any operator A:

$$\hat{p} \rightarrow \hat{A} \quad -(259)$$

and the second quantum Hamilton equation in one format is:

$$\frac{d}{dp}\langle \hat{A} \rangle = -\frac{i}{\hbar}\langle [\hat{x}, \hat{A}] \rangle . \quad -(260)$$

In the special case:

$$\hat{A} = \hat{H} \quad -(261)$$

the second quantum Hamilton equation is:

$$\frac{d}{dp}\langle \hat{H} \rangle = -\frac{i}{\hbar}\langle [\hat{x}, \hat{H}] \rangle \quad -(262)$$

However it is known that:

$$\langle [\hat{x}, \hat{H}] \rangle = -\frac{\hbar}{i}\frac{d\langle \hat{x} \rangle}{dt} \quad -(263)$$

so the second quantum Hamilton equation is:

$$\frac{d\langle \hat{H} \rangle}{dp} = \frac{d}{dt}\langle \hat{x} \rangle \quad -(264)$$

which reduces to its classical counterpart, the second quantum Hamilton equation of classical dynamics, Q. E. D.:

$$\frac{dH}{dp} = \frac{dx}{dt}. \quad -(265)$$

Note carefully that both the quantum Hamilton equations derive directly from the familiar commutator (242) of quantum mechanics. Conversely the Hamilton equations of 1833 imply the commutator (242) given only the Schroedinger postulate in position and momentum representation respectively. In the Hamilton equations of classical dynamics, x and p are simultaneously observable, so they are also simultaneously observable in the quantized Hamilton equations of motion and in quantum mechanics in general. This argument refutes Copenhagen straightforwardly, and the arbitrary assertion that x and p are not simultaneously observable.

The anti commutator method of refuting Copenhagen was also developed in UFT 175 on www.aias.us and is based on the definition of the anti commutator:

$$\{\hat{x}, \hat{p}\}\phi = -i\hbar\left(x\frac{\partial\phi}{\partial x} + \frac{\partial}{\partial x}(x\phi)\right) = -i\hbar\left(\phi + 2x\frac{d\phi}{dx}\right) \quad -(266)$$

In the position representation the anti commutator is:

$$\{\hat{x}, \hat{p}\}\phi = -i\hbar\left(x\frac{\partial\phi}{\partial x} + \frac{\partial}{\partial x}(x\phi)\right) = -i\hbar\left(\phi + 2x\frac{\partial\phi}{\partial x}\right). \quad -(267)$$

Similarly the commutator of $\hat{p}^2$ and $\hat{x}^2$ is defined as:

$$[\hat{x}^2, \hat{p}^2]\phi = \left([\hat{x}^2, \hat{p}]\hat{p} + \hat{p}([\hat{x}^2, \hat{p}])\right)\phi. \quad -(268)$$

Now use the quantum Hamilton equations to find that:

$$[\hat{p}, \hat{x}^2]\phi = -2i\hbar x\phi \quad -(269)$$

$$[\hat{x}^2, \hat{p}]\phi = 2i\hbar x\phi \quad -(270)$$

It follows that:

$$[\hat{x}^2, \hat{p}^2]\phi = 2i\hbar(\hat{p}\hat{x} + \hat{x}\hat{p})\phi \quad -(271)$$

so the following useful equation has been proven in one dimension:

$$[\hat{x}^2, \hat{p}^2]\phi = 2i\hbar\{\hat{x}, \hat{p}\}\phi. \quad -(272)$$

In three dimensions the Schroedinger axiom in position representation is:

$$\hat{p}\phi = -i\hbar\nabla\phi \quad -(273)$$

and in three dimensions the relevant commutator is:

$$[\underset{\sim}{r}, \underline{p}]\phi = -i\hbar\left(\underset{\sim}{r}\cdot\underline{\nabla}\phi - \underline{\nabla}\cdot(\underset{\sim}{r}\phi)\right) \quad -(274)$$

where in Cartesian coordinates:

$$r^2 = X^2 + Y^2 + Z^2 \quad -(275)$$

Therefore:

$$[\underset{\sim}{r}, \underline{p}]\phi = -i\hbar\left(\underset{\sim}{r}\cdot\underline{\nabla}\phi - \phi\,\underline{\nabla}\cdot\underline{r} - \underset{\sim}{r}\cdot\underline{\nabla}\phi\right) \quad -(276)$$

where:

$$\underline{\nabla}\cdot(\underline{r}\phi) = \phi\,\underline{\nabla}\cdot\underline{r} + \underset{\sim}{r}\cdot\underline{\nabla}\phi \quad -(277)$$

in which:

$$\underline{\nabla}\cdot\underline{r} = 3 \quad -(278)$$

So:

$$[\hat{\underset{\sim}{r}}, \hat{\underline{p}}]\phi = 3i\hbar\phi \quad -(279)$$

In three dimensions:

$$[\hat{r}^2, \hat{p}^2]\phi = \left([\hat{r}^2, \underline{\hat{p}}]\cdot\underline{\hat{p}} + \underline{\hat{p}}\cdot\left([\hat{r}^2, \underline{\hat{p}}]\right)\right)\phi \quad -(280)$$

where:

$$[\hat{r}^2, \underline{\hat{p}}]\phi = r^2\hat{p}\phi - \hat{p}(r^2\phi) = i\hbar\nabla r^2\phi \quad -(281)$$

and where:

$$\underline{\nabla} r^2 = \frac{\partial r^2}{\partial X}\underline{i} + \frac{\partial r^2}{\partial Y}\underline{j} + \frac{\partial r^2}{\partial Z}\underline{k} \quad -(282)$$

with:

$$r^2 = X^2 + Y^2 + Z^2 \quad -(283)$$

So:

$$\underline{\nabla} r^2 = 2\underline{r} \quad -(284)$$

and the three dimensional equivalent of Eq. (272) is:

$$[\hat{r}^2, \hat{p}^2]\phi = 2i\hbar\{\underline{r}, \underline{p}\}\phi \quad -(285)$$

The anti commuttator in this equation is:

$$(\hat{\underline{r}}\cdot\hat{\underline{p}} + \hat{\underline{p}}\cdot\hat{\underline{r}})\phi = \hat{\underline{r}}\cdot\hat{\underline{p}}\phi + \hat{\underline{p}}\cdot(\hat{\underline{r}}\phi) \quad -(286)$$

$$= -i\hbar(2\underline{r}\cdot\underline{\nabla}\phi + 3\phi)$$

where:

$$\underline{r}\cdot\underline{\nabla}\phi = X\frac{\partial\phi}{\partial X} + Y\frac{\partial\phi}{\partial Y} + Z\frac{\partial\phi}{\partial Z} \quad -(287)$$

so in Cartesian coordinates:

$$\{\hat{\underline{r}}, \hat{\underline{p}}\}\phi = -i\hbar\left(2\left(X\frac{\partial\phi}{\partial X} + Y\frac{\partial\phi}{\partial Y} + Z\frac{\partial\phi}{\partial Z}\right) + 3\phi\right). \quad -(288)$$

When considering the H atom the relevant anti commutator is:

$$\{\hat{r}, \hat{p}_r\}\phi = -i\hbar\left\{r, \frac{\partial}{\partial r}\right\}\phi. \quad -(289)$$

With these definitions some expectation values:

$$\langle[\hat{r}^2, \hat{p}_r^2]\rangle = 2i\hbar\langle\{\hat{\underline{r}}, \hat{\underline{p}}\}\rangle \quad -(290)$$

are worked out for exact solutions of the Schroedinger equation in the fifteen calculational notes accompanying UFT 175 on www.aias.us. All expectation values were checked by computer algebra and tabulated. The result is a definitive refutation of Copenhagen because expectation values can be zero or non-zero depending on which solution of Schroedinger's equation is used, as discussed already. So this method reduces Copenhagen to absurdity, Q. E. D., a reductio ad absurdum refutation of the Copenhagen interpretation of quantum mechanics.

The force equation of quantum mechanics was first inferred in 2011 in UFT 176 and UFT 177 on www.aias.us and have been very influential. It was derived from the two quantum Hamilton equations:

$$i\hbar \frac{d}{dq}\langle \hat{H} \rangle = \langle [\hat{H}, \hat{p}] \rangle \quad -(291)$$

and

$$i\hbar \frac{d}{dp}\langle \hat{H} \rangle = -\langle [\hat{H}, \hat{q}] \rangle \quad -(292)$$

applied to canonical operators $\hat{p}$ and $\hat{q}$. By using the well known {1 - 10}:

$$\frac{d}{dq}\langle \hat{H} \rangle = \left\langle \frac{d\hat{H}}{dq} \right\rangle, \quad \frac{d}{dp}\langle \hat{H} \rangle = \left\langle \frac{d\hat{H}}{dp} \right\rangle \quad -(293)$$

these equations can be put in to operator format as follows:

$$i\hbar \frac{d\hat{H}}{dq}\psi = [\hat{H}, \hat{p}]\psi \quad -(294)$$

and

$$i\hbar \frac{d\hat{H}}{dp}\psi = -[\hat{H}, \hat{q}]\psi \quad -(295)$$

where ψ is the wave function. If the hamiltonian is defined as:

$$H = \frac{p^2}{2m} + V(x) \quad -(296)$$

then:

$$\frac{dH}{dx} = \frac{dV}{dx} \quad -(297)$$

because in the Hamilton dynamics x and p are independent, canonical variables. Therefore Eq. (293) is satisfied automatically. Using the result:

$$[\hat{H}, \hat{p}]\psi = i\hbar \frac{dV}{dx}\psi = -i\hbar F \psi \quad -(298)$$

where F is force, Eq. (291) gives the force equation of quantum mechanics:

$$-\left(\frac{d\hat{H}}{dx}\right)\psi = F\psi \quad -(299)$$

where the eigenoperator is defined by:

$$\frac{d\hat{H}}{dx} := -\hbar^2 \frac{\partial^3}{\partial x^3} + \frac{dV(x)}{dx}. \quad -(300)$$

In the classical limit, the corresponding principle of quantum mechanics means that Eq. (299) becomes one of the Hamilton equations:

$$F = \frac{dp}{dt} = -\frac{dH}{dx}. \quad -(301)$$

In the momentum representation Eq. (295) gives a second fundamental equation of quantum mechanics:

$$\left(\frac{d\hat{H}}{dp}\right)\phi = v\phi \quad -(302)$$

where the eigenvalues are those of quantized velocity. Here:

$$\frac{dH}{dp} = \frac{p}{m} \quad -(303)$$

and:

$$\left(\frac{d\hat{H}}{dp}\right)\phi = v\phi. \quad -(304)$$

Eq. (302) corresponds in the classical limit to the second Hamilton equation:

$$v = \frac{dx}{dt} = \frac{dH}{dp}. \quad -(305)$$

The general, or canonical, formulation of Eqs. (299) and (302) is as follows:

$$-\left(\frac{d\hat{H}}{dq}\right)\phi = F\phi \quad -(306)$$

and

$$\left(\frac{d\hat{H}}{dp}\right)\phi = v\phi \quad -(307)$$

which reduce to the canonical Hamilton equations:

$$-\frac{dH}{dq} = \frac{dp}{dt} \quad -(308)$$

and

$$\frac{dH}{dp} = \frac{dq}{dt} \quad -(309)$$

The rotational equivalent of Eq. (294) is:

$$i\hbar\left(\frac{d\hat{H}}{d\phi}\right)\phi = [\hat{H}, \hat{J}_Z]\phi \quad -(310)$$

in which the canonical variables are:

$$q = \phi, \; \hat{p} = \hat{J}_Z . \quad -(311)$$

For rotational problems in the quantum mechanics of atoms and molecules, H commutes with $\hat{J}_Z$ so

$$[\hat{H}, \hat{J}_Z] = 0 \quad -(312)$$

in which case:

$$\left(\frac{d\hat{H}}{d\phi}\right)\phi = 0 . \quad -(313)$$

In order for $d\hat{H}/d\phi$ to be non-zero there must be a ϕ dependent potential energy in the hamiltonian:

$$H = \frac{J^2}{2I} + V(\phi) \quad -(314)$$

so the hamiltonian operator must be:

$$\hat{H} = -\frac{\hbar^2}{2I}\hat{\Lambda}^2 + V(\phi) \quad -(315)$$

where $\hat{\Lambda}$ is the lagrangian operator. In this case:

$$\frac{d\hat{H}}{d\phi} = -\frac{\hbar^2}{2I}\hat{\Lambda}^2 + \frac{dV}{d\phi} \quad -(316)$$

and Eq (310) gives the torque equation of quantum mechanics:

$$-\left(\frac{d\hat{H}}{d\phi}\right)\psi = T_q\psi = -\left(\frac{dV}{d\phi}\right)\psi \quad -(317)$$

where T_q are eigenvalues of torque.

There also exist higher order quantum Hamilton equations as discussed in UFT 176, and quantum Hamilton equations for rotation in a plane.

Finally as shown in detail in the influential UFT 177 on www.aias.us the force equation of quantum mechanics can be derived from the quantum Hamilton equations and is:

$$(\hat{H} - E)\frac{d\psi}{dx} = F\psi \quad -(318)$$

where the force is defined by:

$$\frac{d}{dx}\langle\hat{H}\rangle = \frac{dH}{dx} = \frac{dV}{dx} = -F = -\frac{dp}{dt} \quad -(319)$$

In the force equation the hamiltonian operator acts on the derivative of the Schroedinger wave function or in general on the derivative of a quantum mechanical wave function obtained in any way, for example in computational quantum chemistry, and this is a new method of general utility as developed in UT 175.