6. Basic Relativistic Quantum Mechanics

Abstract quantum states projected in configuration space helps bridging the realm from pure mathematics to the applied one thereby allowing for introduction of inertial (Lorentz) frames.

It is at a Fence that the theory of special relativity defines transformation properties between Lorentz frames. Communication protocols permit following events in an I-frame endowed with motion relative to the one singles out as reference; (it can be a laboratory frame for example). Invariance of four-vector norm to these transformations leads to mathematical expressions for rotations and translations in spacetime: Lorentz group. Yet, one may select a family of hyperplanes where all space coordinates are label with the same time parameter; this space is designated as space-time and corresponds to a "simultaneity" space. The configuration spaces used to project abstract quantum states are endowed with this property. From now on we leave abstract representation in the background and work with wave functions that are these projected quantum states.

Now, one would like to introduce relative motion into the picture and calculate quantum states (changes) from the perspective of the I-frame where the experimentalist will fix its measuring devices to get signals from an internal quantum system in motion. Moreover, beyond the energy range where relativistic effects might be relevant, situations occur that are described with variable number of I-frames (particle numbers). The approach to simple 1-system introduced must be reformulated.

So far we have emphasized aspects concerning symmetries and invariance based on space-time homogeneity and isotropy leading to quantum numbers characterizing base states. Now focus is on construction model Hamiltonian operators at the Fence; this means abstract operators projected in configuration space whenever such is the case.

A key point is to keep clearly distinguishing the concepts of quantum states from basis sets. Once the latter base states are found, they remain fixed while it is the amplitude in front of them that can change when a quantum state evolves in time; quantum processes are hence just time evolution of the amplitudes. The material systems (1-systems) sustain quantum states; these latter are the mathematical elements of the theory not the material as such. This perspective fits better than the particle model. The eigen value equations to be constructed are

hence considered as ways-ans-means to get basis (eigen states) function for the material system that appears to be the case.

For charged systems, a new symmetry emerges from charge conjugation that plays a fundamental role. Particle-base and antiparticle-base states can be accommodated in charge conjugated spaces although from a simplified view they come from different operators. Such is the magic of relativistic quantum mechanics.

To get a step forward, a bit more about special relativity is given below so that some progress can be accomplished in the construction of relativistic operators. The relativistic models are given with the aim at illustrating the construction of model Hamiltonians.

E&E-7-1-1. A little more on special relativity

The standard axioms of SR are:

1) All inertial frames are equivalent (but some are more useful than others).

2) There exists a maximum speed signal, c, i.e. speed of light in vacuum.

The point of most interest is that the speed of light is independent of the speed of both source and receptor I-frames. In this context, c is a universal constant; such as electron charge (e) is so far universal constant (see Berzi and Gorini, J.Math,Phys.10(1969)1518 for an in depth analysis of the reciprocity principle).

In a mechanical view, the energy E and frequency ν of an electromagnetic (EM) field are related; it is Planck constant (h) that bridges these quantities: $h\nu$ is exchangeable energy at frequency ν between the EM field and a recorder (material system). Because $\nu\lambda = c$, a momentum can be defined by $1/\lambda = k$ and $hk=p$ has momentum dimension; thus, in relativistic theory energy is proportional to a momentum:

$$E = h\nu = hc/\lambda = p\,c \qquad (6.1)$$

λ gives an idea of extension; it is a characteristic wave concept in optics. Observe then that the higher energy ($h\nu$) you put in the EM field the smaller must be its wave length (λ) in order to keep the fundamental relationship: $\nu\,\lambda = c$.

The special case of an inertial rest frame with a mass M at its origin show a four-momentum $p^{\mu} = (Mc,0,0,0)$; i.e. linear momentum $\vec{p}=\mathbf{0}$. For an isolated I-frame there is no way to know its state of motion from within. This is a typical fence device.

So far we have considered rotation invariances in 3-space. In four-space, boosters are rotations of time-space planes. Boosters and 3-space rotations form Lorentz homogeneous rotation group; inclusion of origin translations (**a**) form the inhomogeneous Poincaré group of transformations.

$$\text{-Translations: } U(\mathbf{a},\underline{1}) = \exp(i\,\mathbf{P}\cdot\mathbf{a}) \qquad (6.2)$$

$$\text{-Rotations: } U(0,\underline{\underline{\Lambda}}) = \exp(iM^{\mu\nu}\,\Lambda_{mn}) \qquad (6.3)$$

The important things here are the commutation relations because we can distinguish the angular momentum vector, $\mathbf{J} = (M_{32},M_{13},M_{21})$ and a second vector $\mathbf{N}=(M_{01},M_{02},M_{03})$ standing for the boosts (relative velocities). These vectors permit defining a new vector **w**:

$$\mathbf{w} = P_o\,\mathbf{J} - \mathbf{P}\cdot\mathbf{N}$$

$$w^{o} = \mathbf{P}\cdot\mathbf{J} \qquad (6.4)$$

The fundamental invariants (Casimir operators) are:

$$P^2 = P_m P^m$$
$$w^2 = w_m w^m \qquad (6.5)$$

Angular momentum and translations lead to conserved quantities, boosts are not conserved that is the reason why they do not provide with quantum labels for base functions.

The eigen values of P^2 and w^2 serve to classify the irreducible representations of the Poincaré group. With c=1:

$$1a)\ P^2 = M^2 > 0 \text{ and } P_o > 0\ ;$$
$$1b)\ P^2 = M^2 > 0 \text{ and } P_o < 0 \qquad (6.6)$$
$$2a)\ P^2 = 0 \text{ and } P_o > 0\ ;$$
$$2b)\ P^2 = 0 \text{ and } P_o < 0 \qquad (6.7)$$

The case 1) with $M \neq 0$ can be transformed to a Lorentz frame where three-momentum $\vec{p}=0$; the material system is said to be at rest in this I-frame. In this rest frame the eigen values of P^m are $p^m = (M,0,0,0)$ and

$$p^2 = p_m p^m = M^2$$
$$-w^2 = w_o^2 + \vec{w}^2 = p_o^2 J^2 = M^2 s(s+1) \qquad (6.8)$$

The eigen values of J^2 in the rest frame are just the value of the total intrinsic angular momentum (spin) of the material system, i.e. s(s+1).

From the above presentation, it follows an important result: in relativistic physics *massive systems can be classified according to their mass and spin*.

A booster transformation is a communication protocol to get coordinates equivalent in two I-frames that are in relative *uniform* motion. There are no accelerations involved.

Now, remember that a quantum state in abstract Hilbert space is independent from the I-frame we select to project it. Thus, the wave function is the same for both frames if we assume the same quantum state is being represented either with configuration coordinates in one of them, say $\{\mathbf{q}\}$, or $\{\mathbf{q}'\}$ in the other. The communication protocol for coordinates is the one obtained from relevant LTs.

E&E-7-2-1 More on special relativity

The abstract quantum state is invariant, by definition, to LTs. However, the projection of this state in the inertial frame coordinates, i.e. a wave function, would look differently if we use two or several frames related by LTs.

In what follows, for the sake of simplicity, we use a unique, privileged, frame wherefrom the communication protocols are applied (LTs). In the privileged frame only the speed of LTs frames can be sensed. It remains to ensure that the form of the time evolution equations is invariant.

Let us now portray Hamiltonian operators for massive systems with spin s=0 and s=1/2, respectively. They would lead to the Klein-Gordon-Schrödinger equation, or KGS for short, and for s=1/2 to the famous Dirac equation. In the standard literature, these equations are taken to describe relativistic particles. In our approach, the equations would permit to calculate complete base set functions in rigged Hilbert space sustained by relativistic material systems. Thus, albeit negative energy states are problematic in the particle view, here because the sign plays the role of a label, the energy is positive always; we will examine some aspects of this problem to help set up the relativistic computer schemes. Once again, the situation brings us to the fence between Hilbert and real space representations.

The presentation of equations is fairly heuristic.

6.1. Klein-Gordon-Schrödinger equation

Quantum states are sustained by material systems. While the formalism is identical to the standard one used in Relativistic Quantum Mechanics, the particle view is eradicated; focus is put on base states required to describe quantum states of systems commonly described as particles that are referred to as 1-systems. This elimination avoids long discussions found in standard literature on "negative energy" states without loses of rigor. A reader not familiar with the subject may take the opportunity to see that it is not as dreadful as one would imagine.

In abstract space, the form of Schrödinger time dependent equation follows from a unitary time evolution operator and continuity conditions (topology). The space part representation is required to construct mappings bridging abstract Hilbert space to projected configuration space, the wave functions. To this end the introduction of an I-frame is essential. From momentum four vector for a material system having total mass M, the scalar product

$$(E/c, p_1, p_2, p_3)\bullet\ [E/c, -p_1, -p_2, -p_3]$$

is equated to the invariant (scalar) product M^2c^2. This is the equation put up by Einstein (1905). The problem now is to get a model Hamiltonian.

From equation (3.2.33) let us take the momentum operator $\hat{p}$ and energy operator derived from eq.(1.3.1.7), namely, $\hat{E} = \mathrm{i}\hbar\,\partial/\partial t$ and *replace* the classical physics symbols. A model four-momentum operator obtains:

$$(E/c\ -p_1, -p_2, -p_3) \rightarrow (\hat{E}/c, -\hat{p}_1, -\hat{p}_2, -\hat{p}_3) \qquad (6.1.1)$$

Constructs the formally invariant scalar product with operator symbols:

$$(\hat{E}/c, -\hat{p}_1, -\hat{p}_2, -\hat{p}_3) \bullet [\hat{E}/c, \hat{p}_1, \hat{p}_2, \hat{p}_3] =$$
$$(\hat{E}/c)^2 - \hat{p}_1{}^2 - \hat{p}_2{}^2 - \hat{p}_3{}^2$$

Note that the scalar product and scalars (numbers) are invariant to Lorentz transformations. Now, subtracts the scalar M^2c^2 and apply the resulting operator to the scalar function $\Psi_M(\mathbf{q},t)$. We get a differential equation:

$$\{\partial^2/\partial(ct)^2 - \{(\partial^2/\partial q_1{}^2 + \partial^2/\partial q_2{}^2 + \partial^2/\partial q_3{}^2) + M^2c^2/\hbar^2\}\Psi_M(\mathbf{q},t) = 0 \qquad (6.1.2)$$

This is the scalar Klein-Gordon equation initially discovered by Schrödinger.

Here comes a key issue: $\Psi_M(\mathbf{q},t)$ is a mathematical function that should satisfy the differential equation and boundary conditions one may endow eq.(6.1.2) with. If you come from the other side of the Fence, it is a supplementary hypothesis that such function would correspond to a wave function, namely, a quantum state projected in coordinate **q**.

Once the hypothesis is retained, this equation as it is written above is used to describe quantum states of a system with both spin and charge zero. This differential equation leads to a calculation of a base set. Quantum states are then linear superpositions over such base states. These quantum states are sustained by the material system to the extent its "materiality" appears in the factor $M^2c^2/\hbar^2$.

For charged system with spin-zero, base states interaction with the electromagnetic field is incorporated via the minimal substitution: $p^\mu \rightarrow p^\mu - (e/c)A^\mu(\mathbf{q})$. The component $A^0(\mathbf{q})$ is a longitudinal field, while $A^1(\mathbf{q})$, $A^2(\mathbf{q})$ and $A^3(\mathbf{q})$ are the components of the transverse electromagnetic field (Cf.Chapt.6); this potential is taken as an external potential to the free particle-state system.

The mass M is indicated as a label to the function. The constants related to real world are gathered in the factor $M^2c^2/\hbar^2$; this factor has dimension of an inverse of length square, i.e. $\mathbf{k}^2$ where **k** is a vector in reciprocal space.

The set of plane waves $\Psi_{M,\mathbf{p}}(\mathbf{q},t) = C \exp(i(\mathbf{p}.\mathbf{q} - Et)/\hbar)$ fulfill eq.(6.1.2); replacing it there one gets the relativistic energy expression:

$$(E/c)^2 - \mathbf{p}.\mathbf{p} = M^2c^2 \text{ or } E/c = \pm\sqrt{(M^2c^2 + \mathbf{p}^2)} \qquad (6.1.3)$$

Here pops up the surprise because E/c coincides with the classical mechanics expression for the relativistic energy. The novelty is in the sign of the energy for there seem to be base states with positive and negative energies. Historically, there was a problem because the functions $\Psi_{M,\mathbf{p}}(\mathbf{q},t)$ were endowed with a particle interpretation, and massive free particles with negative energies was unheard of; nowadays this is still a non-sense.

The parameter E must be taken as an eigen label (value) of the time-independent KGS equation; it cannot represent energy at Fence because the relationship $E=Mc^2$ cannot be negative unless the mass is negative which is not an acceptable statement. This double meaning can be easily seen from a perspective of quantum states description: the parameter E used to separate time from space part is a label that may have the dimension of frequency or energy if we introduce Planck constant. As a label we write:

$$E_n(\lambda) = E_{\pm} = \lambda_{\pm}\, p^o$$
$$p^o = +\sqrt{(\, M^2c^4 + \mathbf{p}^2\, c^2)} > 0 \qquad (6.1.4)$$

For base states to be assigned negative or positive energy labels does not make big fuzz. Yet, the Hamiltonian appears to be non-bounded from below. For charged systems this puzzle was solved once charge conjugated states were used to suggest existence of a material system with equal mass and spin but different charge and finally were experimentally detected: the so called anti-particles. For uncharged systems, the particle- and antiparticle-states coincide.

The interesting thing for charged systems, as already noted, is the existence of a new symmetry: *charge conjugation*. This new symmetry allows Klein-Gordon-Schrödinger (KGS) equation to include both types of base states just ordering with an energy-label into positive and negative label states. It is the product energy by times (E·t) that matters.

Following the brilliant idea of Wheeler, properly formulated by Feynman in quantum electrodynamics tells that “negative energy” states represent the states of electrons moving backwards in time. Thus, reversing the direction of proper time amounts to the same as reversing the sign of the charge so that the electron state moving backward in time would look like a positron state moving forward in time (Feynman, Quantum Electrodynamics; page 68).

A negative sign can conventionally be assigned to the direction of time flow that would be opposite to standard one: base states propagating from "future" to "past". Propagation in the negative time direction would have the same state energy as those propagating in the positive direction. The relativistic equation (6.1.2) hides base states that can also incorporate zero charge states. We leave these matters now and focus attention on the non-relativistic limit of this equation.

To get the non-relativistic limit for the scalar KGS equation the energy written as

$$p^o = Mc^2\, (\sqrt{(1+ \mathbf{p}^2/M^2c^2)} \approx\ Mc^2\, (1+ \mathbf{p}^2/2M^2c^2\text{-}\ldots),$$

and taken as a label in absolute value one gets

$$|E| \approx Mc^2 + \mathbf{p}^2/2M - O(1/c^2)\ldots).$$

If we take away the rest mass energy in this expression we recover the classical mechanical kinetic energy of a material system: $\mathbf{p}^2/2M$. A transformation of the wave function is required to accomplish the change. The base function is written as follows:

$$\Psi_M(\mathbf{q},t) = \Phi(\mathbf{q},t)\, \exp(-i\, Mc^2 t/\hbar^2) \qquad (6.1.5)$$

Most of the total mass M is twisted away from the base function $\Phi(\mathbf{q},t)$ and basically taken up by the phase factor. Introducing eq.(6.1.5) into eq.(6.1.2) we come, after some algebra, to eq.(6.1.6)

$$\begin{aligned} & i\hbar\, \partial\, \Phi(\mathbf{q},t)/\partial t = \\ & -(\hbar^2/2M)(\partial^2/\partial q_1^2 + \partial^2/\partial q_2^2 + \partial^2/\partial q_3^2)\, \Phi(\mathbf{q},t) = \\ & \hat{H}(\hat{q})\Phi(\mathbf{q},t) \end{aligned} \qquad (6.1.6)$$

This is the non-relativistic time-dependent Schrödinger equation. The equation yields a model Hamiltonian for eq.(1.3.1.1). There is a term containing the second derivative of time is affected by a 1/c factor (not shown); the non-relativistic case consists in taking $c \to \infty$ limit and, consequently the second time derivative vanishes.

Thus, a dynamic scheme includes a model of the Hamiltonian, i.e.:

$$\begin{aligned} & \hat{H} \to \hat{H}(\hat{q})_{\text{free}} = \\ & -(\hbar^2/2M)(\partial^2/\partial q_1^2 + \partial^2/\partial q_2^2 + \partial^2/\partial q_3^2) \end{aligned} \qquad (6.1.7)$$

This operator permits calculating base states once relevant boundary conditions are given to supplement eq.(6.1.6); periodic boundary conditions (PBC) are commonly used in this context. For a cube of length L on each side one gets:

$$\begin{aligned} & \mathbf{p}_n = (2\pi\hbar/L)\ (n_1, n_2, n_3) \\ & n_i = 0, \pm 1, \pm 2, \ldots \end{aligned} \qquad (6.1.8)$$

The norm is chosen as $N=(2E_nL^3)^{-1/2}$, then the two type of solutions $\phi^{(+)}$ and $\phi^{(-)}$ are ortho-normal:

$$\phi_n^{(\pm)}(\mathbf{q},t) = N \exp(i(\mathbf{p}_n.\mathbf{q} - E_n(\lambda)\, t)/\hbar) \qquad (6.1.9)$$

The energy parameter is quantized:

$$E_n(\lambda) = \lambda \sqrt{(M^2c^2 + \mathbf{p}^2)} \text{ with } \lambda = \pm 1.$$

For us, $E_n(\lambda)$ is a label for base states and the quantum state related to this equation should include a sum over positive and negative label base states.

If we take $A^o = 0$, the transverse EM will be the mechanism prompting for energy exchange between the material system and the EM field; equation (6.1.9) may be seen as representing base states for positive and charge conjugated negative charges for $\lambda = \pm 1$. Thus, $\phi_n^{(-)}(\mathbf{q},t)$ specifies a base state for negative charge system and $\phi_n^{(+)}(\mathbf{q},t)$ would stand for base states of the positive charge, "antiparticle". The energy for both base states is positive and equals to:

$$| E_n(\lambda)| = +\sqrt{(M^2c^2 + \mathbf{p}^2)}.$$

A general quantum state will be a specific linear superposition among the infinite set:

$$\Psi(\mathbf{q},t) = \Sigma_n \{C_n(\Psi)\, \phi_n^{(+)}(\mathbf{q},t) + D_n(\Psi)\, \phi_n^{(-)}(\mathbf{q},t)\} \qquad (6.1.10)$$

The generic quantum state given by eq.(6.1.10) may represent different varieties of particle-state/anti-particle-state situations. Because the base states are always there, the situation here does not involve "physical" particles being created or annihilated, but changes in the quantum state reflected by the amplitudes.

It may well happen that the complete set of amplitudes $\{C_v(\Psi)\}$ is zero at all times so that any experiment designed to probe the response of say positive energy-label states will yield zero relative amplitude. Thus, it is sufficient that at least one amplitude from $D_n(\Psi)$-set be non-zero for the experiment probing negative label states will yield a finite response.

Pair annihilation yields zero amplitudes for both $\{C_v(\Psi)\}$ and $\{D_v(\Psi)\}$ the energy must be put into the EM field. Note that this way of representing quantum states of different material systems can be done because there exists a symmetry relating both Hamiltonians, i.e. charge conjugation. Due to charge conjugation symmetry, Hilbert space is the sum of base states for particle- and antiparticle-states. The representation of arbitrary quantum states must include positive and negative base states always.

The scalar Klein-Gordon equation actually describes spin-zero systems. The real interest (for us) was to find out the form of a non-relativistic Hamiltonian equivalent to the one used by Schrödinger. The result shows consistency. But the spectra of electron states in an external Coulomb field led Schrödinger to results at variance with experiment. The non-relativistic limit equation yields the gross elements of hydrogen atom spectrum only.

The problem is that electron states that must be described with spin 1/2 base states do not fit KGS equation when adapted to describe the spectrum of the hydrogen-like systems. Here we focus attention on Dirac equation where the base states are column vectors in four dimensions named 4- base-vectors. These 4-b-

vectors are multiplied by scalar function that fulfill KGS equations thus the interest to look up first at least to some aspects of this equation.

6.2. Dirac equation

The natural step now is to seek after a relativistic equation for states of spin 1/2. This was not the way followed by the pioneers but is just a shortcut through a forest. A relativistic invariant equation has symmetries built in that in case of charged systems lead to quantum numbers labeling "particle" and "antiparticle states. While quantum base states appear to be related by a charge conjugation operation, in the laboratory they correspond to different material systems with different physical properties. Do not forget this point.

Spin 1/2 functions have dimension two (Cf.Sect.3.5.2 where 2-spinors are examined) and if the base functions for this equation would somehow accommodate charge conjugated states, thus spin dimension may require at least of 4-component base:

$$\Psi = [\Psi_1\ \Psi_2\ \Psi_3\ \Psi_4] = (\Psi_1\ \Psi_2\ \Psi_3\ \Psi_4)^t.$$

Note that KGS equation has square momentum dimensions, while Dirac wanted to have an equation linear in this dimension. The symbol Ψ is a 4x1 matrix (column vector). We need an operator to act on this object that is not going to reduce the dimensions of the basic base vector. Pick up ($\hat{E}$/c, - $\hat{p}_1$, - $\hat{p}_2$, - $\hat{p}_3$) and a vector of fixed 4x4 matrix elements ($\underline{\underline{\alpha}}^0\ \underline{\underline{\alpha}}^1\ \underline{\underline{\alpha}}^2\ \underline{\underline{\alpha}}^3$). The scalar product would represent a momentum operator appropriate for this space:

$$(\underline{\underline{\alpha}}^0\ \underline{\underline{\alpha}}^1\ \underline{\underline{\alpha}}^2\ \underline{\underline{\alpha}}^3)\ [\hat{E}/c,\ \hat{p}_1,\ \hat{p}_2,\ \hat{p}_3] =$$
$$\underline{\underline{\alpha}}^o \hat{E}/c + \underline{\underline{\alpha}}^1 \hat{p}_1 + \underline{\underline{\alpha}}^2 \hat{p}_2 + \underline{\underline{\alpha}}^3 \hat{p}_3.$$

Each term, say $\underline{\underline{\alpha}}^2 \hat{p}_2$, is a 4x4 operator that can act on a 4-vector Ψ: $(\underline{\underline{\alpha}}^2 \hat{p}_2)\Psi$. The scalar product is Lorentz invariant; following a trick similar to KGS equation, complete the special relativity form with $Mc^2\ \underline{\underline{\alpha}}^4$; the matrix $\underline{\underline{\alpha}}^4$, designated by $\underline{\underline{\beta}}$ in the literature, is to be determined as well as ($\underline{\underline{\alpha}}^1\ \underline{\underline{\alpha}}^2\ \underline{\underline{\alpha}}^3$) = $\underline{\underline{\boldsymbol{\alpha}}}$. To alleviate notation, the circumflex over these and other matrix operators is to be understood; they represent fixed matrix operators anyway. Now multiply from the right with Ψ a 4-component vector to get:

$$(\underline{\underline{\alpha}}^o \hat{E}/c + \underline{\underline{\alpha}}^1 \hat{p}_1 + \underline{\underline{\alpha}}^2 \hat{p}_2 + \underline{\underline{\alpha}}^3 \hat{p}_3)\Psi =$$
$$Mc\ \underline{\underline{\alpha}}^4\ \Psi \qquad (6.2.1)$$

This equation is just a form; it does not contain physics yet. Introducing the operators´ definitions as we did with KGS equation and taking $\underline{\underline{\alpha}}^o$ as the unit matrix operator we get a definition of Dirac Hamiltonian:

$$\begin{aligned} & i\hbar\,\partial\Psi/\partial t = \\ & \{c\hbar/i\,(\underline{\underline{\alpha}}^1\,\partial/\partial q_1 + \underline{\underline{\alpha}}^2\,\partial/\partial q_2 + \underline{\underline{\alpha}}^3\,\partial/\partial q_3\,) + Mc^2\,\underline{\underline{\alpha}}^4\}\Psi \equiv \\ & \hat{H}_{Dirac}\Psi \end{aligned} \qquad (6.2.2)$$

The term in round parenthesis can be written as $-i\,c\hbar\,\underline{\underline{\alpha}}\cdot\nabla$, and an inertial frame is involved once ∇ and $i\hbar\partial/\partial t$ are introduced. This equation has the form of Dirac relativistic equation; quantum states sustained by an isolated material system of mass M are determined with Hamiltonian:

$$\hat{H}_{Dirac} = -i\,c\hbar\,\underline{\underline{\alpha}}\cdot\nabla + \underline{\beta}\,Mc^2 \qquad (6.2.3)$$

The energy operator is linear in the momentum if we divide by c above. The electromagnetic field shares this property in so far energy is proportional to the reciprocal space vector **k**: $\omega = |\mathbf{k}|\,c$. Multiply by $\hbar$ to get $\hbar\omega$ equal to energy and $\hbar|\mathbf{k}|\,c$. Observe that Planck constant ($\hbar$) and speed of light (c) turn on physical dimensions on to the abstract operators. The last term has the dimension of energy (Mc^2) and dimension of $c\nabla$ is (1/time) that multiplied by $\hbar$ (energy x time) gives dimension of energy too. In Special Relativity theory use $E/c = p^o = p_o$ as being the time-component of the momentum 4-vector (see eq.(6.1.4)).

The relationships between matrices $\underline{\underline{\alpha}}_1, \underline{\underline{\alpha}}_2, \underline{\underline{\alpha}}_3, \underline{\underline{\alpha}}_4$ are derived by using an iterated eq. (6.2.2). Imposing fulfillment of a Klein-Gordon-Schrödinger equation for each component, the matrices $\underline{\underline{\alpha}}$ and $\underline{\underline{\alpha}}_4$ must satisfy the relations

$$\underline{\underline{\alpha}}^i\,\underline{\underline{\alpha}}^j + \underline{\underline{\alpha}}^j\,\underline{\underline{\alpha}}^i = 2\,g^{ij}\,\underline{\underline{1}} \qquad (6.2.4)$$

$$\underline{\underline{\alpha}}^i\,\underline{\beta} + \underline{\beta}\,\underline{\underline{\alpha}}^i = \underline{0} \qquad (6.2.5)$$

$$\underline{\underline{\alpha}}_4^{\,2} = \underline{\beta}^2 = \underline{1} \qquad (6.2.6)$$

The metric matrix is defined as: $g_{00} = 1$, $g_{11} = g_{22} = g_{33} = -1$, $g_{ij} = 0$ $(i \neq j)$. A representation for these matrices obtain with the set of 2x2 Pauli spin matrices:

$$\begin{aligned} & \underline{\underline{\alpha}}^1 = \begin{bmatrix} \underline{0} & \sigma_1 \\ \sigma_1 & \underline{0} \end{bmatrix}; \quad \underline{\underline{\alpha}}^2 = \begin{bmatrix} \underline{0} & \sigma_2 \\ \sigma_2 & \underline{0} \end{bmatrix}; \\ & \underline{\underline{\alpha}}^3 = \begin{bmatrix} \sigma_3 & \underline{0} \\ \underline{0} & -\sigma_3 \end{bmatrix}; \quad \underline{\underline{\alpha}}^4 = \underline{\beta} = \begin{bmatrix} \underline{1} & \underline{0} \\ \underline{0} & -\underline{1} \end{bmatrix} \end{aligned} \qquad (6.2.7)$$

Note that upper or lower indexes for Pauli matrices are irrelevant: $\sigma^k = \sigma_k$. A simple transformation obtains with gamma matrices: $\gamma^o = \underline{\underline{\beta}}$ and $\gamma^k = \underline{\underline{\beta}}\,\underline{\underline{\alpha}}^k$ leading to a so-called covariant Dirac form:

$$(-i\,\gamma^\mu\,\partial_\mu + M\,c/\hbar\,)\,\Psi = 0 \qquad (6.2.8)$$

We suppress double underline to agree with standard notation. Also, set:

$$p = \gamma\,.\,\hat{p} = \gamma^\mu\,\hat{p}_\mu = \gamma^0\,\hat{p}^0 - \vec{\gamma}\,.\,\vec{p} \qquad (6.2.9)$$

Use short hand notation:

$$\vec{\gamma} = (\gamma^1,\gamma^2,\gamma^3)\;;\;\vec{p} = (\hat{p}^1,\hat{p}^2,\hat{p}^3)\;;\;\gamma_\mu = g_{\mu\nu}\,\gamma^\nu \qquad (6.2.10)$$

The explicit representation of gamma matrices (with notation change to align our writing with standard use) is:

$$\gamma^0 = \begin{bmatrix} \underline{1} & \underline{0} \\ \underline{0} & -\underline{1} \end{bmatrix};\;\gamma^k = \underline{\underline{\beta}}\,\underline{\underline{\alpha}}^k = \begin{bmatrix} \underline{0} & \sigma^k \\ -\sigma^k & \underline{0} \end{bmatrix};$$
$$\gamma^5 = i\,\gamma^0\,\gamma^1\,\gamma^2\gamma^3 = \begin{bmatrix} \underline{0} & \underline{1} \\ \underline{1} & \underline{0} \end{bmatrix} \qquad (6.2.11)$$

Including the 4x4 unit matrix (that implicitly multiplies the term $Mc/\hbar$ in eq.(6.2.8)), the gamma set contains 6 matrices.

In a particle-like perspective, $H = \gamma^0 Mc/\hbar = \underline{\underline{\beta}}\,Mc/\hbar$ is the Hamiltonian in the *rest frame*. For $c=1=\hbar$ the numeric factor $Mc/\hbar$ has dimension of inverse length; in a more rigorous approach it is not possible to use the expression, $p = \gamma\,.\,p = \gamma^\mu\,p_\mu = \gamma^0\,p^0 - \vec{\gamma}\,.\,\vec{p}$, and simply put $\vec{p} = \vec{0}$ to define the rest frame. From our point of view, to do this assignment is equivalent to define a mapping at the fence. The introduction of I-frames incorporates a concept of rest-frame, but if we had a quantum system in Hilbert space that we were projecting onto a frame, this quantum state cannot just vanish. The question is: what is a rest frame at the fence now?

An answer can be cast in the following terms. The rotation group was used to set up base sets able to represent quantum state with the help of an I-frame independently of its linear state of motion. Boosts were not taken into account and, precisely, one thinks that a fence-rest-frame does the job of projecting that part of the abstract quantum state. Because Special Relativity tells us that massive (simple) systems can be classified according to their mass (M) and spin (**S**) we follow the dynamics with the Hamiltonian $H = \gamma^0 M\,c/\hbar$ constructed along semi-classical lines. To make a long

story short, examine the four independent base vectors:

$$u+ = \begin{bmatrix}1\\0\\0\\0\end{bmatrix};\ u- = \begin{bmatrix}0\\1\\0\\0\end{bmatrix};\ v+ = \begin{bmatrix}0\\0\\1\\0\end{bmatrix};\ v- = \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \qquad (6.2.12)$$

They are eigenvectors to the vector spin operator $\vec{\Sigma}$ defined by:

$$\vec{\Sigma} = \begin{pmatrix}\vec{\sigma} & \underline{0}\\ \underline{0} & \vec{\sigma}\end{pmatrix};$$
$$\vec{\sigma} = \underline{\beta}\,(\underline{\alpha}^1, \underline{\alpha}^2, \underline{\alpha}^3) = (\gamma^1, \gamma^2, \gamma^3) \qquad (6.2.13)$$

Note that $(1/2)\hbar\ \vec{\Sigma}$ is the spin angular momentum operator and what we have actually done is to determine the operator for any frame you might consider at rest. For example,

$$\vec{\Sigma}^1\, u^+ = \sigma^1 \begin{bmatrix}1\\0\end{bmatrix};\ \vec{\Sigma}^2\, u^+ = \sigma^2 \begin{bmatrix}1\\0\end{bmatrix};\ \vec{\Sigma}^3\, u^+ = \sigma^3 \begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\0\end{bmatrix}$$
$$\vec{\Sigma}^1\, u^- = \sigma^1 \begin{bmatrix}0\\1\end{bmatrix};\ \vec{\Sigma}^2\, u^+ = \sigma^2 \begin{bmatrix}0\\1\end{bmatrix};\ \vec{\Sigma}^3\, u^+ = \sigma^3 \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\1\end{bmatrix} \qquad (6.2.14)$$

In one word, the two-components of base 4-vectors of eq. (6.2.12) are renamed spinors and belong to Hilbert space.

Pause at this point to introduce some language help. Observe the upper component of u^+ and u^- and for v^+ and v^- the lower components correspond to $|\uparrow>$ and $|\downarrow>$ (α and β) base functions of Section 3.5.2. The 4-spinor admits a partitioning into upper and lower 2-spinor components. This is a useful way to refer to the structure of these mathematical objects; we retain the following definitions:

$$u_1 = \begin{bmatrix}1\\0\end{bmatrix};\ u_2 = \begin{bmatrix}0\\1\end{bmatrix};\ \text{and } v_1 = \begin{bmatrix}1\\0\end{bmatrix};\ v_2 = \begin{bmatrix}0\\1\end{bmatrix} \qquad (6.2.15)$$

Now we move onto Dirac equation to obtain spinors for a general Lorentz frame. This is equivalent to find solutions to eq.(6.3.8). We basically put attention to boosters that will be the intermediate mappings between Hilbert space and real space. Taking the Hamiltonian operator eq. (6.2.3) and the 4-spinor with components u_1 and u_2 times the plane wave with positive energy label, i.e. $\Psi = (u_1\ u_2)^T \exp(i(\mathbf{p}.\mathbf{q}-E(\lambda)\,t)/\hbar)$ a system of equations follows:

$$E(\lambda)\,u_1 = \vec{\sigma}.\,\mathbf{p}\,u_2 + M\,u_1 \qquad (6.2.16a)$$

$$E(\lambda)\,u_2 = \vec{\sigma}.\,\mathbf{p}\,u_1 + M\,u_2 \qquad (6.2.16b)$$

The determinant of this system of equation must equate to zero thereby leading to

$$E(\lambda)^2 = \mathbf{p}^2+M^2 \qquad (6.2.17)$$

Define $E_p = +\sqrt{(\mathbf{p}^2+M^2)}$, then $E(\lambda)= \lambda\, E_p$ and conventionally, equations (6.2.16) describe $\lambda = +1$ case that we name as positive energy-label solutions. For the negative energy-label solutions replace the 2-spinors u by those v and take $\lambda =-1$.

From eq.(6.2.16b) with $\lambda =+1$, one obtains spinor u_2 as a function of u_1 as:

$$u_2 = \vec{\sigma}.\,\mathbf{p}\,u_1/(E_p+M) \qquad (6.2.18)$$

The 4-spinor takes on the form

$$u+= N\begin{bmatrix} u_1 \\ \dfrac{\vec{\sigma}.\vec{p}}{(Ep+M)}u_1 \end{bmatrix} \qquad (6.2.19a)$$

The spinor is now normalized so that one can show:

$$u+= \sqrt{((E_p+M)/2M)}\begin{bmatrix} u_1 \\ \dfrac{\vec{\sigma}.\vec{p}}{(Ep+M)}u_1 \end{bmatrix} \qquad (6.2.19b)$$

The normalization factor $u^\dagger u$ including light velocity reads as E_p/Mc^2 thus, if the kinetic energy is negligible in front of rest mass energy then $E_p=Mc^2$ and the spinors are normalized to one: $u^\dagger u = 1$. The relativistic effect shows up neatly in the so called small component $u_2 = \vec{\sigma}.\,\mathbf{p}\,u_1/(E_p+M)$. The spinor for u- obtains by replacing u_1 by u_2 in the above equations.

We have two interesting vector operators: spin operator $\hat{S}=(1/2)\,\hbar\,\vec{\Sigma}$ and $\hat{p}$. One can form an invariant (scalar) operator measuring the direction of the spin and momentum vectors: This is the helicity operator $\hat{\Lambda}_S= \hat{S}\bullet\hat{p}/|\mathbf{p}|$. This operator commutes with Dirac Hamiltonian and its eigen values can hence be used to label quantum base states.

For an electron base state in the direction $\mathbf{i}_3$, $\mathbf{p}$=(0,0,p) the helicity operator in this direction looks as:

$$\hat{\Lambda}_S = \hat{S}_3 = (1/2)\,\hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad (6.2.20)$$

The eigen values are ±1/2.

The base states along $\mathbf{i}_3$ direction can be denoted as:

$$\Psi_{p,\lambda,+1/2} = \sqrt{((E_p+M)/2M)} \begin{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ \dfrac{\sigma_3 p}{Mc + \Lambda E_p} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{bmatrix} \exp(i(px_3 - \lambda\, E_p t)/\hbar) \qquad (6.2.21a)$$

and

$$\Psi_{p,\lambda,-1/2} = \sqrt{((E_p+M)/2M)} \begin{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \dfrac{\sigma_3 p}{Mc + \Lambda E_p} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{bmatrix} \exp(i(px_3 - \lambda\, E_p t)/\hbar) \qquad (6.2.21b)$$

These equations complete the calculation of base states for a system having mass M, and spin 1/2.

We discover a number of base states larger than those one would imagine for a simple particle system. In fact, this latter concept is not adequate to discuss Dirac's equation. Positive and negative energy labels must now be correlated to laboratory (real) world. But we have not yet included the electric charge into this model and a first step is to do it.

6.3. Hydrogen-like atoms: relativistic models

Hydrogen-like systems are one-electron systems in an external potential generated by a charge Ze; examples are He^{+1}, C^{+5} and U^{+91}.

An external spherically symmetric electrostatic potential A_o =V(r) can be a model to a number of situations found in real life. The case at hand is a nucleus with positive charge Ze located at the origin of the I-frame used to study free electron system; this is a semi-classic model because the nuclei's quantum state (e.g., spin) are not taken into account, only the Coulomb field enters the picture. The units to be used now are e= c = $\hbar$ =1. The electromagnetic four vector looks like [V(r),0,0,0]. Dirac equation interacting with this field is:

$$i\,\partial\psi/\partial t = \hat{H}_{Dirac}\psi = [-i\,\underline{\underline{\alpha}}\cdot\nabla + \underline{\underline{\beta}}\,M + V(r)]\,\psi. \qquad (6.3.1a)$$

We present the solutions to this equation following F.Gross (Relativistic Quantum Mechanics and Field Theory, Wiley, New York, 1993). The solutions can be cast in terms of spinors $\psi^{k}_{jm}(\mathbf{r})\exp(-iEt/\hbar)$ where the space part is given by:

$$\psi^{k}_{jm}(\mathbf{r}) = \begin{bmatrix} F^{k}_{j}(r)\Im^{k}_{jm}(\hat{r}) \\ iG^{k}_{j}(r)\Im^{-k}_{jm}(\hat{r}) \end{bmatrix} \qquad (6.3.2)$$

The symbol $\Im^{k}_{jm}(\hat{r})$ is an angular function that in the spinor components is multiplied by different radial functions. The ansatz (6.3.2) is substituted in (6.3.1a) and two coupled equations follow:

$$(E\,\underline{\underline{1}} - (M + V(r))\underline{\underline{1}})\; F^{k}_{j}(r)\Im^{k}_{jm}(\hat{r}) = -i\,\underline{\underline{\sigma}}\cdot\nabla\; iG^{k}_{j}(r)\Im^{-k}_{jm}(\hat{r}) \qquad (6.3.1b)$$

$$(E\,\underline{\underline{1}} + (M - V(r))\underline{\underline{1}})\; iG^{k}_{j}(r)\Im^{-k}_{jm}(\hat{r}) = -i\,\underline{\underline{\sigma}}\cdot\nabla\; F^{k}_{j}(r)\Im^{k}_{jm}(\hat{r}) \qquad (6.3.1c)$$

The angular function $\Im^{k}_{jm}(\hat{r})$ is a linear superposition of spherical harmonics:

$$\Im^{k}_{jm}(\hat{r}) = -\mathrm{sgn}(k)\sqrt{\frac{k+\frac{1}{2}-m}{2k+1}}\begin{bmatrix}1\\0\end{bmatrix}Y_{\ell,m-1/2} + \sqrt{\frac{k+\frac{1}{2}+m}{2k+1}}\begin{bmatrix}0\\1\end{bmatrix}Y_{\ell,m+1/2} = -\mathrm{sgn}(k)\sqrt{\frac{k+\frac{1}{2}-m}{2k+1}}\,\alpha Y_{\ell,m-1/2} + \sqrt{\frac{k+\frac{1}{2}+m}{2k+1}}\,\beta\, Y_{\ell,m+1/2} \qquad (6.3.3)$$

The 2-spinors α and β are used. The quantum number $k = \pm(j+1/2)$ is positive if $\ell = j+1/2$ implying by this that $k=\ell$. For the negative case, if $\ell=j-1/2$ then $k=-(\ell+1)$. The quantum numbers j and k determine the parity of the quantum base state. Thus, the correct choice of ℓ, for a corresponding j can be seen determining the parity.

To reduce Dirac equations one uses the identity with the unit vector $\hat{r}$:

$$-i\,\underline{\underline{\sigma}}\cdot\nabla = -i\,\underline{\underline{\sigma}}\cdot\,\hat{r}\frac{\partial}{\partial r} + i\,\underline{\underline{\sigma}}\cdot\hat{r}\,\underline{\underline{\sigma}}\cdot\frac{\hat{L}}{r} \qquad (6.3.4)$$

The angular functions have the following properties:

$$\underline{\underline{\sigma}}\cdot\hat{r}\;\Im_{jm}^{\;k}(\hat{r}) = -\;\Im_{jm}^{-k}(\hat{r}) \text{ and}$$
$$\underline{\underline{\sigma}}\cdot\frac{\hat{L}}{r}\;\Im_{jm}^{\;k}(\hat{r}) = -(k+1)/r\;\Im_{jm}^{\;k}(\hat{r}) \qquad (6.3.5)$$

Thus, for eq.(6.3.3c) one gets for the off-diagonal terms

$$i\,c\hbar\,\underline{\underline{\sigma}}\cdot\nabla\;\; F_j^k(r)\Im_{jm}^{\;k}(\hat{r}) =$$
$$(-i\,\underline{\underline{\sigma}}\cdot\,\hat{r}\frac{\partial}{\partial r} + i\,\underline{\underline{\sigma}}\cdot\hat{r}\,\underline{\underline{\sigma}}\cdot\frac{\hat{L}}{r})\,F_j^k(r)\Im_{jm}^{\;k}(\hat{r}) =$$
$$(-i\,\underline{\underline{\sigma}}\cdot\hat{r}\;\Im_{jm}^{\;k}(\hat{r})\;\frac{\partial}{\partial r}F_j^k(\mathrm{r}) +$$
$$i\,\underline{\underline{\sigma}}\cdot\hat{r}(\,\underline{\underline{\sigma}}\cdot\frac{\hat{L}}{r}\Im_{jm}^{\;k}(\hat{r})\,)\;\; F_j^k(\mathrm{r}) =$$
$$(+\,i\;\Im_{jm}^{-k}(\hat{r})\;\frac{\partial}{\partial r}F_j^k(\mathrm{r}) \;\; - i\,\underline{\underline{\sigma}}\cdot\hat{r}\;(k+1)/r\;\Im_{jm}^{\;k}(\hat{r})\,F_j^k(\mathrm{r}) =$$
$$(\frac{\partial}{\partial r}F_j^k(\mathrm{r}) \;\; + (k+1)/r\;F_j^k(\mathrm{r}))\;(i\;\Im_{jm}^{-k}(\hat{r})) \qquad (6.3.6)$$

$$(E\,\underline{\underline{1}} + (\,Mc^2 - V(r))\underline{\underline{1}})\;\; iG_j^k(r)\Im_{jm}^{-k}(\hat{r}) -$$
$$(\frac{\partial}{\partial r}F_j^k(\mathrm{r}) + (k+1)/r\;F_j^k(\mathrm{r}))\;(i\,\Im_{jm}^{-k}(\hat{r})) \qquad (6.3.1c')$$

The phase factor cancels out and multiplying by $(\Im_{jm}^{-k}(\hat{r}))^*$ the angular part is integrated out.

The calculations on eq.(6.3.1b) lead to the coupled differential equations:

$$[E - m - V(r)]\;\; F_j^k(r) \;\; =$$
$$(-(1-k)/r\,)\;\; G_j^k(r) \;\; - \;\mathrm{d}\,G_j^k(r)\,/\mathrm{dr} \qquad (6.3.7a)$$

$$[E + m\text{-}V(r)]\ G_j^k(r) =$$
$$((1+k)/r)\ F_j^k(r) + d\,F_j^k(r)/dr \qquad (6.3.7b)$$

Solving these equations yields the complete spinor for positive energy label state.

The solutions for hydrogen-like atoms are obtained once V(r) is replaced by -Zα/r; where α is the fine structure constant. Power series are used to determine the r-dependence and N is an integer indicating where the series must be terminated to insure convergence. The energy levels are obtained as:

$$E_{N,k} = m\left[1 - \frac{(Z\alpha)^2}{(N+|k|)^2 + 2N\left(\sqrt{k^2-(Z\alpha)^2} - |k|\right)}\right]^{1/2} \qquad (6.3.8)$$

Because |k| = j+1/2 and there is no solution for N=0 & k>0, it is convenient to introduce a new quantum number n as follows:

$$n = N + |k| \geq 1 \quad \& \quad -n \leq k \leq n \qquad (6.3.9)$$

This quantum number coincides with the familiar non-relativistic radial quantum number. Using n and |k| in terms of j, the energy levels can be written

$$E_{nj} = m\sqrt{1 - \frac{(Z\alpha)^2}{n^2 + 2(n-(j+1/2))\left[\sqrt{(j+1/2)^2-(Z\alpha)^2} - (j+1/2)\right]}} \qquad (6.3.10)$$

This is the exact expression for the energy eigen values that depend only on two quantum numbers for Dirac equation (6.3.1) in the spherical symmetric field V(r) = -Zα/r. Take Z=1 and we get the eigen values for the hydrogen atom.

An expansion of the square root leads to:

$$E_{nj} - m \approx -m(Z\alpha)^2/2n^2 -$$
$$m(Z\alpha)^4/2n^4\left[\frac{n}{j+1/2} - 3/4\right] + O((Z\alpha)^6) \qquad (6.3.11)$$

The first term corresponds to Bohr theory; the expression includes fine structure results exactly.

To get a counting of states based on standard orbital and spin angular momentum, let us introduce the spinors $W_\ell^{\ m}(+)$ and $W_\ell^{\ m}(-)$:

$$W_\ell^{\,m}(+) = \begin{bmatrix} \sqrt{\left(\frac{\ell+m}{2\ell+1}\right)}\,Y_\ell^{\,m-1} \\ \sqrt{\left(\frac{\ell-m+1}{2\ell+1}\right)}\,Y_\ell^{\,m} \end{bmatrix}\alpha \;;\quad W_\ell^{\,m}(-) = \begin{bmatrix} \sqrt{\left(\frac{\ell-m+1}{2\ell+1}\right)}\,Y_\ell^{\,m-1} \\ -\sqrt{\left(\frac{\ell+m}{2\ell+1}\right)}\,Y_\ell^{\,m} \end{bmatrix}\beta \qquad (6.3.12)$$

These spinors satisfy the angular momentum equations:

$$\hat{J}^{\,2}\, W_\ell^{\,m}(+) = j(j+1)\, W_\ell^{\,m}(+);\;\; j = \ell + 1/2$$
$$\hat{J}_3\;\; W_\ell^{\,m}(+) = u\, W_\ell^{\,m}(+);\; u = m\text{-}\ell\text{+}1/2 = m\text{-}1/2 \qquad (6.3.13)$$

and

$$\hat{J}^{\,2}\, W_\ell^{\,m}(-) = j(j+1)\, W_\ell^{\,m}(-);\; j = \ell - 1/2$$
$$\hat{J}_3\;\; W_\ell^{\,m}(-) = u\, W_\ell^{\,m}(-);\; u = m\text{-}1/2 \qquad (6.3.14)$$

Possible values for j and u are: j=1/2,3/2,…, u=-j,-j+1,…,j-1,j. The two possible ways to combine spin and orbital angular momenta are given by eqs.(6.3.13) and (6.3.14).

There is some subtlety when counting possible values of u. In $W_\ell^{\,m}(+)$ the index m runs as usual from – l to + l except that it can also take the value ℓ +1 even if the spherical harmonic does not exists. But the amplitude for that component is ℓ–m+1 so that we get zero while the other component is fine, 2ℓ+1, the spherical harmonic being then $Y_\ell^{\,\ell}$. Therefore $W_\ell^{\,\ell+1}(+)$ is well defined. Thus, there are 2j+1 values for u equivalent to 2ℓ+2 different values. For $W_\ell^{\,m}(-)$ the index m goes from - ℓ+1 up to l. The value m= –ℓ is forbidden; similarly m= ℓ+1. Thus the 2j+1 values are covered by 2ℓ different values.

Now count the total number of states for a given n is shown in eq.(6.3.6). The solutions to the differential equations put constraints to the N values. For N=0 we must have k<0. This means that only the value k=-(j+1/2) = -n is allowed and k=n is forbidden. On each level E_{nj} there are 2(2j+1) = 4(j+1/2) = 4 |k| states that correspond to each value of |k|= j+1/2 = 1,2,…,n-1 and for |k|=n there are 2j+1= 2(j+1/2)=2|k|=2n states. Adding all these states for a given quantum number n we get:

$$4\,\Sigma_{|k|=1,n-1}\,|k| + 2n = 4\,n(n-1)/2 + 2n = 2n^2 \text{ states.} \qquad (6.3.15)$$

This is a classical result obtained from counting states derived from the total angular momentum.

Dirac equation represents a tremendous achievement in the quest for understanding the behavior of material systems for which base states with half-integer angular momentum are the building blocks. Yet, it is not a particle equation as initially thought. Furthermore, it is not a representation of a material system, it is rather a model of quantum states the system may show up at the Fence. There is a set of base spinors for the particle-state and another to the anti-particle-state the complete Hilbert space is the direct sum.

The base $[\Psi_1\ \Psi_2\ \Psi_3\ \Psi_4\ \Phi_1\ \Phi_2\ \Phi_3\ \Phi_4]$ has dimension eight and includes both material systems states. The 4-spinor $[\Psi_1\ \Psi_2\ \Psi_3\ \Psi_4.]$ stands for electrons, say, and $[\Phi_1\ \Phi_2\ \Phi_3\ \Phi_4]$ for positrons. A quantum state with amplitudes different from zero only in the particle-state zone would represent a quantum state for the electronic system. We are approaching difficulties in the sense that asymptotically there must be two I-frames describing the complex system. We realize that the level of description attained concerns the quantum states not the particles.

For pair-production the amplitudes at the charge conjugated states are equal and different from zero. The relationships are those found in the relativistic theory with charge-conjugation symmetry.

The elements of the base set are related by conjugation properties as discussed above. Of course, a 4-dimensional representation can be retained if the base set obtained by charge-conjugation is written as $[\Phi_1\ \Phi_2\ \Phi_3\ \Phi_4]$ with the standard rules relating to $[\Psi_1\ \Psi_2\ \Psi_3\ \Psi_4.]$. If you only work to obtaining base states for particle-states, there is no need for 8-dimensional vectors. The 4-spinor refers to only one energy-label case. In the example above $[\Psi_1\ \Psi_2\ \Psi_3\ \Psi_4]$ corresponds to positive energy-label while $[\Phi_1\ \Phi_2\ \Phi_3\ \Phi_4]$ refers to negative-energy-label, Cf. Eq.(6.2.12). Charge conjugation changes the sign of momentum $\mathbf{p}$ into $-\mathbf{p}$ and the energy label; the average values of the spin operators also change sign, s into -s. Now, after charge conjugation negative-label energy spectrum appears as a positive energy label spectrum. For the standard particle interpretation the negative energy solutions of the Dirac equation correspond to the charge-conjugated solutions of positive energy, and vice versa. This symmetry grants a reduction of the 8-diemensional base down to 4-spinors. But do not forget that calculation of the time evolution operator will always require both subspaces. Otherwise, paradoxes will pop up.

Dirac equation provides fundamental corrections in optical spectra. Also, this theory is the only one that describes correctly the angular momentum thereby providing an adequate nomenclature for magnetic states. In fact, as we saw above, it establishes the physical fact that neither the orbital nor spin angular momentum is conserved (constant of motion) and that only the total angular

momentum is conserved. The quantum number characterizing base states differ from the standard L-S coupling as well as from the one obtained from Pauli equation.

Dirac equation does not yield an electron g-factor in full agreement with the experimentally determined one; it also fails to reproduce the splitting of 2p2s base states. These are effects related to missing couplings with the electromagnetic field. Today, they are described in the quantum electrodynamics (QED) framework. In the present context it means a coupling between the conjugated spaces via the quantized electromagnetic field.

6.4. Non-relativistic limit: Pauli equation

Consider the system in an I-frame such that the base spinor fulfils the equation: $\hat{p}\Psi=0$. This state is also known as "electron at rest". The Dirac equation yields:

$$i\hbar\,\partial\psi/\partial t = \underline{\beta}\,Mc^2\,\psi \qquad (6.4.1)$$

Only time dependence is apparent. The four independent base spinors below fulfill the eq. above:

$$u+ = \psi^{(1)} = \begin{bmatrix}1\\0\\0\\0\end{bmatrix} \exp(-iMc^2t/\hbar);$$

$$u- = \psi^{(2)} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \exp(-iMc^2t/\hbar);$$

$$v+ = \psi^{(3)} = \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \exp(iMc^2t/\hbar);$$

$$v- = \psi^{(4)} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \exp(iMc^2t/\hbar) \qquad (6.4.2)$$

These base spinors are equivalent to those found in eq. (6.2.12) and can be normalized if we use eqs.(6.2.21a and b) by putting there the momentum eigen value equal to zero. Note that this spinorial set satisfies Dirac equation with Hamiltonian $(-ic\hbar\underline{\underline{\boldsymbol{\alpha}}}\cdot\nabla + \underline{\beta}Mc^2)$ because in eqs. (6.4.2) has no space dependence: $(-i\,c\,\hbar\,\underline{\underline{\boldsymbol{\alpha}}}\cdot\nabla + \underline{\beta}\,Mc^2)v+ = 0$; the phrase itself, implying that spinors (6.4.2) fulfill Dirac equation, has no meaning. To make progress the spinor ψ

must have space dependence and the system must sense external electromagnetic fields. From our perspective, if there are relativistic quantum states, there must be available base states to construct a representation.

The aim is to show that this equation reproduces the two-component Pauli equation. To do this one has to introduce the electromagnetic four potential

$$A^{\mu} = (A_o(\mathbf{x}),A_1(\mathbf{x}),A_2(\mathbf{x}),A_3(\mathbf{x})) = (A^o(\mathbf{x}),A^1(\mathbf{x}),A^2(\mathbf{x}),A^3(\mathbf{x}))= (A_o(\mathbf{x}), \mathbf{A}(\mathbf{x})) \qquad (6.4.3)$$

In classical electrodynamics $(e/c)A^{\mu}$ is the momentum" transferred" to the field by the charge e so that the canonical momentum $\hat{p}^{\mu}$ must be corrected to get $\hat{p}^{\mu} - (e/c)A^{\mu} \equiv \hat{\Pi}^{\mu}$, that is the kinetic momentum in the minimal coupling model (see Sect. 1.3). Now Dirac equation takes on the form:

$$i\hbar\, \partial\psi /\partial t = (c\underline{\underline{\boldsymbol{\alpha}}} \cdot(\hat{p} -(e/c)\mathbf{A}) + eA_o \underline{\underline{1}} + \underline{\underline{\beta}}\, Mc^2)\psi \qquad (6.4.4)$$

The spinor ψ is partitioned into a pair of two-components spinors $[\tilde{\varphi} \quad \tilde{\xi}]$ and inserted into the above equation. Because the rest energy is the largest energy in a non relativistic limit it is removed with the ansatz:

$$(\tilde{\varphi} \quad \tilde{\xi})^T = (\varphi \quad \xi)^T \exp(-iMc^2t/\hbar);$$

Eq.(6.4.4) takes on the form:

$$i\frac{\partial}{\partial t}\begin{bmatrix}\varphi\\ \xi\end{bmatrix} = c\begin{bmatrix}\hat{\sigma}\cdot\hat{\Pi}\xi\\ \hat{\sigma}\cdot\hat{\Pi}\varphi\end{bmatrix} + eA_o\begin{bmatrix}\varphi\\ \xi\end{bmatrix} - 2\,Mc^2\begin{bmatrix}0\\ \xi\end{bmatrix} \qquad (6.4.5)$$

If the potential term (eA_o) is negligible in front of the rest mass energy, the 2-spinor ξ can be cast in term of the 2-spinor φ as follows: $\xi = \frac{\hat{\sigma}\cdot\hat{\Pi}}{2Mc}\varphi$. From this relation it can be seen that ξ is the small component and $\partial\xi /\partial t = 0$. The equation for the large component reads now:

$$i\hbar\, \partial\varphi /\partial t = \frac{(\hat{\sigma}\cdot\hat{\Pi})(\hat{\sigma}\cdot\hat{\Pi})}{2M}\varphi + eA_o\varphi \qquad (6.4.6)$$

Introducing the definitions from electrodynamics of the magnetic and electric fields, **B** and **E** in terms of the four potential components one gets: **B** = curl **A** = $\nabla\wedge\mathbf{A}$, and eq.(6.4.6) can be transformed into the 2-spinor Pauli equation:

$$i\hbar\,\partial\varphi/\partial t = \{\hat{p}^2/2M - (e/2Mc)(\hat{L} + 2\hat{S})\cdot\mathbf{B} + eA_o\}\,\varphi \quad (6.4.7)$$

The most striking result is that, in the non-relativistic limit, the Dirac equation transforms into the Pauli equation. This latter was already known to be adequate to describe spin 1/2 effects.

For future reference we quote Pauli Hamiltonian below:

$$\hat{H}_{\text{Pauli}} = ((\hat{p}-(e/c)\mathbf{A})^2/2M + eA_o)\,\mathbf{1} - (e/2Mc)\boldsymbol{\sigma}\cdot\mathbf{B} + (e/4M^2c^2)(1/r)(dA_o/dr))\,\boldsymbol{\sigma}\cdot\mathbf{L} \quad (6.4.8)$$

$\mathbf{1}=\boldsymbol{\sigma}^2$ is a 2D unit matrix.

The Pauli Hamiltonian applies to electrically charged 2-spinors including interactions between the charges and a generic transverse electromagnetic field, a magnetic field via Pauli spin matrices and a coupling between orbital and spin angular momenta.

6.5. Effective Hamiltonians

The role played by the small component is crucial to get meaningful effective result. As a matter of fact, the partitioning can be made subtle to actually get an effective Hamiltonian containing most of the relativistic effects in atomic systems found before Dirac proposed his equation. The path to get such operator is not reproduced here, only the final result:

$$H_{\text{eff}} = (\hat{p}-(e/c)\mathbf{A})^2/2M + eA_o - (\hat{p})^4/8M^3c^2 - (e/2Mc)\,\boldsymbol{\sigma}\cdot\mathbf{B} + e[\nabla^2 A_o]/8M^2c^2 + (e/4M^2c^2)(1/r)(dA_o/dr))\,\boldsymbol{\sigma}\cdot\mathbf{L} \quad (6.5.1)$$

Observe that the square bracket means that the operator ∇^2 operates only within brackets.

The terms incorporated by H_{eff} were well known before the discovery of Dirac equation. The derivation from Dirac's equation is to be regarded as a great success and confirmation that the Dirac equation does give a correct description of the interactions of spin 1/2 base states with an EM field.

6.5.1.Fine structure term: $(\hat{p})^4/8M^3c^2$

This is a relativistic correction to the kinetic energy. The correction stems from the expansion of $E/c = (M^2 c^2 + p^2)^{1/2} = Mc(1+ p^2/M^2 c^2)^{1/2}$.

6.5.2. Darwin term

This correction term concerns the value of a wave function at the atomic origin. It reads as:

$$e[\nabla^2 A_o]/8M^2c^2 = e[\nabla^2 V]/8M^2c^2 = -e/8M^2c^2\ \nabla\cdot\mathbf{E}= - Ze^2/8M^2c^2\delta^3(r)$$

Here, $V= A_o$ is the Coulomb potential of a positive charge Ze located at the frame origin; Because of the delta function, this term is non-zero for S-states only. This term reflects positive-negative energy labeled states interferences (Zitterbewegun).

6.5.3.Spin-orbit correction term

The form for this correction in the atomic case reads:

$$(e\hbar/4M^2 c^2)(1/r)(dA_o/dr))\ \boldsymbol{\sigma}\cdot\mathbf{L}= e/(2M^2 c^2)(1/r)(dA_o/dr))\ \mathbf{S}\cdot\mathbf{L}$$

Note the substitution $\mathbf{S} = \hbar\boldsymbol{\sigma}/2$ for the spin operator. This term automatically includes Thomas precession. It is zero for L=0 states (S-states).

The importance for us is that given a 2L+1 multiplet, this operator would mix base states of spin to orbital angular momenta whenever a variation of the Coulomb field is present.

6.5.4. Magnetic field coupling term (Zeeman effect)

The correction term is given by $(e/2Mc)\ \boldsymbol{\sigma}\cdot\mathbf{B}$. This term combined to the linear one coming from expanding $(\hat{p}-(e/c)\mathbf{A})^2/2M$, namely,

$$-e/2Mc\ (\hat{p}\cdot\mathbf{A} + \mathbf{A}\cdot\hat{p}) = -\ e\hbar/2Mc\ \mathbf{B}\cdot\mathbf{L};$$

This leads to the Zeeman effect operator:

$$-(e/2Mc)\ \mathbf{B}\cdot(\hbar\ \mathbf{L}+\boldsymbol{\sigma}\ )=$$
$$-(e\hbar/2Mc)\ \mathbf{B}\cdot(\mathbf{L}+2\mathbf{S})$$

The factor $e\hbar/2Mc = \mu_o$ is Bohr magneton corresponding to 0.58×10^{-8} ev/gauss for the electron.

The importance of the spin-orbit coupling, especially in the context developed in this book, is not the magnitude of the energy corrections, but the fact that it breaks symmetries that hold in non-relativistic quantum theory.

With hindsight gleaned from KGS equation, it is apparent that the Hilbert space for the particle/anti-particle-states must be the direct sum of both elements. Spinors make the formalism somewhat less transparent that the one obtained for scalar base functions. With a little patience you can go through the calculation of the spectra for hydrogen-like atoms.

6.5.5. Hydrogen atom revisited

The 1-system corresponding to an hydrogen atom is used to examine the response of the model operator H_o derived from $(\hat{p}-(e/c)\mathbf{A})^2/2M + eA_o$ for the case where no transverse **A** is present:

$$\hat{H}_o = \hat{p}^2/2M + eA_o \qquad (6.5.5.1)$$

The longitudinal field A_o is taken as -Ze/r. The non-relativistic eigen functions and eigen energies, in particular for hydrogen Z=1 are known.

Consider the fine structure correction: $\hat{H}_1 = (\hat{p}^2)^2/2M^3c^2$. The first thing to do is a comparison of the order of magnitude for the correction: $<\hat{H}_1>/<\hat{H}_o>$.

$$<\hat{H}_1>/<\hat{H}_o> \approx (<\hat{p}^2>/2M^3c^2)/(1/2M)=$$
$$(<\hat{p}^2>/M^2c^2)=(McZ\alpha)^2/M^2c^2)= (Z\alpha)^2 \qquad (6.5.5.2)$$

α is the fine structure constant. For hydrogen, the ratio is about $(1/138)^2$ or 10^{-5}, smaller than the reduced mass effects. The fine structure correction to the energy is hence negligible. Of course, a different result obtains for energy gaps.

More interesting for future applications is the study of a magnetic field on hydrogen-like atoms. The effective Hamiltonian reads:

$$\hat{H}= \hat{p}^2/2M + eA_o - \mu_o\ \mathbf{B}\cdot(\mathbf{L}+2\mathbf{S}) =$$

$$\hat{p}^2/2M + eA_o - \mu_o \nabla\wedge\mathbf{A}\cdot(\mathbf{L}+2\mathbf{S}) \qquad (6.6.5.3)$$

The replacement on the second line uses eq.(6.1.4). The form shown by this operator is valid for a Coulomb Hamiltonian.

For molecular oxygen, the quantum state may have amplitudes at a triplet spin state and, consequently in presence of an electromagnetic field the spin multiplet will be split. This is in fact a first step in the activation process of $O_2(^3\Sigma_g^-)$ found on Earth atmosphere.

6.6. Relativistic "electron-only" theory

Dirac equation hides a place to accommodate charge conjugation symmetry. This makes particle-states and anti-particle-states to become related via charge conjugated Dirac operators. Also, parity-transformed base functions obeys the same Dirac equation as the original base function. In fact, different sets of 4x4 Dirac matrices can be used to show the non-relativistic limit of Dirac's theory, or develop the spinor point of view; e.g. a special set of gamma matrices makes charge conjugation identical with complex conjugation (see e.g. R.H.Good,Jr. Rev. Mod.Phys.27(1955)187-211 for detailed analyses). The important point is that any two sets of 4x4 Dirac matrices are connected by a similarity transformation. This is a theorem known as the fundamental theorem.

In few words, if an abstract quantum state is projected in Dirac-space, the wave function must be invariant to the way Dirac's gamma matrices are chosen so long they are related by the fundamental theorem. Different sets of gamma matrices will elicit different aspects of the same abstract quantum state.

Let us discuss some specific cases. The charge conjugation operator C is defined as the product: $-i\,\gamma^5\,\gamma^1\gamma^3 = -i\,\gamma^0\gamma^2$. Thus, the charge conjugated base function is: $\Psi_c = C\,\overline{\Psi}^t$, where $\overline{\Psi}^t$ is the transpose of the Dirac adjoint spinor,

$$\overline{\Psi} = \Psi^\dagger\gamma^0 .$$

In presence of an electromagnetic field the charge conjugated state fulfils the equation:

$$(\,i\,\hbar\,\gamma^\mu\,\partial_\mu - M\,c/\hbar\,)\,\Psi_c = -e\,\gamma^\mu\,A_\mu\,\Psi_c \qquad (6.6.1)$$

in the same external field Dirac equation for the electron states reads:

$$(\,i\,\hbar\,\gamma^\mu\,\partial_\mu - M\,c/\hbar\,)\,\Psi = +e\,\gamma^\mu\,A_\mu\,\Psi \qquad (6.6.2)$$

The solutions to eq.(6.6.1) for Ψ_c are closely related to that of eq.(6.6.2). Observe that these equations define two different Hamiltonians; one for charge +1, the other –1. Yet, a symmetry operation link both and if we use one equation to describe both charge states, the solutions for positive and negative energy labels transform separately under proper Lorentz transformations as well as under space inversion. Their solutions remain strictly separated from each other (free system).

As Feynman pointed out, the puzzle of negative energies for KGD and Dirac equations showed that the crucial idea necessary to wed quantum mechanics and relativity together was the existence of antiparticles and their base states.

Pair production and pair annihilation are well-established experimental phenomena. This makes Dirac's equation less puzzling.

A spinor for a free solution to the Dirac equation with positive energy label is denoted by u(p,s); the negative energy label case the spinor is denoted as v(p,s). Charge conjugation changes the sign of momentum **p** into –**p** and the energy label; the average values of the spin operators also change sign: s into -s. Now, after charge conjugation negative-label energy spectrum appears as a positive energy label spectrum. For the standard particle interpretation the negative energy solutions of the Dirac equation correspond to the charge-conjugated solutions of positive energy, and vice versa.

Hole theory is not discussed here, although it played an important role in the development of relativistic quantum mechanics, today it is superseded by contemporary field theory. Thus, one should not worry about negative energy solutions if a proper formalism is developed to calculate base states for atoms and molecules at a relativistic level with the help of Dirac equation.

The textbook theory presented above (except for the view expressed in this work concerning quantum states) corresponds to a one-electron model submitted to the Coulomb interaction of a nucleus. So far we focus attention first on the non-relativistic limit for this fundamental equation thereafter hydrogen-like systems are examined. Now, the relativistic theory for many electrons material has developed to a high level of accuracy; we will briefly examine some issues.

The Dirac Hamiltonian in eq.(6.2.3) for one electron is specialized for $\hbar$=1 units:

$$h_D = c\,\underline{\underline{\alpha}} \cdot -i\nabla + (\underline{\underline{\beta}} - 1)c^2 + V_{nuc} \qquad (6.6.3)$$

This operator is applied as a substitute for the Schrödinger one-electron operator in the electronic Hamiltonian for n-electrons and m-nuclei:

$$H_{el,D} = \Sigma_{i=1,n}\, h_{D,i} + \Sigma_{i<j}\, (1/|\mathbf{r}_i - \mathbf{r}_j|) \qquad (6.6.4)$$

$$V_{nuc,i} = \Sigma_{k=1,m}\, (1/|\mathbf{r}_i - \mathbf{R}_k|) \qquad (6.6.5)$$

This four-component formulation covers the whole periodic table of elements.

As commented by Reither, one should not mix up large and small component with “particle” and “ antiparticle” states. From the presentation given here it is clear that each type of base function is represented by 4-vectors each. The Hamiltonian operator eq.(6.6.3) corresponds to a semi-classic situation. For V_{nuc} is the nucleus-electron interaction operator where the quantum system standing for a nucleus is replaced by a positive charge acting as a source of Coulomb potential for electrons.

The reader is invited to visit specialized sources such as: M.Reither, Theor.Chem. Acc.116(2006)241-252); R.Mastalerz et al., J.Chem.Phys. 127(2007) 074105); and references therein. MOLCAS quantum chemistry package version 7 is available and many of its features published in: Aquilante et al., J.Comp.Chem. 31 (2009) 224-247.

The computation procedures never mix up base states of particle/anti-particle material systems. In this manner one can keep the idea associated to matter conseving scheme characteristic of the non-relativistic models. This is not a dis-advantage only that one has to be careful not mixing different levels of presentation. The relativistic effects are translated to the conservation of total angular momentum. However, standard probabilistic interpretation of wave functions coming fromthe family of quantum Euler-Lagrange equation is not granted.

6.7. Towards a Field Theory Framework

The construction of the non-relativistic approach in preceding chapters (as well as following ones) is based on conservation assumption of the material basic elements; electrons and nuclei numbers do not change. In the relativistic approach the number of material elements (particles and anti-particles) can change in many different manners. Furthermore, spin (S) and space (L) quantities can vary independently while, as we saw above, the relativistic case the total angular momentum J=L+S provides quantum numbers.

Experimentally, positrons can be prepared in any free momentum p and spin direction with no correlation whatsoever to an electron with which we want it to collide. In principle, there is need for two I-frames in the laboratory environment. Consider the “chemical reaction”:

$$|e^+> + |e^-> \rightarrow |\text{photon(s)}>$$

First, at the right-hand-side there corresponds to two possible spin states, singlet (S=0) and triplet spin (S=1) states that determines the number of photons produced in an event of real space. The feature with Dirac equation is that by including charge conjugation symmetry, the quantum states are independently described as correlated spin 1/2 state. The particle model is not consistent with Dirac equation.

Creation and annihilation particle-states together with the introduction of a vacuum state are hence required to construct a quantum field model. See Freeman Dyson, Advanced Quantum Mechanics, World Scientific, New Jersey, 2007, for a clear and detailed presentation.

The point is the following: we have to show that if there are quantum states in real space then there must exist a quantum evolution equation. And because one is not describing the material system as such, there is no need to call for the duality pervading present literature pointing to wave-like/particle-like behavior. Such duality arises as a result of imposing classical pictures to quantum mechanical results.

A quantum field theory scheme requires much more mathematics and physics than it is possible for us to deliver here. Yet, some glimpses can be given to help seizing the type of requirements.

The I-frame system evolves in space-time continuum; from a fixed laboratory frame the origin is located at **r**. At this point, one can think of having a set of possible frames $P_{\mathbf{r}}$ attached to the point **r**. Let these possible frames be related, two-by-two, by an element g of a symmetry group G; for example a rotation group as we saw in Chapt.2. We speak of the wave function $\phi(\mathbf{r})$ and seek for the transformation properties when an element p of the set $P_{\mathbf{r}}$ is acted by an element g of the group G; as we already know the wave function belongs to a vector space $\mathcal{V}$ over the field of complex numbers. When g acts on a frame p changing it into another that is designated, as p.g two things have to be taken into account. 1) How does $\mathcal{V}$ change? 2) How does the value of the wave function $\phi(\mathbf{r})$ change with this mapping? To emphasize the relation to the possible frames let us write $\phi(p)$ the value of the wave function at fixed **r** for the selected frame p so that for the transformed frame pg one has $\phi(pg) = g^{-1}\phi(p)$. Because G is a group it is ensured that the inverse to g exists. How does $\mathcal{V}$ change? Let w be another element of $\mathcal{V}$, g transforms $\mathcal{V}$ via the mapping: $w \mapsto g \cdot w$ (it remains to identify the nature of the composition law that for the time being its exact form is not relevant to us).

Now, let us change (move) **r** over the space K with respect to laboratory-frame as we want to describe the dynamics of this system. At each different point in space-time there are sets of possible frames and we want to study if there is any relationship between them. A concatenation P of various $P_{\mathbf{r}}$ as **r** ranges over K is known by the name: *principal fiber bundle*; it is then said that $P_{\mathbf{r}}$ is the fiber over **r**. The situation differs from the one found in Chapters 2 and 3 where concatenation via translation operators only required homogeneity of real space; and for rotations, the origin was kept fixed. Now, the situation is akin to a "trajectory-like" description for the I-frame system with *fixed* internal quantum state.

Select now a frame $p \in P_{\mathbf{r}}$, the mapping $g \mapsto pg$ gives a topological equivalence of G with $P_{\mathbf{r}}$. The concatenation P is not equivalent to the product space K×G; the reason is that P may be twisted. It is the space P that interests us. The wave function ϕ is to be regarded as a function on P. The point is to make a continuous choice of reference frame; such mapping is known as a *gauge*. To define this gauge, let U be a sub-region of K, then the function s_u: U→P, such that $s_u(y) \in P_y$ for all y belonging to U is called a gauge. It is not difficult to see that the wave function change under a change of gauge (even if you cannot see the exact form that for the time being is not relevant). Thus, going around in a closed loop you will end up with a wave function differing from the initial one. If such is the case this means that there are external potentials that will produce such type of response. We are no longer in the business of constructing base sets but now since we are at a Fence there is need to include characteristic elements of such special region.

At the Fence, physically meaningful quantities should be independent of the choice of gauge. The action introduced above is to be generalized into an action density wherefrom equation of motions are to be constructed. The important point is that such an action density is not sufficient. What is needed is a connection defined on P, i.e. it is a gauge potential, that transform in such a way that when incorporated into the proposed action density it leads to a gauge-invariant action density. Once such procedure is achieved one can get at constructing a model as shown in the section below using a very elementary approach. What we are after is to make plausible the construction of a wave function $\phi(\mathbf{r})$ that is not a projection from an abstract quantum state on the real space configuration coordinates. Now, one is moving from real space projected towards abstract space projected wave functions.

6.7.1. Feynman Path Integral Method

We use here Feynman procedure to construct a $\phi(\mathbf{r})$ function that could be related to a quantum state. If one can do that then the construction of field theory objects will be simplified. As a matter of fact, the base functions can be turned on to field operators. We will not do the complete transaction but only suggests the type of procedure.

From special relativity theory any material system associated to an inertial frame may also show intrinsic half-integer angular momentum (spin). The frame systems as a whole may then have integer or half-integer spin: bosonic and fermionic frame systems. Here, we stick to the non-relativistic limit; relativistic schemes to construct base states are examined in chapter 7.

The space of abstract $|\Psi>$-states is a Hilbert space. Now, take real space coordinates for a given I-frame system to get the base states $|R_i>$ just as we did with the system "inside" the I-frame. The wave function is given by the map $\Psi(R_i,t) \Leftrightarrow <R_i| \Psi ,t>$. The linear superposition principle reads:

$$|\Psi,t> = \int d^3R_i \, |R_i><R_i| \, \Psi,t> = \int d^3R_i |R_i> \Psi(R_i,t) \qquad (6.7.1.1)$$

The wave function of the I-frame at the point in real space R_{io} at initial time t_o is given as a datum: $\Psi(R_{io},t_o) = \Psi_o$; the problem is the construction of the wave function at another point $\mathbf{R}_i$ at time t: $\Psi(\mathbf{R}_i,t)$. The latter is a mathematical function derived from Ψ_o. The issue is the nature of su ch a function. It can be just a numerical function related via an algorithm to the datum function or it can be a projection of the quantum state we are studying.

Let us insist on the issue: observe that $\Psi(\mathbf{R}_i,t)$ and $\Psi(R_i,t) = <R_i| \Psi,t>$ are different in the following sense anyway. The latter is the projection of an abstract quantum state on to configuration space at point R_i. While $\Psi(\mathbf{R}_i,t)$ will be the value of a mathematical function derived from an initial value of a function Ψ_o evaluated at $\mathbf{R}_i$. Thus, $\mathbf{R}_i$ and R_i are endowed with different meanings. These spaces are isometric however; they differ in their ideologic content, namely, $\mathbf{R}_i$ indicates the position coordinate of a material system while R_i is element of an abstract mathematical space.

E&E-6.7.1-1. Try to sense the subtle difference

Use of $<R_i|\Psi,t>$ implies the existence of an abstract quantum state that is projected onto a space that has nothing to do with such state. When we use $\Psi(\mathbf{R}_i,t)$ it is implied that this functions obtains from a mathematical procedure after imposing initial and particular boundary conditions; it is the calculated function which is important. Unfortunately we call them both a wave function. Try to keep in mind the conceptual difference.

Let $G(\mathbf{R},\mathbf{R}',t)$ be a kernel such that starting with a wave function $\Psi(\mathbf{R}_{io},t_o=0)$ taken as a datum $\Psi_o(\mathbf{R}_i)$ (initial condition) leads to the function $\Psi(\mathbf{R}_i,t)$; let us see what does it take to construct the wave function $\Psi(\mathbf{R}_i,t)$, formally:

$$\Psi(\mathbf{R}_i,t) = \int G(\mathbf{R}_i,\mathbf{R}_i',t) \, \Psi_o(\mathbf{R}'_i) \, d^3\mathbf{R}'_i \qquad (6.7.1.2)$$

Therefore, all what we need is a rule to calculate the propagator $G(\mathbf{R},\mathbf{R}', t)$. This mathematical object is known as Green function. Path Integral prescription introduced by Feynman leads to the Green function in terms of the system's classical (mechanical) action, $dt \, L(\mathbf{R}_i,d\mathbf{R}_i/dt) = dA$ (Cf.eq.(6.7.A-5) :

$$G(\mathbf{R}_i,\mathbf{R}_i', t) = \Sigma_{paths} \exp(i \, A[l_i]/\hbar) =$$

$$\Sigma_{\text{paths}} \exp\{i/\hbar \int_0^{t_1} dt\, L(\mathbf{R}_i, d\mathbf{R}_i/dt)\} =$$
$$\Sigma_{\text{paths}} \exp\{i/\hbar \int_{R_i',0}^{R,t} \mathbf{P}\cdot d\mathbf{R}_i - H\, dt\} \qquad (6.7.1.3)$$

This symbolic sum is taken over all paths $\{ l_i \}$ connecting the initial space time point (R'_i,t_o) to the final one (R_i,t). Feynman let you imagine that at the initial point at $t_o=0$ and domain $d\mathbf{R}_i$ around position coordinate $\mathbf{R}_i'$ start taking all possible paths linking that domain to another characterized by time t and position $\mathbf{R}$. The terms found in this equation are just weights for each $G(\mathbf{R}_i,\mathbf{R}_i',t)$; another way is to take these functions as base functions we use to expand the initial quantum state with the caveat that you may produce a change of quantum state at the end of the day. In so doing, the algorithm pick up the information in the neighborhood of the wave function, namely, $G(\mathbf{R}_i,\mathbf{R}_i',t)\ \Psi_o(\mathbf{R}'_i)\ d^3\mathbf{R}'_i$ and sum over the range $d^3\mathbf{R}'_i$ that is of course a lot of work; don´t try by yourself, let the formalism do the job.

Each path has a characteristic contribution related to an energy change so that picking all paths would mean that the system has the possibility to count all possible actions (energy balances), e.g. $\mathbf{P}\cdot d\mathbf{R}_i - H\, dt$).

The formula must be read as a set of slices when one sets $\Delta t=t/N$ and define the function:

$$G_N = (M_i/2\pi\, i\hbar\Delta t)^{3(N+1)/2} \int \exp(iA_N/\hbar) d^3\mathbf{R}_i(1)\ldots d^3\mathbf{R}_i(N-1) \qquad (6.7.1.4)$$

The function A_N:

$$A_N = (M_i/2\Delta t)\Sigma_{j=1,N}(\mathbf{R}_i(j)-\mathbf{R}'_i(j))^2 - V(\mathbf{R}_i(j),t_j)\Delta t \qquad (6.7.1.5)$$

It is at this point the characteristic interactions are included via the term $V(\mathbf{R}_i(j),t_j)$. The time slice t_j equals $j\Delta t$. One should get the exact Green function by taking the limit $N\to\infty$ so that one gets:

$$\Psi(\mathbf{R}_i,t) = \int(\lim_{N\to\infty} G_N(\mathbf{R}_i,\mathbf{R}_i',t)\ \Psi_o(\mathbf{R}'_i)\ d^3\mathbf{R}' \qquad (6.7.1.6)$$

The wave function calculated with the above formula requires information along all possible paths connecting the starting to the end points. The method would be useless if you have to take the infinite family of paths; the point is that only some specific sets of paths sharing some variational property would contribute most to the algorithm. For the present case what one is doing is to make possible the calculation of the quantum state of an I-frame system sustaining an initial quantum state $\Psi_o(\mathbf{R}'_{io})$. We *are not* calculating the material system as a particle but the quantum states when an external potential $V(\mathbf{R}_i(j), t_j)$ is present.

The question is: what relationship has this quantum state evolving in time with Schrödinger equation?

The most spectacular achievement Feynman got in his PhD thesis (Rev.Mod.Phys.) was to show that $\Psi(\mathbf{R}_i,t+\Delta t)$ fulfils the estimate:

$$\Psi(\mathbf{R}_i,t+\Delta t) = \Psi(\mathbf{R}_i,t) - i\Delta t/\hbar\ V\ \Psi(\mathbf{R}_i,t) + i(\hbar\Delta t/2M_i)\nabla_{\mathbf{R}i}^2\ \Psi(\mathbf{R}_i,t) + o(\Delta t)$$

Rearranging the terms of this estimate multiplying by $i\hbar$ and dividing by Δt:

$$i\hbar(\Psi(\mathbf{R}_i,t+\Delta t) - \Psi(\mathbf{R}_i,t))/\Delta t = -(\hbar^2/2M_i)\nabla_{\mathbf{R}i}^2\ \Psi(\mathbf{R}_i,t) + V\ \Psi(\mathbf{R}_i,t) + o(\Delta t)$$

Taking the limit $\Delta t \to 0$ he got Schrödinger differential equation, that for the present case corresponds to quantum states sustained by the I-frame carrying a mass M_i:

$$i\hbar\ \partial\Psi(\mathbf{R}_i,t)/\partial t = -(\hbar^2/2M_i)\nabla_{\mathbf{R}i}^2\ \Psi(\mathbf{R}_i,t) + V(\mathbf{R}_i)\ \Psi(\mathbf{R}_i,t) \qquad (6.7.1.7)$$

The result obtained by Feynman is another way to arrive at Schrödinger equation but this time in real space.

Observe that the actual "position" of the mass is irrelevant because the operator $\nabla_{\mathbf{R}i}^2$ senses the wave function curvature. Here, the mass position entering the amplitude A_N is fixed (Cf.Eq.6.7.1.5). So you can stick to the idea developed in this work and think the quantum state is sustained by the material system, of course, but not as a (classical) particle if you keep "inside" the I-frame where eq.(6.7.1.7) is derived. The quantum system is expressed in its own space so to speak. The existence of the wave function is granted by the presence of the material system inside the volume used for carrying out integrations. Actual position is not an issue.

The integration implied by the calculation of the Green function (6.7.1.4) is a mathematical operation; results obtained by computing are validated against experimental data. What imports is the propagation of $\Psi_o(\mathbf{R}'_i)$ not the "paths". Thus, $\Psi(\mathbf{R}_i,t)$ describes the quantum state sustained by a material system in the external potential $V(\mathbf{R}_i)$. If $\Psi_o(\mathbf{R}'_i)$ stands for data concerning a given quantum state in a domain (ball) around $\mathbf{R}'_i$, the algorithm permits constructing a (different) wave function for the quantum state at domain around another point; of course it ought to be the whole domain to get an exact result for $\Psi(\mathbf{R}_i,t)$ which means we introduce more and more domains for $\Psi_o(\mathbf{R}'_i)$.

The material system sustaining that state can be described as an I-frame system with mass M_i at the origin but the quantum state is evaluated in an open domain around that origin which is *displaced along classical paths*. This is another view; the result concerning the quantum state is independent from such pictures if carried out exactly.

This is an amazing way to look at quantum mechanics. It is understood that the potential $V(\mathbf{R}_i)$ generates transitions in a way to be determined later on. Here, two aspects are highlighted:

-1) The constructive procedure is ensured by the fact that $\Psi_o(R_i,t_o)$ in a domain around R_i should contain enough information about the quantum state in Hilbert space that was prepared at t_o and projected in this configuration space. The set of square integrable complex functions over real space is a realization of Hilbert space. And the solutions to eq. (6.7.1.7) belong to this set provided the space is rigged with some limits allowing for generalized functions such as Dirac delta function.

Lemma: *A wave function is the projection of a quantum state on the configuration space that for the present case happens to be* R^3*, namely* $<R_i|\Psi,t>$.

-2) The potential $V(\mathbf{R}_i)$ is a resource. A number of laboratory situations can be model with the help of specific potentials to the extent that external forces acting on the I-frame system can be simulated with $V(\mathbf{R}_i)$. The quantum states obtained from Schrödinger Eq.(6.7.1.7) are then those the material system will expose to interactions of many kinds. You can see that a classic system (I-frame) "dissolves" into a representative set of quantum base states incorporating the external potential; this statement simply means that again one focus attention on pertinent quantum states that are sustained by the material system this time including its internal quantum state. Today, atoms can be slowed and subsequently trapped in laboratory space. The slowing can be achieved electromagnetically, laser cooling for example. Any response from the I-frame system is mediated by changes of its quantum state.

The I-frame as such can always be seen as a classical system (object). If you have a manner to record its classical coordinates (origin) then follow the trajectory say with velocity **v** with respect to another I-frame where you might be sitting. In this case, the classical linear momentum M**v** is well defined. This situation does not eliminate the sources for quantum mechanical response to appropriate probes. There is nothing strange if you keep clear distinctions between these two levels of description. The two-fold-ness belongs to the knowledge available.

The I-frame system may have "internal" quantum states ruled by eq.(6.7.1.7). Thus, for example, a hydrogen atom moving in real space sustains quantum electronic states with respect to the inertial frame also. Note that if the material system were at the "border" of the (classical) universe its quantum states will be the same as those determined in your laboratory. One can detect hydrogen atoms in galaxies far distant from the one we are moving with.

The mixing of classical and quantum elements on one and the same material system is one of the mechanisms allowing for proper descriptions of molecular machines. The import for designing molecular machines (Barbara, P.F. (editor) Acc.Chem.Res.**34**, Issue 6: Molecular Machines Special Issue) cannot be overlooked.

In spectroscopy, recorded from a fixed frame, the velocity of the source will show up as Doppler type effects that are so useful in Astronomical Spectroscopy. The base states of this composite system are direct products of internal and global base states. So long we keep accelerations out of the analysis, inertial frames permit setting the basis to analyze quantum processes far back in the past.

Once the analysis in absence of acceleration (forces acting at the origin of the I-frame) is done one can start examining situations where trapping external potentials are set up. A first analysis starts by letting aside couplings with the internal degrees of freedom to incorporate them when they become central to the understanding of processes (phenomena).

We conciliate now the abstract configuration space used in preceding chapters (see sect. 4.1.4) with a real configuration one where the coordinates are labels that support the material space and can be mapped to a position configuration space. In order to get a consistent approach one assigns a given set of coordinates and keep the order all along. Only the base states supported by such coordinate can be changed. The configuration space retains its invariant character assigned to it in the abstract model; with this caveat, the “Lemma” presented above holds.

6.9. From here to a quantum field model

We close this chapter at this point.