

## Path Integrals in Relativistic Quantum Mechanics

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**Abstract :** This paper is a review of path integral representations for semigroups  $\{\exp -t H_r/\hbar\}_{t \geq 0}$  where  $H_r$ 's are relativistic quantum Hamiltonians. We consider three different cases: in the first one  $H_r$  is a relativistic Schrödinger operator, in the second is the Hamiltonian associated to Klein-Gordon equation and in the third is that coming from the Dirac one. The paths are trajectories of diffusion processes and, for the Dirac case, they differ from previous constructions based on jump Markov processes. All formulas describe *one* relativistic particle in an external static electromagnetic field therefore they are relativistic versions of the Feymann-Kac representation for Schrödinger semigroups.

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## §1. Introduction

Since the discovery of the atomic nucleus by E. Rutheford, a sensible model of matter depicts ordinary bodies as collections of pointlike electrons and nuclei attracting and repelling each other by Coulomb forces. Such a model is troublesome in classical physics which is unable to account for the very existence of atoms: why don't electrons fall into the nucleus and radiate all their energy away? In 1925 wave mechanics provided a solution by showing that atoms have a *ground state* namely a state with a minimal energy  $E_{\min} > -\infty$  and it became clear that atoms with  $Z$  electrons each with charge  $e < 0$  and nuclear charge  $-Ze > 0$  could not have an energy lower than  $-Z^3 R_y$  where  $R_y$  is the Rydberg constant related to  $e$ ,  $\hbar$  and  $m$  (the mass of the electron) through  $R_y = me^4/2\hbar^2$ . This result solved the problem of stability for *individual* atoms but not for matter in bulk. Due to the long range of Coulomb interaction, why two separated pieces of matter do not feel each other's influence? The point is that even if bodies are globally neutral, it is not obvious that they do not become polarized in such a way as to attract or repel each other. An important facet of stability for matter in bulk is the saturation property of the binding energy per particle i.e. the requirement that, for a system of  $N$  particles, not only the ground state energy  $E_{\min}$  is finite (stability of the first kind) but also that  $E_{\min} \sim -C_0 N R_y$  (stability of the second kind) for a suitable positive constant  $C_0$ . In order to appreciate this point, let suppose for instance that  $E_{\min} \sim -C_0 N^r R_y$  with  $r > 1$ . Then bringing together two large pieces of matter each containing say  $10^{23}$  particles, would release an energy  $\Delta E = C_0(2^r - 2)10^{23r} R_y$  which could be rather huge and matter should collapse under Coulomb interaction! The problem of stability of quantum mechanical systems consisting of point charges was explicitly raised about 41 years after the birth of quantum mechanics in a paper by Fisher and Ruelle<sup>1</sup> and the answer was given only in the late sixties and early seventies beginning with the work of Dyson and Lenard<sup>2,3</sup> (see<sup>4</sup> for a succinct but valuable review which contains further references). One can simplify the problem of  $N$  electrons interacting with  $K$  nuclei with charges  $-Z_1 e, \dots, -Z_K e$  by using the Born-Oppenheimer approximation where nuclei are assumed to have infinite mass (allowing the mass to be finite only raises the energy) and are located at fixed but arbitrary space points  $\mathbf{R}_1, \dots, \mathbf{R}_K$ . Now we have a system in which the only quantum objects are  $N$  electrons with a Hamiltonian  $H_N$  given by

$$(1.1) \quad H_N = -\frac{\hbar^2}{2m} \sum_{i=1}^N \Delta_i - \sum_{i=1}^N \sum_{j=1}^K \frac{Z_j e^2}{\|\mathbf{r}_i - \mathbf{R}_j\|} + \sum_{1 \leq i < j \leq N} \frac{e^2}{\|\mathbf{r}_i - \mathbf{r}_j\|} + \sum_{1 \leq i < j \leq K} \frac{Z_i Z_j e^2}{\|\mathbf{R}_i - \mathbf{R}_j\|}$$

and Dyson and Lenard demonstrated that the infimum  $E_{\min}$  of the spectrum of  $H_N$  satisfies the inequality  $E_{\min} \geq -C_0 N R_y$  for all  $\mathbf{R}_1, \dots, \mathbf{R}_K$  *provided* that electrons behave as fermions. If electrons obeyed Bose-Einstein statistics matter would definitely not be stable under Coulomb forces as in that case  $E_{\min} \sim -C_1 N^{7/5} R_y$ . The key to understanding the stability of a system of  $N$  fermions is the fact well known to physicists that the kinetic energy  $T$  grows with the electron density  $\rho_\psi$ , indeed  $T_\psi \geq \text{const.} \int_{\mathbb{R}^3} \rho_\psi(\mathbf{r})^{5/3} d^3 \mathbf{r}$  for each<sup>4</sup> quantum state  $\psi \in AL^2(\mathbb{R}^3 N)$  (physicists already knew that the energy of a degenerate gas of  $N$  Fermi particles confined in a

volume  $V$  is proportional to  $N(N/V)^{2/3}$ ). The previous theorems proceed from non-relativistic quantum mechanics embodied in the Schrödinger operator (1.1) however the Schrödinger theory is not physically reliable when binding or Fermi energies become greater than rest energy contributions because relativistic corrections become relevant. Some of them proceeds from relativistic kinematic which modify the relation between kinetic energy and momentum and this fact has important consequences. For instance, the previous mentioned result that the minimal available kinetic energy for  $N$  fermions is related to the density  $\rho_\psi$  by  $T_{\min} = \text{const.} \int_{\mathbb{R}^3} \rho_\psi(\mathbf{r})^{5/3} d^3\mathbf{r}$ , besides Fermi statistics, is a consequence of the non-relativistic equality  $T = |\mathbf{p}|^2/2m$  between kinetic energy and momentum  $\mathbf{p}$ . However, due to the relativistic relation  $T = \sqrt{c^2|\mathbf{p}|^2 + m^2c^4}$ , in the extreme relativistic region, the energy of a degenerate Fermi gas is proportional to  $\int_{\mathbb{R}^3} \rho_\psi^{4/3}(\mathbf{r}) d^3\mathbf{r}$  and therefore the contribution of electron gas to the total energy  $E$  of a white dwarf of mass  $M$  is proportional to  $M^{4/3}/R$  which depends on the radius  $R$  of the star in the same way as the gravitational energy which is proportional to  $-GM^2/R$ . Since the total energy is  $E(M, R) = (C_1 M^{4/3} - C_2 GM^2)/R = C_3(M)/R$ , the Fermi pressure of the degenerate electron gas is unable to prevent the collapse of the star when  $C_3(M) < 0$  and this happens for  $M \geq 1.45M$  which is the famous limit of Chandrasekhar. This is at variance with what would happen in a non-relativistic Universe where the energy of a degenerate Fermi gas is always proportional to  $N(N/V)^{2/3}$  and the total energy is  $E(M, R) = (C_1 M^{5/3}/R^2 - C_2 GM^2/R)$  which, as a function of  $R$ , has a finite minimum for any  $M$ . By coming back to Coulomb interaction between nuclei and electrons, it is well known that relativistic corrections becomes significant when nuclei have high atomic number since they are of order  $(\alpha Z)^2$  where  $\alpha = e^2/\hbar c$  is the fine structure constant. Therefore relativistic corrections are important for heavy elements for which  $\alpha Z$  is not much less than unity but they arise not only from relativistic kinematic but also from spin-orbit coupling and Darwin “fluctuation” term related to the Zitterbewegung of relativistic electrons. Strictly speaking, theorems on the stability of matter should proceed from Quantum Electrodynamics which is the relativistic theory describing the interaction between charged particles and the quantized electromagnetic field. Unfortunately Q.E.D., although physically well founded, is not under full mathematical control and there is a real need for quantum models of relativistic charged point particles interacting via electromagnetic forces which would both suitable for rigorous mathematical treatments and physically transparent as reasonable approximations of the full quantum electrodynamics. In the existing literature<sup>5</sup> on the stability of matter the adopted solution incorporates relativistic effects only through a modification of kinematic consisting in replacing everywhere the nonrelativistic kinetic energy by the relativistic one  $\sum_{i=1}^N \sqrt{-\hbar^2 c^2 \Delta_i + m_i^2 c^4}$ . This modification captures only a part of relativistic corrections to the Schrödinger theory with Coulomb forces. It produces “relativistic Schrödinger operators” which, for one “electron” with potential energy  $V(\cdot)$ , are of form  $H_1 = \sqrt{-\hbar^2 c^4 \Delta + m^2 c^4} + V(\cdot)$ . They differ significantly from the usual Schrödinger Hamiltonians  $H = -(\hbar^2/2m) \Delta + V(\cdot)$ . For instance, in the Coulomb field of a nucleus, the infimum of the spectrum of  $H_1$  collapses<sup>6</sup> to  $-\infty$  when the atomic number  $Z$  exceeds a critical value  $Z_c$  of the order of magnitude of the inverse fine constant  $\alpha$  (by the way, the ground state energy is finite for all values of  $Z$  in the Schrödinger theory however, for  $Z$  greater than  $(e^2/\hbar c)^{-1}$ , the binding energy exceeds the rest energy  $mc^2$  which is a physically suspect result). For a system of  $N$  electrons in the Coulomb field of  $K$  infinitely massive nuclei located at  $\mathbf{R}_1, \dots, \mathbf{R}_K$ , the relativistic analogous (1.1) becomes

$$\begin{aligned}
 H_N = & \sum_{i=1}^N \sqrt{-\hbar^2 c^2 \Delta_i + m^2 c^4} - \sum_{i=1}^N \sum_{j=1}^K \frac{Z_j e^2}{\|\mathbf{r}_i - \mathbf{R}_j\|} + \\
 (1.2) \quad & + \sum_{1 \leq i < j \leq N} \frac{e^2}{\|\mathbf{r}_i - \mathbf{r}_j\|} + \sum_{1 \leq i < j \leq K} \frac{Z_i Z_j e^2}{\|\mathbf{R}_i - \mathbf{R}_j\|}
 \end{aligned}$$

and there is a simple theorem<sup>5</sup> which relates the stability of the many body system described by  $H_N$  to the stability of just one electron in presence of an atomic nucleus. In this latter case, the spectrum of  $H_1$  (with  $V(\mathbf{r}) = -Ze^2/\|\mathbf{r}\|$ ) is bounded from below provided that  $Z \leq Z_c = 2/\pi\alpha$ , now let suppose that  $Z_j \leq Z_c$  for all  $j = 1, \dots, K$ , then the quantum Hamiltonian  $H_N$  is stable for fermions when  $q\alpha \leq 1/47$  where  $q$  is the number of spin states ( $q = 2$  for electrons and the actual value of  $\alpha$  is roughly  $1/137$ ). From the previous discussion it would seem that the theory of relativistic Schrödinger operators is in a good shape but what about its physical status? In other words what approximation of Quantum Electrodynamics leads to quantum Hamiltonians of the form (1.2)? Now we come back to Quantum Electrodynamics which includes many physical effects related to the interaction between matter and photons. Apart creation and annihilation of pairs and, of course, emission and absorption of photons, two important features of Q.E.D. are radiative corrections and vacuum polarization. Radiative corrections modify the magnetic moment of electrons and generate small displacements of atomic energy levels with respect to the previsions of Dirac theory which accounts for the interaction of electrons (or positrons) with an external (i.e. unquantized) e.m. field. In the Coulomb field of an infinitely massive nucleus with atomic number  $Z < \alpha^{-1}$  the Dirac theory provides energy levels given by

$$\begin{aligned}
 E_{n,1} = mc^2 \left[ n + \left( \frac{Z\alpha}{n - (J + \frac{1}{2}) + \sqrt{(J + \frac{1}{2})^2 - Z^2\alpha^2}} \right)^2 \right]^{-\frac{1}{2}} = \\
 (1.3) \quad = mc^2 - \frac{mc^2}{2} \frac{(\alpha Z)^2}{n^2} + mc^2 (\alpha Z)^4 \left( \frac{3}{8n^4} - \frac{1}{2(J + \frac{1}{2})n^3} \right) + O((\alpha Z)^6)
 \end{aligned}$$

with  $n = 1, 2, \dots$   $J = 1/2, 1, 3/2, \dots$ . The first term is the rest energy, the second is the nonrelativistic (Schrödinger) contribution while the term proportional to  $(\alpha Z)^4$  provides the most relevant relativistic corrections to Schrödinger theory which are not only of pure kinematical origin. Since the Dirac energy depends on the principal quantum number  $n$  and on the total angular momentum  $J$  but not on the orbital angular momentum  $l$ , in the hydrogen atom, the levels  $2S_{1/2}$  ( $n = 2, l = 0, J = 1/2$ ) and  $2P_{1/2}$  ( $n = 2, l = 1, J = 1/2$ ) should be degenerate but in 1947 was experimentally found a small energy difference corresponding to an emission or an absorption of photons with a frequency of  $1057 \text{ Mc sec}^{-1}$ , therefore  $\Delta E/E \sim 1.4 \cdot 10^{-3}$ . This Lamb-Retherford shift breaks the degeneracy of levels with the same  $n$  and  $J$  but differing  $l$  and it is almost entirely due to radiative corrections. A simple qualitative description in terms of the interaction of electrons with the vacuum quantum fluctuations of the electromagnetic field is the following: although the average field strengths are zero in vacuum, their mean square values are non vanishing and drive mean square fluctuations in the electron's position which, in turns, produce a smearing out of the Coulomb potential as seen by the particle. The net effect, for atomic hydrogen, is a shift of the  $2S_{1/2}$  levels upward relative to the  $2P_{1/2}$  lines. The vacuum polarization originates from the presence of virtual pairs in the vacuum of Q.E.D since a bare test charge  $Q_0$  surrounds itself by a cloud of virtual electrons and positrons. Some of these, with net charge  $\delta Q$  of the same sign as  $Q_0$ , are repelled away leaving a charge  $-\delta Q$  in the part

of the cloud which is closely bound to the test body i.e. within the distance  $\hbar/mc$ . If one observes the charge of the body from a distance which is large compared with  $\hbar/mc$ , he would see an effective charge  $Q = Q_0 - \delta Q$  (the renormalized one). However, as one inspects within distances much less than  $\hbar/mc$ , the charge that will be seen is the bare one  $Q_0$ . This means that the biggest part of vacuum polarization is unobservable since can be incorporated in the charge renormalization as the bare electric charge is meaningless, nevertheless it remain small observable consequences namely nonlinear effects as scattering of light by light and a modification of the Coulomb field at short distances. This last effect produces a relative shift of energy levels because in  $S$  states electrons get closer to the nucleus inside the surrounding polarization cloud and see a positive electric charge greater than the one seen in  $P$  states. By vacuum polarization, the  $2S_{1/2}$  levels are lowered by  $27 \text{ Mc sec}^{-1}$  relative to the  $2P_{1/2}$  ones and this constitutes a direct proof that vacuum polarization effects are real since the agreement between theory and experiment is within  $0.2 \text{ Mc sec}^{-1}$ . Now let consider relativistic electrons in presence of an *external* electromagnetic field, for instance the Coulomb field of one or several infinitely massive atomic nuclei. In the Furry picture of Q.E.D. with an external field, the unperturbed Hamiltonian  $H_0$  of matter is that of the second quantized Dirac theory or of the Klein-Gordon one (for matter composed by spinless charges as pions) in the external field. The "external field approximation"  $H_0$  of Q.E.D. is a rough picture since accounts only for the interaction of each particle with the external field but not with photons which, by exchanging energy-momentum, are responsible for the electromagnetic interaction between the particles themselves and it may not a theory in which the number of particles is conserved as external fields could create pairs<sup>7</sup> at non-zero rate also in the static limit but, if the *electric* field is below a critical value  $E_c \approx \frac{m^2 c^3}{e \hbar}$  the "Klein Paradox" can't occur and the external field approximation of Q.E.D. becomes a respectable *linear* quantum field theory in which the number of particles is conserved with an energy operator  $H_0$  which is the direct sum of the one particle Hamiltonian  $H_1$ , the two particle Hamiltonian  $H_2$  and so on and therefore the only relevant operator is exactly  $H_1$  because  $H_2 = H_1 \oplus H_1, H_3 = H_1 \oplus H_1 \oplus H_1 \oplus H_1, H_n = H_1 \oplus \dots \oplus H_1$  as particles do not interact among themselves. In the case of the Dirac theory, the operator  $H_1$  should not be confused with the Dirac Hamiltonian  $H_D$  itself indeed  $H_D = H_1 \oplus (-\bar{H}_1)$  where  $\bar{H}_1$  is that of the positron. This decomposition corresponds to the splitting of the spectrum of  $H_D$  in positive and negative part and can be obtained in principle by the Foldy-Wouthuysen transformation<sup>8,51</sup> which is an unitary map  $U$  in the Hilbert space  $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$  which displays explicitly the new equivalent Hamiltonian  $H'_D = U H_D U^{-1}$  as a direct sum of two operators  $H_1$  and  $\bar{H}_1$  each in  $L^2(\mathbb{R}) \otimes \mathbb{C}^2$  which are the true one-electron and one-positron quantum Hamiltonians. Unfortunately the FW transformation is available in a closed form only in the free case and in that with a purely magnetic external field<sup>9</sup>, however  $H_1$  and  $\bar{H}_1$  are well defined operators for *all* subcritical electric fields and we *always* assume that this condition is satisfied. The Coulomb field of a nucleus is subcritical when  $Z < \alpha^{-1}$  but the Dirac theory *breaks down* when  $Z/geq\alpha^{-1}$  as it is clear from the formula (1.3). For the general meaning of invariant wave equations in presence of on external field see<sup>11,12</sup>. Now we come back to the full Q.E.D. where the quantum Hamiltonian is  $H = H_0 + H_R + H_I$  i.e. the sum of  $H_0$ , of the Hamiltonian  $H_R$  of the free quantum electromagnetic field and of  $H_I$  which represents the interaction between matter and photons. In the radiation gauge, the interaction Hamiltonian  $H_I$  splits in two pieces  $H_I = H_I^{(1)} + H_I^{(2)}$  the first containing only the contributions from the transverse part of the e.m. field while the second picks up the contributions from scalar and longitudinal modes. Formally

$$H_I^{(2)} = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{\|\mathbf{x} - \mathbf{y}\|} d\mathbf{x}d\mathbf{y}$$

where  $\rho(\cdot)$  is the electric charge density operator given by  $\rho(\mathbf{x}) = e : \psi^*(\mathbf{x})\psi(\mathbf{x}) :$

for the quantized Dirac field  $\psi(\cdot)$  where  $::$  is the Wick ordering.  $H_I^{(2)}$  looks as the Coulomb self-energy of a cloud of electric charges with density  $\rho(\cdot)$  but it should not be interpreted too literally as representing the instantaneous Coulomb interaction between particles as it contains also effects related to the vacuum polarization since  $H_I^{(2)}$  acting on the bare (Fock) vacuum  $|0\rangle$  creates pairs (in general, one can think about vacuum polarization as the fact that the physical vacuum and the bare one are distinguishable from one another<sup>13</sup>). In order to separate the "true" Coulomb interaction  $H_C$  between particles from the remaining parts of  $H_I^{(2)}$ , let observe that  $\rho(\cdot)$  has a splitting  $\rho(\cdot) = \rho_1(\cdot) + \rho_2(\cdot)$  with  $\rho_1(\cdot)|0\rangle = 0$ ,  $Q = \int \rho(\mathbf{x}) d\mathbf{x} = \int \rho_1(\mathbf{x}) d\mathbf{x}$  while  $\int \rho_2(\mathbf{x}) d\mathbf{x} = 0$ . Clearly  $\rho_2(\cdot)$  is the part of the charge density which accounts for the contribution of pairs and one can take  $H_C = \int \int : \rho_1(\mathbf{x}) \rho_1(\mathbf{y}) : / \|\mathbf{x} - \mathbf{y}\| d\mathbf{x} d\mathbf{y}$  as the wanted Coulomb interaction. In the Dirac theory  $\rho_1(\cdot) = e(\psi_+^*(\cdot)\psi_+(\cdot) + \psi_-^*(\cdot)\psi_-(\cdot))$  where  $\psi(\cdot) = \psi_+(\cdot) + \psi_-(\cdot)$  is the decomposition of the Dirac field in the positive frequency part (containing only annihilation operators of electrons) and the negative frequency one (containing only creation operators of positrons). Now the full quantum Hamiltonian looks

$$H = H_0 + H_C + H_R + (H_I^{(1)} + H_I^{(2)} - H_C)$$

and  $H_0|0\rangle = H_C|0\rangle = 0$ ,  $H_C|1\rangle = 0$  and one can assume that  $H_M = H_0 + H_C$  is the "dressed" quantum Hamiltonian of matter which accounts for the biggest part of electromagnetic interaction between particles. Of course,  $H_M$  is still a roughening of Q.E.D. in which particles are decoupled from radiation therefore emission or absorption of real photons is forbidden but this last fact is not important if one is only interested in the ground state of "cold" matter with no photons incoming from outside. The physical meaning of the previous roughening consists, therefore, in neglecting the Lamb shift and the small observable effects of vacuum polarization since the biggest part is already included in the charge renormalization. In Quantum Electrodynamics there is also a renormalization of the mass related to the electromagnetic self-interaction of particles but the definition of  $H_C$  through a further Wick ordering implies that this operator annihilates not only the Fock vacuum  $|0\rangle$  but also all vectors  $|1\rangle$  in the one-particle subspace as we imagine to have already included the electromagnetic self-interaction in the mass renormalization. The "matter" Hamiltonian  $H_M = H_0 + H_C = H_0 + \int \int : \rho_1(\mathbf{x}) \rho_1(\mathbf{y}) / \|\mathbf{x} - \mathbf{y}\| d\mathbf{x} d\mathbf{y}$  conserves the number of particle (or of antiparticles) and it could be an interesting mathematical problem to study how the ground state energy  $E_N^0$  of  $H_M^{(N)}$  (which is the restriction of  $H_M$  to the  $N$  particle subspace) depends on  $N$ . It would be also interesting to compare such a restriction with the relativistic Schrödinger operator (1.2). Let start from the simplest case of just one particle which in the relativistic Schrödinger model is already significant for stability. Because  $H_C|1\rangle = 0$ , the operator  $H_M^{(1)}$  is just the one particle Hamiltonian  $H_1$  of the Dirac or Klein-Gordon theory in the external field and must be compared with the one body relativistic Schrödinger operator  $\tilde{H} = \sqrt{-\hbar^2 c^2 \Delta + m^2 c^4} + V(\cdot)$ . The quickest way of making such a comparison is through the corresponding Feymann-Kac formulas. The famous Feymann-Kac formula<sup>13,14</sup> originated the study of Schrödinger operators via probabilistic techniques and is an important tool in nonrelativistic quantum mechanics. It provides a path integral representation of Schrödinger semigroups  $\{\exp -tH/\hbar\}_{t \geq 0}$  in  $L^2(\mathbb{R}^\nu)$  with  $H = -(\hbar^2/2m) \Delta_\nu + V$  through

$$((1.4)) \quad (e^{-tH/\hbar} \psi)(\mathbf{x}) = \mathbb{E}_{\mathbf{x}}(\psi(\mathbf{X}_t) \exp -\frac{1}{\hbar} \int_0^t V(\mathbf{X}_s) ds)$$

where  $s \in [0, +\infty) \mapsto \mathbf{X}_t$  is a  $\nu$ -dimensional Brownian motion. When a magnetic field  $\mathbf{B} = \text{rot} \mathbf{A}$  is present, the Schrödinger operator  $H$  gets modified by the minimal

coupling  $(-i\hbar\nabla \rightarrow -i\hbar\nabla - (e/\hbar c)\mathbf{A})$  and (1.4) gets replaced<sup>14</sup> by the Feymann-Kac-Itô formula

$$(1.5) \quad (e^{-tH(\mathbf{A})/\hbar} \psi)(\mathbf{x}) = \mathbf{E}_{\mathbf{x}} \left( \psi(\mathbf{X}_t) e^{-\frac{1}{\hbar} \left\{ \int_0^t V(\mathbf{X}_s) ds + \frac{ie}{c} \int_0^t \mathbf{A}(\mathbf{X}_s) \cdot d\mathbf{X}_s + \frac{ie\hbar}{2mc} \int_0^t (\operatorname{div} \mathbf{A})(\mathbf{X}_s) ds \right\}} \right)$$

Since  $(\exp -tH(\mathbf{A})/\hbar)$  depends on  $\mathbf{A}(\cdot)$  only through a phase factor, (1.5) implies the diamagnetic inequality  $|(e^{-tH(\mathbf{A})/\hbar} \psi)(\mathbf{x})| \leq (e^{-tH(\mathbf{0})/\hbar} |\psi|)(\mathbf{x})$  and this means that the energy of a Schrödinger particle (or a system of such a particles) can only rise when the magnetic field is turned on and, therefore, the stability of nonrelativistic matter is preserved when magnetic fields are present. We remark an import fact: it follows by Itô Lemma in stochastic calculus that  $\exp -tH(\mathbf{A})/\hbar$  is invariant up to an unitary transformation (which is a simple  $\mathbf{x}$  dependent rephasing of wave functions) under the gauge transformation  $\mathbf{A} \rightarrow \mathbf{A} + \operatorname{grad} f$ . This is a check of consistence for (1.5) since gauge invariance can't be given up in a physical theory. A part from its usefulness<sup>16,17,18,19,20,21</sup> in the spectral theory of Schrödinger operators, the right side of (1.4) defines<sup>(21,22,23,2)</sup> a bounded continous semigroup  $\{P^t\}_{t \geq 0}$  of self-adjoint operators in  $L^2(\mathbf{R}^\nu)$  for fairly general potentials  $V(\cdot)$  and it is perfectly possible to define the quantum Hamiltonian  $H$  itself as its negative infinitesimal generator providing a unique selfadjoint extension of the formal differential operator  $-(\hbar^2/2m)\Delta + V(\cdot)$ . It is interesting that an analogous<sup>24,25</sup> of (1.4) holds also for the one body relativistic Schrödinger operator  $\tilde{H}_1 = \sqrt{-\hbar^2 c^2 \Delta + m^2 c^4} + V$ , namely

$$(1.6) \quad (e^{-t\tilde{H}_1/\hbar} \psi)(\mathbf{x}) = e^{-tmc^2/\hbar} \mathbf{E}_{\mathbf{x}} \left( \psi(\xi_t) \exp -\frac{1}{\hbar} \int_0^t V(\xi_s) ds \right)$$

where  $s \mapsto \xi_s$  is a suitable *jump* Markov process in  $\mathbf{R}^\nu$ . Formula (1.6) can be generalized<sup>26</sup> when a magnetic field is present providing a gauge-invariant relativistic version of (1.5) which we shall describe later because it displays an interesting asymmetry between the contribution of the electric field and that of the magnetic one. We remark, however, that in the literature there exist<sup>27</sup> different "Feymann-Kac-Itô" formulas for semigroups of operators arising not via minimal coupling from relativistic Schrödinger models but through Weyl quantization<sup>28</sup> of classical relativistic Hamiltonians. Unfortunately such operators are *definitely* not gauge-invariant and therefore are the *wrong* ones as physically meaningful quantum Hamiltonians. Let us come back to the comparison between the one-body relativistic Schrödinger operator  $\tilde{H}_1 = \sqrt{-\hbar^2 c^2 \Delta + m^2 c^4} + V$  and the one-particle Hamiltonian  $H_1$  provided, say, by the Klein-Gordon theory which, as  $\tilde{H}_1$ , doesn't include spin-orbit coupling. The Klein-Gordon Hamiltonian  $H_1$  in an external electric field is not explicitly known but there is a simple device for obtaining a "Feymann-Kac" formula for its semigroup  $\exp -tH_1/\hbar$ . In an external (static electric) field  $\mathbf{E} = -e^{-1} \operatorname{grad} V$  the Klein-Gordon equations in  $d = 1 + \nu$  space-time dimensions is

$$(1.7) \quad \frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} - \Delta_\nu \varphi + \frac{2iV}{\hbar c^2} \frac{\partial \varphi}{\partial t} + \frac{(m^2 c^4 - V^2)}{\hbar^2 c^2} \varphi = 0$$

and the one-particle Hilbert space  $\mathfrak{D}_1$  of the second quantized theory can be identified with the linear space of its positive-frequency solutions endowed with a suitable Hilbert norm related to the Klein-Gordon conserved current. Since we want exactly the "imaginary-time" evolution, we must enter into the Euclidean region through the Wick rotation  $t \rightarrow -it, t > 0$  where the (hyperbolic) Klein-Gordon equation becomes the elliptic one

$$(1.8) \quad -\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \Delta_\nu u - \frac{2V}{\hbar c^2} \frac{\partial u}{\partial t} + \frac{(m^2 c^4 - V^2)}{\hbar^2 c^2} u = 0$$

In the Euclidean region negative frequency solutions explode for  $t \uparrow +\infty$  while positive frequency ones vanish exponentially and by imposing the condition of vanishing  $u(t, \cdot)$  for  $t \uparrow +\infty$  we get a well posed Dirichlet problem in the half-space  $D = \{(t, \mathbf{x}) \in \mathbb{R}^d : t > 0\} \subset \mathbb{R}^d$ . Since  $V(\cdot)$  doesn't depend on  $t$ , such a Dirichlet problem defines a semigroup  $\{P^t\}_{t \geq 0}$  on the space  $\mathfrak{D}_1$  of its boundary data which exhibits the solution  $u(t, \cdot)$  with  $u|_{\partial D} = u_0(\cdot)$  by  $u(t, \cdot) = (P^t u_0)(\cdot)$ .  $\{P^t\}_{t \geq 0}$  translates positive frequency solutions forward in the time direction and is precisely the Hamiltonian semigroup  $\exp -tH_1/\hbar|_{t \geq 0}$  which we search for. By exploiting well known<sup>47</sup> stochastic processes techniques for solving Dirichlet problems and Girsanov's formula<sup>47</sup>, the result is

$$(1.9) \quad (e^{-tH_1/\hbar} u_0)(\mathbf{x}) = e^{-tmc^2\hbar} \mathbf{E}_{(\mathbf{x},0)}(u_0(\mathbf{X}_{\tau_t}) \exp -\frac{1}{\hbar} \int_0^{\tau_t} V(\mathbf{X}_s) dX_s^d)$$

Here  $s \mapsto \mathbf{X}_s = (X_s^1, X_s^2, \dots, X_s^{d-1})$  is again a  $d-1 = \nu$ -dimensional Brownian motion with diffusion coefficient  $\hbar/m$  while  $dX_s^d = cds + \sqrt{\hbar/m} dW_s^d$  where  $s \mapsto W_s^d$  is an extra one-dimensional Wiener process *independent* on  $s \mapsto \mathbf{X}_s$ . This last diffusion  $s \mapsto X_s^d$  on the Euclidean time axis defines the Markov time  $\tau_t = \inf\{s \geq 0 : X_s^d = ct\}$  namely the first hitting time of the hyperplane  $\Sigma_t = \{(x^1, \dots, x^d) \in \mathbb{R}^d : x^d = ct\}$  by the  $d$ -dimensional Markov process  $s \mapsto (\mathbf{X}_s, X_s^d)$ . It is known<sup>24</sup> that  $t \mapsto \xi_t$  can be represented as  $\xi_t = \mathbf{X}_{\tau_t}$  and therefore

$$(1.10) \quad (e^{-tH_1/\hbar} u_0)(\mathbf{x}) = e^{-tmc^2\hbar} \mathbf{E}_{\mathbf{x}}(u_0(\xi_t) \exp -\frac{1}{\hbar c} \int_0^{\tau_t} V(\mathbf{X}_s) dX_s^d)$$

This last formula coincides with (1.6) only in the free case  $V = 0$  but is subtly different when the electric field is not trivial. We remark the following interesting fact: in presence of a magnetic field, the formula (1.10) becomes

$$(1.12) \quad (e^{-tH_1/\hbar} u_0)(\mathbf{x}) = e^{-tmc^2/\hbar} \mathbf{E}_{\mathbf{x}}(u_0(\xi_t) \exp -\frac{1}{\hbar} \{ \frac{e}{c} \int_0^{\tau_t} \mathcal{A}_i(\mathbf{X}_s) dX_s^i + \frac{e\hbar}{2mc} \int_0^{\tau_t} \partial_i \mathcal{A}^i(\mathbf{X}_s) ds \})$$

where  $e\mathcal{A}^d = e\mathcal{A}_d = eA^0 = V$  while  $\mathcal{A}^1 = \mathcal{A}_1 = iA^1, \dots, \mathcal{A}^{d-1} = \mathcal{A}_{d-1} = iA^{d-1}$  if  $\mathbf{A} = (A^1, \dots, A^{d-1})$  is the magnetic vector potential in  $d-1 = \nu$  space-dimensions. Formula (1.12) looks more "covariant" and symmetric than

$$(1.13) \quad (e^{-t(\tilde{H}(\mathbf{A})/\hbar} \psi)(\mathbf{x}) = e^{-tmc^2/\hbar} \mathbf{E}_{\mathbf{x}}(\psi(\xi_t) \exp -\frac{1}{\hbar} \{ \int_0^t V(\xi_s) ds + S_{mag}(\tau_t, \mathcal{A}_i, \mathbf{X}) \})$$

with

$$S_{mag}(\tau_t, \mathcal{A}_i, \mathbf{X}) = \frac{e}{c} \sum_{i=1}^{d-1} \int_0^{\tau_t} \mathcal{A}_i(\mathbf{X}_s) dX_s^i + \frac{e\hbar}{2mc} \sum_{i=1}^{d-1} (\partial - i\mathcal{A}^i)(\mathbf{x}_s) ds$$

which holds for relativistic Schrödinger semigroups obtained via minimal coupling with the magnetic field and it may be interesting to understand the deep reasons of the difference between (1.10) and (1.11) (or (1.12) and (1.13)) which embodies that between Klein-Gordon theory and the relativistic Schrödinger operator model. Magnetic fields may have subtle effects. In nonrelativistic quantum mechanics we remarked that (1.5) implies diamagnetic inequalities for Schrödinger particles, however electrons have an intrinsic magnetic moment associated to their spin. This magnetic moment is not accounted for by the Schrödinger theory which must be replaced by the Pauli one in the nonrelativistic domain. The paramagnetic coupling of the magnetic field with the spin implies important differences<sup>31</sup> for the stability of matter namely the existence of a critical atomic number  $Z_c^{mag}$  also in the nonrelativistic theory. This critical number is very high and physically unrealistic since, for high  $Z$ , relativistic



corrections become important. Therefore we must turn to the Dirac theory in an external e.m. field. It is possible<sup>83</sup> to derive a "Feymann-Kac" formula also for the one-electron (or the one-positron) Hamiltonian  $H_1$ . It looks

$$(1.14) \quad (e^{-t(H_1/\hbar)} \psi)(\mathbf{x}) = e^{-tmc^2/\hbar} E_{\mathbf{x}} \left( M_{\tau_t} \psi(\xi_t) \exp - \frac{e}{\hbar c} \int_0^{\tau_t} \mathcal{A}_i(\mathbf{X}_s) dX_s^i + \frac{e\hbar}{2mc} \int_0^{\tau_t} \partial_i \mathcal{A}^i(\mathbf{X}_s) ds \right)$$

where  $\psi(\cdot) \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$  is a two component (Pauli) spinor and the matrix valued stochastic process  $s \rightarrow M_s$ , acting on its component, is defined by the differential equation

$$\dot{M}_s = \frac{e}{2mc} M_s \Lambda(\mathbf{X}_s)$$

where  $\Lambda(\mathbf{x}) = \boldsymbol{\sigma} \cdot (\mathbf{B}(\mathbf{x}) + i\mathbf{E}(\mathbf{x}))$  with  $M_0 = \mathbf{I}$ . Through its dependence on  $\mathbf{E}$ , the matrix  $M_{\tau_t}$  accounts for the spin-orbit coupling which is a relativistic effect and (1.14) gives a non perturbative control, through its semigroup, on the one-electron relativistic Hamiltonian  $H_1$  which is the positive part of the Dirac one after the Foldy-Wouthuysen transformation. Formula (1.14) has the right<sup>32,33</sup> nonrelativistic limit and It would be interesting to investigate how the critical atomic number  $Z_c^{\text{mag}}$  gets modified in the relativistic domain.

## §2. Relativistic Schrödinger Operators and their Path Integrals

When the nonrelativistic kinetic energy  $T = \sum_{i=1}^N |\mathbf{p}_i|^2/2m_i$  gets replaced by the relativistic one  $T = \sum_{i=1}^N \sqrt{c^2|\mathbf{p}_i|^2 + m^2c^4}$ , the usual Schrödinger theory becomes that of relativistic Schrödinger operators<sup>5</sup> which, for just one "electron" in a field of force with potential energy  $V$ , look

$$(2.1) \quad H = \sqrt{-c^2\hbar^2\Delta + m^2c^4} + V$$

The formula (2.1) defines in a formal way a self-adjoint operator in  $L^2(\mathbb{R}^\nu)$  which is assumed representing the quantum Hamiltonian of a relativistic spinless particle in  $\nu$  space dimensions. For  $\nu = 3$  and  $V(\mathbf{x}) = -Ze^2/|\mathbf{x}|$  (the potential energy in the Coulomb field of a nucleus with atomic number  $Z$ ), such operators were studied by Herbst which proved that  $H$  is a bona fide self-adjoint operator with positive spectrum *provided* that  $Z \leq 2/\pi\alpha$  where  $\alpha = e^2/\hbar c$  is the fine structure constant. There is a simple device<sup>5</sup> for handling  $H$ . Since  $c|\mathbf{p}| \geq (c^2|\mathbf{p}|^2 + m^2c^4)^{1/2} - mc^2 \geq c|\mathbf{p}| - mc^2$ , the stability of  $H = \sqrt{-c^2\hbar^2\Delta + m^2c^4} - mc^2 - Ze^2/r$  is the same as that of

$$(2.2) \quad \tilde{H} = \hbar c \sqrt{-\Delta} - Ze^2/r$$

and it is enough to study the operator

$$(2.3) \quad H_1 = \sqrt{-\Delta} - Z\alpha/r$$

which is homogeneous under length scaling and, therefore,  $E_0 = \inf \text{spec}(H_1)$  is either 0 or  $-\infty$  by the scaling  $\psi(\mathbf{x}) \rightarrow \lambda^{3/2}\psi(\lambda\mathbf{x})$ . The latter alternative holds, as Herbst showed<sup>6</sup>, when  $Z\alpha > 2/\pi$ . Such critical atomic numbers exist also in the Dirac and Klein-Gordon theories ( $Z_c = \alpha^{-1}$  in the Dirac case<sup>54</sup> and  $Z_c = 1/2\alpha$  for the Klein-Gordon one<sup>46</sup>). We remark that  $-\sqrt{-\Delta_\nu}$  is the infinitesimal generator of the  $\nu$ -dimensional Cauchy process<sup>8</sup>  $t \mapsto \xi_t$  which solves the Dirichlet problem  $\Delta_\nu u = 0$ ,  $u|_{\partial D} = u_0$  in a half-space  $D = \{x \in \mathbb{R}^d : x^d > 0\}$ ,  $d = \nu + 1$  through its probability

transition density density  $p_t^C(\mathbf{x}, \mathbf{y}) = p_t^C(|\mathbf{x} - \mathbf{y}|)$  which defines the Poisson integral  $(P^t * u_0)(\mathbf{x}) = u(\mathbf{x}, t) = \int_{\mathbb{R}^\nu} p_t^C(|\mathbf{x} - \mathbf{y}|) u_0(\mathbf{y}) d^\nu \mathbf{y}$  and, for  $\nu = 3$ , it is related to the Dirichlet form<sup>5</sup>

$$\mathcal{E}(u, u) = (2\pi^2)^{-1} \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|u(x) - u(y)|^2}{|\mathbf{x} - \mathbf{y}|^4} d\mathbf{x} d\mathbf{y}$$

whose jumping measure<sup>12</sup> is (in  $\nu = 3$ )  $J(d\mathbf{x} d\mathbf{y}) = (2\pi)^{-2} |\mathbf{x} - \mathbf{y}|^{-4} d\mathbf{x} d\mathbf{y}$ . Also  $L_0 = \mu - \sqrt{-\Delta_\nu + \mu^2}$  is the infinitesimal generator of a Markov jump process  $t \mapsto \xi_t$  and the corresponding Dirichlet form has a jumping measure of the form  $J(d\mathbf{x} d\mathbf{y}) = (2\pi)^{-2} \mu^2 |\mathbf{x} - \mathbf{y}|^{-2} K(\mu|\mathbf{x} - \mathbf{y}|)$  where  $K(\cdot)$  is a Bessel function. Such a stochastic process is one with stationary and independent increments and can be obtained by a time change of Brownian motion<sup>24</sup> namely, as the Cauchy process itself, it is subordinate to the Brownian motion in the sense of Bochner. From this remark one can understand why a Feymann-Kac formula holds for  $\exp -tH$  when  $H = \sqrt{-\Delta + \mu^2} + V$ , indeed it is clear that

$$(2.4) \quad (e^{-tH} \psi)(\mathbf{x}) = e^{-t\mu} \mathbf{E}_\mathbf{x}(\psi(\xi_t) \exp - \int_0^t V(\xi_s) ds)$$

essentially by Trotter-Kato formula. When one perturb the nonrelativistic quantum free Hamiltonians  $H_0 = -(1/2) \Delta_\nu$  by the multiplication operator  $V$ , it is known<sup>15</sup> in which Kato class one should choose  $V(\cdot)$  in order to get a self-adjoint operator bounded from below. When  $H_0 = \sqrt{-\Delta + \mu^2}$ , the analogous result is the following<sup>25</sup>: let  $V(\cdot) : \mathbb{R}^\nu \mapsto \mathbb{R}$  a locally integrable function such that its negative part  $V^-(\mathbf{x}) = -\min\{0, V(\mathbf{x})\}$  satisfies

$$(2.5) \quad \lim_{t \downarrow 0} \sup_{\mathbf{x} \in \mathbb{R}^\nu} \mathbf{E}_\mathbf{x} \left( \int_0^t V^-(\xi_s) ds \right) = 0$$

while its positive part satisfies the same assumption locally, then  $H_0 + V$  is essentially self-adjoint on the space  $C_0^\infty(\mathbb{R}^\nu)$  and the corresponding semigroup can be expressed by<sup>24,25</sup> the Feymann-Kac formula (2.4). The condition (2.5) is equivalent to

$$\lim_{\delta \downarrow 0} \sup_{\mathbf{x} \in \mathbb{R}^\nu} \int g_\lambda(|\mathbf{x} - \mathbf{y}|) V^-(\mathbf{y}) d\mathbf{y} = 0$$

where  $g_\lambda(|\mathbf{x}|) = \int_0^{+\infty} e^{-\lambda t} p_t(|\mathbf{x}|) dt$  is the “ $\lambda$ -potential” for the process  $s \mapsto \xi_s$  and a potential function  $V = V^+ - V^-$  will be said of the “Kato class” whenever  $V^-$  and (locally)  $V^+$  satisfy the condition above. Such a “Kato class” is the same both for  $H_0 = \sqrt{-\Delta}$  and  $H_0 = \sqrt{-\Delta + \mu^2} - \mu$  and, by the Herbst result, it is obvious that the Coulomb potential is not included at variance with the non-relativistic case. Now we want to explain the subordination of the process  $t \mapsto \xi_t$  to the Brownian motion  $s \mapsto \mathbf{W}_s$ . In order to do that let  $s \mapsto W_s^d$  an extra one-dimensional Wiener process independent on  $s \mapsto \mathbf{W}_s$  and, for  $\alpha \geq 0$  and  $\beta \geq 0$ ,  $\tau_{\alpha, \beta} = \inf\{s \geq 0 : \beta s + W_s^d > \alpha\}$ . Each hitting time  $\tau_{\alpha, \beta}$  is an optional time finite a.s., moreover, for each  $\beta \geq 0$ , the jump process  $\alpha \in [0, +\infty) \mapsto \tau_{\alpha, \beta}$  is right-continuous and nondecreasing with independent and stationary increments. By the optional stopping theorem applied to the continuous exponential martingale  $s \mapsto \exp\{\theta W_s^d - s\theta^2/2\}$ , one can check that<sup>8</sup>

$$(2.6) \quad \mathbf{E}(\exp -\gamma \tau_{\alpha, \beta}) = \exp -(\alpha(\sqrt{\beta^2 + 2\gamma} - \beta))$$

which generalize the well known result  $\mathbf{E}(\exp -\gamma \tau_{\alpha, 0}) = \exp -\alpha\sqrt{2\gamma}$ . It is expedient to choose (for  $t \geq 0$ )  $\alpha = t\sqrt{mc^2/\hbar}$  and  $\beta = \sqrt{mc^2/\hbar}$ . Let  $\tau_t = \inf\{s \geq 0 :$

$cs + \sqrt{\hbar/m} W_s^d > ct\}$  then

$$(2.7) \quad e^{-tmc^2/\hbar} \mathbf{E}(\exp -\gamma\tau_t/\hbar) = \exp -t\sqrt{2mc^2\gamma + m^2c^4}/\hbar$$

Therefore, if  $\Gamma_0$  is any nonnegative self-adjoint operator, by the spectral theorem

$$(2.8) \quad e^{-tmc^2/\hbar} \mathbf{E}(\exp -\tau_t\Gamma_0/\hbar) = \exp -t\sqrt{2mc^2\Gamma_0 + m^2c^4}/\hbar$$

In other words the semigroup  $t \mapsto \exp -tH_0/\hbar$  for  $H_0 = \sqrt{2mc^2\Gamma_0 + m^2c^4}$  can be constructed<sup>26</sup> as the averaged semigroup of  $\Gamma_0$  after replacing the deterministic time  $t$  by the random one  $\tau_t$ . It may be interesting to observe that when the speed of light  $c \uparrow +\infty$ , the random process  $t \rightarrow \tau_t$  converges in probability to the deterministic time  $t$  uniformly on bounded intervals<sup>30</sup>. By this remark one can easily grasp the probabilistic mechanism behind the nonrelativistic limit. By choosing  $\Gamma_0 = -(\hbar^2/2m)\Delta$  (the nonrelativistic free quantum Hamiltonian)  $H_0 = \sqrt{-\hbar^2c^2\Delta + m^2c^4}$  is exactly the free relativistic one. Since

$$(e^{-\tau\Gamma_0/\hbar} \psi)(\mathbf{x}) = \mathbf{E}_{\mathbf{x}}(\psi(\mathbf{X}_{\tau}))$$

where  $s \mapsto \mathbf{X}_s$  is a  $\nu$ -dimensional Brownian motion with infinitesimal generator  $(\hbar/2m)\Delta$ , one gets

$$(2.9) \quad (e^{-tH_0/\hbar} \psi)(\mathbf{x}) = e^{-tmc^2/\hbar} \mathbf{E}_{\mathbf{x}}(\psi(\xi_t)) = e^{-tmc^2/\hbar} \mathbf{E}_{(\mathbf{x},0)}(\psi(\mathbf{X}_{\tau_t}))$$

where  $s \mapsto X_s^i = (\mathbf{X}_s, X_s^d)$  is the  $d = \nu + 1$ -dimensional diffusion given by  $d\mathbf{X}_s = \sqrt{\hbar/md} d\mathbf{W}_s$ ,  $dX_s^d = cds + \sqrt{\hbar/md} dW_s^d$  while  $\tau_t = \inf\{s \geq 0 : X^d = ct\}$  and we can make the identification  $\xi_t = \mathbf{X}_{\tau_t}$ . The “space-time” diffusion  $s \mapsto X_s^i = (\mathbf{X}_s, X_s^d)$  is, in some sense, the “ground state process” for a free relativistic spinless particle with rest mass  $m$ . The formula (2.8) can be exploited also when a magnetic field is present<sup>26</sup>. Indeed, if  $\Gamma_0 = (1/2m)(-i\hbar\nabla - (e/c)\mathbf{A})^2$  which makes sense as positive self-adjoint operator when  $\mathbf{A} \in L_{\text{loc}}^2(\mathbb{R}^\nu)$ ,  $\text{div } \mathbf{A} = 0$ , it is well known that

$$(2.10) \quad (e^{-t\Gamma_0/\hbar} \psi)(\mathbf{x}) = \mathbf{E}_{\mathbf{x}}(\psi(\mathbf{X}_t) \exp -i\frac{e}{\hbar c} \int_0^t \mathbf{A}(\mathbf{X}_s) \cdot d\mathbf{X}_s)$$

and therefore

$$(2.11) \quad (e^{-tH_0(\mathbf{A})/\hbar} \psi)(\mathbf{x}) = e^{-tmc^2/\hbar} \mathbf{E}_{\mathbf{x}}(\psi(\mathbf{X}_{\tau_t}) \exp -i\frac{e}{\hbar c} \int_0^{\tau_t} \mathbf{A}(\mathbf{X}_s) \cdot d\mathbf{X}_s)$$

for  $H_0(\mathbf{A}) = \sqrt{c^2(-i\hbar\nabla - (e/c)\mathbf{A})^2 + m^2c^4}$ . If  $H_0(\mathbf{A})$  is perturbed by  $V = eA_0$  (where  $A_0$  is the electric potential) and  $H = H_0(\mathbf{A}) + eA_0$ , the (2.11) becomes

$$(2.12) \quad (e^{-tH/\hbar} \psi)(\mathbf{x}) = e^{-tmc^2/\hbar} \mathbf{E}_{\mathbf{x}}(\psi(\mathbf{X}_{\tau_t}) \exp -\frac{1}{\hbar} \{e \int_0^t A^0(\xi_s) ds + i\frac{e}{c} \int_0^{\tau_t} \mathbf{A}(\mathbf{X}_s) \cdot d\mathbf{X}_s\})$$

which is<sup>26</sup> a gauge-invariant formula, at variance with others found in the literature<sup>27,28</sup>, but displays an unpleasant asymmetry between  $A^0$  and  $\mathbf{A}$  which are time and space components of a four-vector.

### §3. The Klein-Gordon Semigroup and its Path Integral

This section and the following one on Dirac semigroups are related to the so called “external field problem”<sup>10,11</sup> where particles and quantum fields of which particles are quanta interact with an “external field” or an “external source”. The problem of quantum fields with “external sources” has a very long story related to the names

of Feynmann, Matthews and Salam, Schwinger and other people. External sources or fields are *given* functions of space-time coordinates and this means, physically, that one neglects the back reaction of the quantum field upon the source itself. This assumption is reasonable when the source is related to a macroscopic object. If the quantum field is, say, the electromagnetic one, the source could be a macroscopic electric current or, if the quantum field describes charged elementary particles as electrons, positrons, pions and so on, the external electromagnetic field may be a classical one controlled by macroscopic devices as superconducting coils and microwave frequency cavities or the magnetic field surrounding pulsars and other astrophysically interesting bodies in the Galaxy. In some cases one can take as source also microscopic objects but with size much larger than field quanta for instance atomic nuclei with their Coulomb field. Due to the large mass ratio between nucleons and electrons it is not physically unreasonable to use the Born-Oppenheimer approximation in which nuclei are considered as infinitely massive point particles which interact with electrons in a "recoiless" manner. Therefore, quantum field theories with external fields have a genuine physical interest in many important circumstances but they are useful also in connection with the more fundamental theories of interacting quantum fields (see, for instance<sup>11</sup>) and they give a taste of the difficulties encountered in interacting (i.e. nonlinear) quantum field theories. For instance, the Van Hove<sup>35</sup> model is a caricature of nuclear interaction via Yukawa theory of nuclear forces drawn in a way that emphasizes the influence of a nucleon on the meson field describing the surrounding cloud of pions. In this model a neutral scalar field interacts with a classical source mimicking a recoiless nucleon and exhibits renormalization effects which, in the limit of a pointlike source, generate the disquieting Van Hove phenomenon namely the fact that the quantum Hamiltonian of the meson field cannot be a bona fide operator acting in the Fock space of the free theory. This last fact is an intriguing general feature of interacting quantum field theories embodied in the Haag theorem. Quantum field with external sources exhibit other unexpected behaviors. From a mathematical point of view they correspond to *linear* field equations but with space-time dependent coefficients. When the external field is a static one, due to "Klein paradox", the theory may break if the external field is too strong as it will be explained in the next section. If one restricts himself to space-time dependent external fields with fast decrease or even with compact support, especially suited for the purpose of the scattering theory because the quantum field will be free in the distant regions of space-time, one can use the Källen-Yang-Feldman equations<sup>10,36</sup> in order to construct the interpolating quantum field but other unpleasant surprises come now because, for certain relativistic wave equations, for instance the Rarita-Schwinger one describing 3/2 spin particles (say the  $N^*$  (1516) resonance) and for certain innocent looking external fields, the anticommutator or the commutator of quantum field operators do not vanish for casually disjoint points<sup>37,11</sup>. Picturesquely speaking, the particles will move at speeds greater than that light where the external field is nonvanishing and sufficiently strong. Classically this means that signals exhibit group velocities greater than light which is possible for wave propagation in a dispersive medium but contrast the locality requirements of special relativity in which speed of physical signals must not exceed  $c$  and if the initial data for the Cauchy problem of a wave equation have compact support, then the support of the solution must be contained in the future light cone generated by the initial one. This is true for free relativistic wave equations which are hyperbolic systems (in the modern meaning of the term) with a cone of hyperbolicity which, by relativistic invariance, coincides with the light cone but may be false when an external field is present. Since quantum field commutators (for integer spin) or anticommutators (for half integer spin) are proportional to  $i(S_A(x, y) - S_R(x, y))$  where  $S_A$  and  $S_R$  are the retarded and advanced elementary solutions of the classical field equation, it is clear that the Velo-Zwanziger phenomenon is due to the fact that a sufficiently strong and inhomogeneous external field may destroy or seriously modify the hyperbolic nature of free relativistic wave equations. The deep roots of the difficulty is related to the circumstances that relativistic wave equations, are "singular" hyperbolic systems highly sensible to perturbations. Now

we come to Klein-Gordon theory in an external electromagnetic field but we bound ourselves only to a static one in order to preserve time-translation invariance and keep quantum Hamiltonians (for Klein-Gordon equation in time-dependent external fields see<sup>38</sup>) and we shall consider only electric fields of small strength in order to avoid the Klein paradox<sup>8,39</sup>. We begin with the free equation  $(\square + M^2)\varphi = 0$  in order to make clear some important points about its quantum meaning. After the wave equation itself  $\square\varphi = 0$  and Maxwell's ones in the free space, it is the oldest invariant wave equation and the simplest. It was already considered in the year 1926 by E. Schrödinger together with the famous nonrelativistic equation which bears his name and in the same year was independently proposed by W. Gordon, O. Klein, V. Fock and others. Such second order hyperbolic partial differential linear equation admits, by very inspection, the conserved current  $J_\varphi^\mu = (c\rho_\varphi, \mathbf{J}_\varphi) = ic(\bar{\varphi}\partial^\mu\varphi - \varphi\partial^\mu\bar{\varphi})$  but, since the  $\varphi$  and its time derivative  $\partial_t\varphi$  can be specified arbitrary at any give time, the density  $\rho_\varphi$  is not positive in general and  $J^\mu$  cannot be interpreted as a "probability current". This fact is at variance with the Schrödinger equation which admits the probability current  $J_\psi^\mu = (\rho_\psi, \mathbf{J}_\psi) = (|\psi|^2, (i\hbar/2m)(\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}))$ . Under such circumstances, Klein-Gordon equation was temporarily discarded in favour of the Dirac one (1928) in the first period of relativistic quantum mechanics. It was considered again after the new interpretation of *all* relativistic equation to be described in the next section as a free quantum field theory but now with  $J_{op}^\mu = (iec/\hbar)(\varphi_{op}^*\partial^\mu\varphi_{op} - \varphi_{op}\partial^\mu\varphi_{op}^*)$  as electric current operator. The second quantized theory turned out to describe massive spinless particles, for instance pions, with mass  $m$  related to  $M$  by  $M = mc/\hbar$  which are neutral i.e. coincide with their own antiparticles when the quantum field  $\varphi_{op}$  is hermitian, otherwise carry a charge and, as in the Dirac case, the quantum theory describes the antiparticles as well. Apart from such a field theoretical aspect, after the famous paper by E.P. Wigner<sup>40</sup>, one can check the *single* particle quantum interpretation of the unquantized Klein-Gordon equation by focusing one's attention only on its normalizable positive frequency solutions which, in  $d = \nu + 1$  space-time dimensions, are the tempered distributions

$$(3.1) \quad \varphi(x) = (2\pi)^{-\frac{\nu}{2}} \int_{H_M^+} \psi(p) e^{-ip_\mu x^\mu} \Omega_M(dp)$$

where  $H_M^+$  is the positive hyperboloid  $H_M^+ = \{p = (p^0, \mathbf{p}) \in \mathbb{R}^{1+3} : p^\mu p_\mu = M^2, p^0 \geq M\}$ ,  $\Omega_M(dp) \equiv d^3\mathbf{p}/2p^0$  the natural Lorentz invariant positive measure on  $H_M^+$  and  $\psi \in L^2(H_M^+, \Omega_M(dp))$ . For these solutions, the charge  $\int_{x^0=ct} \rho_\varphi d^3\mathbf{x}$  associated to the Klein-Gordon conserved current defines a Hilbert norm  $\|\varphi\|$  through  $\|\varphi\|^2 = \int_{x^0=ct} \rho_\varphi d^3\mathbf{x}$  indeed  $\|\varphi\|^2 = \int_{H_M^+} |\psi(p)|^2 \Omega_M(dp)$ . The resulting complex Hilbert space  $\mathfrak{D}$  carries a continuous unitary irreducible representation of the Poincaré group with mass  $M$  and spin  $s = 0$  therefore, according to Wigner's analysis,  $\mathfrak{D}$  describes the pure states of a massive free spinless particle which has the vectors  $\psi(\cdot) \in L^2(H_M^+, \Omega_M(dp))$  as wave functions in the momentum space. The generator  $P^\mu$  of space-time translations are self-adjoint operators which represent the component of the momentum-energy four vector of the particle, in particular  $H_1 = cP^0$  is the single-particle free quantum Hamiltonian. The second quantized theory to which we alluded before lives on the symmetric Fock space  $\mathcal{F}_s(\mathfrak{D}) = \bigoplus_{n=0}^{\infty} S\mathfrak{D}^{\otimes n}$  builded up on the single particle Hilbert space when the quantum field is hermitian while, in the case of a charged field, the Fock space is  $\mathcal{F}_s(\mathfrak{D}) \otimes \mathcal{F}_s(\overline{\mathfrak{D}})$  where  $\overline{\mathfrak{D}}$  is the one-antiparticle Hilbert space constructed by charge conjugation and which can be identified with the space of negative frequency solutions. We remark that positive frequency solutions can be also defined as solutions of the Cauchy problem  $\square\varphi + M^2\varphi = 0$ ,  $\varphi(t=0, \mathbf{x}) = \varphi_0(\mathbf{x})$ ,  $\partial_t\varphi(t=0, \mathbf{x}) = \dot{\varphi}_0(\mathbf{x})$  with initial data re-

stricted by  $\varphi_0 \in H^{1/2}(\mathbf{R}^\nu)$  and  $\dot{\varphi}_0 = -icH_0\varphi_0$  where  $H_0$  is the pseudodifferential operator  $H_0 = \sqrt{-\Delta_\nu + M^2}$ . Moreover  $\|\varphi\|^2 = \|H_0^{1/2}\varphi_0\|_{L^2}^2$ . This suggest a new representation of the single particle Hilbert space in which  $\mathfrak{D}$  is identified with the Sobolev space  $H^{1/2}(\mathbf{R}^\nu)$  endowed with the Hilbert norm  $\|\varphi_0\| = \|H_0^{1/2}\varphi_0\|_{L^2}$ . In this new representation (which will turn to be natural from the standpoint of the Feymann-Kac formula) the one particle quantum Hamiltonian is exactly  $H_1 = \hbar c H_0$  as self-adjoint operator in  $H^{1/2}(\mathbf{R}^\nu)$ . By the way,  $\rho_\varphi(t, \mathbf{x}) = |(H_0^{1/2}\varphi)(t, \mathbf{x})|^2 \geq 0$  so it is, after all, a *probability density* if  $\varphi$  is a *positive frequency solution* properly normalized. This density has a well defined quantum meaning because  $\int_B \rho_\varphi(t, \mathbf{x}) d\mathbf{x}$  is exactly the probability that the particle shall be localized in  $B \subset \mathbf{R}^\nu$  in the sense of Newton e Wigner<sup>41</sup> hence the possibility of a relativistic extension<sup>42,43</sup> of Nelson's stochastic mechanics. Up to now we encountered *four* isomorphic versions of the one particle Hilbert space  $\mathfrak{D}_1$ . The first one  $\mathfrak{D}_1 = L^2(H_M^+, \Omega_M(dp))$  defines a representation which "diagonalizes" the momentum-energy operators  $P^\mu$  therefore its vectors  $\psi(\cdot)$  are wave functions in the momentum space. This Hilbert space is immediately related to the theory of unitary representations of the Poincaré group and the description of free particles as elementary relativistic quantum systems in the sense of Wigner<sup>40</sup>. The second representation is strictly connected with the Klein-Gordon equation itself. In this case  $\mathfrak{D}_1$  is the linear space of positive frequency solutions  $\varphi$  normed by  $\|\varphi\|^2 = \int_{x^0=ct} \rho_\varphi d\mathbf{x}$  and carries the obvious representation of the Poincaré group in which  $P^\mu = i\hbar\partial^\mu$  generates space-time translations of solutions and  $P^\mu P_\mu = m^2 c^2$  is the Klein-Gordon equation itself. In the third representation  $\mathfrak{D}_1 = H^{1/2}(\mathbf{R}^\nu)$  (the space of initial values  $\varphi_0$  for  $\varphi$ ) normed by  $\|\varphi_0\|^2 = \|H_0^{1/2}\varphi_0\|_{L^2}^2$ . Now  $P^0 = c^{-1}H_1 = \hbar H^0$  and  $\mathbf{P} = -i\hbar\nabla$ . Finally we can take  $\mathfrak{D}_1 = L^2(\mathbf{R}^\nu)$  normed in the usual honest way. This last representation is the configuration space version of the first one indeed is exactly the representation which "diagonalizes" the Newton-Wigner position operators  $q_1, \dots, q_\nu$ . Unfortunately the relativistic invariance looks complicated in this representation owing to the fact that space localization of the particle has not an invariant meaning in space-time. But there exists also a *fifth useful version* of  $\mathfrak{D}_1$  which until now (at the best of our knowledge) *escaped notice*. This new representation is exactly the *Euclidean* analogous of the second one namely its vectors  $u$  are solutions of the "Euclidean" Klein-Gordon equation  $(-\Delta_d + M^2)u = 0$  and are normed in a very natural way. In order to understand this construction of one-particle quantum states we remark that positive frequency solutions are boundary values of holomorphic functions in a suitable complex domain  $\Omega \subset \mathbb{C}^d$ . Indeed, by looking at (3.1), it is easy to see that the function of complex variables  $z = (z^0, z^1, \dots, z^\nu)$   $\tilde{\varphi}(z) = (2\pi)^{-d/2} \int_{H_M^+} \psi(p) e^{-ip_\mu z^\mu} \Omega_M(dp)$  is well defined and holomorphic when  $\text{Im } z$  belongs to the past open light cone  $V_- = \{\eta \in \mathbf{R}^d : \eta_\mu \eta^\mu > 0, \eta^0 < 0\}$  and that  $\langle \varphi, f \rangle = \lim_{\eta \rightarrow 0, \eta \in V_-} \int_{\mathbf{R}^d} \tilde{\varphi}(x + i\eta) f(x) dx$  for all positive frequency solution  $\varphi$  and for all test function  $f$ . The complex domain  $\Omega = \{z \in \mathbb{C}^d : \text{Im } z \in V_-\}$  contain all Schwinger points  $z = (ix^d, x^1, \dots, x^\nu)$ ,  $x = (x^1, x^2, \dots, x^d) \in \mathbf{R}^d$  with  $x^d < 0$  and from now on we shall denote by  $D$  the open half  $d$ -dimensional space  $D = \{x = (x^1, \dots, x^d) \in \mathbf{R}^d : x^d < 0\}$  and, for all positive frequency solution  $\varphi$  of Klein-Gordon equation, by  $u(\cdot)$  the associated function on  $D$  defined by

$$u(x^1, \dots, x^d) = \tilde{\varphi}(ix^d, x^1, \dots, x^\nu) = (2\pi)^{-\frac{d}{2}} \int_{H_M^+} \psi(p) e^{(p_0 x^d + i\mathbf{p} \cdot \mathbf{x})} \Omega_M(dp)$$

where  $\tilde{\varphi}$  is the analytic continuation of  $\varphi$ . The function  $u$  is, so speaking, the Klein-Gordon "wave function" in the Euclidean region while  $\varphi$  is the Klein-Gordon wave function in the physical space-time. Euclidean wave functions  $u$  are exponentially

vanishing for  $x^d \rightarrow -\infty$  moreover, by transition from the hyperbolic to the elliptic case through complex domains<sup>51</sup> they satisfy the elliptic equation

$$(3.2) \quad (-\Delta_d + M^2)u = 0$$

which is the free Euclidean Klein-Gordon equation. It easy to check that Euclidean wave functions belong to the Sobolev space  $H^1(D)$  which is the natural one to be considered<sup>45</sup> in searching for weak (or generalized) solutions of the Dirichlet problem

$$(3.3) \quad \begin{cases} Lu = 0 & \text{in } D \\ u|_{\partial D} = u_0 \end{cases}$$

when  $L$  is a second order linear elliptic operator with  $L^\infty$  coefficients. Of course, the boundary datum  $u_0$  must belong to the trace of  $H^1(D)$  on the boundary  $\partial D$  of the domain which, when  $D$  is the half-space  $\mathbb{R}_-^d$  and, therefore,  $\partial D = \mathbb{R}^\nu$ , is precisely the Sobolev space  $H^{1/2}(\mathbb{R}^\nu)$  which we already encountered. By using Plancherel's theorem and elementary integrations it follows that

$$(3.4) \quad \|\varphi\|_{\mathfrak{D}_1}^2 = \int_D \left( \sum_{i=1}^d |\partial_i u|^2 + M^2 |u|^2 \right) dx$$

for all positive frequency solution  $\varphi$  with squared norm  $\|\varphi\|_{\mathfrak{D}_1}^2 = \int_{x^0=ct} \rho_\varphi d\mathbf{x}$ . The left hand side of (3.4) is the natural squared Hilbert norm in  $H^1(D)$  and, therefore, positive frequency solutions of the free Klein-Gordon equation can be elegantly characterized in the Euclidean region as those functions in  $H^1(D)$  which, for a given trace  $u_0 \in H^{1/2}(\mathbb{R}^\nu)$  on the boundary  $\partial D = \mathbb{R}^\nu$ , minimizes the functional  $u \in H^1(D) \mapsto \|u\|_{H^1(D)}^2 = \int_D \left( \sum_{i=1}^d |\partial_i u|^2 + M^2 |u|^2 \right) dx$ . Now we got a new version of the one-particle (free) Hilbert space in which  $\mathfrak{D}_1^0$  is identified with the closed linear subspace of  $H^1(D)$  of all weak solutions of (3.2) normed in its natural way

$$(3.5) \quad \|u\|_{\mathfrak{D}_1^0}^2 = \int_D \left( \sum_{i=1}^d |\partial_i u|^2 + M^2 |u|^2 \right) dx$$

This representation is especially fitted for the free Hamiltonian semigroup  $\{P^t\}_{t \geq 0} = \{\exp -tH_1^0/\hbar\}_{t \geq 0}$  which replaces the free unitary group  $\{\exp -itH_1^0/\hbar\}_{t \in \mathbb{R}}$  of the physical region. This last group acts on Klein-Gordon wave functions by translating them in time  $\varphi(x^0, \dots, x^\nu) \rightarrow \varphi(x^0 + ct, x^1, \dots, x^\nu)$  which, after Wick rotation, becomes

$$(3.6) \quad (P^t u)(x^1, \dots, x^d) = u(x^1, \dots, x^{d-1}, x^d - ct)$$

and it is clear *at once* by (3.5) that  $\{P^t\}_{t \geq 0}$  is a reality preserving *contractive* semigroup  $\|P^t u\|_{\mathfrak{D}_1^0} \leq \|u\|_{\mathfrak{D}_1^0}$  in  $H^1(D)$  but it is not difficult to check that *on its subspace*  $\mathfrak{D}_1^0$ ,  $P^t$  is *also* self-adjoint. In order to prove that we can restrict to real functions in  $H^1(D)$  as  $P^t$  is reality preserving and let be  $u^t \in v^\tau$  the time-translated by  $t$  and  $\tau$  of  $u$  and  $v$ . If  $F(t, \tau) = \langle P^t u, P^\tau v \rangle_{H^1} = \int_D \left( \sum_{i=1}^d \partial_i u^t \partial_i v^\tau + M^2 u^t v^\tau \right) dx$ , then

$$\frac{\partial F}{\partial t} - \frac{\partial F}{\partial \tau} = c \int_D \left( (-\Delta_d u^t + M^2 u^t) \partial_d v^\tau - (-\Delta_d v^\tau + M^2 v^\tau) \partial_d u^t \right) dx = 0$$

and, therefore,  $F(t, \tau) = G(t + \tau) \Rightarrow \langle P^t u, P^\tau v \rangle_{H^1} = \langle P^\tau u, P^t v \rangle_{H^1}$  for all  $t, \tau > 0$ . Because  $\lim_{t \downarrow 0} \|P^t u\|_{\mathfrak{D}_1^0} = \|u\|_{\mathfrak{D}_1^0}$  by monotone convergence theorem, it follows that

$\{P^t\}_{t \geq 0}$  is a strongly continuous self-adjoint semigroup and therefore has a positive self-adjoint generator  $H_1^0$  ( $P^t = \exp -tH_1^0/\hbar$ ) which is the free one-particle Hamiltonian in our representation. We come now at the more interesting case of the Klein-Gordon equation in a (static) external electromagnetic field  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ , by minimal coupling  $\partial_\mu \rightarrow \partial_\mu + i(e/\hbar c)A_\mu$ , this equation is

$$(3.7) \quad \square_d \varphi + \frac{2ie}{\hbar c} A^\mu \partial_\mu \varphi + (M^2 - \frac{e^2}{\hbar^2 c^2} A_\mu A^\mu) \varphi + \frac{ie}{\hbar c} (\partial_\mu A^\mu) \varphi = 0$$

which, in the Lorentz gauge  $\partial_\mu A^\mu = 0$  becomes

$$(3.8) \quad \square_d \varphi + \frac{2ie}{\hbar c} A^\mu \partial_\mu \varphi + (M^2 - \frac{e^2}{\hbar^2 c^2} A_\mu A^\mu) \varphi = 0$$

If the external field  $F_{\mu\nu}$  is not too strong, the field equation (3.7), together with the canonical commutation relations, defines a respectable linear quantum field theory but we must still identify its one-particle Hilbert space  $\mathfrak{D}_1$  and its one-particle quantum Hamiltonian  $H_1$  (of course there is also a one-antiparticle Hilbert space  $\overline{\mathfrak{D}}_1$  and a one-antiparticle Hamiltonian  $\overline{H}_1$ ). Inspired by the previous remarks on the free case, we follow the Euclidean strategy by considering the Euclidean version of (3.7) namely

$$(3.9) \quad -\Delta_d u + \frac{2e}{\hbar c} \mathcal{A}^j \partial_j u + (M^2 - \frac{e^2}{\hbar^2 c^2} \mathcal{A}_j \mathcal{A}^j) u = 0$$

where  $\mathcal{A}_d = \mathcal{A}^d = A^0$  and  $\mathcal{A}_j = \mathcal{A}^j = iA^j$ ,  $j = 1, \dots, d-1$  are the Euclidean electromagnetic potentials. The elliptic equation (3.9) defines again a Dirichlet problem in the half-space  $D$  from which we define the one-particle Hilbert space  $\mathfrak{D}_1$  and the one-particle Hamiltonian  $H_1$ . The analogous Dirichlet problem in the upper half-space  $\overline{D} = \mathbb{R}_+^d$  is related to the one-antiparticle structure but it is clear that it is enough to make the change  $\mathcal{A}_i \rightarrow -\mathcal{A}_i$  by time-reversal and charge conjugation. In the sequel, for the sake of simplicity, we shall consider a purely electric external field as the effect of a magnetic one is quite trivial. If  $V = eA^0 = e\mathcal{A}^d$ , we got the Dirichlet problem

$$\begin{cases} -\Delta_d u + \frac{2V}{\hbar c} \partial_d u + (M^2 - \frac{V^2}{\hbar^2 c^2}) u = 0 & \text{in } D \\ u|_{\partial D} = u_0 \end{cases}$$

but we didn't explain how weak the electric field  $\mathbf{E} = e^{-1} \text{grad} V$  should be in order that (3.7) be an honest external field problem for the Klein-Gordon equation. From the point of view of the Euclidean approach, the strenght of the electric field should be judged<sup>46</sup> through the quadratic form

$$(3.11) \quad Q(u, u) = \int_D \left( \sum_{i=1}^d |\partial_i u|^2 + (M^2 - \frac{V^2}{\hbar^2 c^2}) |u|^2 \right) dx$$

which is related to the classical energy functional and, for  $V(\cdot) \in L_{\text{loc}}^2(\mathbb{R}^{d-1})$ , the natural condition is the positivity of the form on its natural domain in  $L^2(D)$ . In  $d = 4$  with  $V(\mathbf{x}) = Ze^2/|\mathbf{x}|$  this positivity condition is *not* satisfied if  $Z \geq \frac{1}{2}\alpha^{-1}$  where  $\alpha = e^2/\hbar c \sim \frac{1}{137}$  since the form (3.11) is not bounded from below when  $Z \geq \frac{1}{2}\alpha^{-1}$ . In order to simplify the matter, we shall suppose in the sequel that  $V \in L^\infty$  and  $\|V\|_\infty < mc^2 - \epsilon$ . Therefore, as in the free case, we search for solutions of (3.10) again in the Sobolev space  $H^1(D)$  but we equip it by the new Hilbert norm

$$(3.12) \quad \|u\|_{H^1}^2 = \int_D \left( \sum_{i=1}^d |\partial_i u|^2 + (M^2 - \frac{V^2}{\hbar^2 c^2}) |u|^2 \right) dx$$



which is equivalent to the old one. Now we *define* the one-particle Hilbert space  $\mathfrak{D}_1$  as the closed subspace of  $H^1(D)$  consisting of all weak solutions of (3.10) *normed* by (3.12). In order to check the physical consistency of such a Hilbert norm, we remark that the density  $\rho_\varphi$  for a solution  $\varphi$  of (3.7) in the purely electric case is now

$$(3.13) \quad \rho_\varphi = i(\bar{\varphi}\partial_0\varphi - \varphi\partial_0\bar{\varphi} + \frac{2iV}{\hbar c}\bar{\varphi}\varphi)$$

Therefore the squared Hilbert norm of a positive frequency solution  $\varphi$  should be

$$(3.14) \quad \|\varphi\|^2 = i \int_{x^0=ct} ((\bar{\varphi}\partial_0\varphi - \varphi\partial_0\bar{\varphi} + \frac{2iV}{\hbar c}\bar{\varphi}\varphi)) dx$$

where, by charge conservation, the right hand side of (3.14) doesn't depend on  $t$  and can be evaluated for  $t = 0$ . On the other hand, by the *divergence theorem*, it easy to check that

$$(3.15) \quad \|u\|_{H^1}^2 = \lim_{x^d \uparrow 0} \int_{\mathbb{R}^{d-1}} (\bar{u}\partial_d u + u\partial_d \bar{u} - \frac{2V}{\hbar c}|u|^2) dx$$

for solutions  $u$  of (3.10), a formula which can be easily compared with (3.14) by formal analytic continuation from  $\varphi$  to  $u$ . Having got our Hilbert space  $\mathfrak{D}_1$ , we pick up the right one-particle Hamiltonian  $H_1$  by defining its semigroup  $P^t = \exp -tH_1/\hbar$  still through (3.6). This definition is sensible because, due to the assumption of a *static field*, solutions translated in time are still solutions. By *exactly* the same procedure of the free case, it turns out that  $\{P^t\}_{t \geq 0}$  is a self-adjoint, strongly continuous reality preserving contractive semigroup on  $\mathfrak{D}_1$  and, , the one-particle quantum Hamiltonian  $H_1$  is its generator. We have now an honest one-particle quantum mechanics extracted from the once (before 1930) discarded Klein-Gordon equation also in the case of an external static field not too strong. But now we come to the Feymann-Kac formula namely a path integral representation of the Hamiltonian semigroup  $P^t = \exp -tH_1/\hbar$ . Admittedly, the representation of states by means of Euclidean space-time functions isn't very natural especially for the sake of comparison with Schrödinger quantum mechanics in the nonrelativistic limit and it should be better to represent them by wave functions  $u_0(\cdot)$  on  $\mathbb{R}^\nu$ . There is an easy possibility which exploits the one to one correspondence between boundary data  $u_0(\cdot)$  and solution of the Dirichlet problem (3.10) when a theorem of existence and uniqueness holds. Because we assumed  $V \in L^\infty$  we can exploit standard theorems if  $|V|_\infty$  is suitably small. By the rescaling

$$(3.16) \quad u(x^1, \dots, x^d) = M^{\frac{d-2}{2}} \tilde{u}(Mx^1, \dots, Mx^d)$$

our Euclidean equation becomes

$$(3.17) \quad -\Delta_d u + 2\tilde{V}\partial_d u + (1 - \tilde{V}^2)u = 0$$

where  $\tilde{V}(\mathbf{x}) = V(M\mathbf{x})/M\hbar c = V(M\mathbf{x})/mc^2$  and the squared norm is

$$(3.18) \quad \|u\|_{H^1}^2 = \int_D \left( \sum_{i=1}^d |\partial_i u|^2 + (1 - \tilde{V}^2)|u|^2 \right) dx$$

Now, by Stampacchia's theorem, it follows that if  $\|\tilde{V}\|_\infty < (\sqrt{2} - 1)$  (i.e., in the original units,  $|V|_\infty < (\sqrt{2} - 1)mc^2$ ) for each  $u_0 \in H^{1/2}(\mathbb{R}^\nu)$  there is one and only one solution  $u(\cdot)$  of (3.17) with  $u|_{\partial D} = u_0$  and we can identify the one-particle Hilbert space  $\mathfrak{D}_1$  with the Sobolev space  $H^{1/2}(\mathbb{R}^\nu)$  endowed with the norm  $\|u_0\|_{\mathfrak{D}_1} = \|u\|_{H^1}$  where  $u$  is the unique solution of (3.17) with  $u_0$  as trace on the boundary. Apparently we reverted to the third representation of the free case but there is a difference because

the new Hilbert structure is not the old one as it is defined through a Dirichlet problem containing the potential  $V$ , as in interacting field theories, the Hilbert structure depends on the interaction  $V$ . The Hamiltonian semigroup  $P^t$  previously defined is carried on the new Hilbert space of boundary data in a very simple way, indeed  $P^t u_0$  is the trace of the solution  $u$  issued from  $u_0$  after backward time-translation. We remark that also a Dirichlet problem in a half-space for elliptic operators with "time independent" coefficients, may generate a semigroup in the vector space of its boundary data while, usually, semigroups are connected to Cauchy problems for parabolic equations as the heat equation or the imaginary-time Schrödinger one (in which case the semigroup is given by the Feymann-Kac formula). Now it is easy to get a path integral representation of  $\{P^t\}_{t \geq 0}$  because there are path integral formulas for solving Dirich-

let problems. Let  $D$  be a domain of  $\mathbb{R}^d$  and  $L = - \sum_{i,j} a^{ij}(\cdot) \partial_i \partial_j - 2 \sum_{i=1}^d b^i(\cdot) \partial_i + c(\cdot)$  a second order elliptic partial differential operator namely one in which the real and symmetric matrix valued function  $(a^{ij}(\cdot))$  is positive definite in each point  $x$  of a domain  $D$  and it may be represented as  $(a^{ij}(\cdot)) = \sigma(\cdot) \sigma^T(\cdot)$ . Now let us consider the  $d$ -dimensional diffusion  $s \mapsto Y_s = (Y_s^1, \dots, Y_s^d) = (\mathbf{Y}_s, Y_s^d)$  defined by the Itô stochastic differential equation

$$(3.19) \quad dY_s^i = b^i(Y_s) ds + \sum_{j=1}^d \sigma^{ij}(Y_s) dW_s^j \quad i = 1, \dots, d$$

where  $s \rightarrow (W_s^1, \dots, W_s^d)$  is the  $d$ -dimensional Wiener process namely the  $d$ -dimensional Brownian motion with generator  $(1/2) \Delta_d$ . The solution  $u$  of the Dirichlet problem

$$(3.20) \quad \begin{cases} Lu(x) = 0 & \text{for } x \in D \\ u|_{\partial D} = u_0 \end{cases}$$

is given by<sup>47</sup>

$$(3.21) \quad u(x) = \mathbb{E}_x(u_0(Y_{\tau_D}) \exp - \frac{1}{2} \int_0^{\tau_D} c(Y_s) ds)$$

where  $\tau_D$  is the first hitting time of the boundary  $\partial D$  of the domain by the stochastic process  $s \mapsto Y_s$ . Of course some hypotheses on the coefficients  $a^{ij}(\cdot)$ ,  $b^i(\cdot)$ ,  $c(\cdot)$  must be satisfied and, moreover, for unbounded domains (as our half-space) it is important<sup>47</sup> that  $\tau_D^x < +\infty$  a.s and, also,  $\mathbb{E}_x(\tau_D) < +\infty \forall x \in D$ . In order to pick up a more convenient Dirichlet problem, we make the change

$$(3.22) \quad u(x^1, \dots, x^d) = v(x^1, \dots, x^d) \exp x_d$$

and the new function  $v$  (which has the same boundary datum as  $u$ ) satisfies now the equation

$$(3.23) \quad -\Delta_d v - 2(1 - \tilde{V}) \partial_d v + \tilde{V}(2 - \tilde{V}) v = 0$$

The advantage of (3.23) is related to the fact that the new drift  $b^i$  is  $(b^1, \dots, b^d) = (0, \dots, 0, (1 - \tilde{V}))$  and, because we assumed  $\|\tilde{V}\|_\infty < (\sqrt{2} - 1)$ , the only nonzero component, namely the  $d$ -one, satisfies  $b^d = 1 - \tilde{V} > \sqrt{2}$ . Therefore the vector field  $b^i(\cdot)$  has always the right direction namely it points towards the boundary  $\partial D$  of half-space. Picturesquely we can say that particles travel forward in time while antiparticles go backward (at least for an external potential not too strong). By comparing the hitting time  $\tau_D$  of  $s \mapsto Y_s$  with the one  $\tilde{\tau}_D$  of the diffusion  $s \mapsto \tilde{Y}_s$  satisfying  $d\tilde{Y}_s^d = \sqrt{2} ds + dW_s^d$ ,  $d\tilde{Y}_s^i = dW_s^i, i = 1, \dots, d-1$  it is very easy to see that

$\tau_D^x < +\infty$  a.s. and  $E_x(\tau_D) < +\infty \forall x \in D$ . Therefore we are in a good shape and we can apply to  $v$  the formula (3.21) by obtaining, after its definition

$$(3.24) \quad u(x^1, \dots, x^d) = e^{x^d} E_{(x^1, \dots, x^d)}(u_0(Y_{\tau_D}^1, \dots, Y_{\tau_D}^{d-1}) \exp - \frac{1}{2} \int_0^{\tau_D} \tilde{V}(\mathbf{Y}_s)(2 - \tilde{V}(\mathbf{Y}_s)) ds)$$

Now we use Girsanov's formula<sup>47</sup> by choosing as reference process the "free" ( $\tilde{V} = 0$ ) one  $s \mapsto X_s = (\mathbf{X}_s, X_s^d)$  which satisfies

$$(3.25) \quad \begin{aligned} dX_s^i &= dW_s^i \quad i = 1, \dots, d-1 \\ dX_s^d &= ds + dW_s^d \end{aligned}$$

and, by coming back to original units

$$(3.26) \quad \begin{aligned} dX_s^i &= \sqrt{\hbar/m} dW_s^i \quad i = 1, \dots, d-1 \\ dX_s^d &= cds + \sqrt{\hbar/m} dW_s^d \end{aligned}$$

The Girsanov formula is a change of variables in path integrals. When two diffusions  $s \mapsto X_s = (\mathbf{X}_s, X_s^d)$  and  $s \mapsto Y_s = (\mathbf{Y}, Y_s^d)$  in  $\mathbf{R}^d$  are defined by

$$(3.27) \quad dY_s^i = b^i(Y_s)ds + \sum_{j=1}^d \sigma_j^i(Y_s) dW_s^j \quad i = 1, \dots, d$$

and

$$(3.28) \quad dX_s^i = (b^i(X_s) - \delta b^i(X_s))ds + \sum_{j=1}^d \sigma_j^i(X_s) dW_s^j \quad i = 1, \dots, d$$

namely have the same Brownian noise but different drifts, than the corresponding measures  $\mu_x \mathcal{D}(Y_s)$  and  $\mu_x \mathcal{D}(X_s)$  on their paths starting from  $x \in \mathbf{R}^d$  are absolutely continuous with a Radon-Nykodim derivative given by ( $0 \leq s \leq \tau$ )

$$(3.29) \quad \frac{\mu_x \mathcal{D}(Y_s)}{\mu_x \mathcal{D}(X_s)}(X) = \exp \int_0^\tau \sum_{i=1}^d \phi^i(X_s) dW_s^i - \frac{1}{2} \int_0^\tau \sum_{i=1}^d (\phi^i(X_s))^2 ds$$

where

$$(3.30) \quad \delta b^i(x) = \sum_{j=1}^d \sigma_j^i(x) \phi^j(x)$$

After simple calculations, the Girsanov formula gives us

$$(3.31) \quad u(x^1, \dots, x^d) = e^{x^d} E_{(x^1, \dots, x^d)}(u_0(\mathbf{X}_{\tau_D}) \exp - \int_0^{\tau_D} \tilde{V}(\mathbf{X}_s) dX_s^d)$$

where  $\tau_D$  is now the first hitting time of the boundary of  $D$  by  $s \mapsto X_s$ . The result (3.31) remind us of the usual Feymann-Kac formula but with the big difference that  $\int_0^t \tilde{V}(\mathbf{X}_s) ds$  is replaced by  $\int_0^{\tau_D} \tilde{V}(\mathbf{X}_s) dX_s^d$  which is a stochastic integral with a random upper limit of integration. Now we perform a forward translation in time in order to display explicitly the dependence of  $P^t u_0$  on  $t$ . By coming back to the original unit we get

$$(3.31) \quad ((\exp - \frac{tH_1}{\hbar})u_0)(\mathbf{x}) = e^{-\frac{mc^2 t}{\hbar}} E_{\mathbf{x},0)}(u_0(\mathbf{X}_{\tau_t}) \exp - \frac{e}{\hbar c} \int_0^{\tau_t} \mathcal{A}^d(\mathbf{X}_s) dX_s^d)$$

where  $\tau_t$  is, now, the first hitting time of the hyperplane  $\Sigma_t = \{x \in \mathbb{R}^d : x^d = ct\}$  by the free diffusion  $s \mapsto X_s$  given by (3.26). The (3.31) shows, at once, that  $P^t$  is a positivity improving operator. In presence of a magnetic field the formula must be modified according to:

$$(3.32) \quad \begin{aligned} & ((\exp - \frac{tH_1}{\hbar})u_0)(\mathbf{x}) = \\ & = e^{-\frac{m\xi^2 t}{\hbar}} E_{(\mathbf{x},0)} \left( u_0(\mathbf{X}_{\tau_t}) \exp - \left( \frac{e}{\hbar c} \int_0^{\tau_t} \mathcal{A}_i(\mathbf{X}_s) dX_s^I + \frac{e}{2mc} \int_0^{\tau_t} (\partial_i \mathcal{A}^i)(\mathbf{X}_s) ds \right) \right) \end{aligned}$$

which is a “Feymann-Kac-Ito” formula more elegant and symmetrical than that one true for relativistic Schrödinger operators in a magnetic field. Because

$$\tau_t = \inf \{ s \geq 0 : cs + \sqrt{\frac{\hbar}{m}} W_s^d = ct \}$$

it is not difficult to see that in the nonrelativistic limit  $c \uparrow +\infty$ , the jump process  $t \mapsto \tau_t$  converges in probability to the deterministic time  $t$  uniformly on compact intervals and, therefore,  $t \mapsto \xi_t = \mathbf{X}_{\tau_t}$ , in the same limit, converges to the Brownian motion  $t \mapsto \mathbf{x}_t$  of the usual Feynman-Kac formula. By subtracting from  $H_1$  the rest energy  $mc^2$ , it is now quite clear that the nonrelativistic limit of (3.32) is the right one.

#### §4. The Dirac Semigroup and its Path Integral

The first approaches to a path integral representation of Dirac’s propagator were based on zigzag paths in space-time along which particles travel at the speed of light. The key point of this approach lies in the fact that the  $1+1$  dimensional free Dirac equation, after analytical continuation of constants, becomes the *telegrapher* equation which has a well known probabilistic meaning. Such a path integral representation started by Feymann and Riazanov<sup>70,71</sup> but, in spite of many improvements<sup>72–81</sup>, it has not given a completely satisfactory answer. The main reason of this failure is that the connection between Dirac and telegrapher equation is purely  $1+1$  dimensional while, in higher dimensions, it seems very hard to find similar probabilistic interpretations (however, see<sup>80,81</sup>). Therefore, the  $3+1$  dimensional case can be treated only in very special situations by this method (for example central electric field and spherically symmetric wavefunction, a case which is essentially  $1+1$  dimensional). Our approach is radically different since it is based on Brownian motion. Our construction starts by observing that the right semigroup to be considered should non involve *directly* the Dirac Hamiltonian  $H_D = H_{e-} \oplus (-H_{e+})$  but only its positive part  $H_{e-}$  (corresponding to the positive half of the spectrum) or minus its negative part  $-H_{e+}$  (corresponding to negative energy levels). The physical reason is the following: although the Dirac equation  $(-i \not{\partial} + M + (e/\hbar c) \not{A})\psi = 0$  was, at the outset, treated as a relativistic version of the Schrödinger one namely a partial differential equation for the wave function  $\psi$  of a relativistic electron in the external electromagnetic field  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ , it was soon realized that such an interpretation was plagued with negative energy solutions. They are quite innocuous for a free electron but not in presence of an external field because particles with positive energy can be scattered into unphysical negative energy states and there is no adequate resolution of this “Klein Paradox” (O. Klein 1928) within the framework of a single particle theory. Dirac himself advocated (1930) a new interpretation of his equation by means of the “hole theory” by supposing that all negative energy levels were filled according to the Pauli exclusion principle. A “hole” in this infinite sea of negative energy electrons behaves as a positively charged particle with the same mass. The first antiparticle,

the positron, disquieting herald of the antimatter, was actually discovered by C.D. Anderson (1932) in the secondary cosmic radiation and P.A.M. Dirac was awarded the Nobel prize in the year 1933 (together with E. Schrödinger). The hole theory marks a transition from a single particle theory to a many bodies one describing particles of both signs of charge. Therefore the period 1930/1936 saw a fundamental transformation in the interpretation of relativistic wave equations. What was formerly a single particle theory was transformed to a many particles one which shows the symmetric appearance of particles and antiparticles by associating positive energy solutions with annihilation operators for particles and negative energies with creation operators for antiparticles (at variance with the original hole theory with its highly asymmetric vacuum). Whereas in the single particle interpretation, the Dirac theory was a differential equation for the electron wave function, in the many particle theory it became an equation for the field operator  $\psi$ . What was formerly a conserved probability current became a conserved electric current and what was formerly a nonvanishing probability for a transition from positive to negative energies turned out to be related to a probability for the creation of particle-antiparticle pairs by the external field, a physically possible phenomenon which solves the Klein paradox<sup>39</sup> in the new frame. It must be stressed that *static* external fields poses a problem if they are so strong to eliminate the energy gap between the positive and negative halves of Dirac spectrum. Indeed, in this situation, the external field will become capable of creating pairs at non zero rate<sup>49</sup> also in the static limit and, because the external field has been assumed static, this process has been going on for an infinite time and should have created an infinite number of particles. The Fock space formulation of the second quantized theory is not set up to handle such a possibility, it should break down and does so (in the Coulomb field of a nucleus with atomic number  $Z$  the critical value is  $Z = \alpha^{-1}$  where  $\alpha$  is the fine structure constant). One can see here the importance of the survival of the spectral gap. If a spectral gap survives the perturbation of the free Dirac Hamiltonian  $H_D^0$  by the external field, then a reasonable field theory is on hand<sup>50</sup> in which there is no interaction between particles but only between each particle and the external field and all relevant physics is fully contained in the one particle (or the one antiparticle) Hamiltonian from which the full Hamiltonian of the field can be constructed by second quantization in a straightforward way. Therefore we have justified our approach since the one electron Hamiltonian  $H_{e-}$  is precisely the positive part of the Dirac one  $H_D$  while the one positron Hamiltonian  $H_{e+}$  is minus the negative part of this operator. The decomposition  $H_D = H_{e-} \oplus (-H_{e+})$  can be obtained in principle by means of the well known Foldy-Wouthuysen transformation<sup>82,48,51</sup> however this task can be performed in a closed form only when the external field is purely magnetic<sup>9</sup> because in presence of an electric field (not so strong to eliminate the energy gap), the Foldy-Wouthuysen transformation, which exists by general arguments<sup>52</sup>, is not known in an explicit form but only as a perturbative expansion and so for the single particle Hamiltonians. This means that the operator  $H_{e-}$  is not explicitly given, nevertheless we are able to bypass the problem and to give an *explicit* path integral representation of its semigroup  $\exp -t H_{e-} / \hbar$  which holds for an electrons (or positrons) in an external field which is not sufficiently strong<sup>53,54,55</sup> to eliminate the spectral gap. We wish to add some other considerations about the importance of the Dirac Hamiltonian  $H_D$  which is the differential linear operator

$$(4.1) \quad H_D = \boldsymbol{\alpha} \cdot \left( -i\hbar \nabla - \frac{e}{c} \mathbf{A} \right) + mc^2 \beta + eA_0 = H_D^0 \mathbf{A} + cA^0$$

acting on the complex Hilbert space  $\mathcal{H} = L^2(\mathbf{R}^3) \otimes \mathbb{C}^4$  of square integrable four component spinors  $\psi : \mathbf{R}^3 \rightarrow \mathbb{C}^4$ . Here  $A^0 = A_0$  and  $\mathbf{A}$  are time independent electromagnetic potential in the gauge  $\nabla \cdot \mathbf{A} = 0$  (therefore the external electric  $\mathbf{E}$  and magnetic field  $\mathbf{B}$  are given by  $\mathbf{E} = -\nabla A^0$ ,  $\mathbf{B} = \text{rot } \mathbf{A}$ ) while the four  $4 \times 4$  matrices  $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$  and  $\beta$  are hermitian and obey the anticommutation relations  $\alpha_i \alpha_j + \alpha_j \alpha_i = \delta_{ij} 1$ ,  $\alpha_i \beta + \beta \alpha_i = 0$ ,  $\beta^2 = 1$ . There exists a wide literature on the

selfadjointness, the essential selfadjointness of Dirac Hamiltonians and on the existence of a spectral gap<sup>53,54,55,56</sup> in a more general context. Indeed the matrices  $\alpha_1, \alpha_2, \alpha_3$  generate the Clifford algebra  $\text{Cliff}(\text{Cliff}(E^3))$  over the real three-dimensional Euclidean space and this means that the free Dirac operator can be naturally defined in a more abstract setting on a smooth  $\nu$ -dimensional Riemannian manifold  $M^\nu$  endowed with a spin structure<sup>57,58</sup>. We will denote with  $D$  such a general Dirac operator which, for  $\nu = 3$  and  $M^3 = E^3$ , is nothing else than the free Dirac Hamiltonian  $D = -i\alpha \cdot \nabla$  with  $m = 0$  but one can think of it also as the operator  $-i \not{\partial}$  appearing in the Dirac equation  $(-i \not{\partial} + M)\psi = 0$  on a  $d$ -dimensional space-time namely a smooth Hausdorff manifold with a Lorentzian metric *provided* that there exists for it a spin structure<sup>58</sup> and, with this last interpretation,  $D$  is related to the coupling of a massless Dirac field with the gravitational one. The operator  $D$  on a Riemannian spin manifold  $M$  is an elliptic partial differential operator acting on sections  $\Gamma(S)$  of a suitable complex vector bundle  $\pi : S \rightarrow M$  over the manifold (such sections being smooth spinor fields on  $M$ ) and its selfadjointness or essential self adjointness on compact Riemannian manifold or, more generally, on paracompact and complete ones is well known<sup>56</sup> and generalizes analogous property for the Laplace-Beltrami operator<sup>59</sup>. There are deep relations between the Dirac operator  $D$  on a Riemannian spin manifold  $M$  and some metric and topological properties of  $M$ . For instance, by considering the scalar curvature (the simplest geometric invariant), there are examples<sup>60,61</sup> of manifolds which do not carry metrics with positive scalar curvature related to the Dirac operator. Aside from that, there are many papers on the index of Dirac operators which have a natural splitting

$$D = \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix}$$

with  $D_+^* = D_-$ ,  $D_-^* = D_+$ , corresponding to the splitting of the space of spinor fields into eigenspaces of chirality  $\pm 1$  and it is well known the interest of the index  $\text{Ind}(D) = \dim \ker D_+ - \dim \ker D_- = n_+ - n_-$  which, in physics, is a problem related to the so called “zero-modes” of  $D$  since  $n_\pm =$  number of chirality  $\pm 1$  normalizable zero-energy Dirac spinors. This index can be evaluated by the famous Atiyah-Singer theorem<sup>62</sup> for which there exists “heat equation”<sup>63</sup> and path integral<sup>64</sup> proofs related to ideas of E. Witten<sup>65,66</sup>. We remark that some of this considerations can be extended in infinite dimensional cases<sup>67</sup>. After this short plunge into the general setting for Dirac operators, we come back to our problem of finding a Feymann-Kac formula for the Dirac Hamiltonian (4.1), therefore we dive into the Euclidean region ( $x^0 \rightarrow ix^4$ ,  $x^4 \in \mathbb{R}$ ) where, by transition from the hyperbolic to the elliptic case through complex domains<sup>44</sup>, the Dirac operator  $-i\gamma^\mu \partial_\mu + M$  becomes the elliptic one  $-e^\alpha \partial_\alpha + M$  where ( $e^1 = i\gamma^1, \dots, e^3 = i\gamma^3$ ,  $e^4 = \gamma^0 \Rightarrow e^\alpha e^\beta + e^\beta e^\alpha = 2\delta^{\alpha\beta} 1$ ) and the Dirac equation looks

$$(4.2) \quad \left( \sum_{\alpha=1}^4 -e^\alpha \left( \partial_\alpha + \frac{e}{\hbar c} \mathcal{A}_\alpha \right) + M \right) \psi = 0$$

where  $\mathcal{A}_1 = \mathcal{A}^1 = iA^1, \dots, \mathcal{A}_3 = \mathcal{A}^3 = iA^3$ ,  $\mathcal{A}_4 = \mathcal{A}^4 A^0 = A_0$ . We start by writing the (4.2) in the “heat equation form” ( $x^4 = -ct$ )

$$(4.3) \quad \hbar \frac{\partial \psi}{\partial t} = -H_D \psi$$

with the important proviso that, *at variance* with the heat equation on a Riemannian manifold, the self-adjoint elliptic operator  $H_D$  is *not* positive. We always assume that the external field  $F_{\mu\nu}$  is not too strong in such a way that a spectral gap  $(-mc^2 + k, mc^2 - l)$  (with  $l < mc^2$  and  $k < mc^2$ ) survives the perturbation of  $H_D^0 = -i\hbar c \alpha \cdot \nabla + mc^2 \beta$  by the external potential  $A^\mu = (A^0, \mathbf{A})$  and we call  $\mathcal{H}_+$  and  $\mathcal{H}_-$  the

closed subspaces of  $\mathcal{H} = L^2(\mathbf{R}^3) \otimes \mathbb{C}^4$  corresponding respectively to the positive part (included in  $[mc^2 - el, +\infty)$ ) and the negative one (included in  $(-\infty, -mc^2 + k]$ ) of the spectrum of  $H_D$ , therefore  $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ . The Foldy-Wouthuysen transformation maps isometrically  $\mathcal{H}$  onto itself in such a way that  $\mathcal{H}_+$  is mapped on the subspace of Dirac spinors of the form

$$\psi = \begin{pmatrix} \psi_+ \\ 0 \end{pmatrix}$$

with  $\psi_+ \in L^2(\mathbf{R}^3) \otimes \mathbb{C}^2$  while  $\mathcal{H}_-$  is mapped isometrically onto the subspace of spinors

$$\psi = \begin{pmatrix} 0 \\ \psi_- \end{pmatrix}$$

with  $\psi_-$  in the same space, therefore  $H_D$  goes into  $H'_D$  where

$$H'_D = \begin{pmatrix} H_{e-} & 0 \\ 0 & -H_{e+} \end{pmatrix}$$

in which  $H_{e-}$  and  $H_{e+}$  are positive selfadjoint operators in the Hilbert space  $L^2(\mathbf{R}^3) \otimes \mathbb{C}^2$  of two component (Pauli) spinors. Of course  $H_{e-}$  is the Hamiltonian of a relativistic electron while  $H_{e+}$  is that of a positron and the quantum field theory obtained via second quantization of the Dirac equation in the external

fields  $A^\mu$  lives in the Fock space  $\mathcal{F} = \bigoplus_{n,m=0}^{\infty} A\mathcal{H}_+^{\otimes n} \otimes A\mathcal{H}_-^{\otimes m} = \mathcal{F}_A(\mathcal{H}_+) \otimes \mathcal{F}_A(\mathcal{H}_-)$

with a field Hamiltonian  $H$  which is  $d\Gamma(H_{e-}) \otimes 1 + 1 \otimes d\Gamma(H_{e+})$  where, if  $\mathfrak{D}$  is some Hilbert space then  $\mathcal{F}_A(\mathfrak{D})$  the antisymmetric Fock space over  $\mathfrak{D}$ ,  $d\Gamma(A)$  means the second quantization of the selfadjoint operator  $A$  which lives in  $\mathfrak{D}$ . Physically  $H = d\Gamma(H_{e-}) \otimes 1 + 1 \otimes d\Gamma(H_{e+})$  means that the energy of the field is simply the sum of energies of electrons and positrons since they do not interact. A positive frequency solution  $\psi(t, \mathbf{x})$  of (4.3) is a solution with "initial" data (namely on the boundary  $\mathbf{R}^3$  of the domain  $D = \mathbf{R}^+ \times \mathbf{R}^3$ )  $\psi_0(\mathbf{x}) = \psi(t=0, \mathbf{x})$  in  $\mathcal{H}_+$  while a negative frequency solution has its "initial" data in the orthogonal subspace  $\mathcal{H}_-$ . Since we are in the Euclidean region, positive frequency solutions vanish exponentially when  $t \uparrow +\infty$  while the negative ones explode. It is interesting to notice that positive frequency solutions can be characterized in a different manner. Indeed, if  $\psi$  solves (4.3), then it is easy to see after some trivial algebra, that  $\psi$  is also a solution of a second order elliptic equation  $P(D)\psi = 0$  where  $P(D)$  is the elliptic (matrix) operator given by ( $x_4 = ct$ )

$$(4.4) \quad P(D) = -\frac{\hbar}{2m} \sum_{\alpha=1}^4 \left( \partial_\alpha + \frac{e}{\hbar c} \mathcal{A}_\alpha \right)^2 + \frac{mc^2}{2\hbar} - \frac{e}{2mc} \boldsymbol{\alpha} \cdot (\mathbf{B} + i\mathbf{E})$$

Therefore, every positive frequency solution of (4.3) is also a solution of the Dirichlet problem in the half-space  $D = \mathbf{R}^+ \times \mathbf{R}^3 \subset \mathbf{R}^4$

$$(4.5) \quad \begin{cases} P(D)\psi = 0 & \text{for } t > 0 \\ \psi(t=0, \mathbf{x}) = \psi_0(\mathbf{x}) \in \mathcal{H}_+ \subset L^2(\mathbf{R}^3) \otimes \mathbb{C}^4 \\ \lim_{t \uparrow +\infty} \psi(t, \mathbf{x}) = 0 \end{cases}$$

This Dirichlet problem with  $L^2$  boundary data<sup>68</sup> has a unique solution and, therefore, positive frequency imaginary-time wave functions can be also defined through the Dirichlet problem (4.5) *provided* that the boundary datum  $\psi_0$  is chosen in the subspace  $\mathcal{H}_+$ : the equivalence between two different Dirichlet problem, one of the first order and the other of second order under a suitable *constraint* on boundary data is a classical one. In order to explain this fact we simplify the matter by considering, instead of

the (Euclidean) Dirac equation (4.3), a simpler first order elliptic system namely the Cauchy-Riemann equations

$$(4.6) \quad \begin{cases} \frac{\partial u_1}{\partial t} + \frac{\partial u_2}{\partial x} = 0 \\ \frac{\partial u_2}{\partial t} - \frac{\partial u_1}{\partial x} = 0 \end{cases}$$

which is exactly the free, massless, Euclidean Dirac equation in  $d = 2$ . This system defines a self-adjoint *contractive* semigroup  $P^t = \exp -tH$  on  $\mathcal{H} = L^2(\mathbf{R}) \otimes \mathbb{C}^2$  *provided* that the boundary data  $u_0 = (u_1^0, u_2^0)$  for the associated Dirichlet problem in the half plane  $D = \mathbf{R}^+ \times \mathbf{R} \subset \mathbf{R}^2$  are suitably restricted to a subspace of  $\mathcal{H}$ . Indeed let  $u_1(t, x) = (P^t * u_1^0)(x)$  and  $u_2(t, x) = (P^t * u_2^0)(x)$  be the Poisson integrals<sup>69</sup> of  $u_1^0$  and  $u_2^0 \in L^2(\mathbf{R})$  namely

$$(P^t * f)(x) = \int_{\mathbf{R}} p(t, x - y) f(y) dy = (e^{-t\sqrt{-\Delta}} f)(x)$$

then the following theorem holds<sup>69</sup>: a *necessary* and *sufficient* conditions that  $u(t, x) = (u_1(t, x), u_2(t, x))$  be a solution of the second order Dirichlet problem (4.5) in the half-plane  $D = \{(t, x) : t > 0\}$  with boundary data  $u^0 = (u_1^0, u_2^0)$  is that  $u_2^0 = (Ru)_1^0$  where  $R$  is the Riesz transform in  $L^2(\mathbf{R})$  and this linear constraint determines a subspace  $\mathcal{H}_+$  of  $L^2(\mathbf{R}) \otimes \mathbb{C}^2$  which, by remembering that  $R = (-\Delta)^{-1/2} \partial_x$ , easily shows that  $\mathcal{H}_+$  is precisely the subspace of  $L^2(\mathbf{R}^3) \otimes \mathbb{C}^2$  corresponding to the positive part of the spectrum for the "Dirac Hamiltonian"

$$H_D = \begin{pmatrix} 0 & \partial_x \\ -\partial_x & 0 \end{pmatrix}$$

by performing explicitly the "Foldy-Wouthuysen" transformation which brings  $H_D$  to the diagonal form

$$H'_D = \begin{pmatrix} \sqrt{-\Delta} & 0 \\ 0 & -\sqrt{-\Delta} \end{pmatrix}$$

By the previous considerations, the problem of controlling the Hamiltonian semigroup  $\{\exp -tH_D/\hbar\}_{t \geq 0}$  *restricted* to the subspace  $\mathcal{H}_+$  of positive energy states is now related to the solution of the second order Dirichlet problem (4.5). If the matrix valued function  $\mathbf{x} \in \mathbf{R}^3 \mapsto \Lambda(\mathbf{x}) = \boldsymbol{\alpha} \cdot \mathbf{F}(\mathbf{x})$  (with  $\mathbf{F}(\mathbf{x}) = (e/2mc)(\mathbf{B}(\mathbf{x}) + i\mathbf{E}(\mathbf{x}))$ ) were diagonal, one could employ the standard probabilistic formula which we used for the Klein-Gordon equation to solve also the Dirichlet problem (4.5), nevertheless in the non-diagonal case, one can generalize such a formula and the result is the following path integral representation (with the rest energy explicitated)

$$(4.7) \quad \psi(t, \mathbf{x}) = e^{-\frac{mc^2 t}{\hbar}} \mathbf{E} \left( M_{\tau_t} \psi_0(\mathbf{X}_{\tau_t}) e^{-\frac{S(\tau_t)}{\hbar}} \right)$$

with

$$(4.8) \quad S(\tau) = \frac{e}{\hbar c} \int_0^\tau \mathcal{A}_i(\mathbf{X}_s) dX_s^i$$

where the stochastic processes  $s \mapsto X_s^i = (\mathbf{X}_s, X_s^4)$  and the Markov time  $\tau_t$  are the same as in the Klein-Gordon equation and  $s \mapsto M_s$  is the matrix valued stochastic process which solves the equation

$$(4.9) \quad \dot{M}_s = M_s \Lambda(\mathbf{X}_s)$$

with the initial condition  $M_0 = 1$ . In this form, our path integral representation involves only diffusions and it reminds the Feymann-Kac formula<sup>32</sup> for the Pauli equation (2.25). The main difference lies in the fact that an extra Wiener process  $s \mapsto W_s^4$



appears in (2.9) and that the deterministic time  $t$  is replaced by the Markov one  $\tau_t$  constructed by  $s \mapsto W_s^4$ . Only a last problem remains to be settled at this point. The formal solution of the equation (2.11) is the anti-ordered exponential

$$(4.10) \quad M_\tau = T^* \exp \int_0^\tau \Lambda(\mathbf{X}_s) ds$$

defined as a product of  $\exp \Lambda(\mathbf{X}_s) ds$  with increasing values of  $s$  from the left to the right. Unfortunately the above expression can be made explicit only when  $\mathbf{F}$  has a constant direction. In this case, in fact, the matrices  $\Lambda(\mathbf{X}_s)$  commute at different times and the anti-ordered exponential becomes an ordinary one. It would be useful to give a compact probabilistic representation of (2.12) also in the case in which  $\mathbf{F}$  is not constant in direction. This is indeed possible. Suppose that the four matrices  $\alpha$  and  $\beta$  are in the spinorial representation

$$(4.11) \quad \alpha = \begin{pmatrix} \sigma & 0 \\ 0 & -\sigma \end{pmatrix} \quad \beta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

where  $\sigma = (\sigma_x, \sigma_y, \sigma_z)$  are the three Pauli matrices. By using a Poisson process  $s \mapsto N_s$  with parameter 1, we get the following probabilistic representation for  $s \mapsto M_s$

$$(4.12) \quad M_\tau = \begin{pmatrix} M_+(\tau) & 0 \\ 0 & M_-(\tau) \end{pmatrix}$$

where the  $M_\sigma(\tau)$  ( $\sigma$  is an auxiliary dichotomic variable taking values in  $\{-1, 1\}$ ) are two 2 by 2 matrices given by

$$(4.13) \quad M_\sigma(\tau) = E \left( \begin{array}{cc} \frac{1+(-1)^{N_\tau}}{2} L_+^\sigma(\tau) & \frac{1-(-1)^{N_\tau}}{2} L_+^\sigma(\tau) \\ \frac{1-(-1)^{N_\tau}}{2} L_-^\sigma(\tau) & \frac{1+(-1)^{N_\tau}}{2} L_-^\sigma(\tau) \end{array} \right)$$

where the expectation is taken with respect to the Poisson process and

$$(4.14) \quad \begin{aligned} L_\pm^\sigma(\tau) = & \exp \left\{ \int_0^\tau [1 \pm \sigma(-1)^{N_s} F_3(\mathbf{X}_s)] ds \right\} \times \\ & \times \exp \left\{ \int_0^\tau \ln [F_1(\mathbf{X}_s) \pm i\sigma(-1)^{N_s} F_2(\mathbf{X}_s)] dN_s \right\} \end{aligned}$$

where  $F_1, F_2, F_3$  are the three component of  $\mathbf{F}$ . If we insert the above expression into (2.9) we get a path integral representation of the semigroup  $\{\exp -tH_e/\hbar\}_{\{t \geq 0\}}$  for completely general subcritical external fields where the contribution of the electromagnetic field is completely explicit since it is entirely contained in the factors  $\exp -S/\hbar$  and  $s \mapsto M_s$ . The formula contains a "spin-orbit coupling" because  $s \mapsto M_s$  depends on the electric field too and it can be compared with the probabilistic representation<sup>33</sup> of Pauli semigroups which is its nonrelativistic limit. It turns out that  $\exp -S/\hbar$  takes into account the interaction of the point particle with the field as it were spinless, while the matrix  $M$  contains the contributions due to the interaction of the spin with the magnetic and electric fields. The Hamiltonian semigroup for the positron can be obtained exactly in the same way by looking at the Dirichlet problem (4.15) in the domain  $t < 0$ . The result is a path integral which is identical to (4.16) except that the four potential  $\mathcal{A}_i$  is replaced by  $-\mathcal{A}_i$  or, equivalently,  $e \rightarrow -e$ . The description of electron states through four component spinors  $\psi$  restricted by the condition  $\psi \in \mathcal{H}_+$  is not completely natural by the physical reason that an electron (or a positron) has only two spin degrees of freedom as it is clearly displayed by the Foldy-Wouthuysen transformation to which we alluded before. As explained in<sup>86</sup> this redundancy may be eliminated by using, instead of (4.5), the (Euclidean) Feymann and Gell-Mann equation<sup>85</sup> by which one obtains, by the same technique, a representation of the one-electron Hamiltonian semigroup acting on two-component spinors to which we alluded

in the introduction and which is directly related to the Foldy-Wouthuysen transformation.

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